Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:56 PM GMT

PDB ID	:	1HV5
Title	:	CRYSTAL STRUCTURE OF THE STROMELYSIN-3 (MMP-11) CATALYTIC DOMAIN COMPLEXED WITH A PHOSPHINIC INHIBITOR
Authors	:	Gall, A.L.; Ruff, M.; Kannan, R.; Cuniasse, P.; Yiotakis, A.; Dive, V.; Rio, M.C.; Basset, P.; Moras, D.
Deposited on	:	2001-01-08
Resolution	:	2.60 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:

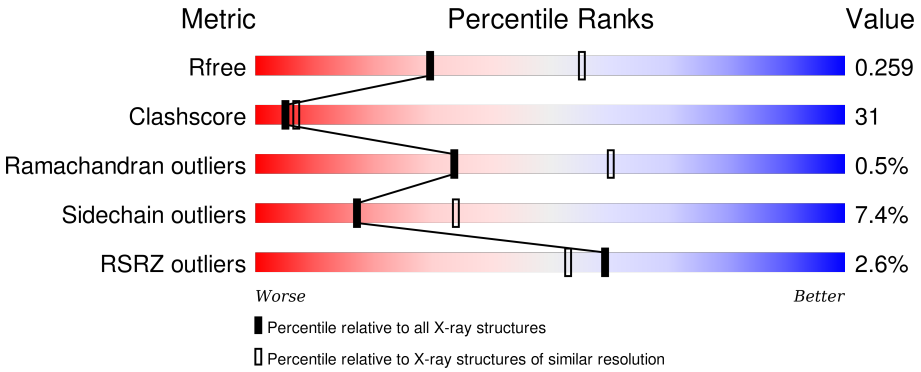
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	165	63% 31%
1	B	165	5% 53% 39% 6%
1	C	165	64% 30%
1	D	165	66% 24% 6%
1	E	165	58% 34% 6%

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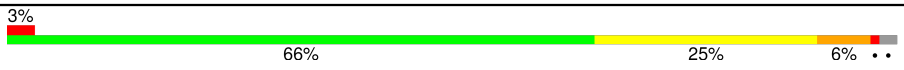
Mol	Chain	Length	Quality of chain
1	F	165	

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
4	CPS	B	5002	-	-	-	X
4	CPS	E	5005	-	-	-	X
4	CPS	F	5091	-	-	X	X
5	RXP	A	6001	-	-	-	X
5	RXP	B	6002	-	-	-	X
5	RXP	C	6003	-	-	-	X
5	RXP	D	6004	-	-	-	X
5	RXP	E	6005	-	-	-	X
5	RXP	F	6006	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10772 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 STROMELYSIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1342	863	236	240	3			
1	C	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	D	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	E	165	Total	C	N	O	S	0	0	0
			1352	868	238	243	3			
1	F	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			

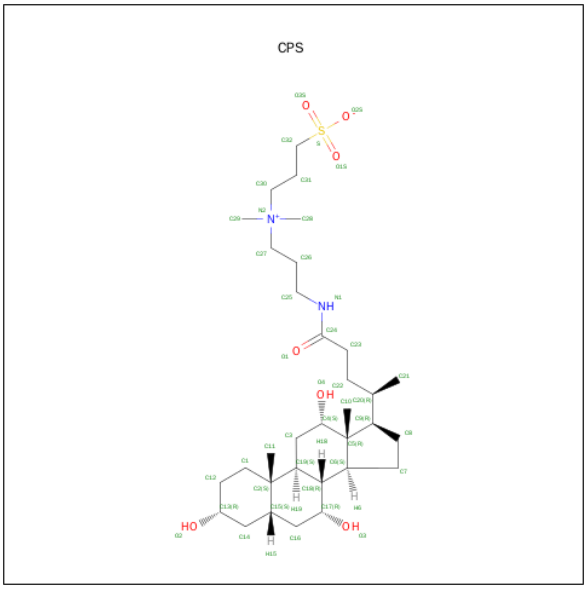
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	C	1	Total C O 26 23 3	4	0
4	D	1	Total C O 26 23 3	4	0
4	E	1	Total C O 26 23 3	4	0

