Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BHW
Title	:	PEA LIGHT-HARVESTING COMPLEX II AT 2.5 ANGSTROM RESOLUTION
Authors	:	Standfuss, J.; Terwisscha Van Scheltinga, A.C.; Lamborghini, M.; Kuehlbrandt, W.
Deposited on	:	2005-01-19
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

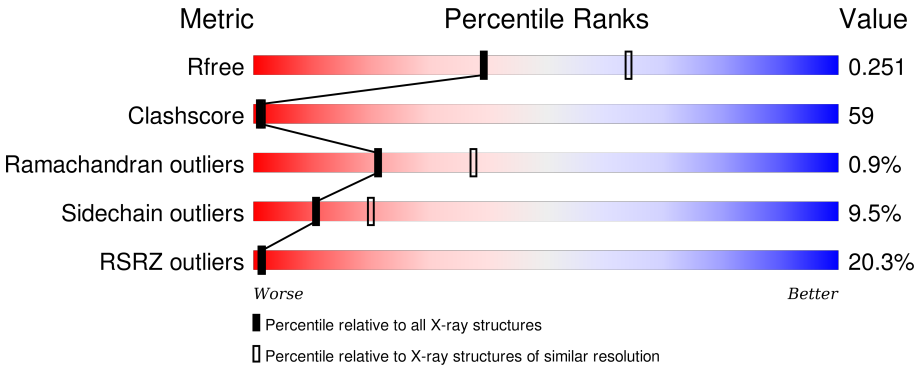
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	22% 55% 38%
1	B	232	18% 52% 40% 5%
1	C	232	19% 54% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LUX	A	501	X	-	X	-
2	LUX	A	502	X	-	X	-
2	LUX	B	501	X	-	X	-
2	LUX	B	502	X	-	-	X
2	LUX	C	501	X	-	X	-
2	LUX	C	502	X	-	-	X
3	NEX	A	503	-	-	-	X
3	NEX	B	503	-	-	-	X
3	NEX	C	503	-	-	-	X
4	XAT	A	504	X	-	-	-
4	XAT	B	504	X	-	-	-
4	XAT	C	504	X	-	-	-
5	CLA	A	601	X	-	X	-
5	CLA	A	602	X	-	-	-
5	CLA	A	603	X	-	-	-
5	CLA	A	604	X	-	X	-
5	CLA	A	605	X	-	X	X
5	CLA	A	606	X	-	-	-
5	CLA	A	607	X	-	-	-
5	CLA	A	608	X	-	-	-
5	CLA	B	601	X	-	X	-
5	CLA	B	602	X	-	-	-
5	CLA	B	603	X	-	X	-
5	CLA	B	604	X	-	X	-
5	CLA	B	605	X	-	X	X
5	CLA	B	606	X	-	-	-
5	CLA	B	607	X	-	-	-
5	CLA	B	608	X	-	X	-
5	CLA	C	601	X	-	X	-
5	CLA	C	602	X	-	-	-
5	CLA	C	603	X	-	-	-
5	CLA	C	604	X	-	-	X
5	CLA	C	605	X	-	X	X
5	CLA	C	606	X	-	-	-
5	CLA	C	607	X	-	-	-
5	CLA	C	608	X	-	-	-
6	CHL	A	609	-	-	X	-
6	CHL	A	610	-	-	X	-
6	CHL	A	611	-	-	X	-
6	CHL	A	612	X	-	-	X
6	CHL	A	614	-	-	-	X
6	CHL	B	609	-	-	X	-
6	CHL	B	610	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CHL	B	611	-	-	X	-
6	CHL	B	612	X	-	X	-
6	CHL	B	614	-	-	-	X
6	CHL	C	609	-	-	X	-
6	CHL	C	610	-	-	X	-
6	CHL	C	611	-	-	X	-
6	CHL	C	612	X	-	X	-
6	CHL	C	614	-	-	-	X
8	DGD	A	802	X	-	-	X
8	DGD	B	802	X	-	-	X
8	DGD	C	802	X	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8373 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

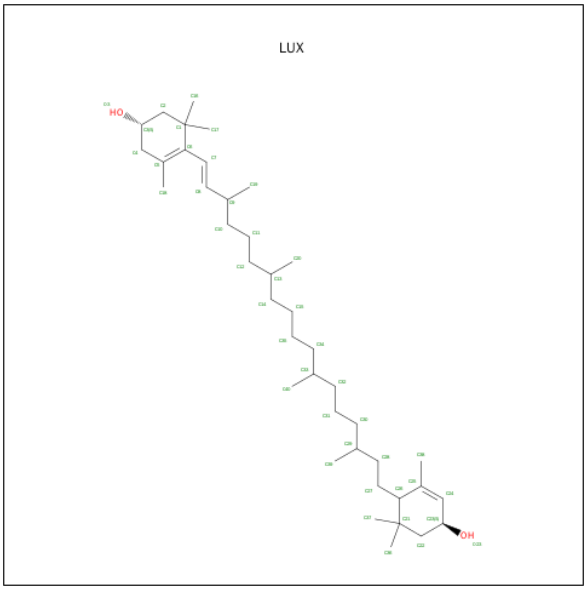
- Molecule 1 is a protein called CHLOROPHYLL A-B BINDING PROTEIN AB80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	B	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	C	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			

There are 3 discrepancies between the modelled and reference sequences:

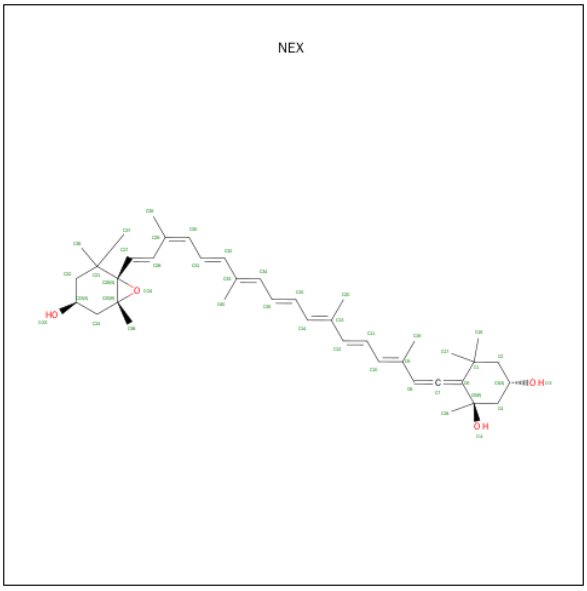
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	CYS	CONFLICT	UNP P07371
B	79	SER	CYS	CONFLICT	UNP P07371
C	79	SER	CYS	CONFLICT	UNP P07371

- Molecule 2 is (3R,3'R,6'S,9R,9'R,13R,13'S)-4',5'-DIDEHYDRO-5',6',7',8',9,9',10,10',11,11',12,12',13,13',14,14',15,15'-OCTADECAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUX) (formula: $C_{40}H_{72}O_2$).



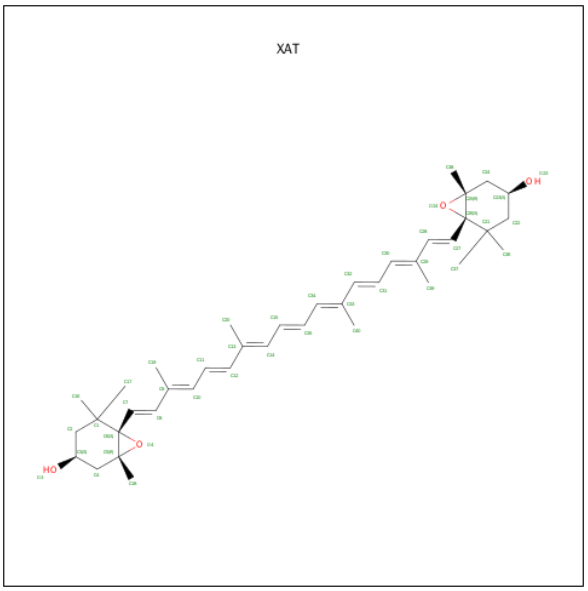
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 42 40 2	0	0
2	A	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0

- Molecule 3 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



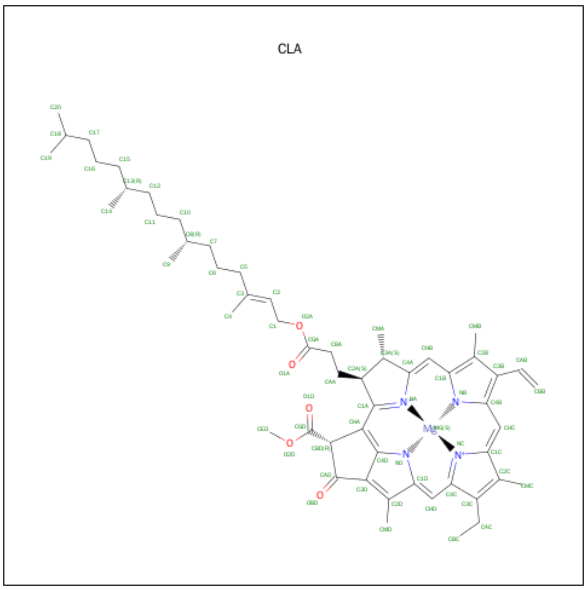
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 44 40 4	0	0
3	B	1	Total C O 44 40 4	0	0
3	C	1	Total C O 44 40 4	0	0

- Molecule 4 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 44 40 4	0	0
4	B	1	Total C O 44 40 4	0	0
4	C	1	Total C O 44 40 4	0	0

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		

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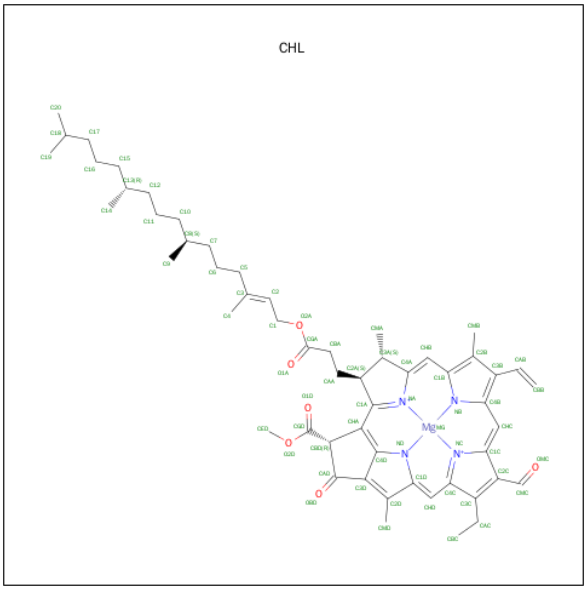
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		

- Molecule 6 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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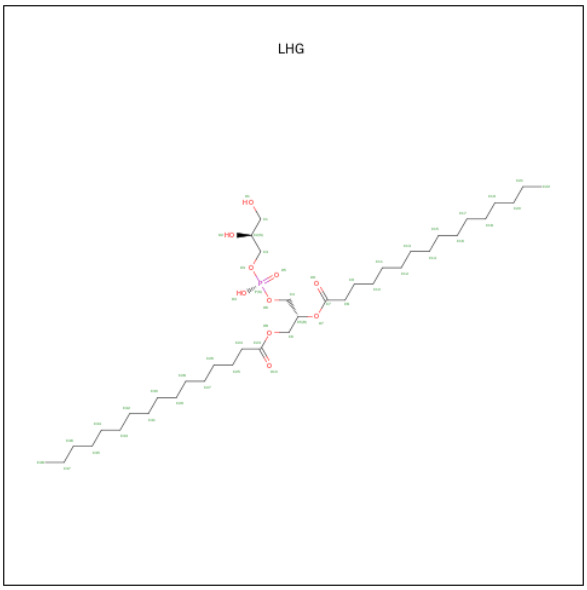
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		

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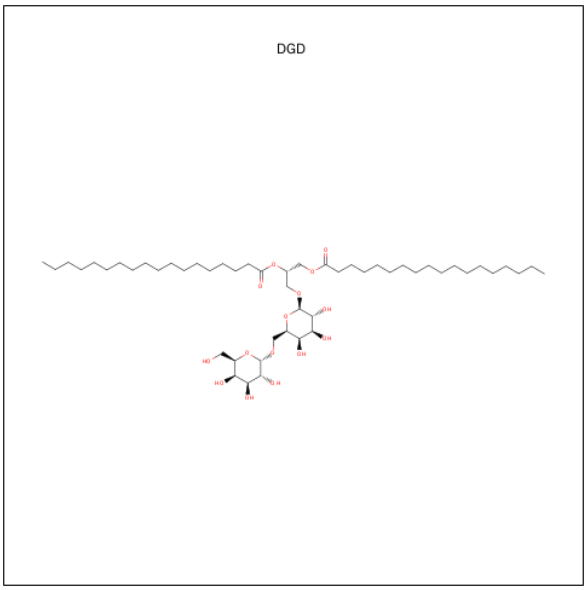
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 8 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			38	25	13		
8	B	1	Total	C	O	0	0
			38	25	13		
8	C	1	Total	C	O	0	0
			38	25	13		

- Molecule 9 is water.

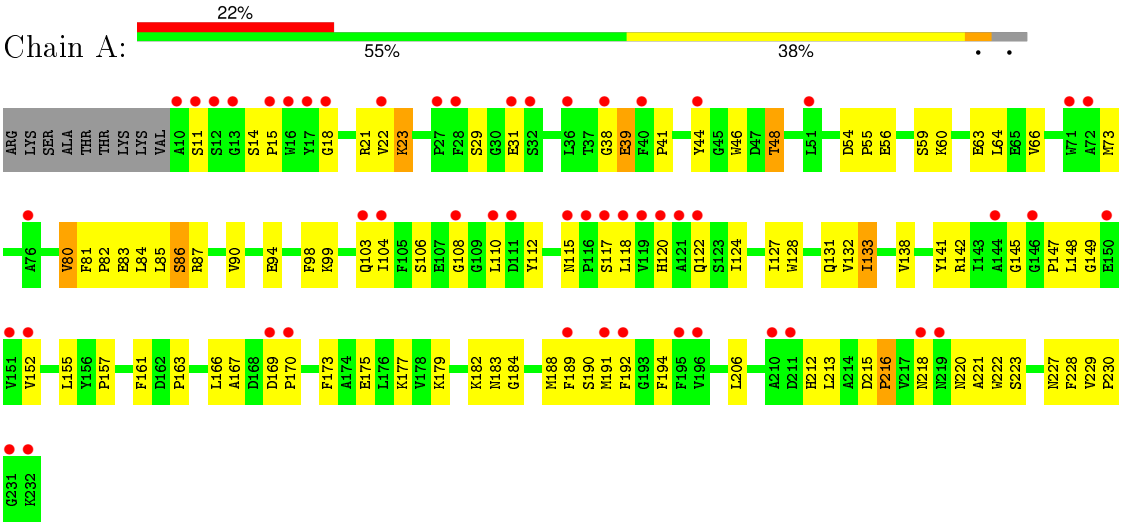
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	7	Total	O	0	0
			7	7		
9	C	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

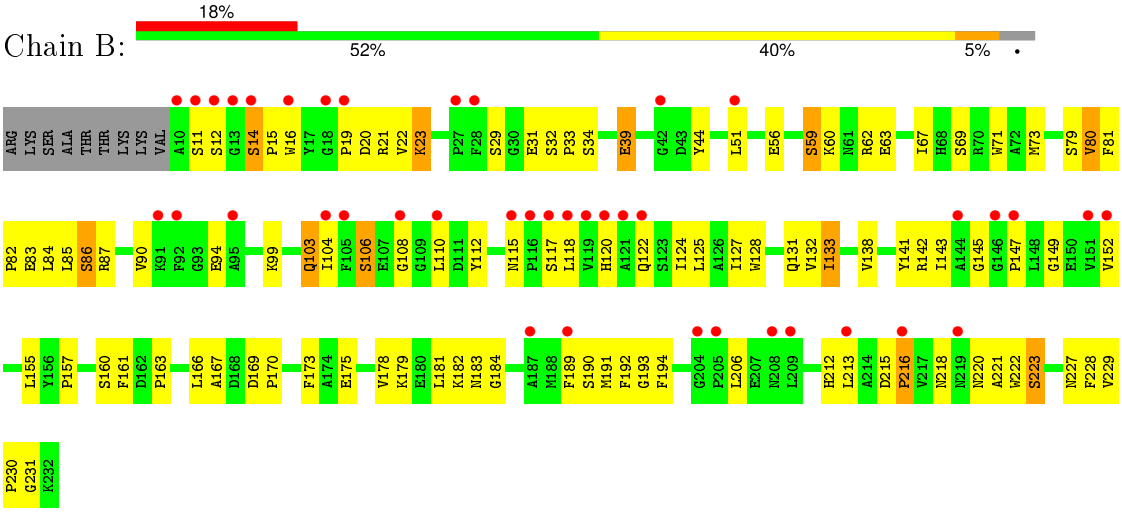
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain A:



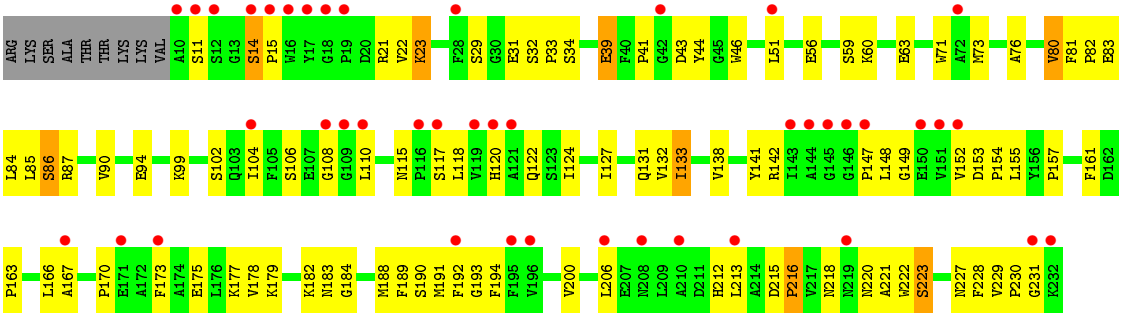
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain B:



- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain C:


ARG LYS SER ALA THR THR LYS LYS VAL A10 S11 S12 G13 S14 P15 W16 Y17 G18 P19 D20 R21 V22 K23 F28 S29 G30 E31 S32 P33 S34 E39 F40 P41 G42 D43 Y44 G45 W46 L51 E56 S59 K60 E63 W71 A72 M73 A76 W80 F81 P82 E83
L84 L85 S86 R87 V90 E94 K99 S102 Q103 I104 F105 S106 E107 G108 G109 L110 N115 P116 S117 L118 V119 H120 A121 Q122 S123 I124 I127 Q131 V132 I133 V138 Y141 R142 I143 A144 G145 G146 P147 L148 G149 E150 V151 V152 D153 P154 L155 Y156 P157 F161 D162
P163 L166 A167 P170 E171 A172 F173 A174 E175 L176 K177 V178 K179 K182 N183 G184 M188 F189 S190 M191 F192 G193 F194 F195 V196 V200 L206 E207 N208 L209 A210 D211 H212 L213 A214 D215 P216 V217 N218 N219 N220 A221 W222 S223 N227 F228 V229 P230 G231 K232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.40Å 128.00Å 62.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 85.7 (48.22-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.51Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.220 , 0.241 0.232 , 0.251	Depositor DCC
R_{free} test set	990 reflections (2.11%)	DCC
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 103.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 47843 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8373	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, LUX, XAT, CHL, CLA, NEX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/1735	0.66	0/2363
1	B	0.53	0/1735	0.69	0/2363
1	C	0.52	0/1735	0.66	0/2363
All	All	0.51	0/5205	0.67	0/7089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1683	0	1601	127	0
1	B	1683	0	1601	138	0
1	C	1683	0	1601	135	0
2	A	84	0	134	50	0
2	B	84	0	134	49	0
2	C	84	0	134	50	0
3	A	44	0	56	4	0
3	B	44	0	56	4	0
3	C	44	0	56	4	0
4	A	44	0	56	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	56	16	0
4	C	44	0	56	16	0
5	A	490	0	508	133	0
5	B	490	0	508	141	0
5	C	490	0	508	131	0
6	A	352	0	338	114	0
6	B	352	0	338	112	0
6	C	352	0	338	114	0
7	A	49	0	74	12	0
7	B	49	0	74	13	0
7	C	49	0	74	13	0
8	A	38	0	40	4	0
8	B	38	0	40	2	0
8	C	38	0	40	4	0
9	A	9	0	0	1	0
9	B	7	0	0	1	0
9	C	5	0	0	1	0
All	All	8373	0	8421	982	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (982) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:CLA:HMB1	5:A:604:CLA:HBB1	1.22	1.18
5:B:601:CLA:HMB1	5:B:601:CLA:HBB1	1.21	1.18
5:B:604:CLA:HMB1	5:B:604:CLA:HBB1	1.22	1.16
6:B:613:CHL:HBB1	6:B:613:CHL:HMB1	1.27	1.16
6:C:613:CHL:HBB1	6:C:613:CHL:HMB1	1.28	1.16
5:C:604:CLA:HBB1	5:C:604:CLA:HMB1	1.22	1.15
1:A:220:ASN:HB2	5:A:608:CLA:HED1	1.24	1.14
5:A:607:CLA:H121	5:A:607:CLA:H91	1.29	1.14
5:A:605:CLA:H41	5:C:605:CLA:H51	1.29	1.13
5:B:606:CLA:HBB1	5:B:606:CLA:HMB1	1.23	1.12
5:A:601:CLA:HMB1	5:A:601:CLA:HBB1	1.29	1.12
6:A:610:CHL:H92	6:A:612:CHL:H162	1.31	1.12
5:C:602:CLA:H91	5:C:602:CLA:H121	1.21	1.11
6:A:613:CHL:HMB1	6:A:613:CHL:HBB1	1.27	1.11
5:C:607:CLA:H121	5:C:607:CLA:H91	1.26	1.11
5:A:606:CLA:HMB1	5:A:606:CLA:HBB1	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:603:CLA:HMB1	5:A:603:CLA:HBB1	1.26	1.10
5:C:603:CLA:HMB1	5:C:603:CLA:HBB1	1.28	1.09
5:B:602:CLA:H121	5:B:602:CLA:H91	1.19	1.09
1:C:73:MET:HG2	2:C:501:LUX:H352	1.34	1.09
5:A:602:CLA:H121	5:A:602:CLA:H91	1.22	1.08
5:B:607:CLA:H91	5:B:607:CLA:H121	1.30	1.08
5:C:606:CLA:HMB1	5:C:606:CLA:HBB1	1.20	1.08
5:B:603:CLA:HMB1	5:B:603:CLA:HBB1	1.33	1.07
1:B:220:ASN:HB2	5:B:608:CLA:HED1	1.31	1.05
6:C:610:CHL:H92	6:C:612:CHL:H162	1.36	1.05
5:C:601:CLA:HBB1	5:C:601:CLA:HMB1	1.36	1.05
5:A:605:CLA:H51	5:B:605:CLA:H41	1.39	1.04
5:B:605:CLA:H51	5:C:605:CLA:H41	1.39	1.04
1:A:73:MET:HG2	2:A:501:LUX:H352	1.38	1.03
6:B:612:CHL:H152	6:B:612:CHL:H192	1.40	1.03
6:B:610:CHL:H92	6:B:612:CHL:H162	1.37	1.03
1:A:118:LEU:HA	6:A:614:CHL:CED	1.89	1.03
1:B:73:MET:HG2	2:B:501:LUX:H352	1.40	1.02
5:A:605:CLA:H52	5:B:604:CLA:H91	1.43	1.00
1:C:83:GLU:HB3	1:C:206:LEU:HD12	1.42	1.00
1:A:194:PHE:CZ	2:A:501:LUX:H383	1.96	1.00
1:A:83:GLU:HB3	1:A:206:LEU:HD12	1.43	1.00
6:A:612:CHL:H192	6:A:612:CHL:H152	1.41	1.00
1:C:194:PHE:HZ	2:C:501:LUX:H383	1.24	1.00
1:C:194:PHE:CZ	2:C:501:LUX:H383	1.97	1.00
5:B:605:CLA:H52	5:C:604:CLA:H91	1.41	0.99
1:C:118:LEU:HA	6:C:614:CHL:CED	1.92	0.98
1:B:118:LEU:HA	6:B:614:CHL:CED	1.93	0.98
1:C:220:ASN:HB2	5:C:608:CLA:HED1	1.45	0.98
6:A:610:CHL:H142	6:A:612:CHL:H72	1.43	0.98
6:A:610:CHL:HBA1	1:B:229:VAL:HG22	1.45	0.97
6:C:612:CHL:H152	6:C:612:CHL:H192	1.42	0.97
1:C:132:VAL:HG12	1:C:133:ILE:HD13	1.46	0.97
1:B:83:GLU:HB3	1:B:206:LEU:HD12	1.42	0.97
1:B:132:VAL:HG12	1:B:133:ILE:HD13	1.45	0.96
1:B:194:PHE:HZ	2:B:501:LUX:H383	1.29	0.96
1:B:194:PHE:CZ	2:B:501:LUX:H383	2.01	0.96
1:A:194:PHE:HZ	2:A:501:LUX:H383	1.25	0.95
5:B:602:CLA:H141	5:B:607:CLA:H112	1.48	0.95
5:A:604:CLA:H91	5:C:605:CLA:H52	1.48	0.95
6:A:610:CHL:H201	6:B:609:CHL:H62	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:602:CLA:H121	5:B:602:CLA:C9	1.95	0.94
5:C:602:CLA:C9	5:C:602:CLA:H121	1.97	0.94
6:C:611:CHL:H192	6:C:611:CHL:H151	1.50	0.94
1:C:14:SER:HB2	1:C:15:PRO:HD2	1.47	0.93
6:B:610:CHL:H142	6:B:612:CHL:H72	1.46	0.93
6:B:610:CHL:HBA1	1:C:229:VAL:HG22	1.48	0.93
6:B:611:CHL:H151	6:B:611:CHL:H192	1.52	0.92
2:C:501:LUX:H373	5:C:603:CLA:C2B	2.00	0.92
5:B:607:CLA:H92	5:B:607:CLA:H52	1.48	0.91
2:A:501:LUX:H373	5:A:603:CLA:C2B	2.01	0.91
6:A:609:CHL:H62	6:C:610:CHL:H201	1.52	0.91
6:C:610:CHL:H142	6:C:612:CHL:H72	1.50	0.91
2:C:502:LUX:C36	5:C:606:CLA:HMB3	2.02	0.90
5:A:602:CLA:H121	5:A:602:CLA:C9	2.00	0.90
2:A:502:LUX:C36	5:A:606:CLA:HMB3	2.00	0.90
1:A:81:PHE:HB3	1:A:82:PRO:HD3	1.53	0.90
5:A:607:CLA:H92	5:A:607:CLA:H52	1.53	0.89
5:C:607:CLA:H92	5:C:607:CLA:H52	1.51	0.89
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.53	0.89
2:B:501:LUX:H373	5:B:603:CLA:C2B	2.02	0.89
2:B:502:LUX:C36	5:B:606:CLA:HMB3	2.02	0.89
6:C:611:CHL:H192	6:C:611:CHL:HAA2	1.54	0.89
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.55	0.88
8:B:802:DGD:O2E	8:B:802:DGD:HD61	1.73	0.88
1:A:220:ASN:CB	5:A:608:CLA:HED1	2.03	0.87
5:B:607:CLA:H91	5:B:607:CLA:C12	2.05	0.87
6:A:610:CHL:C9	6:A:612:CHL:H162	2.05	0.87
1:C:163:PRO:HD2	2:C:501:LUX:H3	1.55	0.87
5:A:607:CLA:C12	5:A:607:CLA:H91	2.06	0.86
1:C:81:PHE:HB3	1:C:82:PRO:HD3	1.58	0.86
5:A:605:CLA:C19	6:A:612:CHL:H71	2.06	0.86
1:B:104:ILE:HD12	1:B:127:ILE:HD12	1.54	0.86
1:A:132:VAL:HG12	1:A:133:ILE:HD13	1.58	0.86
5:C:607:CLA:H121	5:C:607:CLA:C9	2.05	0.85
8:A:802:DGD:O2E	8:A:802:DGD:HD61	1.73	0.85
1:B:220:ASN:CB	5:B:608:CLA:HED1	2.06	0.85
1:A:229:VAL:HG22	6:C:610:CHL:HBA1	1.57	0.85
6:B:610:CHL:H201	6:C:609:CHL:H62	1.59	0.85
5:A:602:CLA:HBB1	5:A:602:CLA:HHC	1.59	0.84
1:A:118:LEU:HA	6:A:614:CHL:HED1	1.59	0.84
1:B:163:PRO:HD2	2:B:501:LUX:H3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:606:CLA:CBB	5:C:606:CLA:HMB1	2.07	0.84
1:B:118:LEU:HA	6:B:614:CHL:HED2	1.59	0.84
5:B:602:CLA:HBB1	5:B:602:CLA:HHC	1.59	0.84
6:A:611:CHL:H192	6:A:611:CHL:H151	1.59	0.84
6:C:610:CHL:C9	6:C:612:CHL:H162	2.07	0.84
5:A:602:CLA:H141	5:A:607:CLA:H112	1.58	0.84
1:B:192:PHE:CE2	5:B:604:CLA:H171	2.13	0.84
5:C:607:CLA:C12	5:C:607:CLA:H91	2.08	0.84
1:A:104:ILE:HD12	1:A:127:ILE:HD12	1.60	0.84
1:C:104:ILE:HD12	1:C:127:ILE:HD12	1.60	0.84
6:B:610:CHL:C9	6:B:612:CHL:H162	2.07	0.83
1:A:163:PRO:HD2	2:A:501:LUX:H3	1.61	0.83
1:B:14:SER:HB2	1:B:15:PRO:CD	2.07	0.83
8:C:802:DGD:O2E	8:C:802:DGD:HD61	1.76	0.83
1:A:14:SER:HB2	1:A:15:PRO:CD	2.08	0.82
1:C:14:SER:HB2	1:C:15:PRO:CD	2.07	0.82
1:B:81:PHE:HB3	1:B:82:PRO:HD3	1.62	0.82
1:C:85:LEU:HB3	1:C:90:VAL:HG21	1.61	0.82
1:C:118:LEU:HD13	5:C:606:CLA:C12	2.10	0.82
5:B:603:CLA:H92	5:B:608:CLA:HMD1	1.63	0.81
5:A:605:CLA:H191	6:A:612:CHL:H71	1.63	0.81
5:B:605:CLA:C19	6:B:612:CHL:H71	2.11	0.81
6:B:609:CHL:H141	6:B:609:CHL:H172	1.62	0.80
6:A:610:CHL:CBA	1:B:229:VAL:HG22	2.11	0.80
1:B:122:GLN:HB2	6:B:614:CHL:CBB	2.12	0.80
1:C:118:LEU:HA	6:C:614:CHL:HED2	1.62	0.80
6:A:611:CHL:H192	6:A:611:CHL:HAA2	1.62	0.80
1:C:117:SER:O	6:C:614:CHL:HED2	1.82	0.80
1:A:118:LEU:HA	6:A:614:CHL:HED2	1.62	0.79
4:B:504:XAT:O4	6:B:609:CHL:H192	1.82	0.79
5:C:602:CLA:HHC	5:C:602:CLA:HBB1	1.63	0.79
4:A:504:XAT:O4	6:A:609:CHL:H192	1.82	0.79
1:B:132:VAL:HG12	1:B:133:ILE:CD1	2.12	0.79
1:A:117:SER:O	6:A:614:CHL:HED2	1.83	0.79
5:A:607:CLA:H121	5:A:607:CLA:C9	2.09	0.79
5:B:605:CLA:H191	6:B:612:CHL:H71	1.65	0.79
1:C:220:ASN:CB	5:C:608:CLA:HED1	2.13	0.79
2:B:502:LUX:H362	5:B:606:CLA:HMB3	1.65	0.78
1:A:192:PHE:CD2	5:A:604:CLA:H18	2.18	0.78
1:A:85:LEU:HB3	1:A:90:VAL:HG21	1.66	0.78
6:A:609:CHL:H172	6:A:609:CHL:H141	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:CLA:H122	5:B:601:CLA:C9	2.14	0.78
6:B:611:CHL:HAA2	6:B:611:CHL:H192	1.65	0.78
1:A:213:LEU:HD11	5:A:608:CLA:HMC3	1.65	0.78
5:C:603:CLA:H92	5:C:608:CLA:HMD1	1.64	0.78
1:C:192:PHE:CD2	5:C:604:CLA:H18	2.19	0.78
1:C:118:LEU:HA	6:C:614:CHL:HED1	1.65	0.78
5:C:605:CLA:C19	6:C:612:CHL:H71	2.15	0.77
1:B:85:LEU:HB3	1:B:90:VAL:HG21	1.66	0.77
6:B:613:CHL:CBB	6:B:613:CHL:HMB1	2.13	0.77
5:B:602:CLA:OBD	5:B:607:CLA:HBA2	1.84	0.77
1:C:192:PHE:CE2	5:C:604:CLA:H171	2.20	0.77
1:A:229:VAL:HG22	6:C:610:CHL:CBA	2.15	0.76
2:C:502:LUX:H362	5:C:606:CLA:HMB3	1.66	0.76
2:B:502:LUX:H321	5:B:605:CLA:HMC2	1.66	0.76
4:C:504:XAT:O4	6:C:609:CHL:H192	1.86	0.76
2:C:502:LUX:H111	5:C:604:CLA:HMC2	1.68	0.76
5:C:604:CLA:HBB1	5:C:604:CLA:CMB	2.11	0.76
2:A:502:LUX:H362	5:A:606:CLA:HMB3	1.67	0.75
1:A:118:LEU:HD13	5:A:606:CLA:C12	2.16	0.75
2:A:501:LUX:H373	5:A:603:CLA:CMB	2.16	0.75
5:A:604:CLA:HBB1	5:A:604:CLA:CMB	2.12	0.75
6:C:609:CHL:H172	6:C:609:CHL:H141	1.67	0.75
1:B:118:LEU:HD13	5:B:606:CLA:C12	2.17	0.75
5:B:608:CLA:HBB1	5:B:608:CLA:HHC	1.69	0.75
1:C:132:VAL:HG12	1:C:133:ILE:CD1	2.16	0.75
5:B:601:CLA:C12	5:B:601:CLA:H92	2.17	0.74
5:A:603:CLA:CHB	5:A:608:CLA:HMD3	2.15	0.74
5:B:601:CLA:CBB	5:B:601:CLA:HMB1	2.06	0.74
5:B:605:CLA:H121	5:B:605:CLA:H92	1.70	0.74
6:B:610:CHL:CBA	1:C:229:VAL:HG22	2.17	0.74
5:A:601:CLA:C9	5:A:601:CLA:H122	2.17	0.74
4:B:504:XAT:H242	6:B:609:CHL:CMC	2.18	0.74
4:B:504:XAT:H361	7:B:801:LHG:HC92	1.69	0.74
6:C:611:CHL:HBB1	6:C:611:CHL:HHC	1.67	0.74
2:A:502:LUX:H321	5:A:605:CLA:HMC2	1.70	0.74
6:A:610:CHL:H201	6:B:609:CHL:C6	2.17	0.74
6:B:612:CHL:HHC	6:B:612:CHL:HBB1	1.69	0.74
5:C:602:CLA:OBD	5:C:607:CLA:HBA2	1.87	0.74
1:B:192:PHE:CD2	5:B:604:CLA:H18	2.22	0.74
2:B:501:LUX:H381	2:B:501:LUX:C28	2.17	0.74
6:A:609:CHL:HHD	6:A:609:CHL:HBC2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:611:CHL:H151	6:C:611:CHL:C19	2.17	0.73
6:B:609:CHL:HBB1	6:B:609:CHL:HHC	1.70	0.73
1:B:118:LEU:HA	6:B:614:CHL:HED1	1.71	0.73
2:C:501:LUX:H122	5:C:601:CLA:HHC	1.71	0.73
2:B:501:LUX:H122	5:B:601:CLA:HHC	1.71	0.73
5:C:603:CLA:CHB	5:C:608:CLA:HMD3	2.19	0.73
4:C:504:XAT:H242	6:C:609:CHL:CMC	2.18	0.73
5:B:601:CLA:H122	5:B:601:CLA:H92	1.71	0.73
1:C:73:MET:HG2	2:C:501:LUX:C35	2.13	0.73
1:B:73:MET:HG2	2:B:501:LUX:C35	2.18	0.72
1:A:192:PHE:CE2	5:A:604:CLA:H171	2.24	0.72
2:A:501:LUX:H122	5:A:601:CLA:HHC	1.72	0.72
1:A:73:MET:HG2	2:A:501:LUX:C35	2.18	0.72
5:A:604:CLA:CBB	5:A:604:CLA:HMB1	2.08	0.72
5:A:606:CLA:HMB1	5:A:606:CLA:CBB	2.11	0.72
4:A:504:XAT:H242	6:A:609:CHL:CMC	2.20	0.72
1:A:222:TRP:CH2	6:C:610:CHL:HBC2	2.25	0.71
2:A:501:LUX:H381	2:A:501:LUX:C28	2.19	0.71
1:A:122:GLN:HB2	6:A:614:CHL:CBB	2.20	0.71
6:C:609:CHL:H101	6:C:609:CHL:H142	1.72	0.71
6:B:611:CHL:HHC	6:B:611:CHL:HBB1	1.72	0.71
5:A:605:CLA:H92	5:A:605:CLA:H121	1.71	0.71
5:B:602:CLA:C14	5:B:607:CLA:H112	2.19	0.71
5:B:603:CLA:H172	5:B:608:CLA:HBA1	1.71	0.71
5:C:605:CLA:H191	6:C:612:CHL:H71	1.72	0.71
2:C:501:LUX:H373	5:C:603:CLA:CMB	2.19	0.71
2:C:502:LUX:H373	5:C:606:CLA:C2B	2.20	0.71
6:A:609:CHL:H142	6:A:609:CHL:H101	1.72	0.71
6:A:611:CHL:HHC	6:A:611:CHL:HBB1	1.72	0.71
1:B:117:SER:O	6:B:614:CHL:HED2	1.90	0.71
1:C:94:GLU:HG2	1:C:99:LYS:HB3	1.70	0.71
5:A:607:CLA:C9	5:A:607:CLA:C12	2.68	0.71
6:A:610:CHL:C14	6:A:612:CHL:H72	2.21	0.70
2:B:501:LUX:H373	5:B:603:CLA:CMB	2.21	0.70
5:A:602:CLA:OBD	5:A:607:CLA:HBA2	1.90	0.70
1:B:166:LEU:HD12	2:B:501:LUX:O3	1.92	0.70
6:B:611:CHL:H151	6:B:611:CHL:C19	2.22	0.70
2:C:501:LUX:H381	2:C:501:LUX:C28	2.21	0.70
5:C:607:CLA:HBB1	5:C:607:CLA:HHC	1.73	0.70
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.26	0.70
5:B:605:CLA:HBB1	5:B:605:CLA:HHC	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:609:CHL:C6	6:C:610:CHL:H201	2.22	0.70
6:A:612:CHL:HHC	6:A:612:CHL:HBB1	1.73	0.70
5:B:603:CLA:C9	5:B:608:CLA:HMD1	2.20	0.70
5:A:602:CLA:OBD	5:A:607:CLA:HBD	1.91	0.70
5:A:605:CLA:C4	5:C:605:CLA:H51	2.16	0.70
5:C:601:CLA:H122	5:C:601:CLA:C9	2.22	0.69
1:B:118:LEU:HD22	5:B:606:CLA:C12	2.22	0.69
5:A:601:CLA:H92	5:A:601:CLA:C12	2.23	0.69
1:C:167:ALA:HB1	1:C:173:PHE:CD1	2.27	0.69
1:C:142:ARG:NH2	6:C:612:CHL:O1D	2.24	0.69
5:B:607:CLA:C12	5:B:607:CLA:C9	2.68	0.69
2:C:501:LUX:C24	2:C:501:LUX:H363	2.22	0.69
2:A:501:LUX:H363	2:A:501:LUX:C24	2.21	0.69
5:A:602:CLA:C12	5:A:602:CLA:H91	2.12	0.69
1:A:142:ARG:NH2	6:A:612:CHL:O1D	2.19	0.69
1:C:131:GLN:HE22	6:C:610:CHL:HMC	1.58	0.69
5:B:604:CLA:H41	5:B:605:CLA:HBA1	1.75	0.69
5:B:606:CLA:HMB1	5:B:606:CLA:CBB	2.09	0.69
1:A:132:VAL:HG12	1:A:133:ILE:CD1	2.22	0.69
3:A:503:NEX:H403	6:A:613:CHL:O1A	1.93	0.68
5:B:604:CLA:HMB1	5:B:604:CLA:CBB	2.09	0.68
6:C:609:CHL:HHC	6:C:609:CHL:HBB1	1.75	0.68
1:A:86:SER:HA	1:A:90:VAL:O	1.93	0.68
5:B:601:CLA:C12	5:B:601:CLA:C9	2.72	0.68
5:B:602:CLA:OBD	5:B:607:CLA:HBD	1.94	0.68
1:C:122:GLN:HB2	6:C:614:CHL:CBB	2.24	0.68
5:C:601:CLA:H92	5:C:601:CLA:C12	2.24	0.68
1:A:131:GLN:HE22	6:A:610:CHL:HMC	1.59	0.68
5:A:602:CLA:C14	5:A:607:CLA:H112	2.23	0.68
5:C:605:CLA:H121	5:C:605:CLA:H92	1.76	0.68
1:C:166:LEU:HD12	2:C:501:LUX:O3	1.94	0.68
2:B:501:LUX:C24	2:B:501:LUX:H363	2.24	0.67
1:A:213:LEU:HD21	5:A:608:CLA:CHC	2.25	0.67
4:A:504:XAT:H361	7:A:801:LHG:HC92	1.75	0.67
4:C:504:XAT:H361	7:C:801:LHG:HC92	1.74	0.67
5:C:605:CLA:C15	5:C:605:CLA:H192	2.25	0.67
5:B:604:CLA:H41	5:B:605:CLA:CBA	2.24	0.67
2:C:502:LUX:H321	5:C:605:CLA:HMC2	1.77	0.67
5:B:607:CLA:HHC	5:B:607:CLA:HBB1	1.76	0.67
5:C:607:CLA:C5	5:C:607:CLA:H92	2.24	0.67
5:B:605:CLA:H152	5:B:605:CLA:H192	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:609:CHL:H101	6:B:609:CHL:H142	1.77	0.67
1:B:131:GLN:HE22	6:B:610:CHL:HMC	1.59	0.67
5:A:605:CLA:HHC	5:A:605:CLA:HBB1	1.75	0.67
1:B:131:GLN:HE22	6:B:610:CHL:CMC	2.07	0.67
6:C:609:CHL:HHD	6:C:609:CHL:HBC2	1.77	0.67
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.77	0.67
5:A:601:CLA:H92	5:A:601:CLA:H122	1.77	0.66
5:A:603:CLA:H92	5:A:608:CLA:HMD1	1.77	0.66
6:A:610:CHL:HBB1	6:A:610:CHL:HHC	1.76	0.66
1:C:131:GLN:HE22	6:C:610:CHL:CMC	2.07	0.66
6:B:610:CHL:C14	6:B:612:CHL:H72	2.24	0.66
1:C:22:VAL:CG2	6:C:609:CHL:HBC3	2.26	0.66
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.77	0.66
5:B:605:CLA:H192	5:B:605:CLA:C15	2.25	0.66
5:C:602:CLA:H141	5:C:607:CLA:H112	1.77	0.66
5:B:603:CLA:CHB	5:B:608:CLA:HMD3	2.25	0.66
6:B:610:CHL:H201	6:C:609:CHL:H8	1.77	0.66
2:B:502:LUX:H373	5:B:606:CLA:C2B	2.26	0.66
5:C:603:CLA:H172	5:C:608:CLA:HBA1	1.77	0.66
6:C:612:CHL:HBB1	6:C:612:CHL:HHC	1.77	0.66
1:B:22:VAL:CG2	6:B:609:CHL:HBC3	2.26	0.66
5:B:602:CLA:H91	5:B:602:CLA:C12	2.13	0.66
1:B:142:ARG:NH2	6:B:612:CHL:O1D	2.22	0.66
6:B:610:CHL:H201	6:C:609:CHL:C6	2.26	0.66
3:C:503:NEX:H403	6:C:613:CHL:O1A	1.95	0.66
1:A:131:GLN:HE22	6:A:610:CHL:CMC	2.09	0.65
6:A:613:CHL:CMB	6:A:613:CHL:HBB1	2.15	0.65
1:B:80:VAL:HG12	1:B:81:PHE:N	2.11	0.65
6:A:609:CHL:HBB1	6:A:609:CHL:HHC	1.78	0.65
5:B:604:CLA:CMB	5:B:604:CLA:HBB1	2.10	0.65
6:B:610:CHL:HBC2	1:C:222:TRP:CH2	2.31	0.65
5:C:608:CLA:HBB1	5:C:608:CLA:HHC	1.77	0.65
6:A:610:CHL:HBA1	1:B:229:VAL:CG2	2.23	0.65
3:B:503:NEX:H403	6:B:613:CHL:O1A	1.96	0.65
6:B:612:CHL:HBC1	6:B:613:CHL:HBB2	1.78	0.65
5:A:607:CLA:H92	5:A:607:CLA:C5	2.25	0.65
5:B:605:CLA:C9	5:B:605:CLA:C12	2.75	0.65
6:C:612:CHL:C15	6:C:612:CHL:H192	2.21	0.65
1:A:80:VAL:HG12	1:A:81:PHE:N	2.11	0.65
6:A:609:CHL:H41	7:A:801:LHG:H162	1.79	0.65
6:C:610:CHL:C14	6:C:612:CHL:H72	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.31	0.65
2:B:502:LUX:H111	5:B:604:CLA:HMC2	1.79	0.64
1:B:104:ILE:CD1	1:B:127:ILE:HD12	2.25	0.64
5:A:601:CLA:C9	5:A:601:CLA:C12	2.74	0.64
5:A:602:CLA:HMD2	5:A:607:CLA:C1D	2.27	0.64
1:B:149:GLY:O	6:B:611:CHL:HMC	1.97	0.64
5:A:607:CLA:HHC	5:A:607:CLA:HBB1	1.79	0.64
5:A:608:CLA:HHC	5:A:608:CLA:HBB1	1.79	0.64
5:C:603:CLA:C9	5:C:608:CLA:HMD1	2.26	0.64
2:A:502:LUX:H111	5:A:604:CLA:HMC2	1.80	0.64
6:B:612:CHL:H192	6:B:612:CHL:C15	2.24	0.64
5:C:601:CLA:H111	5:C:601:CLA:H162	1.80	0.64
5:C:606:CLA:CMB	5:C:606:CLA:HBB1	2.10	0.64
6:C:610:CHL:HBB2	6:C:612:CHL:HBC1	1.78	0.64
4:C:504:XAT:H403	7:C:801:LHG:H121	1.79	0.64
5:C:601:CLA:H92	5:C:601:CLA:H122	1.80	0.64
2:A:502:LUX:H193	5:A:604:CLA:H141	1.80	0.63
5:C:604:CLA:CBB	5:C:604:CLA:HMB1	2.09	0.63
1:A:104:ILE:HD12	1:A:127:ILE:CD1	2.28	0.63
1:B:73:MET:HG2	2:B:501:LUX:H142	1.80	0.63
5:C:605:CLA:HHC	5:C:605:CLA:HBB1	1.80	0.63
1:B:213:LEU:HD21	5:B:608:CLA:CHC	2.27	0.63
6:B:610:CHL:HBB1	6:B:610:CHL:HHC	1.80	0.63
4:C:504:XAT:H3	6:C:609:CHL:C19	2.29	0.63
2:A:502:LUX:H361	5:A:606:CLA:HMB3	1.79	0.63
4:B:504:XAT:H371	7:B:801:LHG:H362	1.81	0.63
6:C:610:CHL:HBB1	6:C:610:CHL:HHC	1.80	0.63
1:A:118:LEU:HD22	5:A:606:CLA:C12	2.29	0.62
1:B:115:ASN:HB3	1:B:118:LEU:HD12	1.80	0.62
2:C:501:LUX:H101	5:C:601:CLA:H72	1.80	0.62
2:B:502:LUX:C24	2:B:502:LUX:H363	2.29	0.62
1:B:94:GLU:HG2	1:B:99:LYS:HB3	1.80	0.62
5:B:605:CLA:C12	5:B:605:CLA:H92	2.29	0.62
5:C:602:CLA:OBD	5:C:607:CLA:HBD	1.99	0.62
2:B:502:LUX:H102	5:B:604:CLA:CHC	2.29	0.62
1:C:213:LEU:HD21	5:C:608:CLA:CHC	2.28	0.62
1:A:166:LEU:HD12	2:A:501:LUX:O3	2.00	0.62
1:C:94:GLU:HG2	1:C:99:LYS:CB	2.30	0.62
1:A:115:ASN:HB3	1:A:118:LEU:HD12	1.81	0.62
5:C:605:CLA:H192	5:C:605:CLA:H152	1.81	0.62
1:C:133:ILE:N	1:C:133:ILE:HD13	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:LUX:H381	2:C:502:LUX:C28	2.30	0.62
1:C:84:LEU:CD2	5:C:607:CLA:H191	2.30	0.62
1:C:21:ARG:HH11	1:C:21:ARG:HG2	1.64	0.62
5:A:605:CLA:C15	5:A:605:CLA:H192	2.30	0.61
1:C:86:SER:HA	1:C:90:VAL:O	2.00	0.61
5:C:601:CLA:C9	5:C:601:CLA:C12	2.77	0.61
2:A:501:LUX:H101	5:A:601:CLA:H72	1.83	0.61
5:C:602:CLA:C12	5:C:602:CLA:C9	2.78	0.61
5:C:605:CLA:C12	5:C:605:CLA:C9	2.78	0.61
1:A:81:PHE:HB3	1:A:82:PRO:CD	2.28	0.61
1:B:94:GLU:HG2	1:B:99:LYS:CB	2.30	0.61
5:B:601:CLA:H111	5:B:601:CLA:H162	1.82	0.61
5:C:607:CLA:C12	5:C:607:CLA:C9	2.70	0.61
6:A:611:CHL:C19	6:A:611:CHL:H151	2.28	0.61
5:C:605:CLA:H92	5:C:605:CLA:C12	2.30	0.61
2:A:502:LUX:H363	2:A:502:LUX:C24	2.30	0.61
5:A:603:CLA:HMB1	5:A:603:CLA:CBB	2.13	0.61
5:A:605:CLA:C12	5:A:605:CLA:C9	2.78	0.61
5:B:604:CLA:H142	5:B:604:CLA:H101	1.82	0.61
5:B:606:CLA:H102	6:B:614:CHL:CED	2.30	0.61
5:B:608:CLA:HHD	5:B:608:CLA:HBC2	1.83	0.61
1:A:229:VAL:CG2	6:C:610:CHL:HBA1	2.29	0.61
2:A:501:LUX:H281	2:A:501:LUX:H381	1.82	0.61
1:A:222:TRP:HH2	6:C:610:CHL:HBC2	1.63	0.61
2:A:501:LUX:H101	5:A:601:CLA:H52	1.82	0.61
6:A:610:CHL:HBC2	1:B:222:TRP:CH2	2.35	0.61
2:C:502:LUX:H361	5:C:606:CLA:HMB3	1.82	0.60
2:A:502:LUX:C28	2:A:502:LUX:H381	2.32	0.60
2:A:502:LUX:H373	5:A:606:CLA:C2B	2.31	0.60
1:C:81:PHE:HB3	1:C:82:PRO:CD	2.31	0.60
5:A:605:CLA:H152	5:A:605:CLA:H192	1.83	0.60
4:A:504:XAT:H371	7:A:801:LHG:H362	1.84	0.60
5:B:607:CLA:C5	5:B:607:CLA:H92	2.25	0.60
1:B:133:ILE:N	1:B:133:ILE:HD13	2.16	0.60
1:C:149:GLY:O	6:C:611:CHL:HMC	2.02	0.60
4:A:504:XAT:H3	6:A:609:CHL:C19	2.31	0.60
5:C:603:CLA:CMB	5:C:603:CLA:HBB1	2.15	0.60
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.81	0.60
1:C:80:VAL:HG12	1:C:81:PHE:N	2.17	0.59
1:A:216:PRO:HB3	5:A:608:CLA:C1B	2.32	0.59
5:C:606:CLA:H102	6:C:614:CHL:HED1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:CG	2:B:501:LUX:H352	2.23	0.59
2:B:502:LUX:H361	5:B:606:CLA:HMB3	1.82	0.59
1:B:104:ILE:HD12	1:B:127:ILE:CD1	2.28	0.59
5:B:602:CLA:C9	5:B:602:CLA:C12	2.76	0.59
5:C:606:CLA:H91	6:C:614:CHL:O2D	2.02	0.59
1:B:86:SER:HA	1:B:90:VAL:O	2.03	0.59
6:B:610:CHL:HBA1	1:C:229:VAL:CG2	2.27	0.59
1:B:108:GLY:O	1:B:122:GLN:NE2	2.32	0.59
1:B:182:LYS:HE2	5:B:607:CLA:O1D	2.03	0.59
6:A:610:CHL:H72	6:A:612:CHL:H172	1.84	0.58
1:B:84:LEU:CD2	5:B:607:CLA:H191	2.33	0.58
5:C:604:CLA:H101	5:C:604:CLA:H142	1.85	0.58
5:A:604:CLA:H142	5:A:604:CLA:H101	1.86	0.58
1:A:22:VAL:CG2	6:A:609:CHL:HBC3	2.33	0.58
5:A:603:CLA:H172	5:A:608:CLA:HBA1	1.84	0.58
6:C:611:CHL:C19	6:C:611:CHL:HAA2	2.28	0.58
2:C:502:LUX:H363	2:C:502:LUX:C24	2.34	0.58
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.84	0.58
1:A:182:LYS:NZ	7:A:801:LHG:O4	2.31	0.58
1:A:84:LEU:CD2	5:A:607:CLA:H191	2.34	0.58
1:A:104:ILE:CD1	1:A:127:ILE:HD12	2.33	0.58
5:B:606:CLA:H91	6:B:614:CHL:O2D	2.04	0.58
1:C:104:ILE:CD1	1:C:127:ILE:HD12	2.32	0.58
6:C:610:CHL:H72	6:C:612:CHL:H172	1.86	0.58
5:A:605:CLA:C12	5:A:605:CLA:H92	2.32	0.58
2:B:501:LUX:H281	2:B:501:LUX:H381	1.84	0.58
6:B:609:CHL:HHD	6:B:609:CHL:HBC2	1.86	0.58
6:B:610:CHL:HBB2	6:B:612:CHL:HBC1	1.86	0.58
1:C:115:ASN:HB3	1:C:118:LEU:HD12	1.86	0.58
2:C:502:LUX:H122	5:C:604:CLA:HHC	1.86	0.58
4:B:504:XAT:H3	6:B:609:CHL:C19	2.34	0.57
6:A:611:CHL:C19	6:A:611:CHL:HAA2	2.33	0.57
1:A:133:ILE:N	1:A:133:ILE:HD13	2.18	0.57
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.68	0.57
5:A:602:CLA:C12	5:A:602:CLA:C9	2.78	0.57
5:B:601:CLA:HBC1	6:B:611:CHL:H201	1.86	0.57
5:B:603:CLA:H172	5:B:608:CLA:CBA	2.35	0.57
2:A:501:LUX:H373	5:A:603:CLA:HMB3	1.85	0.57
5:B:606:CLA:H102	6:B:614:CHL:HED1	1.85	0.57
5:B:601:CLA:CMB	5:B:601:CLA:HBB1	2.12	0.57
1:B:73:MET:HG2	2:B:501:LUX:C15	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:607:CLA:C4C	7:C:801:LHG:HC61	2.35	0.57
1:A:149:GLY:O	6:A:611:CHL:HMC	2.04	0.57
6:B:610:CHL:HBC2	1:C:222:TRP:HH2	1.69	0.57
1:A:85:LEU:HB3	1:A:90:VAL:CG2	2.34	0.57
6:A:610:CHL:HBB2	6:A:612:CHL:HBC1	1.86	0.57
1:A:194:PHE:CE1	2:A:501:LUX:H383	2.38	0.56
6:A:610:CHL:H201	6:B:609:CHL:H8	1.87	0.56
2:B:501:LUX:C37	5:B:603:CLA:HMB3	2.34	0.56
2:B:502:LUX:H193	5:B:604:CLA:H141	1.86	0.56
2:B:502:LUX:C28	2:B:502:LUX:H381	2.35	0.56
6:B:610:CHL:H201	6:C:609:CHL:C8	2.34	0.56
5:A:605:CLA:H51	5:B:605:CLA:C4	2.26	0.56
2:B:501:LUX:H101	5:B:601:CLA:H52	1.87	0.56
5:B:602:CLA:HMD2	5:B:607:CLA:C1D	2.35	0.56
2:A:502:LUX:H122	5:A:604:CLA:HHC	1.88	0.56
1:B:213:LEU:HD11	5:B:608:CLA:HMC3	1.86	0.56
2:B:501:LUX:H101	5:B:601:CLA:H72	1.86	0.56
1:B:147:PRO:HG2	6:B:611:CHL:HBB2	1.88	0.56
5:C:606:CLA:H102	6:C:614:CHL:CED	2.35	0.56
1:C:73:MET:HG2	2:C:501:LUX:C15	2.35	0.56
2:C:501:LUX:H381	2:C:501:LUX:H281	1.86	0.56
1:C:22:VAL:HG22	6:C:609:CHL:HBC3	1.87	0.56
1:A:22:VAL:HG22	6:A:609:CHL:HBC3	1.88	0.56
5:B:607:CLA:C4C	7:B:801:LHG:HC61	2.35	0.56
5:C:603:CLA:HMB1	5:C:603:CLA:CBB	2.16	0.56
1:C:85:LEU:HB3	1:C:90:VAL:CG2	2.33	0.56
6:A:613:CHL:CBB	6:A:613:CHL:HMB1	2.13	0.56
2:C:502:LUX:H102	5:C:604:CLA:CHC	2.36	0.56
1:B:216:PRO:HB3	5:B:608:CLA:C1B	2.36	0.56
2:C:502:LUX:H373	5:C:606:CLA:C3B	2.36	0.56
5:C:603:CLA:C1B	5:C:608:CLA:HMD3	2.36	0.56
1:A:73:MET:HE2	1:A:183:ASN:C	2.26	0.55
2:A:502:LUX:H102	5:A:604:CLA:CHC	2.35	0.55
6:B:609:CHL:H41	7:B:801:LHG:H162	1.88	0.55
2:C:501:LUX:H373	5:C:603:CLA:HMB3	1.88	0.55
1:C:147:PRO:HG2	6:C:611:CHL:HBB2	1.88	0.55
1:C:182:LYS:NZ	7:C:801:LHG:O4	2.35	0.55
1:C:213:LEU:HD11	5:C:608:CLA:HMC3	1.87	0.55
5:A:606:CLA:H91	6:A:614:CHL:O2D	2.06	0.55
1:C:83:GLU:CD	1:C:206:LEU:HB2	2.26	0.55
5:A:603:CLA:C1B	5:A:608:CLA:HMD3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:LUX:H373	5:B:603:CLA:HMB3	1.88	0.55
6:C:613:CHL:CMB	6:C:613:CHL:HBB1	2.16	0.55
6:C:613:CHL:CBB	6:C:613:CHL:HMB1	2.14	0.55