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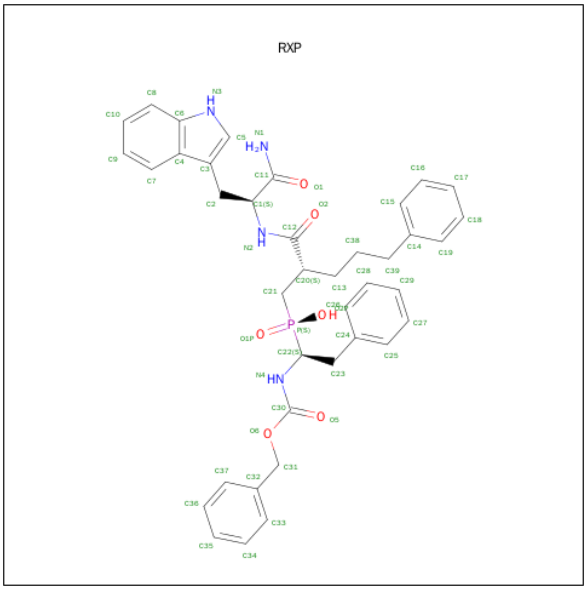
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	C	1	Total C O 26 23 3	4	0
4	D	1	Total C O 26 23 3	4	0
4	E	1	Total C O 26 23 3	4	0
4	F	1	Total C O 26 23 3	4	0
4	F	1	Total C N O S 42 32 2 7 1	0	0

- Molecule 5 is 1-BENZYLOXYCARBONYLAMINO-2-PHENYL-ETHYL)-{2-[1-CARBAMOYL-2-(1H-INDOL-3-YL)-ETHYLCARBAMOYL]-5-PHENYL-PENTYL}-PHOSPHINIC ACID (three-letter code: RXP) (formula: $C_{39}H_{43}N_4O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 50 39 4 6 1	0	0
5	B	1	Total C N O P 50 39 4 6 1	0	0
5	C	1	Total C N O P 50 39 4 6 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	E	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	F	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

- Molecule 6 is water.

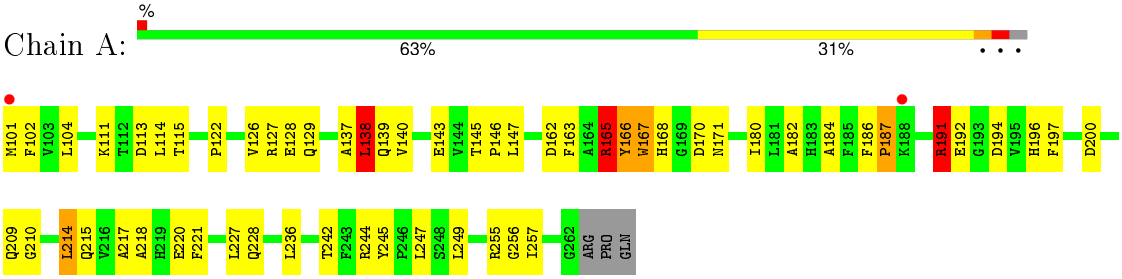
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	376	Total	O	0	0
			376	376		
6	B	318	Total	O	0	0
			318	318		
6	C	367	Total	O	0	0
			367	367		
6	D	341	Total	O	0	0
			341	341		
6	E	353	Total	O	0	0
			353	353		
6	F	381	Total	O	0	0
			381	381		

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.

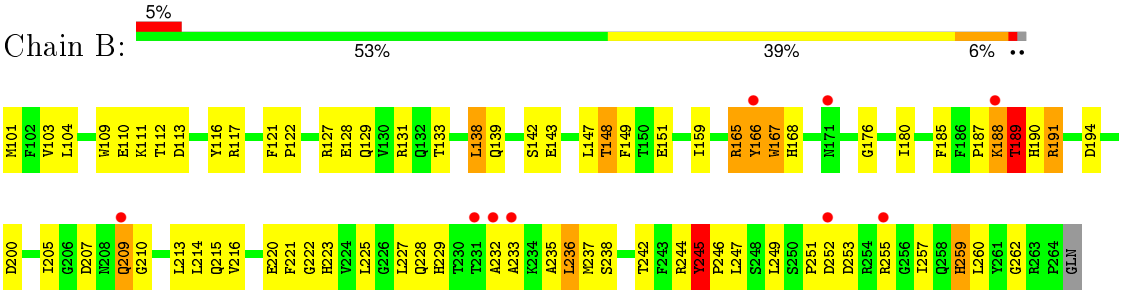
- Molecule 1: STROMELYSIN 3

Chain A:



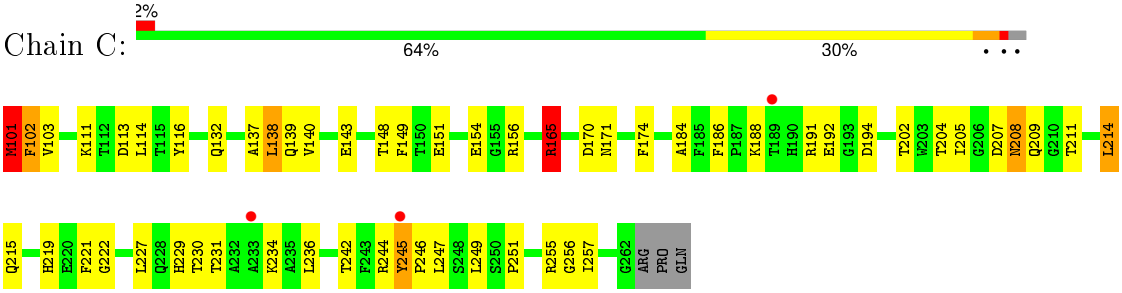
- Molecule 1: STROMELYSIN 3

Chain B:



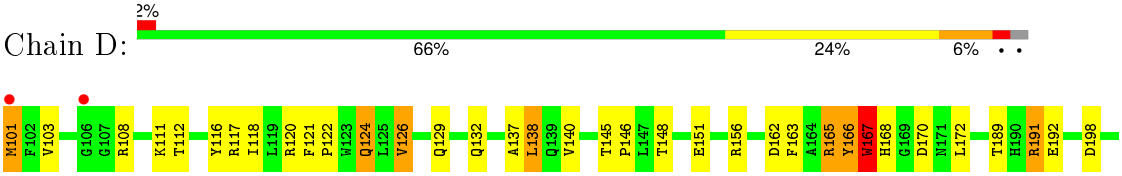
- Molecule 1: STROMELYSIN 3

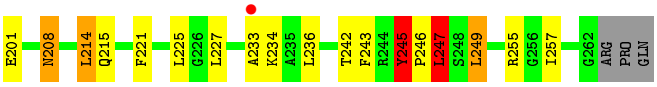
Chain C:



- Molecule 1: STROMELYSIN 3

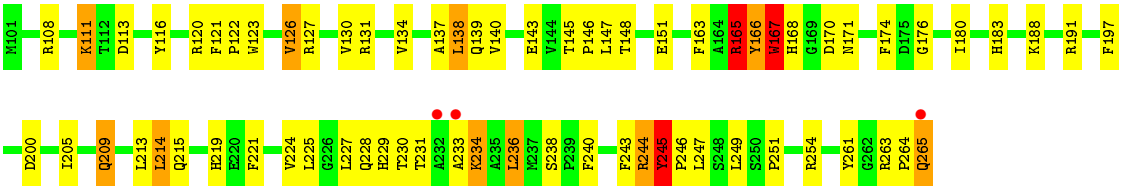
Chain D:





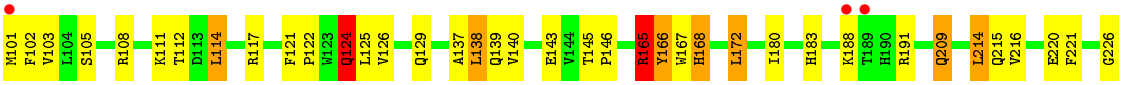
• Molecule 1: STROMELYSIN 3

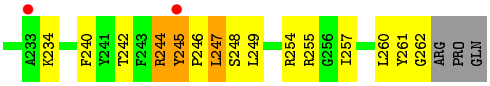
Chain E:



• Molecule 1: STROMELYSIN 3

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.10Å 148.50Å 91.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.60 19.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.89-2.60) 96.7 (19.89-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.262 0.213 , 0.259	Depositor DCC
R_{free} test set	5828 reflections (10.16%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 59596 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10772	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% 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: RXP, ZN, CPS, CA