4:B:504:XAT:H403	7:B:801:LHG:H121	1.88	0.54
1:C:118:LEU:HD22	5:C:606:CLA:C12	2.37	0.54
1:A:221:ALA:HB3	4:A:504:XAT:H193	1.89	0.54
6:B:614:CHL:HHC	6:B:614:CHL:HBB1	1.88	0.54
1:B:179:LYS:HD3	5:B:602:CLA:HAA2	1.90	0.54
2:B:501:LUX:H381	2:B:501:LUX:H282	1.86	0.54
2:A:501:LUX:C37	5:A:603:CLA:HMB3	2.36	0.54
4:C:504:XAT:H3	6:C:609:CHL:H191	1.89	0.54
6:B:610:CHL:C20	6:C:609:CHL:H8	2.37	0.54
5:C:604:CLA:H41	5:C:605:CLA:HBA1	1.89	0.54
6:C:614:CHL:HHC	6:C:614:CHL:HBB1	1.88	0.54
5:A:606:CLA:H102	6:A:614:CHL:CED	2.38	0.54
1:C:108:GLY:O	1:C:122:GLN:NE2	2.36	0.54
1:C:216:PRO:HB3	5:C:608:CLA:C1B	2.38	0.54
1:A:147:PRO:HB2	6:A:611:CHL:HBB2	1.90	0.54
5:B:601:CLA:CBC	6:B:611:CHL:H201	2.37	0.54
1:B:22:VAL:HG21	6:B:609:CHL:CBC	2.38	0.54
2:C:501:LUX:C37	5:C:603:CLA:HMB3	2.38	0.54
6:A:609:CHL:H8	6:C:610:CHL:H201	1.90	0.54
1:A:94:GLU:HG2	1:A:99:LYS:CB	2.37	0.54
1:B:85:LEU:HB3	1:B:90:VAL:CG2	2.35	0.53
4:A:504:XAT:H3	6:A:609:CHL:H191	1.91	0.53
5:B:606:CLA:H91	6:B:614:CHL:CED	2.38	0.53
1:A:83:GLU:CD	1:A:206:LEU:HB2	2.27	0.53
5:A:606:CLA:CMB	5:A:606:CLA:HBB1	2.14	0.53
1:B:118:LEU:HD23	6:B:614:CHL:CED	2.38	0.53
5:C:605:CLA:OBD	6:C:612:CHL:HBA2	2.08	0.53
2:B:502:LUX:H373	5:B:606:CLA:C3B	2.39	0.53
1:B:23:LYS:HB3	1:B:29:SER:OG	2.08	0.53
2:B:502:LUX:H122	5:B:604:CLA:HHC	1.90	0.53
6:B:610:CHL:H142	6:B:612:CHL:C7	2.31	0.53
6:B:611:CHL:C19	6:B:611:CHL:C15	2.87	0.53
1:A:108:GLY:O	1:A:122:GLN:NE2	2.36	0.53
6:A:610:CHL:HBC2	1:B:222:TRP:HH2	1.74	0.53
6:B:612:CHL:C19	6:B:612:CHL:H152	2.25	0.53
1:C:73:MET:HE1	1:C:184:GLY:N	2.24	0.53
1:C:161:PHE:O	2:C:501:LUX:H4C2	2.08	0.53
1:B:19:PRO:HD2	1:B:20:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:CG2	6:B:609:CHL:CBC	2.87	0.53
6:C:609:CHL:H41	7:C:801:LHG:H162	1.91	0.53
5:A:601:CLA:H162	5:A:601:CLA:H111	1.91	0.53
5:B:603:CLA:HBB2	7:B:801:LHG:H292	1.89	0.53
1:C:220:ASN:CG	5:C:608:CLA:HED1	2.29	0.53
5:A:605:CLA:OBD	6:A:612:CHL:HBA2	2.10	0.52
1:B:22:VAL:HG22	6:B:609:CHL:HBC3	1.91	0.52
5:B:605:CLA:OBD	6:B:612:CHL:HBA2	2.10	0.52
1:C:118:LEU:HD23	6:C:614:CHL:CED	2.40	0.52
1:C:22:VAL:CG2	6:C:609:CHL:CBC	2.87	0.52
6:C:611:CHL:H192	6:C:611:CHL:CAA	2.34	0.52
5:A:604:CLA:HBC3	5:A:604:CLA:HMC1	1.92	0.52
6:B:609:CHL:C14	6:B:609:CHL:H172	2.35	0.52
5:C:602:CLA:C14	5:C:607:CLA:H112	2.39	0.52
6:A:609:CHL:C14	6:A:609:CHL:H172	2.38	0.52
1:A:39:GLU:HG3	1:A:39:GLU:O	2.08	0.52
1:B:81:PHE:HB3	1:B:82:PRO:CD	2.37	0.52
6:B:610:CHL:H203	6:C:609:CHL:H101	1.91	0.52
6:C:609:CHL:H142	6:C:609:CHL:C10	2.38	0.52
5:C:606:CLA:H91	6:C:614:CHL:CED	2.40	0.52
2:A:502:LUX:H202	5:A:604:CLA:H202	1.92	0.52
6:A:611:CHL:C19	6:A:611:CHL:C15	2.88	0.52
1:C:115:ASN:HB3	1:C:118:LEU:CD1	2.40	0.52
5:C:608:CLA:HHD	5:C:608:CLA:HBC2	1.92	0.52
6:C:611:CHL:C19	6:C:611:CHL:CAA	2.88	0.52
5:C:601:CLA:HBC1	6:C:611:CHL:H201	1.91	0.52
1:A:115:ASN:HB3	1:A:118:LEU:CD1	2.40	0.52
1:C:73:MET:HE3	1:C:183:ASN:C	2.30	0.52
5:A:606:CLA:H102	6:A:614:CHL:HED1	1.92	0.51
2:A:501:LUX:H282	2:A:501:LUX:H381	1.91	0.51
6:A:609:CHL:H142	6:A:609:CHL:C10	2.39	0.51
6:A:614:CHL:HBB1	6:A:614:CHL:HHC	1.92	0.51
1:A:118:LEU:HD23	6:A:614:CHL:CED	2.40	0.51
2:A:502:LUX:C20	5:A:604:CLA:H202	2.41	0.51
4:A:504:XAT:H403	7:A:801:LHG:H121	1.92	0.51
1:B:73:MET:HE3	1:B:183:ASN:C	2.30	0.51
5:B:601:CLA:H122	5:B:601:CLA:H91	1.93	0.51
5:B:601:CLA:H92	5:B:601:CLA:H121	1.91	0.51
5:B:604:CLA:H3A	5:B:604:CLA:CGA	2.41	0.51
6:B:610:CHL:H201	6:C:609:CHL:C7	2.40	0.51
1:C:73:MET:HG2	2:C:501:LUX:H142	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:604:CLA:HBC3	5:C:604:CLA:HMC1	1.92	0.51
6:A:612:CHL:H192	6:A:612:CHL:C15	2.24	0.51
5:A:606:CLA:H91	6:A:614:CHL:CED	2.41	0.51
1:B:59:SER:O	1:B:63:GLU:HG3	2.11	0.51
2:B:501:LUX:H111	5:B:601:CLA:HMC2	1.91	0.51
1:C:73:MET:CE	1:C:183:ASN:CB	2.89	0.51
1:B:133:ILE:CD1	1:B:133:ILE:N	2.73	0.51
1:A:118:LEU:O	1:A:120:HIS:N	2.38	0.51
2:C:501:LUX:H101	5:C:601:CLA:H52	1.93	0.51
6:C:611:CHL:C15	6:C:611:CHL:C19	2.84	0.51
1:B:227:ASN:O	1:B:228:PHE:HB2	2.11	0.51
1:A:56:GLU:O	1:A:60:LYS:HG2	2.10	0.51
5:B:603:CLA:C1B	5:B:608:CLA:HMD3	2.40	0.51
5:B:608:CLA:CHD	5:B:608:CLA:HBC2	2.41	0.51
6:A:610:CHL:H201	6:B:609:CHL:C8	2.40	0.51
6:A:609:CHL:CHD	6:A:609:CHL:HBC2	2.40	0.51
5:B:605:CLA:H51	5:C:605:CLA:C4	2.28	0.51
1:C:179:LYS:HD3	5:C:602:CLA:HAA2	1.93	0.51
5:B:607:CLA:C3C	7:B:801:LHG:HC61	2.40	0.50
1:B:147:PRO:CG	6:B:611:CHL:HBB2	2.41	0.50
1:A:73:MET:HG2	2:A:501:LUX:C15	2.39	0.50
1:B:194:PHE:CE1	2:B:501:LUX:H383	2.46	0.50
1:C:22:VAL:HG21	6:C:609:CHL:CBC	2.42	0.50
1:C:102:SER:HB3	6:C:610:CHL:HED2	1.93	0.50
1:A:73:MET:HE3	1:A:184:GLY:N	2.26	0.50
1:A:189:PHE:HE1	6:A:609:CHL:HED2	1.75	0.50
1:A:212:HIS:O	1:A:216:PRO:N	2.44	0.50
1:A:182:LYS:HE2	5:A:607:CLA:O1D	2.12	0.50
1:B:15:PRO:O	1:B:22:VAL:HG12	2.11	0.50
2:C:501:LUX:H101	5:C:601:CLA:C7	2.41	0.50
2:C:501:LUX:C37	5:C:603:CLA:CMB	2.90	0.50
1:A:215:ASP:CG	1:A:218:ASN:HD22	2.15	0.50
6:A:609:CHL:C7	6:C:610:CHL:H201	2.41	0.50
1:A:120:HIS:HD2	6:A:614:CHL:HMB3	1.77	0.50
1:B:115:ASN:HB3	1:B:118:LEU:CD1	2.41	0.50
5:B:603:CLA:CMB	5:B:603:CLA:HBB1	2.21	0.50
1:B:22:VAL:HG21	6:B:609:CHL:HBC1	1.94	0.50
1:B:212:HIS:O	1:B:216:PRO:N	2.45	0.50
1:A:104:ILE:HG12	1:A:104:ILE:O	2.11	0.50
1:B:83:GLU:O	1:B:87:ARG:HG3	2.11	0.50
1:A:179:LYS:HD3	5:A:602:CLA:HAA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:CHL:H203	6:B:609:CHL:H101	1.93	0.50
1:C:220:ASN:O	1:C:223:SER:OG	2.29	0.50
1:C:192:PHE:CZ	5:C:604:CLA:H171	2.47	0.50
1:B:83:GLU:CD	1:B:206:LEU:HB2	2.33	0.50
2:A:501:LUX:C37	5:A:603:CLA:CMB	2.89	0.49
4:B:504:XAT:H363	7:B:801:LHG:C7	2.42	0.49
1:C:148:LEU:HD12	1:C:161:PHE:CZ	2.47	0.49
5:C:605:CLA:H122	5:C:605:CLA:C9	2.42	0.49
1:C:227:ASN:O	1:C:228:PHE:HB2	2.12	0.49
1:C:147:PRO:CG	6:C:611:CHL:HBB2	2.42	0.49
1:A:133:ILE:N	1:A:133:ILE:CD1	2.75	0.49
1:C:21:ARG:HD2	1:C:43:ASP:O	2.11	0.49
1:A:148:LEU:HD12	1:A:161:PHE:CZ	2.47	0.49
6:A:609:CHL:C8	6:C:610:CHL:H201	2.42	0.49
2:B:501:LUX:H102	5:B:601:CLA:CHC	2.43	0.49
6:B:610:CHL:H72	6:B:612:CHL:H172	1.94	0.49
5:A:606:CLA:CHA	5:A:606:CLA:HBA1	2.42	0.49
1:A:191:MET:HG2	2:A:502:LUX:H322	1.93	0.49
6:A:610:CHL:H2	8:A:802:DGD:C4B	2.42	0.49
1:C:157:PRO:HB3	6:C:611:CHL:HBC2	1.94	0.49
1:C:120:HIS:HD2	6:C:614:CHL:HMB3	1.76	0.49
2:A:501:LUX:H101	5:A:601:CLA:C7	2.42	0.49
6:B:610:CHL:H172	6:B:610:CHL:H141	1.93	0.49
1:C:191:MET:HG2	2:C:502:LUX:H322	1.93	0.49
1:C:229:VAL:HG12	1:C:230:PRO:O	2.12	0.49
2:C:501:LUX:H111	5:C:601:CLA:HMC2	1.94	0.49
1:C:194:PHE:CE1	2:C:501:LUX:H383	2.46	0.49
5:C:601:CLA:H92	5:C:601:CLA:H121	1.94	0.49
1:B:39:GLU:HG3	1:B:39:GLU:O	2.12	0.49
5:A:601:CLA:H121	5:A:601:CLA:H92	1.94	0.49
6:A:610:CHL:H142	6:A:612:CHL:C7	2.29	0.49
6:A:611:CHL:H192	6:A:611:CHL:CAA	2.40	0.49
6:B:609:CHL:H142	6:B:609:CHL:C10	2.43	0.49
1:C:133:ILE:N	1:C:133:ILE:CD1	2.75	0.49
1:B:221:ALA:HB3	4:B:504:XAT:H193	1.95	0.49
1:B:213:LEU:HD21	5:B:608:CLA:HHC	1.94	0.49
1:C:190:SER:OG	2:C:501:LUX:H392	2.13	0.49
5:A:603:CLA:C9	5:A:608:CLA:HMD1	2.41	0.49
6:A:611:CHL:CAA	6:A:611:CHL:C19	2.91	0.49
1:B:192:PHE:CZ	5:B:604:CLA:H171	2.47	0.49
1:A:46:TRP:CZ2	6:A:609:CHL:HBA2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:SER:OG	2:B:501:LUX:H392	2.13	0.49
1:C:56:GLU:O	1:C:60:LYS:HG2	2.12	0.49
1:A:22:VAL:CG2	6:A:609:CHL:CBC	2.91	0.48
5:B:604:CLA:C14	5:B:604:CLA:H101	2.42	0.48
3:C:503:NEX:H35	3:C:503:NEX:H401	1.58	0.48
1:B:147:PRO:HB2	6:B:611:CHL:HBB2	1.94	0.48
1:B:191:MET:O	1:B:194:PHE:HB2	2.13	0.48
5:B:605:CLA:C9	5:B:605:CLA:H122	2.43	0.48
2:C:502:LUX:C37	5:C:606:CLA:C2B	2.91	0.48
6:C:610:CHL:H142	6:C:612:CHL:H101	1.94	0.48
1:A:118:LEU:CA	6:A:614:CHL:HED1	2.39	0.48
5:B:606:CLA:HBA1	5:B:606:CLA:CHA	2.38	0.48
6:C:610:CHL:H142	6:C:612:CHL:C7	2.35	0.48
1:C:83:GLU:O	1:C:87:ARG:HG3	2.13	0.48
1:A:73:MET:CE	1:A:184:GLY:N	2.76	0.48
1:C:104:ILE:HD12	1:C:127:ILE:CD1	2.39	0.48
6:C:611:CHL:OMC	6:C:611:CHL:HHC	2.13	0.48
4:B:504:XAT:H3	6:B:609:CHL:H191	1.95	0.48
1:A:83:GLU:O	1:A:87:ARG:HG3	2.13	0.48
1:B:138:VAL:HB	9:B:2002:HOH:O	2.12	0.48
2:B:501:LUX:C37	5:B:603:CLA:CMB	2.89	0.48
6:C:609:CHL:H143	7:C:801:LHG:H211	1.95	0.48
1:B:69:SER:HB3	1:B:184:GLY:HA3	1.95	0.48
6:C:612:CHL:HBC1	6:C:613:CHL:HBB2	1.95	0.48
5:B:607:CLA:H121	5:B:607:CLA:C9	2.09	0.48
1:B:182:LYS:NZ	7:B:801:LHG:O4	2.39	0.48
4:A:504:XAT:H34	5:A:603:CLA:H122	1.95	0.48
5:A:604:CLA:H101	5:A:604:CLA:C14	2.44	0.48
1:C:104:ILE:HD13	1:C:124:ILE:HB	1.95	0.48
1:B:32:SER:HB3	1:B:33:PRO:HD2	1.95	0.48
6:A:610:CHL:H203	6:B:609:CHL:C10	2.44	0.47
1:B:131:GLN:NE2	6:B:610:CHL:HMC	2.28	0.47
6:C:611:CHL:H162	6:C:611:CHL:H141	1.64	0.47
1:B:56:GLU:O	1:B:60:LYS:HG2	2.14	0.47
5:A:601:CLA:H91	5:A:601:CLA:H122	1.94	0.47
2:B:501:LUX:H372	2:B:501:LUX:H27	1.07	0.47
5:B:601:CLA:H111	5:B:601:CLA:C16	2.44	0.47
6:B:610:CHL:H142	6:B:612:CHL:H101	1.95	0.47
1:C:182:LYS:HE2	5:C:607:CLA:O1D	2.14	0.47
4:A:504:XAT:O4	6:A:609:CHL:H162	2.14	0.47
5:B:603:CLA:H161	5:B:608:CLA:C3D	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:611:CHL:H61	6:B:611:CHL:H2	1.60	0.47
4:A:504:XAT:O23	7:A:801:LHG:HC12	2.14	0.47
6:A:610:CHL:H201	6:B:609:CHL:C7	2.43	0.47
1:B:118:LEU:HD23	6:B:614:CHL:HED2	1.95	0.47
1:B:44:TYR:HB2	5:B:604:CLA:HMD1	1.95	0.47
1:A:161:PHE:O	2:A:501:LUX:H4C2	2.15	0.47
1:A:48:THR:HG21	6:C:612:CHL:HAA1	1.97	0.47
2:A:502:LUX:H373	5:A:606:CLA:C3B	2.44	0.47
6:A:611:CHL:OMC	6:A:611:CHL:HHC	2.15	0.47
1:B:192:PHE:CD2	5:B:604:CLA:H171	2.50	0.47
1:C:73:MET:CE	1:C:184:GLY:N	2.78	0.47
2:C:502:LUX:H381	2:C:502:LUX:H281	1.95	0.47
2:A:501:LUX:H102	5:A:601:CLA:CHC	2.45	0.47
1:C:46:TRP:CZ2	6:C:609:CHL:HBA2	2.49	0.47
5:C:607:CLA:C3C	7:C:801:LHG:HC61	2.45	0.47
1:A:227:ASN:O	1:A:228:PHE:HB2	2.15	0.47
1:C:39:GLU:O	1:C:39:GLU:HG3	2.14	0.47
5:A:601:CLA:O1D	5:A:601:CLA:H2A	2.14	0.47
1:B:73:MET:CE	1:B:183:ASN:CB	2.93	0.47
2:C:502:LUX:H122	5:C:604:CLA:HAB	1.97	0.47
6:A:609:CHL:H101	6:C:610:CHL:H203	1.97	0.47
1:B:215:ASP:CG	1:B:218:ASN:HD22	2.18	0.47
1:B:161:PHE:O	2:B:501:LUX:H4C2	2.15	0.47
5:A:603:CLA:CMB	5:A:603:CLA:HBB1	2.14	0.47
1:A:147:PRO:HG2	6:A:611:CHL:HBB2	1.97	0.47
1:B:73:MET:CE	1:B:183:ASN:HB2	2.45	0.47
2:C:502:LUX:C20	5:C:604:CLA:H202	2.45	0.47
2:A:502:LUX:H281	2:A:502:LUX:H381	1.96	0.46
6:A:612:CHL:HBC1	6:A:613:CHL:HBB2	1.95	0.46
1:B:189:PHE:HE1	6:B:609:CHL:HED2	1.80	0.46
6:B:611:CHL:H8	6:B:611:CHL:H52	1.38	0.46
1:C:131:GLN:NE2	6:C:610:CHL:HMC	2.28	0.46
5:B:603:CLA:H151	5:B:608:CLA:HBA2	1.97	0.46
6:B:610:CHL:C20	6:C:609:CHL:C8	2.93	0.46
6:C:611:CHL:H61	6:C:611:CHL:H2	1.47	0.46
5:A:604:CLA:H41	5:A:605:CLA:HBA1	1.97	0.46
6:A:610:CHL:C20	6:B:609:CHL:H8	2.44	0.46
5:A:601:CLA:HMB1	5:A:601:CLA:CBB	2.16	0.46
5:B:603:CLA:HMB1	5:B:603:CLA:CBB	2.20	0.46
6:B:610:CHL:H203	6:C:609:CHL:C10	2.46	0.46
2:B:502:LUX:C20	5:B:604:CLA:H202	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:613:CHL:HBB1	6:B:613:CHL:CMB	2.16	0.46
1:C:73:MET:CG	2:C:501:LUX:H352	2.25	0.46
5:C:601:CLA:O1A	5:C:601:CLA:H3A	2.16	0.46
1:C:32:SER:HB3	1:C:33:PRO:HD2	1.98	0.46
1:C:22:VAL:HG21	6:C:609:CHL:HBC1	1.97	0.46
1:B:112:TYR:O	1:B:118:LEU:HD12	2.16	0.46
5:C:603:CLA:C1A	5:C:603:CLA:CGA	2.94	0.46
5:C:606:CLA:HBA1	5:C:606:CLA:CHA	2.43	0.46
4:A:504:XAT:H363	7:A:801:LHG:C7	2.46	0.46
1:B:104:ILE:HG12	1:B:104:ILE:O	2.16	0.46
1:A:41:PRO:HG3	1:A:177:LYS:HD2	1.98	0.46
1:A:73:MET:CE	1:A:183:ASN:CB	2.94	0.46
1:A:188:MET:HG2	2:A:502:LUX:H352	1.97	0.46
5:A:601:CLA:HBC1	6:A:611:CHL:H201	1.97	0.46
4:B:504:XAT:H34	5:B:603:CLA:H122	1.98	0.46
1:B:84:LEU:HD23	5:B:607:CLA:H191	1.98	0.46
1:B:73:MET:HE1	1:B:184:GLY:N	2.31	0.46
1:B:63:GLU:O	1:B:67:ILE:HG12	2.16	0.46
5:A:607:CLA:C4C	7:A:801:LHG:HC61	2.46	0.45
5:B:605:CLA:H12	1:C:51:LEU:HD21	1.98	0.45
4:C:504:XAT:H371	7:C:801:LHG:H362	1.98	0.45
1:C:147:PRO:HB2	6:C:611:CHL:HBB2	1.99	0.45
6:B:611:CHL:HHC	6:B:611:CHL:OMC	2.16	0.45
1:C:73:MET:HE2	1:C:183:ASN:HB2	1.99	0.45
2:C:501:LUX:H102	5:C:601:CLA:CHC	2.46	0.45
6:C:609:CHL:CHD	6:C:609:CHL:HBC2	2.46	0.45
1:A:23:LYS:HB3	1:A:29:SER:OG	2.15	0.45
1:C:23:LYS:HB3	1:C:29:SER:OG	2.15	0.45
1:A:190:SER:OG	2:A:501:LUX:H392	2.15	0.45
3:A:503:NEX:H35	3:A:503:NEX:H401	1.70	0.45
5:A:603:CLA:C1A	5:A:603:CLA:CGA	2.94	0.45
2:C:502:LUX:H282	2:C:502:LUX:H381	1.99	0.45
1:B:128:TRP:NE1	4:C:504:XAT:C20	2.78	0.45
5:C:607:CLA:C9	5:C:607:CLA:H52	2.36	0.45
6:A:609:CHL:HED3	7:A:801:LHG:H142	1.99	0.45
5:B:604:CLA:H41	5:B:605:CLA:HBA2	1.99	0.45
7:B:801:LHG:HC62	7:B:801:LHG:H242	1.72	0.45
1:C:115:ASN:HB3	1:C:118:LEU:HG	1.98	0.45
1:C:191:MET:O	1:C:194:PHE:HB2	2.15	0.45
5:C:605:CLA:H191	6:C:612:CHL:H51	1.98	0.45
1:C:215:ASP:CG	1:C:218:ASN:HD22	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:503:NEX:H401	3:B:503:NEX:H35	1.63	0.45
1:B:120:HIS:HD2	6:B:614:CHL:HMB3	1.81	0.45
4:C:504:XAT:H10	7:C:801:LHG:H223	1.98	0.45
6:A:609:CHL:H8	6:C:610:CHL:C20	2.46	0.45
1:C:118:LEU:HD23	6:C:614:CHL:HED2	1.96	0.45
1:A:104:ILE:HD13	1:A:124:ILE:HB	1.98	0.45
1:A:131:GLN:NE2	6:A:610:CHL:HMC	2.30	0.45
2:B:501:LUX:H101	5:B:601:CLA:C7	2.45	0.45
2:B:502:LUX:H202	5:B:604:CLA:H202	1.99	0.45
5:C:608:CLA:CHD	5:C:608:CLA:HBC2	2.47	0.45
6:A:610:CHL:C20	6:B:609:CHL:H62	2.33	0.45
6:B:612:CHL:CBC	6:B:613:CHL:CBB	2.95	0.45
6:B:612:CHL:HAC1	6:B:613:CHL:HBB1	1.98	0.45
2:C:501:LUX:H282	2:C:501:LUX:H381	1.96	0.45
1:B:132:VAL:HG12	1:B:133:ILE:N	2.32	0.45
1:A:112:TYR:O	1:A:118:LEU:HD12	2.17	0.45
5:A:605:CLA:C9	5:A:605:CLA:H122	2.47	0.45
5:B:604:CLA:C4	5:B:605:CLA:HBA2	2.47	0.45
1:C:192:PHE:CD2	5:C:604:CLA:C18	2.96	0.45
3:C:503:NEX:H371	6:C:611:CHL:H171	1.98	0.45
4:C:504:XAT:H11	4:C:504:XAT:H191	1.81	0.45
5:A:601:CLA:O1A	5:A:601:CLA:H3A	2.17	0.45
4:B:504:XAT:C37	7:B:801:LHG:H362	2.47	0.45
5:C:603:CLA:H172	5:C:608:CLA:CBA	2.46	0.45
1:B:16:TRP:CZ3	1:B:22:VAL:HG11	2.52	0.44
5:B:603:CLA:H18	5:B:608:CLA:ND	2.33	0.44
5:C:605:CLA:HMD3	6:C:610:CHL:H192	1.98	0.44
1:B:141:TYR:HA	1:B:145:GLY:O	2.17	0.44
1:A:21:ARG:HD3	1:A:38:GLY:HA3	1.99	0.44
4:A:504:XAT:H201	4:A:504:XAT:H15	1.75	0.44
4:A:504:XAT:H35	4:A:504:XAT:H401	1.63	0.44
1:A:192:PHE:CZ	5:A:604:CLA:H171	2.50	0.44
1:B:73:MET:CE	1:B:184:GLY:N	2.80	0.44
1:B:73:MET:HG2	2:B:501:LUX:C14	2.47	0.44
2:C:502:LUX:H27	2:C:502:LUX:H372	1.34	0.44
1:B:138:VAL:HA	1:B:141:TYR:CD1	2.52	0.44
3:A:503:NEX:H371	6:A:611:CHL:H171	1.98	0.44
1:C:178:VAL:O	1:C:182:LYS:HG3	2.17	0.44
1:A:21:ARG:HH11	1:A:21:ARG:HG2	1.81	0.44
1:C:41:PRO:HG3	1:C:177:LYS:HD2	2.00	0.44
1:A:213:LEU:HD21	5:A:608:CLA:HHC	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG12	1:A:230:PRO:O	2.18	0.44
6:A:611:CHL:H61	6:A:611:CHL:H2	1.49	0.44
6:A:612:CHL:C19	6:A:612:CHL:H152	2.27	0.44
1:B:192:PHE:CD2	5:B:604:CLA:C18	2.96	0.44
4:B:504:XAT:H10	7:B:801:LHG:H223	1.99	0.44
1:C:118:LEU:O	1:C:120:HIS:N	2.47	0.44
1:C:166:LEU:CD1	2:C:501:LUX:H173	2.48	0.44
1:C:189:PHE:HE1	6:C:609:CHL:HED2	1.83	0.44
1:C:212:HIS:O	1:C:216:PRO:N	2.50	0.44
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.82	0.44
1:A:191:MET:O	1:A:194:PHE:HB2	2.18	0.44
5:A:605:CLA:H12	1:B:51:LEU:HD21	1.99	0.44
1:C:44:TYR:HB2	5:C:604:CLA:HMD1	1.99	0.44
6:C:610:CHL:H141	6:C:610:CHL:H172	2.00	0.44
1:B:169:ASP:HA	1:B:170:PRO:HD3	1.82	0.44
1:A:44:TYR:HB2	5:A:604:CLA:HMD1	1.98	0.44
6:A:609:CHL:C10	6:C:610:CHL:H203	2.48	0.44
2:B:502:LUX:H281	2:B:502:LUX:H381	1.99	0.44
5:B:606:CLA:H102	6:B:614:CHL:HED3	1.99	0.44
1:C:188:MET:HB3	2:C:502:LUX:H142	2.00	0.44
5:C:604:CLA:H41	5:C:605:CLA:CBA	2.47	0.44
4:C:504:XAT:H35	4:C:504:XAT:H401	1.76	0.44
1:A:138:VAL:HA	1:A:141:TYR:CD1	2.52	0.44
2:A:501:LUX:H27	2:A:501:LUX:H372	1.05	0.43
6:B:610:CHL:H143	6:B:610:CHL:H112	1.87	0.43
1:C:73:MET:CE	1:C:183:ASN:HB2	2.48	0.43
1:B:118:LEU:O	1:B:120:HIS:N	2.43	0.43
4:C:504:XAT:H363	7:C:801:LHG:C7	2.48	0.43
2:A:502:LUX:H282	2:A:502:LUX:H381	2.00	0.43
5:A:601:CLA:CMB	5:A:601:CLA:HBB1	2.17	0.43
2:A:501:LUX:H111	5:A:601:CLA:HMC2	1.99	0.43
1:A:118:LEU:HD23	6:A:614:CHL:HED2	2.00	0.43
2:B:502:LUX:H122	5:B:604:CLA:HAB	1.99	0.43
1:C:161:PHE:C	1:C:163:PRO:HD3	2.38	0.43
1:C:84:LEU:HD23	5:C:607:CLA:H191	2.01	0.43
1:A:22:VAL:HG21	6:A:609:CHL:HBC1	2.00	0.43
1:A:98:PHE:HB2	6:A:610:CHL:HMA2	2.00	0.43
2:C:501:LUX:H27	2:C:501:LUX:H372	1.17	0.43
1:C:221:ALA:HB3	4:C:504:XAT:H193	2.01	0.43
6:C:612:CHL:C15	6:C:612:CHL:C19	2.91	0.43
1:B:124:ILE:HG23	1:B:125:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.84	0.43
5:A:606:CLA:H112	5:A:606:CLA:H61	2.00	0.43
1:A:147:PRO:CG	6:A:611:CHL:HBB2	2.48	0.43
7:A:801:LHG:H242	7:A:801:LHG:HC62	1.77	0.43
6:B:611:CHL:HAA2	6:B:611:CHL:C19	2.40	0.43
1:C:102:SER:HB3	6:C:610:CHL:CED	2.49	0.43
1:B:128:TRP:HE1	4:C:504:XAT:C20	2.31	0.43
1:C:200:VAL:O	8:C:802:DGD:HE2	2.18	0.43
1:A:22:VAL:HG21	6:A:609:CHL:CBC	2.49	0.43
1:B:193:GLY:HA2	5:B:603:CLA:C3C	2.49	0.43
1:B:160:SER:O	6:B:611:CHL:C6	2.67	0.43
6:B:612:CHL:CBC	6:B:613:CHL:HBB2	2.47	0.43
1:C:71:TRP:CD1	6:C:612:CHL:HMD3	2.54	0.43
1:A:161:PHE:C	1:A:163:PRO:HD3	2.39	0.43
4:B:504:XAT:H403	7:B:801:LHG:C12	2.49	0.43
1:B:220:ASN:CG	5:B:608:CLA:HED1	2.38	0.43
5:B:605:CLA:HBC1	6:B:612:CHL:CBC	2.48	0.43
5:C:601:CLA:CBC	6:C:611:CHL:H201	2.49	0.43
6:C:611:CHL:HBA2	6:C:611:CHL:HBD	2.01	0.43
1:A:169:ASP:HA	1:A:170:PRO:HD3	1.86	0.43
5:A:607:CLA:C3C	7:A:801:LHG:HC61	2.49	0.43
1:B:166:LEU:CD1	2:B:501:LUX:H173	2.48	0.43
3:C:503:NEX:C35	6:C:611:CHL:HMB3	2.48	0.43
6:C:609:CHL:HED3	7:C:801:LHG:H142	2.00	0.43
7:C:801:LHG:H242	7:C:801:LHG:HC62	1.71	0.43
4:A:504:XAT:H11	4:A:504:XAT:H191	1.68	0.43
6:A:610:CHL:HMB1	6:A:610:CHL:HAB	1.85	0.43
4:B:504:XAT:H15	4:B:504:XAT:H201	1.62	0.43
5:C:601:CLA:CBB	5:C:601:CLA:HMB1	2.21	0.43
5:C:607:CLA:C9	5:C:607:CLA:C5	2.93	0.43
1:B:94:GLU:HG2	1:B:99:LYS:HB2	2.01	0.43
1:A:166:LEU:CD1	2:A:501:LUX:H173	2.49	0.43
8:A:802:DGD:HE3	8:A:802:DGD:HD62	2.01	0.43
2:B:502:LUX:C37	5:B:606:CLA:C2B	2.96	0.43
6:C:610:CHL:CBB	6:C:612:CHL:HBC1	2.47	0.43
1:A:66:VAL:HB	1:A:155:LEU:HD13	2.00	0.43
1:B:23:LYS:HB3	1:B:29:SER:CB	2.49	0.43
1:A:142:ARG:HG3	6:A:611:CHL:C1D	2.50	0.42
2:A:502:LUX:H162	2:A:502:LUX:H3	1.69	0.42
6:A:611:CHL:H52	6:A:611:CHL:H8	1.41	0.42
6:A:610:CHL:C20	6:B:609:CHL:C8	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HD2	5:C:601:CLA:OBD	2.18	0.42
1:C:76:ALA:N	1:C:191:MET:HE1	2.34	0.42
8:B:802:DGD:C1E	1:C:231:GLY:H	2.32	0.42
3:A:503:NEX:C35	6:A:611:CHL:HMB3	2.49	0.42
5:B:606:CLA:C10	6:B:614:CHL:HED1	2.47	0.42
1:B:71:TRP:CD1	6:B:611:CHL:HED2	2.54	0.42
1:C:213:LEU:HD21	5:C:608:CLA:HHC	2.02	0.42
5:C:602:CLA:HMD2	5:C:607:CLA:C1D	2.48	0.42
6:C:609:CHL:H172	6:C:609:CHL:C14	2.43	0.42
1:A:138:VAL:HG23	9:A:2003:HOH:O	2.20	0.42
4:C:504:XAT:H15	4:C:504:XAT:H201	1.75	0.42
5:C:601:CLA:H111	5:C:601:CLA:C16	2.46	0.42
6:A:610:CHL:H172	6:A:610:CHL:H141	2.02	0.42
6:A:612:CHL:HAB	6:A:612:CHL:HMB1	1.89	0.42
5:B:601:CLA:H3A	5:B:601:CLA:O1A	2.20	0.42
1:A:120:HIS:CE1	1:A:122:GLN:NE2	2.87	0.42
5:B:601:CLA:HBC2	6:B:611:CHL:O1A	2.18	0.42
5:B:605:CLA:H91	5:B:605:CLA:H122	2.01	0.42
1:C:115:ASN:HB3	1:C:118:LEU:CG	2.50	0.42
1:C:15:PRO:O	1:C:22:VAL:HG12	2.19	0.42
6:B:613:CHL:HAA2	6:B:613:CHL:HBD	2.01	0.42
1:B:128:TRP:NE1	4:C:504:XAT:H202	2.34	0.42
6:C:611:CHL:H52	6:C:611:CHL:H8	1.58	0.42
1:A:192:PHE:HD2	5:A:603:CLA:HMC1	1.84	0.42
5:A:603:CLA:H161	5:A:608:CLA:C3D	2.49	0.42
5:A:605:CLA:C9	5:A:605:CLA:H121	2.42	0.42
1:B:157:PRO:HG2	5:B:601:CLA:OBD	2.20	0.42
5:A:605:CLA:HMB1	5:A:605:CLA:HAB	1.88	0.42
5:A:606:CLA:HMC1	5:A:606:CLA:HBC3	2.01	0.42
1:A:18:GLY:O	1:A:21:ARG:HG2	2.19	0.42
1:B:103:GLN:O	1:B:106:SER:HB3	2.20	0.42
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.92	0.42
5:A:601:CLA:CBC	6:A:611:CHL:H201	2.50	0.41
1:B:213:LEU:CD2	5:B:608:CLA:CHC	2.97	0.41
5:C:601:CLA:H3A	5:C:601:CLA:CGA	2.49	0.41
1:A:128:TRP:NE1	4:B:504:XAT:C20	2.83	0.41
1:A:73:MET:HE1	1:A:183:ASN:HB2	2.02	0.41
2:A:502:LUX:H122	5:A:604:CLA:HAB	2.02	0.41
5:A:603:CLA:H18	5:A:608:CLA:ND	2.35	0.41
1:B:178:VAL:O	1:B:182:LYS:HG3	2.20	0.41
1:B:191:MET:HG2	2:B:502:LUX:H322	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:CLA:H122	5:B:601:CLA:H161	1.88	0.41
6:B:611:CHL:CAA	6:B:611:CHL:H192	2.43	0.41
5:C:604:CLA:CGA	5:C:604:CLA:H3A	2.50	0.41
1:B:19:PRO:CD	1:B:20:ASP:H	2.33	0.41
1:C:120:HIS:CE1	1:C:122:GLN:NE2	2.87	0.41
1:C:138:VAL:HB	9:C:2001:HOH:O	2.20	0.41
1:A:221:ALA:CB	4:A:504:XAT:H193	2.51	0.41
5:A:604:CLA:H3A	5:A:604:CLA:CGA	2.50	0.41
6:A:610:CHL:H142	6:A:612:CHL:H101	2.01	0.41
6:B:614:CHL:HAB	6:B:614:CHL:HMB1	1.89	0.41
2:C:501:LUX:H312	5:C:602:CLA:HMC2	2.01	0.41
5:C:601:CLA:C3A	5:C:601:CLA:CGA	2.98	0.41
1:B:192:PHE:HD2	5:B:603:CLA:HMC1	1.86	0.41
5:B:603:CLA:H61	5:B:603:CLA:H2	1.85	0.41
8:C:802:DGD:HB21	8:C:802:DGD:HB52	1.91	0.41
6:A:609:CHL:C8	6:C:610:CHL:C20	2.98	0.41
6:A:613:CHL:HAA2	6:A:613:CHL:HBD	2.01	0.41
4:B:504:XAT:H401	4:B:504:XAT:H35	1.65	0.41
2:A:501:LUX:C10	5:A:601:CLA:H72	2.50	0.41
1:B:229:VAL:HG12	1:B:230:PRO:O	2.20	0.41
2:B:501:LUX:H371	2:B:501:LUX:H271	1.68	0.41
5:B:603:CLA:C9	5:B:608:CLA:CMD	2.96	0.41
1:B:169:ASP:OD2	1:B:170:PRO:HD2	2.20	0.41
1:A:157:PRO:HB3	6:A:611:CHL:HBC2	2.03	0.41
8:A:802:DGD:C1E	1:B:231:GLY:H	2.33	0.41
1:C:104:ILE:O	1:C:104:ILE:HG12	2.21	0.41
8:C:802:DGD:HE3	8:C:802:DGD:HD62	2.01	0.41
1:C:153:ASP:HA	1:C:154:PRO:HD3	1.92	0.41
5:A:606:CLA:H93	6:A:614:CHL:OBD	2.21	0.41
3:B:503:NEX:C35	6:B:611:CHL:HMB3	2.51	0.41
6:B:611:CHL:C19	6:B:611:CHL:CAA	2.99	0.41
6:B:611:CHL:CHA	6:B:611:CHL:HBA2	2.51	0.41
6:B:612:CHL:HAB	6:B:612:CHL:HMB1	1.92	0.41
5:C:606:CLA:H61	5:C:606:CLA:H112	2.03	0.41
1:A:115:ASN:HB3	1:A:118:LEU:HG	2.01	0.41
5:A:608:CLA:HBC2	5:A:608:CLA:HHD	2.02	0.41
1:C:157:PRO:HG2	5:C:601:CLA:OBD	2.21	0.41
1:C:193:GLY:HA2	5:C:603:CLA:C3C	2.51	0.41
1:A:192:PHE:CD2	5:A:604:CLA:C18	2.97	0.41
5:A:602:CLA:HBB1	5:A:602:CLA:CHC	2.40	0.41
1:A:64:LEU:HD13	5:A:605:CLA:CAA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:604:CLA:H101	5:C:604:CLA:C14	2.49	0.41
1:C:138:VAL:HA	1:C:141:TYR:CD1	2.56	0.41
2:A:501:LUX:H312	5:A:602:CLA:HMC2	2.04	0.40
5:A:608:CLA:HMB1	5:A:608:CLA:HAB	1.92	0.40
1:C:192:PHE:HD2	5:C:603:CLA:HMC1	1.85	0.40
6:C:611:CHL:HBA2	6:C:611:CHL:CHA	2.51	0.40
1:A:15:PRO:O	1:A:22:VAL:HG12	2.21	0.40
4:A:504:XAT:C5	6:A:609:CHL:H192	2.51	0.40
5:C:605:CLA:H122	5:C:605:CLA:H91	2.03	0.40
1:A:141:TYR:HA	1:A:145:GLY:O	2.21	0.40
1:A:157:PRO:HD3	6:A:611:CHL:HMD2	2.03	0.40
1:A:229:VAL:HA	1:A:230:PRO:HD3	1.89	0.40
2:A:502:LUX:H193	5:A:604:CLA:C14	2.50	0.40
1:B:220:ASN:O	1:B:223:SER:OG	2.38	0.40
3:B:503:NEX:H11	3:B:503:NEX:H191	1.88	0.40
5:B:603:CLA:C1A	5:B:603:CLA:CGA	2.99	0.40
1:C:118:LEU:CD2	6:C:614:CHL:CED	3.00	0.40
5:C:601:CLA:H2A	5:C:601:CLA:O1D	2.21	0.40
1:C:132:VAL:HG12	1:C:133:ILE:N	2.35	0.40
5:A:607:CLA:HMB1	5:A:607:CLA:HAB	1.92	0.40
4:A:504:XAT:C37	7:A:801:LHG:H362	2.51	0.40
1:C:194:PHE:HZ	2:C:501:LUX:C38	2.13	0.40
7:C:801:LHG:H312	7:C:801:LHG:H282	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/232 (95%)	210 (95%)	10 (4%)	1 (0%)	34	55
1	B	221/232 (95%)	210 (95%)	9 (4%)	2 (1%)	21	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	221/232 (95%)	208 (94%)	10 (4%)	3 (1%)	14 24
All	All	663/696 (95%)	628 (95%)	29 (4%)	6 (1%)	21 37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	C	14	SER
1	A	216	PRO
1	B	216	PRO
1	C	216	PRO
1	C	170	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/181 (93%)	154 (91%)	15 (9%)	12 23
1	B	169/181 (93%)	150 (89%)	19 (11%)	7 14
1	C	169/181 (93%)	155 (92%)	14 (8%)	14 26
All	All	507/543 (93%)	459 (90%)	48 (10%)	11 20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	23	LYS
1	A	31	GLU
1	A	39	GLU
1	A	48	THR
1	A	59	SER
1	A	80	VAL
1	A	86	SER
1	A	103	GLN