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	0.70	1/1367 (0.1%)	0.87	5/1861 (0.3%)
1	B	0.70	3/1386 (0.2%)	0.99	11/1887 (0.6%)
1	C	0.63	0/1367	0.94	9/1861 (0.5%)
1	D	0.79	3/1367 (0.2%)	0.97	11/1861 (0.6%)
1	E	0.66	1/1396 (0.1%)	0.88	5/1899 (0.3%)
1	F	0.75	3/1367 (0.2%)	0.94	7/1861 (0.4%)
All	All	0.70	11/8250 (0.1%)	0.93	48/11230 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	C-N	-15.08	0.99	1.34
1	E	167	TRP	N-CA	11.29	1.69	1.46
1	A	167	TRP	N-CA	9.55	1.65	1.46
1	F	165	ARG	C-N	-9.54	1.12	1.34
1	F	168	HIS	C-N	-7.49	1.19	1.33
1	B	188	LYS	C-N	-5.82	1.20	1.34
1	D	101	MET	C-N	-5.56	1.21	1.34
1	B	167	TRP	CA-C	-5.18	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	CA-C	-5.15	1.39	1.52
1	F	166	TYR	C-N	-5.12	1.22	1.34
1	B	167	TRP	C-N	-5.00	1.22	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	188	LYS	CB-CA-C	12.47	135.34	110.40
1	F	245	TYR	C-N-CD	10.84	151.17	128.40
1	C	245	TYR	C-N-CD	10.81	151.10	128.40
1	D	101	MET	N-CA-C	8.98	135.24	111.00
1	C	102	PHE	O-C-N	-8.87	108.51	122.70
1	B	245	TYR	C-N-CD	8.84	146.97	128.40
1	D	245	TYR	C-N-CD	8.70	146.66	128.40
1	D	166	TYR	O-C-N	-8.37	109.31	122.70
1	B	245	TYR	N-CA-C	7.77	131.99	111.00
1	A	167	TRP	N-CA-C	7.76	131.96	111.00
1	C	165	ARG	N-CA-C	7.74	131.90	111.00
1	F	168	HIS	N-CA-CB	-7.73	96.68	110.60
1	F	166	TYR	CB-CA-C	-7.65	95.10	110.40
1	C	165	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	E	245	TYR	N-CA-C	7.54	131.35	111.00
1	E	165	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	F	165	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	F	245	TYR	C-N-CA	-7.48	90.59	122.00
1	E	245	TYR	C-N-CD	7.43	144.01	128.40
1	A	165	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	D	165	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	B	191	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	E	167	TRP	N-CA-C	7.12	130.21	111.00
1	B	165	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	D	167	TRP	C-N-CA	6.95	139.08	121.70
1	B	166	TYR	CA-CB-CG	-6.94	100.21	113.40
1	D	245	TYR	N-CA-C	6.71	129.11	111.00
1	A	191	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	E	245	TYR	C-N-CA	-6.59	94.33	122.00
1	F	245	TYR	N-CA-C	6.51	128.58	111.00
1	B	166	TYR	CD1-CG-CD2	6.41	124.95	117.90
1	C	103	VAL	N-CA-C	6.26	127.89	111.00
1	D	101	MET	CG-SD-CE	6.13	110.01	100.20
1	B	166	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	D	167	TRP	N-CA-C	6.02	127.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	245	TYR	N-CA-C	5.96	127.10	111.00
1	B	166	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	C	101	MET	CG-SD-CE	5.79	109.46	100.20
1	D	245	TYR	CA-CB-CG	-5.78	102.42	113.40
1	C	245	TYR	C-N-CA	-5.63	98.34	122.00
1	C	103	VAL	N-CA-CB	-5.62	99.14	111.50
1	A	167	TRP	N-CA-CB	-5.59	100.53	110.60
1	A	138	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	189	THR	N-CA-CB	-5.38	100.07	110.30
1	F	124	GLN	CB-CA-C	-5.37	99.67	110.40
1	B	166	TYR	CG-CD2-CE2	-5.21	117.13	121.30
1	D	247	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	168	HIS	N-CA-C	5.04	124.59	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Peptide
1	D	166	TYR	Mainchain,Peptide
1	D	245	TYR	Sidechain
1	E	166	TYR	Peptide
1	F	165	ARG	Mainchain

5.2 Too-close contacts (i)

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	1324	0	1253	70	0
1	B	1342	0	1272	77	0
1	C	1324	0	1253	77	0
1	D	1324	0	1252	58	0
1	E	1352	0	1281	85	0
1	F	1324	0	1252	68	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	52	0	70	16	0
4	B	52	0	70	15	0
4	C	52	0	70	15	0
4	D	52	0	70	9	0
4	E	52	0	70	16	0
4	F	68	0	91	30	0
5	A	50	0	42	5	0
5	B	50	0	42	4	0
5	C	50	0	42	1	0
5	D	50	0	42	1	0
5	E	50	0	42	9	0
5	F	50	0	42	2	0
6	A	376	0	0	35	0
6	B	318	0	0	30	0
6	C	367	0	0	31	0
6	D	341	0	0	28	0
6	E	353	0	0	31	1
6	F	381	0	0	34	0
All	All	10772	0	8256	517	1

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 31.