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Mol	Chain	Res	Type
1	A	106	SER
1	A	110	LEU
1	A	133	ILE
1	A	152	VAL
1	A	175	GLU
1	A	223	SER
1	B	11	SER
1	B	12	SER
1	B	23	LYS
1	B	31	GLU
1	B	34	SER
1	B	39	GLU
1	B	59	SER
1	B	62	ARG
1	B	79	SER
1	B	80	VAL
1	B	86	SER
1	B	103	GLN
1	B	106	SER
1	B	110	LEU
1	B	133	ILE
1	B	143	ILE
1	B	152	VAL
1	B	175	GLU
1	B	223	SER
1	C	11	SER
1	C	23	LYS
1	C	31	GLU
1	C	34	SER
1	C	39	GLU
1	C	59	SER
1	C	80	VAL
1	C	86	SER
1	C	106	SER
1	C	110	LEU
1	C	133	ILE
1	C	152	VAL
1	C	175	GLU
1	C	223	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	197	GLN
1	A	208	ASN
1	A	218	ASN
1	B	122	GLN
1	B	131	GLN
1	B	197	GLN
1	B	208	ASN
1	B	218	ASN
1	C	122	GLN
1	C	131	GLN
1	C	218	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

60 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LUX	A	501	-	42,43,43	4.31	26 (61%)	55,60,60	3.58	30 (54%)
2	LUX	A	502	-	42,43,43	4.28	24 (57%)	55,60,60	3.57	31 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NEX	A	503	-	39,46,46	2.55	12 (30%)	48,70,70	2.02	11 (22%)
4	XAT	A	504	-	41,47,47	2.45	14 (34%)	48,74,74	2.75	19 (39%)
5	CLA	A	601	1	55,73,73	1.21	6 (10%)	61,113,113	1.75	14 (22%)
5	CLA	A	602	1	50,68,73	1.36	6 (12%)	55,107,113	1.49	9 (16%)
5	CLA	A	603	1	55,73,73	1.10	5 (9%)	61,113,113	1.54	11 (18%)
5	CLA	A	604	1	55,73,73	1.08	4 (7%)	61,113,113	1.56	11 (18%)
5	CLA	A	605	1	55,73,73	1.26	7 (12%)	61,113,113	1.69	10 (16%)
5	CLA	A	606	-	47,65,73	1.21	6 (12%)	50,103,113	1.64	9 (18%)
5	CLA	A	607	7	55,73,73	1.20	7 (12%)	61,113,113	1.64	10 (16%)
5	CLA	A	608	1	38,56,73	1.58	6 (15%)	42,92,113	1.90	11 (26%)
6	CHL	A	609	1	57,74,74	1.43	8 (14%)	56,114,114	1.54	9 (16%)
6	CHL	A	610	9	57,74,74	1.64	10 (17%)	56,114,114	1.51	11 (19%)
6	CHL	A	611	9	57,74,74	1.44	9 (15%)	56,114,114	1.63	11 (19%)
6	CHL	A	612	1	57,74,74	1.53	9 (15%)	56,114,114	1.58	8 (14%)
6	CHL	A	613	-	34,54,74	1.91	4 (11%)	32,90,114	1.75	9 (28%)
6	CHL	A	614	1	32,50,74	1.80	6 (18%)	31,85,114	1.98	10 (32%)
7	LHG	A	801	5	48,48,48	1.62	6 (12%)	49,54,54	1.33	4 (8%)
8	DGD	A	802	-	39,39,67	1.28	3 (7%)	51,51,81	1.99	10 (19%)
2	LUX	B	501	-	42,43,43	4.34	24 (57%)	55,60,60	3.82	31 (56%)
2	LUX	B	502	-	42,43,43	4.38	24 (57%)	55,60,60	3.59	30 (54%)
3	NEX	B	503	-	39,46,46	2.54	11 (28%)	48,70,70	2.08	10 (20%)
4	XAT	B	504	-	41,47,47	2.44	14 (34%)	48,74,74	2.73	18 (37%)
5	CLA	B	601	1	55,73,73	1.18	7 (12%)	61,113,113	1.60	11 (18%)
5	CLA	B	602	1	50,68,73	1.31	7 (14%)	55,107,113	1.55	9 (16%)
5	CLA	B	603	1	55,73,73	1.10	5 (9%)	61,113,113	1.62	11 (18%)
5	CLA	B	604	1	55,73,73	1.19	4 (7%)	61,113,113	1.57	11 (18%)
5	CLA	B	605	1	55,73,73	1.31	7 (12%)	61,113,113	1.63	11 (18%)
5	CLA	B	606	-	47,65,73	1.23	6 (12%)	50,103,113	1.63	9 (18%)
5	CLA	B	607	7	55,73,73	1.22	7 (12%)	61,113,113	1.66	11 (18%)
5	CLA	B	608	1	38,56,73	1.45	5 (13%)	42,92,113	1.78	10 (23%)
6	CHL	B	609	1	57,74,74	1.49	7 (12%)	56,114,114	1.59	9 (16%)
6	CHL	B	610	9	57,74,74	1.64	9 (15%)	56,114,114	1.54	11 (19%)
6	CHL	B	611	9	57,74,74	1.45	8 (14%)	56,114,114	1.60	12 (21%)
6	CHL	B	612	1	57,74,74	1.58	8 (14%)	56,114,114	1.57	9 (16%)
6	CHL	B	613	-	34,54,74	1.80	4 (11%)	32,90,114	1.76	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CHL	B	614	1	32,50,74	1.74	6 (18%)	31,85,114	1.98	9 (29%)
7	LHG	B	801	5	48,48,48	1.58	6 (12%)	49,54,54	1.35	5 (10%)
8	DGD	B	802	-	39,39,67	1.28	4 (10%)	51,51,81	1.96	11 (21%)
2	LUX	C	501	-	42,43,43	4.35	24 (57%)	55,60,60	3.66	30 (54%)
2	LUX	C	502	-	42,43,43	4.30	25 (59%)	55,60,60	3.69	32 (58%)
3	NEX	C	503	-	39,46,46	2.43	9 (23%)	48,70,70	2.14	12 (25%)
4	XAT	C	504	-	41,47,47	2.41	14 (34%)	48,74,74	2.41	15 (31%)
5	CLA	C	601	1	55,73,73	1.28	7 (12%)	61,113,113	1.71	13 (21%)
5	CLA	C	602	1	50,68,73	1.32	6 (12%)	55,107,113	1.49	10 (18%)
5	CLA	C	603	1	55,73,73	1.14	5 (9%)	61,113,113	1.59	10 (16%)
5	CLA	C	604	1	55,73,73	1.01	4 (7%)	61,113,113	1.61	10 (16%)
5	CLA	C	605	1	55,73,73	1.22	6 (10%)	61,113,113	1.61	9 (14%)
5	CLA	C	606	-	47,65,73	1.23	5 (10%)	50,103,113	1.60	10 (20%)
5	CLA	C	607	7	55,73,73	1.18	7 (12%)	61,113,113	1.64	11 (18%)
5	CLA	C	608	1	38,56,73	1.40	6 (15%)	42,92,113	1.81	13 (30%)
6	CHL	C	609	1	57,74,74	1.56	7 (12%)	56,114,114	1.55	11 (19%)
6	CHL	C	610	9	57,74,74	1.58	8 (14%)	56,114,114	1.50	11 (19%)
6	CHL	C	611	9	57,74,74	1.50	9 (15%)	56,114,114	1.61	10 (17%)
6	CHL	C	612	1	57,74,74	1.56	9 (15%)	56,114,114	1.57	10 (17%)
6	CHL	C	613	-	34,54,74	1.78	4 (11%)	32,90,114	1.79	9 (28%)
6	CHL	C	614	1	32,50,74	1.79	6 (18%)	31,85,114	1.98	9 (29%)
7	LHG	C	801	5	48,48,48	1.59	6 (12%)	49,54,54	1.31	4 (8%)
8	DGD	C	802	-	39,39,67	1.36	5 (12%)	51,51,81	2.01	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LUX	A	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	A	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	A	503	-	-	0/27/83/83	0/2/3/3
4	XAT	A	504	-	2/2/12/26	0/31/93/93	0/2/4/4
5	CLA	A	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	602	1	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	604	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	606	-	4/4/18/25	0/28/126/135	0/0/9/9
5	CLA	A	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	A	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	A	609	1	-	0/39/137/137	0/0/9/9
6	CHL	A	610	9	-	0/39/137/137	0/0/9/9
6	CHL	A	611	9	-	0/39/137/137	0/0/9/9
6	CHL	A	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	A	613	-	-	0/13/113/137	0/0/9/9
6	CHL	A	614	1	-	0/10/108/137	0/0/9/9
7	LHG	A	801	5	-	0/53/53/53	0/0/0/0
8	DGD	A	802	-	1/1/11/13	0/24/64/95	0/2/2/2
2	LUX	B	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	B	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	B	503	-	-	0/27/83/83	0/2/3/3
4	XAT	B	504	-	2/2/12/26	0/31/93/93	0/2/4/4
5	CLA	B	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	602	1	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	B	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	604	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	606	-	4/4/18/25	0/28/126/135	0/0/9/9
5	CLA	B	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	B	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	B	609	1	-	0/39/137/137	0/0/9/9
6	CHL	B	610	9	-	0/39/137/137	0/0/9/9
6	CHL	B	611	9	-	0/39/137/137	0/0/9/9
6	CHL	B	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	B	613	-	-	0/13/113/137	0/0/9/9
6	CHL	B	614	1	-	0/10/108/137	0/0/9/9
7	LHG	B	801	5	-	0/53/53/53	0/0/0/0
8	DGD	B	802	-	1/1/11/13	0/24/64/95	0/2/2/2
2	LUX	C	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	C	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	C	503	-	-	0/27/83/83	0/2/3/3
4	XAT	C	504	-	2/2/12/26	0/31/93/93	0/2/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	C	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	602	1	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	C	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	604	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	606	-	4/4/18/25	0/28/126/135	0/0/9/9
5	CLA	C	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	C	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	C	609	1	-	0/39/137/137	0/0/9/9
6	CHL	C	610	9	-	0/39/137/137	0/0/9/9
6	CHL	C	611	9	-	0/39/137/137	0/0/9/9
6	CHL	C	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	C	613	-	-	0/13/113/137	0/0/9/9
6	CHL	C	614	1	-	0/10/108/137	0/0/9/9
7	LHG	C	801	5	-	0/53/53/53	0/0/0/0
8	DGD	C	802	-	1/1/11/13	0/24/64/95	0/2/2/2

All (523) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LUX	C26-C25	-10.98	1.34	1.52
2	B	502	LUX	C26-C25	-10.63	1.34	1.52
2	C	502	LUX	C26-C25	-10.59	1.34	1.52
2	A	501	LUX	C26-C25	-10.33	1.35	1.52
2	A	502	LUX	C26-C25	-9.95	1.35	1.52
2	C	501	LUX	C26-C25	-9.93	1.35	1.52
4	A	504	XAT	C26-C27	-8.29	1.36	1.50
4	B	504	XAT	C26-C27	-8.25	1.37	1.50
3	A	503	NEX	C26-C27	-7.91	1.37	1.50
4	C	504	XAT	C26-C27	-7.90	1.37	1.50
3	B	503	NEX	O24-C25	-7.56	1.34	1.46
3	C	503	NEX	C26-C27	-7.29	1.38	1.50
3	B	503	NEX	C26-C27	-7.14	1.38	1.50
3	C	503	NEX	O24-C25	-7.10	1.35	1.46
2	B	501	LUX	C27-C26	-7.09	1.38	1.54
3	A	503	NEX	O24-C25	-6.99	1.35	1.46
2	C	502	LUX	C27-C26	-6.88	1.38	1.54
2	B	502	LUX	C28-C27	-6.67	1.33	1.53
2	A	502	LUX	C27-C26	-6.62	1.39	1.54
2	A	501	LUX	C28-C27	-6.18	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	LUX	C27-C26	-6.10	1.40	1.54
4	C	504	XAT	O24-C25	-6.08	1.36	1.46
3	B	503	NEX	C12-C13	-6.05	1.32	1.45
4	A	504	XAT	O24-C25	-5.98	1.36	1.46
4	B	504	XAT	O24-C25	-5.96	1.36	1.46
2	A	502	LUX	C28-C27	-5.89	1.35	1.53
2	C	502	LUX	C28-C27	-5.88	1.35	1.53
3	A	503	NEX	C12-C13	-5.83	1.33	1.45
2	B	502	LUX	C10-C9	-5.81	1.35	1.54
2	A	501	LUX	C27-C26	-5.77	1.41	1.54
6	A	613	CHL	C4D-CHA	-5.75	1.37	1.45
2	A	502	LUX	C10-C9	-5.71	1.35	1.54
2	C	502	LUX	C10-C9	-5.56	1.35	1.54
2	A	501	LUX	C10-C9	-5.54	1.35	1.54
2	B	501	LUX	C28-C27	-5.51	1.36	1.53
2	B	501	LUX	C10-C9	-5.44	1.36	1.54
6	B	613	CHL	C4D-CHA	-5.31	1.38	1.45
2	C	501	LUX	C10-C9	-5.28	1.36	1.54
3	C	503	NEX	C12-C13	-5.28	1.34	1.45
2	C	501	LUX	C28-C27	-5.07	1.38	1.53
3	A	503	NEX	C32-C33	-5.02	1.34	1.45
2	A	502	LUX	C9-C8	-5.01	1.34	1.51
6	C	613	CHL	C4D-CHA	-4.94	1.38	1.45
2	C	502	LUX	C18-C5	-4.93	1.42	1.51
3	B	503	NEX	C32-C33	-4.92	1.35	1.45
2	C	502	LUX	C9-C8	-4.92	1.35	1.51
4	A	504	XAT	C32-C33	-4.85	1.35	1.45
5	A	608	CLA	C3B-C2B	-4.85	1.33	1.40
2	C	501	LUX	C27-C26	-4.81	1.43	1.54
6	A	610	CHL	C3B-C2B	-4.73	1.34	1.40
4	C	504	XAT	C32-C33	-4.71	1.35	1.45
6	B	610	CHL	C4D-CHA	-4.70	1.39	1.45
6	B	612	CHL	C4D-CHA	-4.61	1.39	1.45
6	C	609	CHL	C4D-CHA	-4.59	1.39	1.45
2	C	501	LUX	C9-C8	-4.59	1.36	1.51
4	A	504	XAT	C12-C13	-4.57	1.35	1.45
2	B	502	LUX	C9-C8	-4.52	1.36	1.51
6	A	609	CHL	C4D-CHA	-4.52	1.39	1.45
4	B	504	XAT	C32-C33	-4.52	1.35	1.45
2	A	501	LUX	C4-C5	-4.43	1.44	1.51
5	B	608	CLA	C3B-C2B	-4.39	1.34	1.40
4	A	504	XAT	C28-C29	-4.37	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LUX	C9-C8	-4.37	1.36	1.51
3	C	503	NEX	C28-C29	-4.36	1.36	1.45
6	A	610	CHL	C4D-CHA	-4.29	1.39	1.45
4	C	504	XAT	C28-C29	-4.24	1.36	1.45
4	B	504	XAT	C12-C13	-4.23	1.36	1.45
2	B	501	LUX	C9-C8	-4.21	1.37	1.51
5	C	601	CLA	C3B-C2B	-4.13	1.34	1.40
3	C	503	NEX	C32-C33	-4.11	1.36	1.45
6	A	612	CHL	C4D-CHA	-4.10	1.39	1.45
5	B	605	CLA	C3B-C2B	-4.08	1.34	1.40
6	C	610	CHL	C4D-CHA	-4.04	1.40	1.45
6	C	612	CHL	C4D-CHA	-4.03	1.40	1.45
4	B	504	XAT	C28-C29	-4.02	1.37	1.45
6	B	610	CHL	C3B-C2B	-4.02	1.35	1.40
2	C	501	LUX	C4-C5	-4.00	1.45	1.51
2	C	501	LUX	C15-C14	-3.97	1.33	1.52
6	C	611	CHL	C4D-CHA	-3.95	1.40	1.45
2	A	502	LUX	C31-C30	-3.94	1.34	1.52
2	B	501	LUX	C31-C30	-3.94	1.34	1.52
3	B	503	NEX	C28-C29	-3.90	1.37	1.45
2	A	502	LUX	C11-C12	-3.90	1.34	1.52
2	A	502	LUX	C31-C32	-3.85	1.34	1.52
3	A	503	NEX	C11-C10	-3.84	1.31	1.43
5	A	602	CLA	C3B-C2B	-3.84	1.35	1.40
2	B	502	LUX	C11-C12	-3.82	1.34	1.52
2	B	502	LUX	C31-C32	-3.81	1.34	1.52
6	C	610	CHL	C3B-C2B	-3.80	1.35	1.40
6	B	609	CHL	C4D-CHA	-3.79	1.40	1.45
2	C	502	LUX	C15-C14	-3.78	1.34	1.52
4	C	504	XAT	C12-C13	-3.74	1.37	1.45
2	A	501	LUX	C15-C14	-3.72	1.35	1.52
2	C	502	LUX	C11-C12	-3.70	1.35	1.52
5	C	608	CLA	C3B-C2B	-3.69	1.35	1.40
2	B	502	LUX	C31-C30	-3.68	1.35	1.52
2	C	502	LUX	C31-C30	-3.66	1.35	1.52
2	B	502	LUX	C32-C33	-3.65	1.33	1.52
6	A	614	CHL	C4D-CHA	-3.64	1.40	1.45
6	B	611	CHL	C4D-CHA	-3.63	1.40	1.45
3	A	503	NEX	C28-C29	-3.61	1.37	1.45
2	A	501	LUX	C31-C30	-3.61	1.35	1.52
3	C	503	NEX	C15-C14	-3.56	1.32	1.43
2	A	501	LUX	C35-C34	-3.56	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	LUX	C32-C33	-3.54	1.34	1.52
2	B	501	LUX	C11-C12	-3.53	1.35	1.52
2	B	501	LUX	C35-C34	-3.53	1.35	1.52
5	A	605	CLA	C3B-C2B	-3.53	1.35	1.40
6	A	611	CHL	C4D-CHA	-3.52	1.40	1.45
2	C	501	LUX	C35-C34	-3.52	1.36	1.52
2	C	502	LUX	C11-C10	-3.51	1.36	1.52
2	C	502	LUX	C31-C32	-3.47	1.36	1.52
2	B	501	LUX	C15-C14	-3.47	1.36	1.52
2	C	501	LUX	C18-C5	-3.46	1.45	1.51
2	B	501	LUX	C30-C29	-3.45	1.34	1.52
2	C	501	LUX	C32-C33	-3.45	1.34	1.52
6	B	612	CHL	C3B-C2B	-3.44	1.35	1.40
6	B	609	CHL	C3B-C2B	-3.44	1.35	1.40
6	A	612	CHL	C3B-C2B	-3.44	1.35	1.40
6	C	609	CHL	C3B-C2B	-3.43	1.35	1.40
2	A	502	LUX	C15-C14	-3.42	1.36	1.52
2	A	501	LUX	C11-C12	-3.42	1.36	1.52
2	B	502	LUX	C12-C13	-3.41	1.34	1.52
4	B	504	XAT	C8-C9	-3.39	1.38	1.45
3	B	503	NEX	C15-C14	-3.37	1.33	1.43
2	A	502	LUX	C12-C13	-3.36	1.35	1.52
2	A	502	LUX	C32-C33	-3.36	1.35	1.52
6	C	614	CHL	C4D-CHA	-3.35	1.40	1.45
5	C	605	CLA	C3B-C2B	-3.34	1.35	1.40
2	A	501	LUX	C31-C32	-3.34	1.36	1.52
2	B	501	LUX	C14-C13	-3.33	1.35	1.52
2	B	502	LUX	C11-C10	-3.33	1.36	1.52
2	B	501	LUX	C11-C10	-3.32	1.36	1.52
2	C	502	LUX	C14-C13	-3.31	1.35	1.52
2	B	501	LUX	C31-C32	-3.31	1.36	1.52
2	A	501	LUX	C14-C13	-3.31	1.35	1.52
2	B	501	LUX	C4-C5	-3.30	1.46	1.51
5	B	601	CLA	C3B-C2B	-3.30	1.36	1.40
2	B	502	LUX	C18-C5	-3.29	1.45	1.51
2	C	502	LUX	C34-C33	-3.29	1.35	1.52
2	C	501	LUX	C30-C29	-3.28	1.35	1.52
2	B	502	LUX	C35-C34	-3.26	1.37	1.52
2	C	502	LUX	C35-C34	-3.26	1.37	1.52
3	B	503	NEX	C11-C10	-3.26	1.33	1.43
2	C	501	LUX	C28-C29	-3.23	1.35	1.52
2	A	502	LUX	C11-C10	-3.23	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	LUX	C14-C13	-3.23	1.35	1.52
2	C	501	LUX	C31-C30	-3.21	1.37	1.52
2	B	502	LUX	C28-C29	-3.20	1.36	1.52
6	B	614	CHL	C4D-CHA	-3.20	1.41	1.45
2	A	501	LUX	C30-C29	-3.19	1.36	1.52
6	A	614	CHL	C3B-C2B	-3.18	1.36	1.40
2	C	501	LUX	C11-C12	-3.17	1.37	1.52
3	C	503	NEX	C11-C10	-3.17	1.33	1.43
2	C	501	LUX	C14-C13	-3.16	1.36	1.52
2	C	501	LUX	C31-C32	-3.16	1.37	1.52
2	B	501	LUX	C18-C5	-3.16	1.45	1.51
2	B	501	LUX	C32-C33	-3.12	1.36	1.52
2	A	501	LUX	C18-C5	-3.11	1.45	1.51
3	A	503	NEX	C15-C14	-3.11	1.34	1.43
2	A	501	LUX	C28-C29	-3.11	1.36	1.52
2	B	502	LUX	C34-C33	-3.10	1.36	1.52
2	C	502	LUX	C30-C29	-3.10	1.36	1.52
6	A	611	CHL	C3B-C2B	-3.09	1.36	1.40
2	C	501	LUX	C12-C13	-3.09	1.36	1.52
2	A	501	LUX	C11-C10	-3.09	1.37	1.52
2	B	502	LUX	C4-C5	-3.09	1.46	1.51
6	C	611	CHL	C3B-C2B	-3.08	1.36	1.40
5	A	607	CLA	C3B-C2B	-3.08	1.36	1.40
3	C	503	NEX	C35-C34	-3.06	1.34	1.43
2	A	501	LUX	C12-C13	-3.05	1.36	1.52
2	C	502	LUX	C12-C13	-3.05	1.36	1.52
2	B	502	LUX	C15-C14	-3.04	1.38	1.52
2	A	502	LUX	C30-C29	-3.03	1.36	1.52
5	C	602	CLA	C3B-C2B	-3.01	1.36	1.40
2	B	501	LUX	C12-C13	-3.00	1.37	1.52
2	A	502	LUX	C35-C34	-2.99	1.38	1.52
6	C	612	CHL	C3B-C2B	-2.98	1.36	1.40
2	A	502	LUX	C7-C6	-2.97	1.34	1.45
2	A	501	LUX	C34-C33	-2.97	1.37	1.52
4	C	504	XAT	C15-C14	-2.93	1.34	1.43
2	A	502	LUX	C14-C13	-2.92	1.37	1.52
2	C	502	LUX	C28-C29	-2.91	1.37	1.52
5	B	602	CLA	C3B-C2B	-2.91	1.36	1.40
5	C	607	CLA	C3B-C2B	-2.90	1.36	1.40
2	A	501	LUX	C32-C33	-2.90	1.37	1.52
2	A	502	LUX	C28-C29	-2.89	1.37	1.52
5	B	607	CLA	C3B-C2B	-2.88	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	611	CHL	C3B-C2B	-2.88	1.36	1.40
2	C	501	LUX	C11-C10	-2.87	1.38	1.52
2	B	501	LUX	C34-C33	-2.86	1.37	1.52
2	B	501	LUX	C28-C29	-2.85	1.37	1.52
2	C	501	LUX	C34-C33	-2.83	1.38	1.52
4	A	504	XAT	C15-C14	-2.81	1.35	1.43
4	C	504	XAT	C11-C10	-2.80	1.35	1.43
2	A	501	LUX	C7-C6	-2.79	1.35	1.45
2	A	502	LUX	C34-C33	-2.79	1.38	1.52
3	B	503	NEX	C31-C30	-2.76	1.35	1.43
4	C	504	XAT	C8-C9	-2.75	1.39	1.45
5	A	606	CLA	C3B-C2B	-2.75	1.36	1.40
2	B	502	LUX	C30-C29	-2.74	1.38	1.52
2	C	501	LUX	C7-C6	-2.74	1.35	1.45
2	B	502	LUX	C7-C6	-2.69	1.35	1.45
2	A	502	LUX	C18-C5	-2.69	1.46	1.51
2	B	501	LUX	C7-C6	-2.68	1.35	1.45
3	A	503	NEX	C31-C30	-2.67	1.35	1.43
5	A	601	CLA	C3B-C2B	-2.66	1.36	1.40
2	C	501	LUX	C35-C15	-2.65	1.36	1.51
5	B	606	CLA	C3B-C2B	-2.64	1.36	1.40
2	C	502	LUX	C4-C5	-2.62	1.47	1.51
3	B	503	NEX	C35-C34	-2.60	1.35	1.43
2	B	502	LUX	C16-C1	-2.57	1.48	1.53
2	B	501	LUX	C35-C15	-2.56	1.36	1.51
2	C	502	LUX	C7-C6	-2.56	1.36	1.45
2	A	501	LUX	C35-C15	-2.55	1.36	1.51
2	A	501	LUX	C17-C1	-2.55	1.48	1.53
3	A	503	NEX	C35-C34	-2.51	1.35	1.43
2	C	502	LUX	O23-C23	-2.51	1.38	1.43
4	B	504	XAT	C31-C30	-2.49	1.36	1.43
4	B	504	XAT	C15-C14	-2.47	1.36	1.43
2	C	502	LUX	C35-C15	-2.43	1.37	1.51
7	B	801	LHG	O7-C5	-2.42	1.40	1.46
4	C	504	XAT	C31-C30	-2.40	1.36	1.43
5	B	605	CLA	C3B-CAB	-2.39	1.42	1.47
3	C	503	NEX	C31-C30	-2.39	1.36	1.43
2	A	502	LUX	C4-C5	-2.38	1.47	1.51
6	A	610	CHL	C3D-C2D	-2.37	1.34	1.40
4	A	504	XAT	C35-C34	-2.36	1.36	1.43
5	C	606	CLA	C3B-C2B	-2.35	1.37	1.40
4	A	504	XAT	C31-C30	-2.33	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	XAT	C8-C9	-2.31	1.40	1.45
4	A	504	XAT	C2-C1	-2.30	1.50	1.54
4	B	504	XAT	C20-C13	-2.29	1.46	1.50
6	A	609	CHL	C3B-C2B	-2.29	1.37	1.40
4	B	504	XAT	C35-C34	-2.29	1.36	1.43
4	B	504	XAT	C11-C10	-2.28	1.36	1.43
6	C	614	CHL	C3B-C2B	-2.28	1.37	1.40
4	C	504	XAT	C35-C34	-2.28	1.36	1.43
6	B	614	CHL	C3B-C2B	-2.27	1.37	1.40
2	A	502	LUX	C35-C15	-2.26	1.38	1.51
3	A	503	NEX	C37-C21	-2.25	1.49	1.53
2	B	502	LUX	C35-C15	-2.25	1.38	1.51
4	C	504	XAT	C16-C1	-2.25	1.49	1.53
3	B	503	NEX	C37-C21	-2.24	1.49	1.53
3	A	503	NEX	C10-C9	-2.23	1.32	1.35
5	C	603	CLA	C3D-C2D	-2.20	1.34	1.40
2	C	502	LUX	C16-C1	-2.19	1.49	1.53
4	A	504	XAT	C11-C10	-2.18	1.37	1.43
2	A	502	LUX	C16-C1	-2.16	1.49	1.53
5	C	608	CLA	C3B-CAB	-2.15	1.43	1.47
7	C	801	LHG	O7-C5	-2.15	1.41	1.46
2	A	501	LUX	C16-C1	-2.15	1.49	1.53
5	B	602	CLA	C3B-CAB	-2.13	1.43	1.47
5	A	605	CLA	C3B-CAB	-2.09	1.43	1.47
5	A	606	CLA	C3D-C2D	-2.08	1.35	1.40
6	A	611	CHL	C1-C2	-2.07	1.42	1.49
7	A	801	LHG	O7-C5	-2.07	1.41	1.46
4	A	504	XAT	C24-C25	-2.07	1.49	1.52
6	A	610	CHL	C3B-CAB	-2.06	1.43	1.47
6	B	609	CHL	O2A-CGA	2.00	1.39	1.33
6	B	611	CHL	C1A-CHA	2.01	1.41	1.37
6	B	612	CHL	CHD-C4C	2.01	1.41	1.35
6	A	612	CHL	CHD-C4C	2.03	1.41	1.35
5	B	601	CLA	C3C-C2C	2.03	1.41	1.36
6	C	611	CHL	O2A-CGA	2.03	1.39	1.33
6	A	610	CHL	CAC-C3C	2.04	1.56	1.51
6	A	612	CHL	O1D-CGD	2.04	1.26	1.21
5	B	604	CLA	O2A-CGA	2.05	1.39	1.33
5	B	601	CLA	O2A-CGA	2.05	1.39	1.33
8	C	802	DGD	C4E-C3E	2.05	1.57	1.52
5	C	604	CLA	O2A-CGA	2.05	1.39	1.33
5	C	601	CLA	CHC-C1C	2.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	610	CHL	CHD-C4C	2.06	1.41	1.35
6	A	611	CHL	CHD-C4C	2.06	1.41	1.35
5	A	604	CLA	O2A-CGA	2.06	1.39	1.33
5	C	607	CLA	O1D-CGD	2.06	1.26	1.21
5	B	607	CLA	O1D-CGD	2.07	1.26	1.21
7	B	801	LHG	O7-C7	2.08	1.40	1.34
6	B	612	CHL	CBA-CGA	2.11	1.56	1.50
6	C	612	CHL	O1D-CGD	2.11	1.26	1.21
6	A	611	CHL	C1A-CHA	2.12	1.42	1.37
5	A	608	CLA	CHC-C1C	2.12	1.41	1.35
5	C	607	CLA	CHC-C1C	2.13	1.41	1.35
6	C	614	CHL	C1A-CHA	2.13	1.42	1.37
6	A	609	CHL	O1D-CGD	2.13	1.26	1.21
6	C	611	CHL	C3D-C4D	2.14	1.44	1.41
6	A	609	CHL	O2A-CGA	2.14	1.39	1.33
5	A	606	CLA	O1D-CGD	2.15	1.26	1.21
5	C	601	CLA	O2A-CGA	2.15	1.39	1.33
6	C	611	CHL	C4-C3	2.17	1.56	1.50
6	B	611	CHL	CHD-C4C	2.17	1.42	1.35
6	B	610	CHL	C4C-NC	2.17	1.41	1.37
6	B	610	CHL	CHD-C4C	2.18	1.42	1.35
6	B	609	CHL	CHD-C4C	2.18	1.42	1.35
5	B	601	CLA	CMC-C2C	2.18	1.55	1.50
6	A	609	CHL	C2-C3	2.19	1.37	1.33
5	A	607	CLA	CHC-C1C	2.20	1.42	1.35
5	A	605	CLA	O2A-CGA	2.20	1.39	1.33
8	B	802	DGD	O6D-C1D	2.20	1.47	1.41
5	C	605	CLA	O2A-CGA	2.20	1.39	1.33
8	B	802	DGD	O6E-C1E	2.21	1.47	1.41
6	C	612	CHL	CBA-CGA	2.22	1.57	1.50
2	B	501	LUX	C23-C24	2.22	1.52	1.50
5	B	606	CLA	O2A-CGA	2.22	1.40	1.33
5	B	605	CLA	O2A-CGA	2.23	1.40	1.33
6	C	611	CHL	C1A-CHA	2.23	1.42	1.37
8	C	802	DGD	O6E-C1E	2.25	1.47	1.41
5	B	603	CLA	O1D-CGD	2.27	1.26	1.21
6	C	612	CHL	C1A-CHA	2.27	1.42	1.37
5	C	608	CLA	CHC-C1C	2.28	1.42	1.35
5	B	606	CLA	O1D-CGD	2.29	1.27	1.21
5	A	603	CLA	O2A-CGA	2.29	1.40	1.33
5	B	603	CLA	O2A-CGA	2.29	1.40	1.33
5	A	602	CLA	O2A-CGA	2.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	CLA	CMC-C2C	2.32	1.55	1.50
5	A	601	CLA	O1D-CGD	2.33	1.27	1.21
5	A	607	CLA	O1D-CGD	2.34	1.27	1.21
6	B	611	CHL	C3D-C4D	2.34	1.45	1.41
5	C	606	CLA	C2-C3	2.34	1.37	1.33
6	A	614	CHL	C1A-CHA	2.36	1.42	1.37
6	A	611	CHL	C3D-C4D	2.36	1.45	1.41
6	A	609	CHL	CHD-C4C	2.36	1.42	1.35
4	C	504	XAT	C8-C7	2.37	1.37	1.32
3	A	503	NEX	C28-C27	2.37	1.37	1.32
5	A	605	CLA	O1D-CGD	2.38	1.27	1.21
5	B	602	CLA	O2A-CGA	2.40	1.40	1.33
4	B	504	XAT	C8-C7	2.40	1.37	1.32
5	A	606	CLA	C2-C3	2.40	1.37	1.33
4	A	504	XAT	C8-C7	2.41	1.37	1.32
5	B	608	CLA	CMC-C2C	2.42	1.56	1.50
8	C	802	DGD	O3G-C1D	2.42	1.44	1.40
5	A	607	CLA	CMC-C2C	2.42	1.56	1.50
4	C	504	XAT	C4-C5	2.42	1.55	1.52
5	C	607	CLA	CMC-C2C	2.42	1.56	1.50
5	C	602	CLA	O2A-CGA	2.42	1.40	1.33
6	C	609	CHL	O2A-CGA	2.42	1.40	1.33
8	A	802	DGD	O6D-C1D	2.43	1.48	1.41
7	A	801	LHG	O7-C7	2.43	1.41	1.34
6	B	614	CHL	CHD-C4C	2.45	1.43	1.35
5	C	601	CLA	C2-C3	2.45	1.37	1.33
8	B	802	DGD	C4E-C3E	2.45	1.58	1.52
6	B	613	CHL	O1D-CGD	2.45	1.27	1.21
3	B	503	NEX	C28-C27	2.46	1.37	1.32
5	C	603	CLA	CMC-C2C	2.47	1.56	1.50
4	B	504	XAT	C4-C3	2.49	1.56	1.52
6	B	611	CHL	O1D-CGD	2.50	1.27	1.21
5	B	607	CLA	CHC-C1C	2.52	1.43	1.35
5	B	603	CLA	C2-C3	2.52	1.37	1.33
5	B	607	CLA	CMC-C2C	2.52	1.56	1.50
5	B	603	CLA	CMC-C2C	2.54	1.56	1.50
6	C	609	CHL	O1D-CGD	2.54	1.27	1.21
4	B	504	XAT	C4-C5	2.54	1.55	1.52
5	A	603	CLA	C2-C3	2.56	1.38	1.33
5	C	603	CLA	C2-C3	2.56	1.38	1.33
5	A	608	CLA	O2A-CGA	2.56	1.41	1.33
6	C	609	CHL	OMC-CMC	2.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	CLA	CMC-C2C	2.58	1.56	1.50
5	A	604	CLA	CMC-C2C	2.58	1.56	1.50
4	A	504	XAT	C4-C5	2.58	1.55	1.52
5	B	608	CLA	O2A-CGA	2.59	1.41	1.33
8	C	802	DGD	O6D-C1D	2.59	1.48	1.41
5	A	608	CLA	O1D-CGD	2.59	1.27	1.21
5	B	606	CLA	C2-C3	2.59	1.38	1.33
5	B	601	CLA	O2D-CGD	2.60	1.39	1.33
5	C	602	CLA	C2-C3	2.60	1.38	1.33
5	C	608	CLA	O1D-CGD	2.60	1.27	1.21
5	C	606	CLA	O1D-CGD	2.61	1.27	1.21
6	B	610	CHL	O1D-CGD	2.61	1.27	1.21
6	A	610	CHL	O2A-CGA	2.61	1.41	1.33
8	A	802	DGD	O3G-C1D	2.61	1.44	1.40
5	A	601	CLA	C2-C3	2.62	1.38	1.33
5	C	603	CLA	O1D-CGD	2.62	1.27	1.21
6	B	610	CHL	O2A-CGA	2.62	1.41	1.33
6	C	610	CHL	O2A-CGA	2.62	1.41	1.33
6	A	611	CHL	O1D-CGD	2.63	1.27	1.21
5	C	605	CLA	C2-C3	2.64	1.38	1.33
5	C	604	CLA	O1D-CGD	2.68	1.27	1.21
5	C	608	CLA	O2A-CGA	2.68	1.41	1.33
5	C	602	CLA	CMC-C2C	2.69	1.56	1.50
6	C	613	CHL	O1D-CGD	2.70	1.28	1.21
5	A	601	CLA	O2A-CGA	2.70	1.41	1.33
5	B	602	CLA	CMC-C2C	2.70	1.56	1.50
6	B	609	CHL	O1D-CGD	2.71	1.28	1.21
5	C	606	CLA	CMC-C2C	2.71	1.56	1.50
6	A	612	CHL	C1A-CHA	2.71	1.43	1.37
5	C	604	CLA	CMC-C2C	2.72	1.56	1.50
5	A	606	CLA	CMC-C2C	2.72	1.56	1.50
5	A	605	CLA	CMC-C2C	2.72	1.56	1.50
7	C	801	LHG	O7-C7	2.73	1.42	1.34
5	B	605	CLA	CMC-C2C	2.74	1.56	1.50
5	C	605	CLA	CMC-C2C	2.76	1.56	1.50
4	C	504	XAT	C4-C3	2.76	1.56	1.52
6	A	613	CHL	O1D-CGD	2.78	1.28	1.21
5	A	607	CLA	O2A-CGA	2.79	1.41	1.33
5	B	605	CLA	O1D-CGD	2.80	1.28	1.21
5	C	605	CLA	O1D-CGD	2.81	1.28	1.21
5	A	605	CLA	C2-C3	2.81	1.38	1.33
6	C	612	CHL	O2A-CGA	2.82	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	614	CHL	O1D-CGD	2.82	1.28	1.21
5	B	604	CLA	CMC-C2C	2.83	1.56	1.50
5	C	607	CLA	O2A-CGA	2.83	1.41	1.33
5	C	607	CLA	C2-C3	2.86	1.38	1.33
5	B	605	CLA	C2-C3	2.87	1.38	1.33
5	A	604	CLA	O1D-CGD	2.87	1.28	1.21
6	A	614	CHL	O1D-CGD	2.87	1.28	1.21
5	A	602	CLA	C2-C3	2.89	1.38	1.33
5	C	601	CLA	O1D-CGD	2.90	1.28	1.21
6	A	612	CHL	O2A-CGA	2.90	1.42	1.33
5	B	602	CLA	C2-C3	2.92	1.38	1.33
5	A	607	CLA	C2-C3	2.95	1.38	1.33
5	A	602	CLA	CMC-C2C	2.95	1.57	1.50
6	B	612	CHL	C2-C3	2.97	1.38	1.33
6	A	610	CHL	O1D-CGD	2.97	1.28	1.21
5	B	602	CLA	O1D-CGD	2.98	1.28	1.21
5	B	607	CLA	C2-C3	3.01	1.38	1.33
5	B	607	CLA	O2A-CGA	3.03	1.42	1.33
5	B	608	CLA	O1D-CGD	3.03	1.28	1.21
6	B	612	CHL	O2A-CGA	3.06	1.42	1.33
6	B	614	CHL	O1D-CGD	3.06	1.28	1.21
5	A	603	CLA	O1D-CGD	3.07	1.28	1.21
5	C	602	CLA	O1D-CGD	3.09	1.29	1.21
6	C	611	CHL	O1D-CGD	3.11	1.29	1.21
6	A	612	CHL	C2-C3	3.11	1.39	1.33
7	B	801	LHG	P-O6	3.12	1.73	1.59
2	A	501	LUX	C23-C24	3.12	1.52	1.50
6	C	612	CHL	C2-C3	3.17	1.39	1.33
5	A	601	CLA	CMC-C2C	3.17	1.57	1.50
5	B	604	CLA	O1D-CGD	3.20	1.29	1.21
5	A	602	CLA	O1D-CGD	3.20	1.29	1.21
6	A	610	CHL	C2-C3	3.22	1.39	1.33
5	B	601	CLA	O1D-CGD	3.23	1.29	1.21
6	C	610	CHL	C2-C3	3.25	1.39	1.33
5	A	604	CLA	O2D-CGD	3.29	1.41	1.33
6	C	610	CHL	O1D-CGD	3.29	1.29	1.21
7	C	801	LHG	P-O6	3.30	1.74	1.59
8	B	802	DGD	O5D-C1E	3.33	1.46	1.40
6	B	613	CHL	O2D-CGD	3.35	1.41	1.33
6	A	612	CHL	O2D-CGD	3.36	1.41	1.33
5	C	601	CLA	CMC-C2C	3.36	1.57	1.50
5	B	607	CLA	O2D-CGD	3.37	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	CLA	C2-C3	3.38	1.39	1.33
6	C	612	CHL	O2D-CGD	3.40	1.41	1.33
5	B	606	CLA	O2D-CGD	3.43	1.41	1.33
6	A	611	CHL	O2D-CGD	3.43	1.41	1.33
6	B	610	CHL	C2-C3	3.43	1.39	1.33
8	A	802	DGD	O5D-C1E	3.43	1.46	1.40
6	B	609	CHL	O2D-CGD	3.44	1.42	1.33
6	C	613	CHL	O2D-CGD	3.45	1.42	1.33
5	A	606	CLA	O2D-CGD	3.47	1.42	1.33
5	A	608	CLA	CMC-C2C	3.48	1.58	1.50
5	C	607	CLA	O2D-CGD	3.48	1.42	1.33
6	C	609	CHL	O2D-CGD	3.51	1.42	1.33
5	C	604	CLA	O2D-CGD	3.54	1.42	1.33
6	A	609	CHL	O2D-CGD	3.55	1.42	1.33
5	B	608	CLA	O2D-CGD	3.55	1.42	1.33
7	A	801	LHG	P-O6	3.59	1.75	1.59
5	C	606	CLA	O2D-CGD	3.59	1.42	1.33
7	C	801	LHG	O8-C23	3.60	1.44	1.33
5	A	607	CLA	O2D-CGD	3.61	1.42	1.33
5	C	601	CLA	O2D-CGD	3.64	1.42	1.33
2	C	501	LUX	C23-C24	3.65	1.53	1.50
6	A	613	CHL	O2D-CGD	3.71	1.42	1.33
5	C	608	CLA	O2D-CGD	3.72	1.42	1.33
6	B	612	CHL	O2D-CGD	3.74	1.42	1.33
7	A	801	LHG	O8-C23	3.79	1.44	1.33
7	B	801	LHG	O8-C23	3.81	1.44	1.33
6	A	614	CHL	O2D-CGD	3.85	1.43	1.33
8	C	802	DGD	O5D-C1E	3.86	1.47	1.40
6	B	614	CHL	O2D-CGD	3.88	1.43	1.33
5	A	603	CLA	O2D-CGD	3.92	1.43	1.33
6	C	614	CHL	O2D-CGD	3.92	1.43	1.33
5	B	603	CLA	O2D-CGD	4.04	1.43	1.33
5	B	602	CLA	O2D-CGD	4.06	1.43	1.33
5	C	602	CLA	O2D-CGD	4.07	1.43	1.33
6	B	611	CHL	O2D-CGD	4.08	1.43	1.33
5	A	602	CLA	O2D-CGD	4.14	1.43	1.33
5	A	605	CLA	O2D-CGD	4.14	1.43	1.33
5	C	603	CLA	O2D-CGD	4.16	1.43	1.33
6	B	610	CHL	O2D-CGD	4.17	1.43	1.33
5	C	605	CLA	O2D-CGD	4.18	1.43	1.33
6	C	610	CHL	O2D-CGD	4.18	1.43	1.33
6	C	611	CHL	O2D-CGD	4.21	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	610	CHL	O2D-CGD	4.27	1.44	1.33
7	B	801	LHG	P-O3	4.29	1.78	1.59
5	A	601	CLA	O2D-CGD	4.31	1.44	1.33
5	B	605	CLA	O2D-CGD	4.31	1.44	1.33
7	C	801	LHG	P-O3	4.37	1.79	1.59
7	A	801	LHG	P-O3	4.47	1.79	1.59
5	A	608	CLA	O2D-CGD	4.55	1.44	1.33
6	A	609	CHL	CMC-C2C	4.72	1.55	1.45
5	B	604	CLA	O2D-CGD	4.76	1.45	1.33
6	C	611	CHL	CMC-C2C	4.79	1.55	1.45
6	C	610	CHL	CMC-C2C	4.82	1.55	1.45
6	B	611	CHL	CMC-C2C	4.86	1.55	1.45
6	B	610	CHL	CMC-C2C	5.07	1.55	1.45
6	A	614	CHL	CMC-C2C	5.14	1.55	1.45
6	B	614	CHL	CMC-C2C	5.23	1.56	1.45
6	A	611	CHL	CMC-C2C	5.25	1.56	1.45
6	C	613	CHL	CMC-C2C	5.44	1.56	1.45
6	A	612	CHL	CMC-C2C	5.46	1.56	1.45
6	A	610	CHL	CMC-C2C	5.54	1.56	1.45
6	B	613	CHL	CMC-C2C	5.58	1.56	1.45
6	B	612	CHL	CMC-C2C	5.68	1.57	1.45
6	B	609	CHL	CMC-C2C	5.72	1.57	1.45
6	A	613	CHL	CMC-C2C	5.75	1.57	1.45
6	C	609	CHL	CMC-C2C	5.84	1.57	1.45
6	C	614	CHL	CMC-C2C	5.88	1.57	1.45
6	C	612	CHL	CMC-C2C	6.00	1.57	1.45
2	A	501	LUX	C5-C6	6.01	1.43	1.34
2	C	501	LUX	C5-C6	6.74	1.45	1.34
2	C	502	LUX	C5-C6	6.76	1.45	1.34
7	B	801	LHG	P-O5	6.95	1.76	1.51
2	B	501	LUX	C5-C6	6.96	1.45	1.34
7	C	801	LHG	P-O5	7.02	1.76	1.51
2	A	502	LUX	C5-C6	7.10	1.45	1.34
7	A	801	LHG	P-O5	7.22	1.77	1.51
2	B	502	LUX	C5-C6	7.56	1.46	1.34
2	C	502	LUX	C24-C25	16.66	1.54	1.33
2	A	502	LUX	C24-C25	17.39	1.55	1.33
2	B	501	LUX	C24-C25	17.40	1.55	1.33
2	A	501	LUX	C24-C25	17.53	1.56	1.33
2	B	502	LUX	C24-C25	17.69	1.56	1.33
2	C	501	LUX	C24-C25	18.70	1.57	1.33

All (743) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	LUX	C23-C24-C25	-16.95	109.38	125.22
2	A	501	LUX	C23-C24-C25	-15.25	110.96	125.22
2	C	501	LUX	C23-C24-C25	-14.86	111.33	125.22
2	A	502	LUX	C23-C24-C25	-12.43	113.60	125.22
2	C	502	LUX	C23-C24-C25	-11.87	114.12	125.22
2	B	502	LUX	C23-C24-C25	-11.59	114.38	125.22
4	B	504	XAT	C37-C21-C22	-10.07	90.97	108.94
4	A	504	XAT	C37-C21-C22	-10.04	91.02	108.94
2	C	502	LUX	C18-C5-C6	-8.89	115.87	124.61
4	C	504	XAT	C37-C21-C22	-8.07	94.55	108.94
2	A	501	LUX	C37-C21-C26	-7.61	92.99	110.44
2	B	502	LUX	C1-C6-C5	-7.58	111.53	122.66
2	C	501	LUX	C37-C21-C26	-7.21	93.91	110.44
2	C	502	LUX	C1-C6-C5	-6.69	112.83	122.66
2	A	502	LUX	C37-C21-C26	-6.64	95.21	110.44
2	B	501	LUX	C37-C21-C26	-6.31	95.97	110.44
2	B	502	LUX	C18-C5-C6	-6.01	118.70	124.61
4	B	504	XAT	O4-C5-C18	-5.98	108.00	114.99
4	C	504	XAT	C25-C24-C23	-5.90	103.45	113.03
4	A	504	XAT	C25-C24-C23	-5.87	103.49	113.03
2	C	501	LUX	C22-C23-C24	-5.48	105.31	111.75
4	B	504	XAT	C25-C24-C23	-5.36	104.31	113.03
2	A	502	LUX	C1-C6-C5	-5.32	114.84	122.66
2	B	502	LUX	C37-C21-C26	-5.31	98.28	110.44
2	A	502	LUX	C18-C5-C6	-5.27	119.43	124.61
4	A	504	XAT	C19-C9-C10	-5.17	115.27	122.90
2	C	502	LUX	C37-C21-C26	-5.12	98.69	110.44
5	C	601	CLA	CAA-C2A-C3A	-5.05	98.69	113.22
2	B	501	LUX	C22-C23-C24	-4.92	105.97	111.75
3	B	503	NEX	C39-C29-C30	-4.77	115.86	122.90
2	B	501	LUX	C36-C21-C26	-4.70	99.67	110.44
5	A	601	CLA	CMB-C2B-C1B	-4.63	120.71	128.36
3	C	503	NEX	C40-C33-C34	-4.61	116.09	122.90
4	C	504	XAT	O4-C5-C18	-4.56	109.66	114.99
3	A	503	NEX	O24-C25-C38	-4.53	109.69	114.99
5	B	601	CLA	CAA-C2A-C3A	-4.48	100.34	113.22
2	A	501	LUX	C36-C21-C26	-4.48	100.17	110.44
5	C	601	CLA	CMB-C2B-C1B	-4.47	120.96	128.36
3	A	503	NEX	C39-C29-C30	-4.44	116.35	122.90
3	B	503	NEX	O24-C26-C25	-4.33	52.49	59.95
5	B	604	CLA	CAA-C2A-C3A	-4.31	100.81	113.22
8	C	802	DGD	C3G-O3G-C1D	-4.26	106.49	113.94
3	C	503	NEX	C39-C29-C30	-4.25	116.62	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	LUX	C36-C21-C26	-4.22	100.76	110.44
4	B	504	XAT	C15-C14-C13	-4.21	121.11	127.20
5	A	604	CLA	CAA-C2A-C3A	-4.17	101.24	113.22
2	B	502	LUX	C37-C21-C22	-4.12	102.07	109.35
4	A	504	XAT	O4-C5-C18	-4.12	110.18	114.99
2	A	501	LUX	C22-C23-C24	-4.05	106.99	111.75
5	C	604	CLA	CAA-C2A-C3A	-4.03	101.62	113.22
4	A	504	XAT	C40-C33-C34	-4.03	116.95	122.90
5	B	608	CLA	C3B-CAB-CBB	-4.02	118.10	126.32
3	C	503	NEX	O24-C26-C25	-3.98	53.08	59.95
8	B	802	DGD	C3G-O3G-C1D	-3.94	107.06	113.94
3	A	503	NEX	O24-C26-C25	-3.93	53.16	59.95
5	C	603	CLA	CMB-C2B-C1B	-3.93	121.86	128.36
5	B	605	CLA	OBD-CAD-CBD	-3.87	120.10	125.94
2	B	501	LUX	C18-C5-C6	-3.84	120.83	124.61
5	C	605	CLA	OBD-CAD-CBD	-3.84	120.14	125.94
5	B	603	CLA	CMB-C2B-C1B	-3.84	122.01	128.36
5	B	602	CLA	C3B-CAB-CBB	-3.82	118.50	126.32
4	B	504	XAT	C19-C9-C10	-3.81	117.28	122.90
5	C	604	CLA	OBD-CAD-CBD	-3.80	120.21	125.94
3	A	503	NEX	C18-C5-C4	-3.78	106.25	110.97
5	A	601	CLA	CAA-C2A-C3A	-3.78	102.36	113.22
5	A	606	CLA	CMB-C2B-C1B	-3.77	122.12	128.36
2	C	502	LUX	C37-C21-C22	-3.77	102.69	109.35
5	A	603	CLA	CMB-C2B-C1B	-3.75	122.16	128.36
2	B	501	LUX	C1-C6-C5	-3.75	117.16	122.66
2	C	501	LUX	C18-C5-C6	-3.74	120.93	124.61
3	B	503	NEX	C40-C33-C34	-3.67	117.48	122.90
3	B	503	NEX	O24-C25-C38	-3.67	110.71	114.99
5	A	602	CLA	C3B-CAB-CBB	-3.64	118.88	126.32
2	B	502	LUX	C2-C3-C4	-3.64	103.88	110.32
5	C	606	CLA	CMB-C2B-C1B	-3.59	122.42	128.36
3	B	503	NEX	C35-C34-C33	-3.59	122.02	127.20
5	C	604	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
6	B	612	CHL	OBD-CAD-CBD	-3.54	120.59	125.94
6	A	610	CHL	C3B-CAB-CBB	-3.53	119.10	126.32
5	A	605	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
5	A	607	CLA	CAA-C2A-C3A	-3.49	103.18	113.22
8	A	802	DGD	C3G-O3G-C1D	-3.49	107.85	113.94
5	B	607	CLA	CAA-C2A-C3A	-3.49	103.19	113.22
5	C	602	CLA	C3B-CAB-CBB	-3.48	119.20	126.32
2	B	502	LUX	C22-C23-C24	-3.46	107.68	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	XAT	C35-C34-C33	-3.45	122.22	127.20
2	C	502	LUX	C1-C2-C3	-3.44	105.33	113.41
5	C	607	CLA	CAA-C2A-C3A	-3.44	103.32	113.22
5	A	603	CLA	CAA-C2A-C3A	-3.42	103.39	113.22
6	A	611	CHL	CAA-C2A-C3A	-3.42	103.39	113.22
4	C	504	XAT	O24-C26-C25	-3.41	54.06	59.95
4	A	504	XAT	C35-C34-C33	-3.40	122.28	127.20
6	A	611	CHL	OBD-CAD-CBD	-3.40	120.81	125.94
5	B	605	CLA	O1D-CGD-CBD	-3.40	119.75	124.62
3	C	503	NEX	C35-C34-C33	-3.38	122.31	127.20
4	B	504	XAT	C40-C33-C34	-3.38	117.91	122.90
5	B	606	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
3	A	503	NEX	C35-C34-C33	-3.38	122.32	127.20
5	B	603	CLA	CAA-C2A-C3A	-3.36	103.55	113.22
6	C	611	CHL	OBD-CAD-CBD	-3.35	120.88	125.94
5	B	607	CLA	OBD-CAD-CBD	-3.33	120.91	125.94
5	A	607	CLA	OBD-CAD-CBD	-3.33	120.92	125.94
6	B	610	CHL	O1D-CGD-CBD	-3.32	119.86	124.62
6	B	611	CHL	CAA-C2A-C3A	-3.32	103.67	113.22
5	A	608	CLA	O1D-CGD-CBD	-3.32	119.87	124.62
3	C	503	NEX	C37-C21-C36	-3.30	102.43	107.35
6	C	611	CHL	C3B-CAB-CBB	-3.30	119.57	126.32
5	A	602	CLA	OBD-CAD-CBD	-3.30	120.96	125.94
5	B	604	CLA	O1D-CGD-CBD	-3.30	119.90	124.62
4	B	504	XAT	O24-C26-C25	-3.30	54.27	59.95
5	A	608	CLA	CAA-C2A-C3A	-3.28	103.78	113.22
6	C	612	CHL	CAA-C2A-C3A	-3.27	103.81	113.22
5	B	604	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
5	C	605	CLA	O1D-CGD-CBD	-3.26	119.95	124.62
4	B	504	XAT	C17-C1-C2	-3.26	103.13	108.94
5	B	602	CLA	OBD-CAD-CBD	-3.23	121.06	125.94
6	B	612	CHL	CAA-C2A-C3A	-3.22	103.94	113.22
4	C	504	XAT	C15-C14-C13	-3.19	122.59	127.20
5	C	603	CLA	CAA-C2A-C3A	-3.18	104.07	113.22
4	C	504	XAT	C19-C9-C10	-3.18	118.20	122.90
6	B	609	CHL	C3B-CAB-CBB	-3.18	119.81	126.32
2	A	502	LUX	C37-C21-C22	-3.18	103.73	109.35
6	A	612	CHL	CAA-C2A-C3A	-3.18	104.08	113.22
2	C	502	LUX	C7-C6-C5	-3.18	114.10	121.37
6	B	610	CHL	C3B-CAB-CBB	-3.17	119.83	126.32
5	B	605	CLA	C3B-CAB-CBB	-3.16	119.85	126.32
4	A	504	XAT	O24-C26-C25	-3.16	54.50	59.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	604	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
6	A	614	CHL	O1D-CGD-CBD	-3.15	120.10	124.62
6	C	610	CHL	C3B-CAB-CBB	-3.15	119.88	126.32
5	A	608	CLA	CMB-C2B-C1B	-3.14	123.17	128.36
6	C	612	CHL	C3B-CAB-CBB	-3.11	119.95	126.32
5	A	604	CLA	CMB-C2B-C1B	-3.10	123.23	128.36
5	C	608	CLA	CBC-CAC-C3C	-3.10	102.92	112.39
6	B	612	CHL	C3B-CAB-CBB	-3.10	119.98	126.32
5	A	605	CLA	O1D-CGD-CBD	-3.05	120.25	124.62
5	C	608	CLA	CMB-C2B-C1B	-3.04	123.33	128.36
2	C	502	LUX	C36-C21-C26	-3.04	103.47	110.44
4	C	504	XAT	C40-C33-C34	-3.02	118.44	122.90
5	C	602	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
5	C	607	CLA	CMB-C2B-C1B	-3.02	123.36	128.36
5	C	607	CLA	C3B-CAB-CBB	-3.02	120.15	126.32
5	A	608	CLA	C2C-C1C-NC	-3.01	108.00	110.24
5	B	607	CLA	C2C-C1C-NC	-3.00	108.01	110.24
6	B	611	CHL	C3B-CAB-CBB	-2.99	120.19	126.32
5	C	608	CLA	CAA-C2A-C3A	-2.99	104.63	113.22
5	B	601	CLA	CMB-C2B-C1B	-2.99	123.42	128.36
6	B	613	CHL	OBD-CAD-CBD	-2.99	121.43	125.94
5	A	605	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
5	B	608	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
5	B	607	CLA	C3B-CAB-CBB	-2.96	120.27	126.32
5	B	607	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
4	B	504	XAT	C31-C30-C29	-2.95	122.94	127.20
6	B	614	CHL	O1D-CGD-CBD	-2.95	120.40	124.62
6	C	611	CHL	OMC-CMC-C2C	-2.94	118.03	125.58
6	A	612	CHL	C3B-CAB-CBB	-2.94	120.31	126.32
4	B	504	XAT	C20-C13-C14	-2.93	118.57	122.90
6	B	611	CHL	OMC-CMC-C2C	-2.93	118.05	125.58
5	C	604	CLA	O1D-CGD-CBD	-2.92	120.44	124.62
6	C	611	CHL	CAA-C2A-C3A	-2.92	104.83	113.22
5	A	608	CLA	OBD-CAD-CBD	-2.92	121.53	125.94
6	B	611	CHL	OBD-CAD-CBD	-2.91	121.54	125.94
2	A	502	LUX	C2-C3-C4	-2.91	105.16	110.32
5	A	601	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
6	B	609	CHL	OBD-CAD-CBD	-2.90	121.57	125.94
5	B	606	CLA	O1D-CGD-CBD	-2.90	120.47	124.62
6	C	612	CHL	O1D-CGD-CBD	-2.89	120.49	124.62
5	B	603	CLA	O1D-CGD-CBD	-2.87	120.51	124.62
5	A	601	CLA	C2C-C1C-NC	-2.86	108.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	XAT	C15-C14-C13	-2.85	123.08	127.20
6	A	611	CHL	C3B-CAB-CBB	-2.84	120.50	126.32
6	C	613	CHL	OBD-CAD-CBD	-2.84	121.65	125.94
5	B	608	CLA	CAA-C2A-C3A	-2.84	105.05	113.22
5	B	608	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
6	C	609	CHL	C3B-CAB-CBB	-2.83	120.53	126.32
6	A	613	CHL	OBD-CAD-CBD	-2.82	121.68	125.94
5	A	601	CLA	CAA-CBA-CGA	-2.82	105.06	113.32
6	B	612	CHL	O1D-CGD-CBD	-2.80	120.61	124.62
6	B	611	CHL	O1D-CGD-CBD	-2.79	120.62	124.62
6	C	610	CHL	OMC-CMC-C2C	-2.78	118.44	125.58
5	C	601	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
5	A	601	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
5	C	601	CLA	O2A-CGA-O1A	-2.76	116.37	123.49
6	C	610	CHL	O1D-CGD-CBD	-2.75	120.68	124.62
5	A	604	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
5	A	607	CLA	C2C-C1C-NC	-2.75	108.20	110.24
2	A	502	LUX	C1-C2-C3	-2.75	106.97	113.41
6	C	612	CHL	OBD-CAD-CBD	-2.75	121.80	125.94
4	A	504	XAT	C17-C1-C2	-2.74	104.05	108.94
6	C	614	CHL	O1D-CGD-CBD	-2.74	120.70	124.62
6	B	614	CHL	OBD-CAD-CBD	-2.74	121.81	125.94
5	C	607	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
5	B	601	CLA	OBD-CAD-CBD	-2.72	121.84	125.94
2	A	501	LUX	C18-C5-C6	-2.71	121.94	124.61
5	A	607	CLA	C3B-CAB-CBB	-2.70	120.79	126.32
5	C	606	CLA	OBD-CAD-CBD	-2.70	121.87	125.94
2	B	502	LUX	C36-C21-C26	-2.69	104.26	110.44
6	C	609	CHL	OBD-CAD-CBD	-2.69	121.88	125.94
6	C	610	CHL	OBD-CAD-CBD	-2.69	121.88	125.94
6	A	614	CHL	CAA-C2A-C3A	-2.68	109.78	116.20
6	A	610	CHL	OBD-CAD-CBD	-2.67	121.91	125.94
6	A	614	CHL	OBD-CAD-CBD	-2.66	121.92	125.94
5	C	607	CLA	O1D-CGD-CBD	-2.66	120.81	124.62
5	C	608	CLA	OBD-CAD-CBD	-2.65	121.93	125.94
5	A	607	CLA	CMB-C2B-C1B	-2.65	123.97	128.36
5	A	603	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
6	C	609	CHL	OMC-CMC-C2C	-2.63	118.82	125.58
5	B	605	CLA	CMB-C2B-C1B	-2.63	124.02	128.36
5	B	601	CLA	O2A-CGA-O1A	-2.61	116.75	123.49
5	C	607	CLA	C2C-C1C-NC	-2.61	108.30	110.24
5	B	606	CLA	OBD-CAD-CBD	-2.60	122.01	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	CLA	CMB-C2B-C1B	-2.60	124.07	128.36
6	A	611	CHL	OMC-CMC-C2C	-2.59	118.92	125.58
6	A	612	CHL	OBD-CAD-CBD	-2.59	122.03	125.94
3	A	503	NEX	C40-C33-C34	-2.58	119.09	122.90
6	A	612	CHL	O1D-CGD-CBD	-2.58	120.93	124.62
5	A	601	CLA	O2A-CGA-O1A	-2.57	116.85	123.49
6	A	613	CHL	O1D-CGD-CBD	-2.57	120.93	124.62
5	B	607	CLA	CMB-C2B-C1B	-2.57	124.11	128.36
5	A	607	CLA	O1D-CGD-CBD	-2.56	120.96	124.62
5	A	606	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
5	A	606	CLA	O1D-CGD-CBD	-2.54	120.98	124.62
5	C	605	CLA	C3B-CAB-CBB	-2.54	121.13	126.32
5	C	608	CLA	C4B-CHC-C1C	-2.54	123.81	129.26
6	A	609	CHL	OBD-CAD-CBD	-2.53	122.12	125.94
5	C	601	CLA	CBC-CAC-C3C	-2.52	104.69	112.39
6	C	614	CHL	OBD-CAD-CBD	-2.52	122.14	125.94
5	B	603	CLA	O2A-CGA-O1A	-2.51	117.02	123.49
6	A	609	CHL	C3B-CAB-CBB	-2.51	121.19	126.32
3	C	503	NEX	C37-C21-C26	-2.50	104.71	110.84
5	A	605	CLA	C2C-C1C-NC	-2.49	108.39	110.24
6	C	613	CHL	OMC-CMC-C2C	-2.48	119.22	125.58
5	C	606	CLA	CAA-C2A-C3A	-2.46	106.13	113.22
2	A	502	LUX	C36-C21-C26	-2.46	104.80	110.44
5	C	608	CLA	C3B-CAB-CBB	-2.46	121.29	126.32
6	B	614	CHL	CAA-C2A-C3A	-2.44	110.35	116.20
5	B	606	CLA	CAA-C2A-C3A	-2.44	106.21	113.22
5	C	606	CLA	O1D-CGD-CBD	-2.43	121.14	124.62
6	A	610	CHL	O1D-CGD-CBD	-2.42	121.15	124.62
6	C	613	CHL	O1D-CGD-CBD	-2.42	121.15	124.62
5	C	605	CLA	CMB-C2B-C1B	-2.41	124.37	128.36
6	B	614	CHL	OMC-CMC-C2C	-2.41	119.39	125.58
5	A	606	CLA	CAA-C2A-C3A	-2.40	106.30	113.22
5	C	606	CLA	O2A-CGA-O1A	-2.40	117.31	123.49
6	B	610	CHL	C1D-CHD-C4C	-2.39	124.13	129.26
6	C	611	CHL	O1D-CGD-CBD	-2.39	121.20	124.62
5	C	603	CLA	O2A-CGA-O1A	-2.38	117.34	123.49
2	C	501	LUX	C1-C6-C5	-2.37	119.18	122.66
5	A	606	CLA	O2A-CGA-O1A	-2.36	117.40	123.49
6	B	610	CHL	OMC-CMC-C2C	-2.36	119.51	125.58
5	B	608	CLA	C2C-C1C-NC	-2.35	108.49	110.24
5	A	603	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
5	B	602	CLA	CMB-C2B-C1B	-2.35	124.48	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	801	LHG	O10-C23-C24	-2.34	114.34	123.72
3	B	503	NEX	C10-C11-C12	-2.32	116.05	123.13
7	C	801	LHG	O10-C23-C24	-2.32	114.44	123.72
5	B	604	CLA	CAA-CBA-CGA	-2.31	106.55	113.32
6	B	610	CHL	OBD-CAD-CBD	-2.31	122.46	125.94
6	A	610	CHL	O2A-CGA-O1A	-2.30	117.55	123.49
6	B	613	CHL	C1D-CHD-C4C	-2.30	124.32	129.26
6	A	614	CHL	OMC-CMC-C2C	-2.30	119.68	125.58
5	C	602	CLA	C2C-C1C-NC	-2.29	108.54	110.24
6	C	614	CHL	CAA-C2A-C3A	-2.28	110.73	116.20
6	B	609	CHL	O2D-CGD-O1D	-2.28	119.09	123.79
2	B	502	LUX	C7-C6-C5	-2.27	116.17	121.37
5	B	608	CLA	CMB-C2B-C1B	-2.26	124.62	128.36
6	A	613	CHL	OMC-CMC-C2C	-2.26	119.77	125.58
5	C	604	CLA	CAA-CBA-CGA	-2.26	106.71	113.32
6	C	609	CHL	O2D-CGD-O1D	-2.25	119.14	123.79
5	B	603	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
5	A	608	CLA	C3B-CAB-CBB	-2.23	121.75	126.32
2	A	502	LUX	C7-C6-C5	-2.23	116.26	121.37
5	A	602	CLA	O2A-CGA-O1A	-2.22	117.75	123.49
3	C	503	NEX	C10-C11-C12	-2.21	116.39	123.13
6	C	614	CHL	C3B-CAB-CBB	-2.21	121.81	126.32
5	C	603	CLA	C2C-C1C-NC	-2.20	108.60	110.24
6	B	613	CHL	OMC-CMC-C2C	-2.20	119.92	125.58
6	A	614	CHL	CMA-C3A-C2A	-2.20	110.93	116.20
5	A	604	CLA	O1D-CGD-CBD	-2.20	121.47	124.62
6	B	614	CHL	C3B-CAB-CBB	-2.19	121.84	126.32
5	B	603	CLA	C2C-C1C-NC	-2.19	108.62	110.24
6	A	611	CHL	O1D-CGD-CBD	-2.18	121.50	124.62
5	B	605	CLA	C2C-C1C-NC	-2.18	108.62	110.24
6	A	614	CHL	C3B-CAB-CBB	-2.17	121.87	126.32
3	A	503	NEX	C10-C11-C12	-2.17	116.51	123.13
6	B	609	CHL	C1D-CHD-C4C	-2.17	124.60	129.26
6	B	613	CHL	O1D-CGD-CBD	-2.17	121.51	124.62
6	A	614	CHL	C1D-CHD-C4C	-2.17	124.61	129.26
5	B	602	CLA	O2A-CGA-O1A	-2.17	117.90	123.49
6	C	610	CHL	O2A-CGA-O1A	-2.16	117.92	123.49
6	A	609	CHL	O2D-CGD-O1D	-2.16	119.33	123.79
5	C	602	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
5	C	608	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
5	C	601	CLA	OBD-CAD-CBD	-2.14	122.71	125.94
6	C	613	CHL	C1D-CHD-C4C	-2.13	124.68	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	614	CHL	CMA-C3A-C2A	-2.13	111.11	116.20
4	C	504	XAT	C35-C34-C33	-2.13	124.13	127.20
2	C	502	LUX	C38-C25-C24	-2.12	118.91	123.59
5	A	602	CLA	CMB-C2B-C1B	-2.11	124.87	128.36
6	C	612	CHL	O2A-CGA-O1A	-2.11	118.04	123.49
5	C	604	CLA	O2A-CGA-O1A	-2.11	118.04	123.49
6	C	614	CHL	OMC-CMC-C2C	-2.11	120.16	125.58
5	A	604	CLA	CAA-CBA-CGA	-2.11	107.14	113.32
6	A	611	CHL	C1D-CHD-C4C	-2.10	124.74	129.26
3	A	503	NEX	C15-C14-C13	-2.09	124.17	127.20
5	C	602	CLA	CMB-C2B-C1B	-2.09	124.90	128.36
4	A	504	XAT	C15-C35-C34	-2.09	118.77	123.39
6	C	609	CHL	C1D-CHD-C4C	-2.08	124.78	129.26
6	C	614	CHL	CMA-C3A-C2A	-2.08	111.21	116.20
5	A	604	CLA	O2A-CGA-O1A	-2.07	118.14	123.49
5	B	602	CLA	O1D-CGD-CBD	-2.07	121.66	124.62
2	B	501	LUX	C38-C25-C24	-2.07	119.03	123.59
6	B	610	CHL	O2A-CGA-O1A	-2.06	118.17	123.49
5	C	608	CLA	O2A-CGA-O1A	-2.06	118.17	123.49
6	C	609	CHL	CAA-C2A-C1A	-2.05	105.22	112.47
6	A	610	CHL	OMC-CMC-C2C	-2.05	120.30	125.58
6	A	613	CHL	C1D-CHD-C4C	-2.05	124.85	129.26
5	B	606	CLA	O2A-CGA-O1A	-2.05	118.21	123.49
2	A	501	LUX	C38-C25-C24	-2.04	119.08	123.59
2	C	502	LUX	C2-C3-C4	-2.04	106.70	110.32
6	B	611	CHL	C1D-CHD-C4C	-2.04	124.88	129.26
7	A	801	LHG	O10-C23-C24	-2.04	115.57	123.72
5	C	602	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
4	C	504	XAT	C17-C1-C2	-2.03	105.31	108.94
6	C	610	CHL	C1D-CHD-C4C	-2.03	124.90	129.26
4	A	504	XAT	C20-C13-C14	-2.03	119.91	122.90
5	B	608	CLA	C4B-CHC-C1C	-2.02	124.92	129.26
6	B	612	CHL	O2A-CGA-O1A	-2.02	118.28	123.49
6	A	609	CHL	O1D-CGD-CBD	-2.02	121.73	124.62
5	B	604	CLA	O2A-CGA-O1A	-2.02	118.29	123.49
3	A	503	NEX	C37-C21-C26	-2.01	105.90	110.84
6	C	611	CHL	C1D-CHD-C4C	-2.01	124.94	129.26
5	C	603	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
3	B	503	NEX	C18-C5-C4	-2.01	108.47	110.97
5	B	601	CLA	CMA-C3A-C2A	-2.01	105.47	114.35
6	A	610	CHL	C3B-C4B-NB	-2.00	107.16	110.94
5	A	603	CLA	C2C-C1C-NC	-2.00	108.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	611	CHL	C4B-CHC-C1C	2.00	125.63	122.60
5	A	602	CLA	CED-O2D-CGD	2.01	120.71	115.99
6	C	612	CHL	C1B-CHB-C4A	2.01	129.14	126.07
7	B	801	LHG	O8-C6-C5	2.02	114.13	108.69
6	B	612	CHL	C4B-CHC-C1C	2.03	125.68	122.60
6	A	613	CHL	C3A-C2A-C1A	2.03	104.94	101.50
2	A	501	LUX	C20-C13-C14	2.03	118.89	111.08
6	A	609	CHL	C1B-CHB-C4A	2.04	129.18	126.07
5	C	605	CLA	C2A-C1A-CHA	2.04	127.64	123.89
5	C	601	CLA	CGD-CBD-CAD	2.05	117.56	110.62
2	C	501	LUX	C39-C29-C28	2.05	118.95	111.08
5	A	604	CLA	CMB-C2B-C3B	2.06	129.11	125.09
5	C	606	CLA	C1D-CHD-C4C	2.06	125.72	122.60
5	C	608	CLA	C2A-C1A-CHA	2.06	127.68	123.89
5	A	608	CLA	C1D-CHD-C4C	2.07	125.74	122.60
5	A	603	CLA	C1D-CHD-C4C	2.08	125.74	122.60
6	B	611	CHL	CMB-C2B-C3B	2.08	129.16	125.09
2	C	502	LUX	C40-C33-C32	2.08	119.08	111.08
6	A	612	CHL	C4B-CHC-C1C	2.09	125.76	122.60
2	C	501	LUX	C15-C35-C34	2.09	121.08	113.66
6	C	614	CHL	C1B-CHB-C4A	2.09	129.26	126.07
2	A	502	LUX	C27-C28-C29	2.10	125.89	115.26
5	B	607	CLA	C1D-CHD-C4C	2.10	125.77	122.60
5	B	605	CLA	C3A-C2A-C1A	2.10	105.06	101.50
5	A	605	CLA	C2A-C1A-CHA	2.11	127.76	123.89
5	B	604	CLA	C1D-CHD-C4C	2.11	125.79	122.60
2	B	501	LUX	C15-C35-C34	2.11	121.16	113.66
6	C	612	CHL	C4B-CHC-C1C	2.12	125.81	122.60
4	B	504	XAT	C37-C21-C26	2.12	116.04	110.84
5	A	601	CLA	CGD-CBD-CAD	2.12	117.81	110.62
2	C	502	LUX	C20-C13-C14	2.13	119.25	111.08
6	A	613	CHL	C4B-CHC-C1C	2.13	125.82	122.60
6	B	611	CHL	C4B-CHC-C1C	2.15	125.86	122.60
2	B	502	LUX	C40-C33-C32	2.15	119.35	111.08
5	A	604	CLA	C1D-CHD-C4C	2.16	125.88	122.60
6	A	610	CHL	C4B-CHC-C1C	2.17	125.88	122.60
2	C	502	LUX	C38-C25-C26	2.17	121.85	117.90
8	C	802	DGD	C1E-O6E-C5E	2.17	117.96	113.75
4	C	504	XAT	C36-C21-C22	2.18	112.82	108.94
2	A	501	LUX	C35-C15-C14	2.18	121.40	113.66
2	B	501	LUX	C39-C29-C30	2.18	119.46	111.08
2	B	502	LUX	C39-C29-C28	2.19	119.50	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	613	CHL	C3A-C2A-C1A	2.20	105.23	101.50
5	C	607	CLA	C1D-CHD-C4C	2.20	125.93	122.60
8	A	802	DGD	C1E-O6E-C5E	2.21	118.04	113.75
5	B	605	CLA	C2A-C1A-CHA	2.22	127.97	123.89
2	A	501	LUX	C2-C1-C6	2.22	114.04	110.49
8	A	802	DGD	O3G-C1D-C2D	2.23	110.86	108.04
4	A	504	XAT	C37-C21-C26	2.24	116.34	110.84
6	C	610	CHL	C4B-CHC-C1C	2.25	126.00	122.60
6	B	609	CHL	CBA-CAA-C2A	2.25	120.09	113.73
5	C	608	CLA	CMB-C2B-C3B	2.26	129.50	125.09
4	C	504	XAT	C6-O4-C5	2.27	63.92	61.25
2	C	501	LUX	C40-C33-C32	2.27	119.81	111.08
8	B	802	DGD	O2G-C1B-C2B	2.29	118.87	111.90
6	A	614	CHL	C4B-CHC-C1C	2.29	126.07	122.60
8	C	802	DGD	O2G-C1B-C2B	2.29	118.89	111.90
2	C	501	LUX	C20-C13-C12	2.29	119.89	111.08
2	C	501	LUX	C20-C13-C14	2.30	119.93	111.08
6	B	609	CHL	C4B-CHC-C1C	2.31	126.10	122.60
6	B	610	CHL	C4B-CHC-C1C	2.31	126.10	122.60
2	C	502	LUX	C35-C15-C14	2.31	121.88	113.66
5	B	601	CLA	CGD-CBD-CAD	2.32	118.47	110.62
6	B	614	CHL	C1B-CHB-C4A	2.32	129.61	126.07
2	A	501	LUX	C2-C3-C4	2.32	114.43	110.32
5	B	606	CLA	CMB-C2B-C3B	2.33	129.64	125.09
2	A	502	LUX	C39-C29-C28	2.33	120.04	111.08
5	B	604	CLA	CMB-C2B-C3B	2.34	129.66	125.09
6	B	611	CHL	C17-C16-C15	2.34	124.58	112.99
6	C	611	CHL	C17-C16-C15	2.34	124.59	112.99
4	C	504	XAT	C32-C33-C34	2.36	122.79	118.98
2	A	502	LUX	C20-C13-C14	2.37	120.19	111.08
8	B	802	DGD	C1E-O6E-C5E	2.37	118.35	113.75
2	B	501	LUX	O3-C3-C2	2.37	114.78	109.91
5	C	606	CLA	CMB-C2B-C3B	2.38	129.74	125.09
3	C	503	NEX	C40-C33-C32	2.39	122.08	118.10
8	A	802	DGD	O2G-C1B-C2B	2.39	119.19	111.90
6	C	609	CHL	C4B-CHC-C1C	2.41	126.24	122.60
6	B	610	CHL	CED-O2D-CGD	2.41	121.64	115.99
8	B	802	DGD	O6D-C5D-C4D	2.42	114.22	109.68
2	A	502	LUX	C15-C35-C34	2.42	122.26	113.66
8	A	802	DGD	O6D-C1D-C2D	2.42	115.25	110.28
4	B	504	XAT	C32-C33-C34	2.43	122.90	118.98
2	B	501	LUX	O23-C23-C24	2.44	113.99	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	XAT	C6-O4-C5	2.44	64.13	61.25
2	B	501	LUX	C35-C15-C14	2.45	122.36	113.66
6	A	609	CHL	CBA-CAA-C2A	2.46	120.66	113.73
5	A	601	CLA	CED-O2D-CGD	2.47	121.78	115.99
2	C	501	LUX	C18-C5-C4	2.48	118.76	114.24
2	B	501	LUX	C19-C9-C10	2.48	119.11	111.13
2	B	501	LUX	C1-C2-C3	2.49	119.26	113.41
8	B	802	DGD	O3G-C1D-C2D	2.49	111.19	108.04
6	A	610	CHL	CED-O2D-CGD	2.50	121.85	115.99
5	B	601	CLA	C5-C3-C2	2.50	125.80	121.05
8	B	802	DGD	O5D-C6D-C5D	2.51	113.62	109.08
6	C	610	CHL	CED-O2D-CGD	2.51	121.88	115.99
8	C	802	DGD	O3G-C1D-C2D	2.52	111.22	108.04
2	B	502	LUX	C20-C13-C12	2.53	120.80	111.08
5	C	604	CLA	CMB-C2B-C3B	2.53	130.04	125.09
8	B	802	DGD	O6D-C1D-C2D	2.55	115.51	110.28
6	C	609	CHL	CBA-CAA-C2A	2.55	120.93	113.73
6	A	611	CHL	C17-C16-C15	2.56	125.70	112.99
7	C	801	LHG	O7-C7-C8	2.57	117.11	111.53
5	A	608	CLA	C3A-C2A-C1A	2.57	105.86	101.50
5	A	606	CLA	CMB-C2B-C3B	2.58	130.13	125.09
2	B	502	LUX	C19-C9-C10	2.58	119.42	111.13
2	B	502	LUX	C15-C35-C34	2.58	122.83	113.66
7	A	801	LHG	O7-C7-C8	2.58	117.14	111.53
5	C	601	CLA	CED-O2D-CGD	2.59	122.07	115.99
2	A	501	LUX	C40-C33-C34	2.60	121.06	111.08
5	B	603	CLA	CMB-C2B-C3B	2.60	130.17	125.09
6	B	613	CHL	CMB-C2B-C3B	2.60	130.18	125.09
2	A	501	LUX	C31-C32-C33	2.61	124.15	115.49
4	B	504	XAT	C6-O4-C5	2.62	64.34	61.25
2	A	501	LUX	O23-C23-C22	2.62	116.53	110.47
2	A	502	LUX	C35-C15-C14	2.62	122.97	113.66
2	C	502	LUX	C39-C29-C28	2.62	121.15	111.08
4	B	504	XAT	O3-C3-C4	2.62	115.29	109.91
2	A	501	LUX	C40-C33-C32	2.62	121.16	111.08
2	C	502	LUX	C3-C4-C5	2.63	117.27	111.86
4	C	504	XAT	C12-C13-C14	2.63	123.22	118.98
4	A	504	XAT	C32-C33-C34	2.63	123.23	118.98
6	C	613	CHL	C4B-CHC-C1C	2.66	126.63	122.60
2	A	501	LUX	C19-C9-C10	2.67	119.70	111.13
6	A	613	CHL	CMB-C2B-C3B	2.67	130.31	125.09
2	A	501	LUX	C20-C13-C12	2.69	121.40	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	LUX	C15-C14-C13	2.69	124.42	115.49
2	A	502	LUX	C39-C29-C30	2.70	121.45	111.08
2	B	501	LUX	C31-C32-C33	2.71	124.46	115.49
5	C	601	CLA	CMB-C2B-C3B	2.71	130.39	125.09
5	A	604	CLA	C4A-NA-C1A	2.72	109.87	106.36
2	C	501	LUX	C19-C9-C8	2.72	117.44	110.89
5	A	603	CLA	CMB-C2B-C3B	2.74	130.44	125.09
2	C	502	LUX	C19-C9-C10	2.75	119.97	111.13
2	C	502	LUX	C40-C33-C34	2.75	121.66	111.08
2	B	502	LUX	C40-C33-C34	2.76	121.67	111.08
5	B	607	CLA	O2A-CGA-CBA	2.76	120.32	111.90
2	B	502	LUX	C18-C5-C4	2.76	119.28	114.24
6	B	613	CHL	C4B-CHC-C1C	2.77	126.80	122.60
4	A	504	XAT	O3-C3-C4	2.79	115.63	109.91
4	B	504	XAT	C36-C21-C22	2.79	113.91	108.94
2	C	501	LUX	C39-C29-C30	2.79	121.81	111.08
2	C	501	LUX	C40-C33-C34	2.79	121.81	111.08
6	C	613	CHL	CMB-C2B-C3B	2.81	130.59	125.09
8	C	802	DGD	O6D-C1D-C2D	2.81	116.05	110.28
2	B	501	LUX	C39-C29-C28	2.81	121.89	111.08
5	B	604	CLA	C4A-NA-C1A	2.81	110.00	106.36
2	B	502	LUX	C20-C13-C14	2.82	121.90	111.08
8	A	802	DGD	O5D-C6D-C5D	2.82	114.19	109.08
5	C	607	CLA	O2A-CGA-CBA	2.83	120.53	111.90
5	A	601	CLA	C4A-NA-C1A	2.84	110.03	106.36
2	C	501	LUX	C31-C32-C33	2.85	124.94	115.49
2	B	502	LUX	C11-C12-C13	2.86	124.97	115.49
2	B	501	LUX	C40-C33-C34	2.86	122.08	111.08
5	C	603	CLA	CMB-C2B-C3B	2.87	130.70	125.09
2	C	502	LUX	C39-C29-C30	2.87	122.11	111.08
6	C	612	CHL	O2A-CGA-CBA	2.87	120.66	111.90
5	C	604	CLA	C4A-NA-C1A	2.89	110.10	106.36
2	A	502	LUX	C20-C13-C12	2.90	122.24	111.08
5	A	607	CLA	O2A-CGA-CBA	2.91	120.77	111.90
2	B	502	LUX	C35-C34-C33	2.92	125.19	115.49
6	C	609	CHL	O2A-CGA-CBA	2.96	120.92	111.90
2	B	501	LUX	C20-C13-C12	2.96	122.47	111.08
6	C	611	CHL	O2A-CGA-CBA	2.98	120.97	111.90
6	A	611	CHL	O2A-CGA-CBA	2.99	121.02	111.90
2	A	502	LUX	C19-C9-C10	3.00	120.76	111.13
5	B	601	CLA	C4A-NA-C1A	3.00	110.23	106.36
2	C	502	LUX	C20-C13-C12	3.01	122.66	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	LUX	C39-C29-C30	3.02	122.70	111.08
5	B	608	CLA	C4A-NA-C1A	3.03	110.27	106.36
6	A	609	CHL	O2A-CGA-CBA	3.03	121.15	111.90
2	A	502	LUX	C40-C33-C34	3.04	122.74	111.08
7	B	801	LHG	O7-C7-C8	3.05	118.16	111.53
6	A	612	CHL	O2A-CGA-CBA	3.05	121.20	111.90
5	B	604	CLA	O2A-CGA-CBA	3.07	121.24	111.90
2	B	501	LUX	C18-C5-C4	3.07	119.84	114.24
2	A	501	LUX	C15-C14-C13	3.08	125.70	115.49
5	B	605	CLA	O2A-CGA-CBA	3.08	121.29	111.90
6	B	611	CHL	O2A-CGA-CBA	3.08	121.30	111.90
5	A	601	CLA	C11-C10-C8	3.09	125.72	115.49
2	A	502	LUX	C11-C10-C9	3.09	124.82	114.85
6	B	612	CHL	O2A-CGA-CBA	3.10	121.33	111.90
2	A	501	LUX	C39-C29-C30	3.10	122.98	111.08
2	C	501	LUX	C19-C9-C10	3.11	121.12	111.13
5	C	602	CLA	O2A-CGA-CBA	3.12	121.42	111.90
3	B	503	NEX	C16-C1-C6	3.16	113.31	110.48
4	A	504	XAT	C12-C13-C14	3.17	124.10	118.98
2	B	501	LUX	C35-C34-C33	3.18	126.02	115.49
2	B	501	LUX	C15-C14-C13	3.18	126.04	115.49
2	C	502	LUX	C31-C32-C33	3.19	126.07	115.49
5	B	601	CLA	O2D-CGD-CBD	3.19	115.68	111.30
6	B	609	CHL	O2A-CGA-CBA	3.19	121.63	111.90
5	B	601	CLA	C11-C10-C8	3.20	126.10	115.49
6	A	613	CHL	C4A-NA-C1A	3.21	109.82	106.04
5	A	602	CLA	O2A-CGA-CBA	3.21	121.67	111.90
6	A	610	CHL	C4A-NA-C1A	3.21	109.83	106.04
2	C	502	LUX	C11-C12-C13	3.23	126.19	115.49
5	A	601	CLA	CMB-C2B-C3B	3.23	131.41	125.09
5	A	607	CLA	C11-C10-C8	3.24	126.23	115.49
2	C	501	LUX	C1-C2-C3	3.24	121.01	113.41
5	B	602	CLA	O2A-CGA-CBA	3.25	121.80	111.90
2	B	502	LUX	C11-C10-C9	3.25	125.34	114.85
3	C	503	NEX	C37-C21-C22	3.27	114.76	108.94
4	A	504	XAT	C37-C21-C36	3.27	112.23	107.35
6	B	610	CHL	C4A-NA-C1A	3.27	109.90	106.04
5	B	603	CLA	C4A-NA-C1A	3.27	110.59	106.36
5	A	602	CLA	C4A-NA-C1A	3.27	110.59	106.36
2	C	502	LUX	C35-C34-C33	3.28	126.37	115.49
5	C	603	CLA	C4A-NA-C1A	3.29	110.61	106.36
5	A	603	CLA	O2A-CGA-CBA	3.29	121.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	607	CLA	C11-C10-C8	3.31	126.47	115.49
6	B	613	CHL	C4A-NA-C1A	3.31	109.94	106.04
2	A	502	LUX	C18-C5-C4	3.32	120.29	114.24
5	B	606	CLA	C4A-NA-C1A	3.32	110.65	106.36
5	A	605	CLA	C4A-NA-C1A	3.32	110.66	106.36
5	C	607	CLA	C11-C10-C8	3.32	126.51	115.49
3	C	503	NEX	C16-C1-C6	3.33	113.46	110.48
5	A	603	CLA	CBA-CAA-C2A	3.33	123.12	113.73
2	A	501	LUX	C11-C10-C9	3.34	125.60	114.85
5	C	601	CLA	C11-C10-C8	3.34	126.56	115.49
5	A	603	CLA	C4A-NA-C1A	3.34	110.68	106.36
2	C	501	LUX	C35-C34-C33	3.34	126.58	115.49
5	C	605	CLA	O2A-CGA-CBA	3.35	122.11	111.90
5	A	605	CLA	O2A-CGA-CBA	3.35	122.11	111.90
5	C	601	CLA	C4A-NA-C1A	3.35	110.69	106.36
5	A	604	CLA	O2A-CGA-CBA	3.36	122.14	111.90
3	C	503	NEX	C28-C29-C30	3.36	124.40	118.98
6	B	609	CHL	C4A-NA-C1A	3.37	110.01	106.04
2	A	502	LUX	C19-C9-C8	3.37	119.00	110.89
2	A	502	LUX	C35-C34-C33	3.37	126.68	115.49
5	B	605	CLA	C4A-NA-C1A	3.38	110.73	106.36
5	A	608	CLA	O2A-CGA-CBA	3.38	122.21	111.90
5	B	603	CLA	O2A-CGA-CBA	3.43	122.35	111.90
4	C	504	XAT	O3-C3-C4	3.43	116.95	109.91
5	C	606	CLA	C4A-NA-C1A	3.43	110.80	106.36
6	A	609	CHL	C4A-NA-C1A	3.44	110.09	106.04
5	C	602	CLA	O2D-CGD-CBD	3.44	116.02	111.30
5	C	603	CLA	O2A-CGA-CBA	3.44	122.39	111.90
5	C	602	CLA	C4A-NA-C1A	3.45	110.81	106.36
5	A	606	CLA	O2A-CGA-CBA	3.45	122.40	111.90
5	C	603	CLA	CBA-CAA-C2A	3.45	123.46	113.73
5	A	606	CLA	C4A-NA-C1A	3.45	110.83	106.36
6	C	611	CHL	O2D-CGD-CBD	3.46	116.05	111.30
2	A	501	LUX	C18-C5-C4	3.47	120.56	114.24
5	C	606	CLA	O2A-CGA-CBA	3.47	122.47	111.90
5	A	602	CLA	C11-C10-C8	3.48	127.04	115.49
5	C	601	CLA	O2D-CGD-CBD	3.49	116.09	111.30
5	A	608	CLA	C4A-NA-C1A	3.49	110.88	106.36
5	C	604	CLA	O2A-CGA-CBA	3.50	122.57	111.90
5	B	605	CLA	C11-C10-C8	3.50	127.10	115.49
2	C	501	LUX	O23-C23-C22	3.52	118.62	110.47
5	C	605	CLA	C4A-NA-C1A	3.53	110.92	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	602	CLA	C11-C10-C8	3.53	127.21	115.49
2	A	501	LUX	C35-C34-C33	3.54	127.22	115.49
5	C	607	CLA	C4A-NA-C1A	3.54	110.93	106.36
2	A	501	LUX	C19-C9-C8	3.55	119.43	110.89
5	B	606	CLA	O2A-CGA-CBA	3.56	122.74	111.90
5	C	608	CLA	O2A-CGA-CBA	3.56	122.75	111.90
5	C	602	CLA	C11-C10-C8	3.56	127.30	115.49
5	B	602	CLA	C4A-NA-C1A	3.58	110.99	106.36
2	B	501	LUX	C3-C4-C5	3.59	119.25	111.86
4	A	504	XAT	C19-C9-C8	3.59	124.08	118.10
8	C	802	DGD	O5D-C6D-C5D	3.60	115.59	109.08
2	A	501	LUX	O23-C23-C24	3.60	115.80	110.21
5	A	607	CLA	C4A-NA-C1A	3.60	111.02	106.36
5	B	608	CLA	O2A-CGA-CBA	3.61	122.89	111.90
6	C	610	CHL	O2A-CGA-CBA	3.61	122.89	111.90
6	C	609	CHL	C4A-NA-C1A	3.62	110.30	106.04
8	A	802	DGD	O6E-C5E-C6E	3.62	115.52	106.36
6	C	610	CHL	C4A-NA-C1A	3.63	110.32	106.04
6	C	613	CHL	C4A-NA-C1A	3.65	110.34	106.04
6	A	610	CHL	O2A-CGA-CBA	3.66	123.06	111.90
6	B	610	CHL	O2A-CGA-CBA	3.66	123.06	111.90
2	A	501	LUX	C11-C12-C13	3.67	127.66	115.49
2	B	501	LUX	C11-C10-C9	3.67	126.67	114.85
2	B	502	LUX	C3-C4-C5	3.68	119.43	111.86
5	B	603	CLA	CBA-CAA-C2A	3.68	124.11	113.73
5	A	602	CLA	O2D-CGD-CBD	3.68	116.35	111.30
4	B	504	XAT	C12-C13-C14	3.68	124.91	118.98
2	C	502	LUX	C11-C10-C9	3.68	126.72	114.85
5	B	601	CLA	O2A-CGA-CBA	3.69	123.14	111.90
2	A	502	LUX	C31-C32-C33	3.70	127.75	115.49
8	B	802	DGD	O6E-C5E-C6E	3.70	115.71	106.36
6	B	611	CHL	O2D-CGD-CBD	3.70	116.38	111.30
2	C	501	LUX	C3-C4-C5	3.71	119.50	111.86
2	C	502	LUX	C19-C9-C8	3.71	119.83	110.89
5	B	607	CLA	C4A-NA-C1A	3.73	111.18	106.36
5	A	605	CLA	C11-C10-C8	3.75	127.92	115.49
8	C	802	DGD	O6E-C5E-C6E	3.75	115.83	106.36
5	C	605	CLA	C11-C10-C8	3.76	127.95	115.49
3	A	503	NEX	C28-C29-C30	3.77	125.06	118.98
5	C	601	CLA	O2A-CGA-CBA	3.78	123.43	111.90
5	B	602	CLA	O2D-CGD-CBD	3.78	116.49	111.30
5	A	603	CLA	O2D-CGD-CBD	3.80	116.50	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	LUX	C11-C12-C13	3.81	128.13	115.49
2	B	501	LUX	C19-C9-C8	3.81	120.07	110.89
5	C	608	CLA	C4A-NA-C1A	3.83	111.31	106.36
2	B	501	LUX	C11-C12-C13	3.83	128.18	115.49
2	A	502	LUX	C3-C4-C5	3.85	119.78	111.86
2	A	501	LUX	C3-C4-C5	3.86	119.80	111.86
6	A	611	CHL	O2D-CGD-CBD	3.87	116.61	111.30
2	B	502	LUX	C15-C14-C13	3.89	128.40	115.49
2	C	501	LUX	C11-C10-C9	3.90	127.43	114.85
6	B	612	CHL	C4A-NA-C1A	3.93	110.68	106.04
5	A	601	CLA	O2A-CGA-CBA	3.94	123.92	111.90
2	C	502	LUX	C18-C5-C4	3.95	121.44	114.24
7	A	801	LHG	O8-C23-C24	3.95	123.93	111.90
2	C	501	LUX	C11-C12-C13	3.95	128.60	115.49
6	C	610	CHL	O2D-CGD-CBD	3.98	116.77	111.30
2	B	502	LUX	C31-C32-C33	4.02	128.81	115.49
2	A	502	LUX	C15-C14-C13	4.04	128.88	115.49
6	C	611	CHL	C4A-NA-C1A	4.05	110.81	106.04
4	B	504	XAT	C1-C2-C3	4.07	121.88	115.02
7	B	801	LHG	O8-C23-C24	4.13	124.47	111.90
5	C	608	CLA	O2D-CGD-CBD	4.15	117.00	111.30
3	B	503	NEX	C28-C29-C30	4.17	125.70	118.98
6	A	611	CHL	C4A-NA-C1A	4.17	110.95	106.04
6	B	611	CHL	C4A-NA-C1A	4.18	110.97	106.04
2	B	502	LUX	C10-C9-C8	4.20	119.49	110.21
6	A	614	CHL	C4A-NA-C1A	4.21	111.00	106.04
2	B	501	LUX	C31-C30-C29	4.22	129.50	115.49
2	C	501	LUX	C31-C30-C29	4.22	129.50	115.49
5	B	604	CLA	O2D-CGD-CBD	4.23	117.10	111.30
2	B	502	LUX	C19-C9-C8	4.23	121.06	110.89
2	B	501	LUX	O23-C23-C22	4.27	120.33	110.47
5	C	603	CLA	O2D-CGD-CBD	4.27	117.16	111.30
7	C	801	LHG	O8-C23-C24	4.28	124.95	111.90
2	C	502	LUX	C15-C14-C13	4.29	129.72	115.49
6	C	613	CHL	O2D-CGD-CBD	4.30	117.19	111.30
2	A	501	LUX	C28-C27-C26	4.31	124.92	114.87
2	A	501	LUX	C31-C30-C29	4.33	129.84	115.49
6	B	613	CHL	O2D-CGD-CBD	4.33	117.24	111.30
6	C	614	CHL	C4A-NA-C1A	4.44	111.27	106.04
6	A	610	CHL	O2D-CGD-CBD	4.46	117.42	111.30
6	C	612	CHL	C4A-NA-C1A	4.48	111.33	106.04
5	B	608	CLA	O2D-CGD-CBD	4.51	117.49	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	612	CHL	C4A-NA-C1A	4.52	111.37	106.04
5	A	601	CLA	O2D-CGD-CBD	4.52	117.50	111.30
2	C	502	LUX	C10-C9-C8	4.52	120.21	110.21
2	A	502	LUX	C10-C9-C8	4.54	120.23	110.21
2	C	501	LUX	C36-C21-C22	4.57	117.42	109.35
6	A	613	CHL	O2D-CGD-CBD	4.59	117.60	111.30
6	B	610	CHL	O2D-CGD-CBD	4.61	117.62	111.30
6	B	614	CHL	C4A-NA-C1A	4.65	111.52	106.04
6	C	612	CHL	O2D-CGD-CBD	4.68	117.71	111.30
2	A	501	LUX	C36-C21-C22	4.71	117.66	109.35
2	A	502	LUX	C31-C30-C29	4.73	131.18	115.49
5	C	606	CLA	O2D-CGD-CBD	4.74	117.80	111.30
4	C	504	XAT	C1-C2-C3	4.75	123.03	115.02
5	B	603	CLA	O2D-CGD-CBD	4.77	117.84	111.30
2	B	501	LUX	C10-C9-C8	4.80	120.82	110.21
2	A	501	LUX	C10-C9-C8	4.82	120.86	110.21
5	C	605	CLA	O2D-CGD-CBD	4.84	117.93	111.30
8	B	802	DGD	O5D-C1E-C2E	4.84	114.15	108.04
5	A	606	CLA	O2D-CGD-CBD	4.86	117.97	111.30
8	B	802	DGD	O6D-C5D-C6D	4.87	116.56	106.61
7	B	801	LHG	C25-C24-C23	4.88	132.77	113.59
5	A	608	CLA	O2D-CGD-CBD	4.91	118.04	111.30
5	A	604	CLA	O2D-CGD-CBD	4.91	118.04	111.30
5	C	604	CLA	O2D-CGD-CBD	4.92	118.05	111.30
2	C	501	LUX	O23-C23-C24	4.92	117.85	110.21
7	C	801	LHG	C25-C24-C23	4.94	133.00	113.59
6	C	609	CHL	O2D-CGD-CBD	4.94	118.08	111.30
5	B	605	CLA	O2D-CGD-CBD	4.97	118.12	111.30
6	B	612	CHL	O2D-CGD-CBD	4.98	118.14	111.30
8	C	802	DGD	O5D-C1E-C2E	5.00	114.36	108.04
4	A	504	XAT	C1-C2-C3	5.08	123.59	115.02
2	C	501	LUX	C10-C9-C8	5.08	121.44	110.21
5	B	606	CLA	O2D-CGD-CBD	5.08	118.28	111.30
8	A	802	DGD	O6D-C5D-C6D	5.10	117.04	106.61
8	C	802	DGD	O6D-C5D-C6D	5.13	117.09	106.61
6	A	612	CHL	O2D-CGD-CBD	5.13	118.34	111.30
2	A	502	LUX	C36-C21-C22	5.21	118.55	109.35
7	A	801	LHG	C25-C24-C23	5.24	134.18	113.59
2	B	502	LUX	C31-C30-C29	5.27	132.97	115.49
2	C	502	LUX	C36-C21-C22	5.34	118.78	109.35
6	B	614	CHL	O2D-CGD-CBD	5.42	118.74	111.30
2	C	501	LUX	C28-C27-C26	5.43	127.52	114.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	607	CLA	O2D-CGD-CBD	5.44	118.76	111.30
6	A	614	CHL	O2D-CGD-CBD	5.45	118.77	111.30
2	B	501	LUX	C28-C27-C26	5.51	127.72	114.87
6	A	609	CHL	O2D-CGD-CBD	5.52	118.87	111.30
8	A	802	DGD	O5D-C1E-C2E	5.52	115.01	108.04
5	A	607	CLA	O2D-CGD-CBD	5.52	118.88	111.30
2	A	502	LUX	C28-C27-C26	5.53	127.76	114.87
5	C	607	CLA	O2D-CGD-CBD	5.56	118.93	111.30
6	B	609	CHL	O2D-CGD-CBD	5.62	119.00	111.30
2	C	502	LUX	C31-C30-C29	5.66	134.26	115.49
6	C	614	CHL	O2D-CGD-CBD	5.66	119.07	111.30
2	B	501	LUX	C36-C21-C22	5.67	119.36	109.35
2	B	502	LUX	C28-C27-C26	5.69	128.14	114.87
2	C	502	LUX	C28-C27-C26	5.78	128.35	114.87
5	A	605	CLA	O2D-CGD-CBD	5.83	119.30	111.30
2	B	502	LUX	C36-C21-C22	6.17	120.25	109.35
3	A	503	NEX	C1-C2-C3	6.67	129.06	113.41
3	C	503	NEX	C1-C2-C3	6.71	129.14	113.41
3	B	503	NEX	C1-C2-C3	6.78	129.31	113.41
8	B	802	DGD	O6E-C5E-C4E	8.13	124.94	109.68
8	C	802	DGD	O6E-C5E-C4E	8.15	124.97	109.68
8	A	802	DGD	O6E-C5E-C4E	8.26	125.18	109.68
2	A	501	LUX	C37-C21-C36	8.64	120.92	107.91
2	B	501	LUX	C37-C21-C36	9.12	121.64	107.91
2	C	501	LUX	C37-C21-C36	9.39	122.05	107.91
2	B	502	LUX	C37-C21-C36	9.75	122.59	107.91
2	C	502	LUX	C37-C21-C36	10.04	123.03	107.91
2	A	502	LUX	C37-C21-C36	10.54	123.78	107.91

All (129) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	802	DGD	C5E
6	C	612	CHL	C8
2	A	502	LUX	C13
2	A	502	LUX	C33
2	A	502	LUX	C29
2	A	502	LUX	C26
2	A	502	LUX	C9
5	B	604	CLA	C8
5	B	604	CLA	NC
5	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
5	B	604	CLA	NA
5	A	608	CLA	NC
5	A	608	CLA	ND
5	A	608	CLA	NA
5	C	604	CLA	C8
5	C	604	CLA	NC
5	C	604	CLA	ND
5	C	604	CLA	NA
5	B	601	CLA	C8
5	B	601	CLA	NC
5	B	601	CLA	ND
5	B	601	CLA	NA
2	B	502	LUX	C13
2	B	502	LUX	C33
2	B	502	LUX	C29
2	B	502	LUX	C26
2	B	502	LUX	C9
5	B	606	CLA	C8
5	B	606	CLA	NC
5	B	606	CLA	ND
5	B	606	CLA	NA
5	B	608	CLA	NC
5	B	608	CLA	ND
5	B	608	CLA	NA
5	B	607	CLA	NC
5	B	607	CLA	ND
5	B	607	CLA	NA
5	A	601	CLA	C8
5	A	601	CLA	NC
5	A	601	CLA	ND
5	A	601	CLA	NA
5	C	603	CLA	C8
5	C	603	CLA	NC
5	C	603	CLA	ND
5	C	603	CLA	NA
5	A	607	CLA	NC
5	A	607	CLA	ND
5	A	607	CLA	NA
4	A	504	XAT	C6
4	A	504	XAT	C26
5	C	607	CLA	NC
5	C	607	CLA	ND

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Mol	Chain	Res	Type	Atom
5	C	607	CLA	NA
4	C	504	XAT	C6
4	C	504	XAT	C26
5	C	606	CLA	C8
5	C	606	CLA	NC
5	C	606	CLA	ND
5	C	606	CLA	NA
4	B	504	XAT	C6
4	B	504	XAT	C26
5	B	605	CLA	C8
5	B	605	CLA	NC
5	B	605	CLA	ND
5	B	605	CLA	NA
8	A	802	DGD	C5E
5	C	605	CLA	C8
5	C	605	CLA	NC
5	C	605	CLA	ND
5	C	605	CLA	NA
2	A	501	LUX	C13
2	A	501	LUX	C33
2	A	501	LUX	C29
2	A	501	LUX	C26
2	A	501	LUX	C9
2	B	501	LUX	C13
2	B	501	LUX	C33
2	B	501	LUX	C29
2	B	501	LUX	C26
2	B	501	LUX	C9
5	C	602	CLA	NC
5	C	602	CLA	ND
5	C	602	CLA	NA
5	A	603	CLA	C8
5	A	603	CLA	NC
5	A	603	CLA	ND
5	A	603	CLA	NA
5	B	602	CLA	NC
5	B	602	CLA	ND
5	B	602	CLA	NA
6	B	612	CHL	C8
5	B	603	CLA	C8
5	B	603	CLA	NC
5	B	603	CLA	ND

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Mol	Chain	Res	Type	Atom
5	B	603	CLA	NA
2	C	502	LUX	C13
2	C	502	LUX	C33
2	C	502	LUX	C29
2	C	502	LUX	C26
2	C	502	LUX	C9
5	A	605	CLA	C8
5	A	605	CLA	NC
5	A	605	CLA	ND
5	A	605	CLA	NA
5	A	604	CLA	C8
5	A	604	CLA	NC
5	A	604	CLA	ND
5	A	604	CLA	NA
5	C	601	CLA	C8
5	C	601	CLA	NC
5	C	601	CLA	ND
5	C	601	CLA	NA
6	A	612	CHL	C8
5	C	608	CLA	NC
5	C	608	CLA	ND
5	C	608	CLA	NA
5	A	602	CLA	NC
5	A	602	CLA	ND
5	A	602	CLA	NA
5	A	606	CLA	C8
5	A	606	CLA	NC
5	A	606	CLA	ND
5	A	606	CLA	NA
2	C	501	LUX	C13
2	C	501	LUX	C33
2	C	501	LUX	C29
2	C	501	LUX	C26
2	C	501	LUX	C9
8	B	802	DGD	C5E

There are no torsion outliers.

There are no ring outliers.

60 monomers are involved in 801 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LUX	29	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	LUX	21	0
3	A	503	NEX	4	0
4	A	504	XAT	18	0
5	A	601	CLA	21	0
5	A	602	CLA	13	0
5	A	603	CLA	18	0
5	A	604	CLA	22	0
5	A	605	CLA	21	0
5	A	606	CLA	18	0
5	A	607	CLA	17	0
5	A	608	CLA	16	0
6	A	609	CHL	31	0
6	A	610	CHL	31	0
6	A	611	CHL	22	0
6	A	612	CHL	18	0
6	A	613	CHL	6	0
6	A	614	CHL	15	0
7	A	801	LHG	12	0
8	A	802	DGD	4	0
2	B	501	LUX	31	0
2	B	502	LUX	18	0
3	B	503	NEX	4	0
4	B	504	XAT	16	0
5	B	601	CLA	23	0
5	B	602	CLA	11	0
5	B	603	CLA	24	0
5	B	604	CLA	24	0
5	B	605	CLA	23	0
5	B	606	CLA	17	0
5	B	607	CLA	17	0
5	B	608	CLA	21	0
6	B	609	CHL	27	0
6	B	610	CHL	28	0
6	B	611	CHL	22	0
6	B	612	CHL	22	0
6	B	613	CHL	9	0
6	B	614	CHL	16	0
7	B	801	LHG	13	0
8	B	802	DGD	2	0
2	C	501	LUX	31	0
2	C	502	LUX	19	0
3	C	503	NEX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	XAT	16	0
5	C	601	CLA	23	0
5	C	602	CLA	11	0
5	C	603	CLA	17	0
5	C	604	CLA	20	0
5	C	605	CLA	21	0
5	C	606	CLA	17	0
5	C	607	CLA	19	0
5	C	608	CLA	16	0
6	C	609	CHL	30	0
6	C	610	CHL	31	0
6	C	611	CHL	23	0
6	C	612	CHL	21	0
6	C	613	CHL	5	0
6	C	614	CHL	14	0
7	C	801	LHG	13	0
8	C	802	DGD	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	223/232 (96%)	1.25	52 (23%) 1 1	72, 91, 109, 128	0
1	B	223/232 (96%)	1.10	41 (18%) 2 2	70, 89, 107, 126	0
1	C	223/232 (96%)	1.14	43 (19%) 2 1	73, 91, 109, 129	0
All	All	669/696 (96%)	1.16	136 (20%) 1 1	70, 90, 109, 129	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	SER	10.0
1	B	12	SER	9.6
1	B	10	ALA	8.2
1	C	10	ALA	7.6
1	A	10	ALA	7.0
1	B	11	SER	6.9
1	A	118	LEU	6.3
1	A	232	LYS	6.2
1	B	213	LEU	5.8
1	A	36	LEU	5.5
1	B	118	LEU	5.3
1	C	12	SER	5.1
1	A	121	ALA	5.0
1	C	151	VAL	4.7
1	A	11	SER	4.6
1	C	18	GLY	4.4
1	A	28	PHE	4.4
1	A	119	VAL	4.3
1	C	121	ALA	4.2
1	B	121	ALA	4.2
1	C	110	LEU	4.1
1	B	151	VAL	4.0
1	A	32	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	143	ILE	4.0
1	B	13	GLY	3.9
1	A	12	SER	3.9
1	A	110	LEU	3.9
1	B	116	PRO	3.9
1	C	16	TRP	3.8
1	A	18	GLY	3.8
1	A	146	GLY	3.8
1	C	145	GLY	3.8
1	A	104	ILE	3.8
1	C	213	LEU	3.8
1	C	219	ASN	3.6
1	A	108	GLY	3.6
1	A	17	TYR	3.5
1	A	170	PRO	3.5
1	C	120	HIS	3.5
1	A	122	GLN	3.5
1	B	117	SER	3.5
1	C	117	SER	3.4
1	A	16	TRP	3.4
1	C	208	ASN	3.4
1	B	110	LEU	3.4
1	A	169	ASP	3.4
1	A	44	TYR	3.3
1	A	117	SER	3.3
1	B	115	ASN	3.3
1	B	119	VAL	3.2
1	C	152	VAL	3.2
1	B	18	GLY	3.2
1	A	120	HIS	3.2
1	B	122	GLN	3.1
1	A	210	ALA	3.1
1	C	19	PRO	3.1
1	B	104	ILE	3.0
1	C	147	PRO	3.0
1	C	232	LYS	3.0
1	A	31	GLU	3.0
1	C	196	VAL	3.0
1	A	144	ALA	2.9
1	C	108	GLY	2.9
1	B	95	ALA	2.9
1	B	216	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	2.9
1	B	108	GLY	2.9
1	C	116	PRO	2.9
1	C	119	VAL	2.9
1	A	72	ALA	2.8
1	A	115	ASN	2.8
1	A	231	GLY	2.8
1	C	144	ALA	2.8
1	C	28	PHE	2.8
1	C	173	PHE	2.7
1	A	27	PRO	2.7
1	A	22	VAL	2.7
1	B	92	PHE	2.7
1	B	51	LEU	2.6
1	A	111	ASP	2.6
1	A	51	LEU	2.6
1	B	205	PRO	2.6
1	A	196	VAL	2.6
1	A	13	GLY	2.6
1	B	204	GLY	2.6
1	C	14	SER	2.6
1	A	152	VAL	2.5
1	A	192	PHE	2.5
1	C	109	GLY	2.5
1	C	195	PHE	2.5
1	B	19	PRO	2.5
1	B	209	LEU	2.5
1	A	211	ASP	2.5
1	C	15	PRO	2.5
1	C	210	ALA	2.5
1	C	171	GLU	2.5
1	B	14	SER	2.5
1	A	40	PHE	2.4
1	B	16	TRP	2.4
1	B	120	HIS	2.4
1	C	42	GLY	2.4
1	C	192	PHE	2.4
1	A	218	ASN	2.4
1	A	38	GLY	2.4
1	A	150	GLU	2.4
1	B	42	GLY	2.3
1	B	146	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	104	ILE	2.3
1	B	147	PRO	2.3
1	A	76	ALA	2.3
1	B	91	LYS	2.3
1	B	28	PHE	2.3
1	C	51	LEU	2.3
1	B	189	PHE	2.3
1	A	116	PRO	2.3
1	B	27	PRO	2.2
1	A	195	PHE	2.2
1	B	187	ALA	2.2
1	A	15	PRO	2.2
1	A	103	GLN	2.1
1	B	105	PHE	2.1
1	A	71	TRP	2.1
1	B	152	VAL	2.1
1	C	146	GLY	2.1
1	C	17	TYR	2.1
1	C	167	ALA	2.1
1	A	191	MET	2.1
1	B	208	ASN	2.1
1	B	219	ASN	2.1
1	A	189	PHE	2.1
1	B	144	ALA	2.1
1	C	231	GLY	2.1
1	C	72	ALA	2.0
1	C	206	LEU	2.0
1	C	150	GLU	2.0
1	A	219	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CLA	B	605	65/65	0.93	0.45	6.92	75,84,105,108	0
8	DGD	A	802	38/66	0.49	0.46	5.42	106,119,140,140	0
5	CLA	A	605	65/65	0.91	0.49	5.41	77,86,107,110	0
8	DGD	B	802	38/66	0.41	0.50	3.93	104,118,139,140	0
5	CLA	C	605	65/65	0.92	0.41	3.57	77,86,108,110	0
2	LUX	C	502	42/42	0.88	0.35	3.07	58,79,115,128	0
3	NEX	C	503	44/44	0.65	0.40	3.02	67,98,128,133	0
2	LUX	B	502	42/42	0.84	0.35	2.91	53,76,113,126	0
6	CHL	A	612	66/66	0.83	0.36	2.82	76,85,102,104	0
3	NEX	B	503	44/44	0.81	0.35	2.78	64,96,126,131	0
3	NEX	A	503	44/44	0.80	0.30	2.52	66,97,128,132	0
5	CLA	C	604	65/65	0.85	0.30	2.08	60,72,97,102	0
6	CHL	A	610	66/66	0.92	0.29	1.72	65,80,108,110	0
2	LUX	A	502	42/42	0.89	0.32	1.72	57,78,115,128	0
5	CLA	B	604	65/65	0.87	0.30	1.62	56,69,95,100	0
6	CHL	B	612	66/66	0.91	0.27	1.59	74,83,100,102	0
6	CHL	C	614	42/66	0.83	0.41	1.55	99,107,113,137	0
8	DGD	C	802	38/66	0.58	0.43	1.48	106,119,141,141	0
4	XAT	B	504	44/44	0.88	0.21	1.42	63,89,115,147	0
2	LUX	A	501	42/42	0.92	0.27	1.32	61,87,120,136	0
7	LHG	B	801	49/49	0.85	0.28	1.29	72,88,109,115	0
4	XAT	C	504	44/44	0.87	0.20	1.26	65,91,117,149	0
6	CHL	C	612	66/66	0.83	0.31	1.22	77,85,102,104	0
5	CLA	B	601	65/65	0.86	0.23	1.18	68,77,111,113	0
6	CHL	B	614	42/66	0.86	0.42	1.08	97,105,111,134	0
5	CLA	B	607	65/65	0.84	0.24	1.05	75,88,101,104	0
5	CLA	A	602	60/65	0.91	0.24	1.03	79,87,115,116	0
6	CHL	C	610	66/66	0.90	0.24	1.01	67,81,108,110	0
6	CHL	A	614	42/66	0.88	0.43	0.89	99,106,113,136	0
6	CHL	C	609	66/66	0.87	0.24	0.87	77,85,98,101	0
2	LUX	B	501	42/42	0.90	0.26	0.78	59,86,118,134	0
5	CLA	A	601	65/65	0.88	0.23	0.76	69,79,112,115	0
6	CHL	B	610	66/66	0.92	0.23	0.73	65,79,106,108	0
6	CHL	B	611	66/66	0.91	0.26	0.63	68,82,115,121	0
6	CHL	C	611	66/66	0.89	0.28	0.60	69,85,118,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LUX	C	501	42/42	0.88	0.26	0.56	62,88,120,136	0
4	XAT	A	504	44/44	0.91	0.18	0.55	65,91,117,148	0
5	CLA	C	606	57/65	0.91	0.25	0.50	80,91,107,111	0
5	CLA	C	601	65/65	0.88	0.24	0.49	70,79,113,115	0
5	CLA	C	602	60/65	0.91	0.21	0.40	80,87,116,117	0
5	CLA	A	604	65/65	0.85	0.27	0.37	59,71,96,101	0
5	CLA	B	606	57/65	0.89	0.28	0.37	78,89,105,109	0
6	CHL	A	611	66/66	0.89	0.24	0.30	70,85,117,123	0
6	CHL	B	609	66/66	0.88	0.22	0.26	75,83,95,99	0
6	CHL	A	609	66/66	0.87	0.22	0.04	75,85,97,100	0
5	CLA	C	607	65/65	0.83	0.22	0.00	77,91,104,106	0
5	CLA	A	606	57/65	0.90	0.26	-0.04	79,90,107,110	0
5	CLA	B	602	60/65	0.92	0.19	-0.06	77,85,114,114	0
7	LHG	C	801	49/49	0.90	0.24	-0.07	74,90,111,117	0
5	CLA	C	608	48/65	0.90	0.21	-0.08	90,99,117,119	0
5	CLA	A	603	65/65	0.91	0.21	-0.11	75,85,102,105	0
5	CLA	A	607	65/65	0.83	0.23	-0.20	77,90,103,106	0
5	CLA	C	603	65/65	0.92	0.22	-0.20	75,85,102,105	0
5	CLA	B	608	48/65	0.89	0.22	-0.21	88,97,115,117	0
6	CHL	B	613	46/66	0.91	0.20	-0.25	71,80,106,119	0
5	CLA	A	608	48/65	0.90	0.16	-0.33	90,99,116,118	0
6	CHL	A	613	46/66	0.92	0.20	-0.47	73,81,107,120	0
7	LHG	A	801	49/49	0.89	0.25	-0.59	74,90,110,116	0
6	CHL	C	613	46/66	0.91	0.17	-0.60	73,82,107,121	0
5	CLA	B	603	65/65	0.90	0.20	-0.64	74,83,100,103	0

6.5 Other polymers (i)

There are no such residues in this entry.