All (517) 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)
4:D:5004:CPS:C10	4:D:5004:CPS:C5	1.75	1.65
4:B:5007:CPS:C10	4:B:5007:CPS:C5	1.74	1.64
4:A:5006:CPS:C10	4:A:5006:CPS:C5	1.75	1.63
4:F:5091:CPS:C19	4:F:5091:CPS:C18	1.75	1.63
4:F:5011:CPS:C5	4:F:5011:CPS:C10	1.76	1.61
4:C:5008:CPS:C5	4:C:5008:CPS:C10	1.75	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:5001:CPS:C10	4:A:5001:CPS:C5	1.76	1.60
4:E:5005:CPS:C5	4:E:5005:CPS:C10	1.76	1.59
4:B:5002:CPS:C5	4:B:5002:CPS:C10	1.76	1.59
4:E:5010:CPS:C5	4:E:5010:CPS:C10	1.75	1.59
4:D:5009:CPS:C10	4:D:5009:CPS:C5	1.75	1.56
4:C:5003:CPS:C5	4:C:5003:CPS:C10	1.76	1.56
1:E:167:TRP:CA	1:E:167:TRP:N	1.68	1.55
4:F:5091:CPS:C5	4:F:5091:CPS:C10	1.84	1.53
1:B:189:THR:HG22	6:B:6013:HOH:O	1.22	1.37
1:F:240:PHE:CD2	4:F:5091:CPS:H29B	1.60	1.34
1:D:167:TRP:HZ3	6:F:742:HOH:O	1.00	1.31
4:F:5091:CPS:C29	6:F:1547:HOH:O	1.78	1.25
1:A:217:ALA:HA	6:A:6365:HOH:O	1.36	1.21
5:E:6005:RXP:H231	6:E:6108:HOH:O	1.37	1.20
6:A:6072:HOH:O	1:C:102:PHE:CE1	1.94	1.18
1:D:167:TRP:CZ3	6:F:742:HOH:O	1.77	1.07
1:B:222:GLY:HA3	1:B:237:MET:HE1	1.33	1.04
6:A:6072:HOH:O	1:C:102:PHE:HE1	1.34	1.03
1:F:240:PHE:CD2	4:F:5091:CPS:C29	2.42	1.02
1:C:165:ARG:O	6:C:6105:HOH:O	1.83	0.97
1:F:101:MET:HG3	1:F:112:THR:H	1.29	0.97
1:E:166:TYR:O	1:E:168:HIS:ND1	1.97	0.97
1:F:240:PHE:HD2	4:F:5091:CPS:H29B	1.26	0.96
1:E:131:ARG:HD2	6:E:6031:HOH:O	1.63	0.95
1:B:222:GLY:HA3	1:B:237:MET:CE	1.96	0.95
1:A:197:PHE:CZ	6:A:6365:HOH:O	2.18	0.94
1:C:132:GLN:NE2	6:C:6024:HOH:O	2.01	0.94
1:A:165:ARG:HG2	6:A:6022:HOH:O	1.67	0.94
1:D:245:TYR:O	1:D:247:LEU:N	2.01	0.93
1:C:113:ASP:HA	1:C:148:THR:HG22	1.49	0.92
6:A:6089:HOH:O	1:E:165:ARG:HG2	1.68	0.91
1:B:216:VAL:HB	6:B:6277:HOH:O	1.68	0.91
4:F:5091:CPS:H29	6:F:1547:HOH:O	1.49	0.87
4:C:5008:CPS:C6	4:C:5008:CPS:C10	2.54	0.86
1:B:166:TYR:HB3	1:B:167:TRP:CE3	2.10	0.86
1:E:265:GLN:CD	1:E:265:GLN:H	1.78	0.86
4:A:5006:CPS:C9	4:A:5006:CPS:C10	2.52	0.86
1:C:256:GLY:HA2	6:C:6365:HOH:O	1.75	0.86
4:C:5003:CPS:C9	4:C:5003:CPS:C10	2.54	0.85
4:D:5009:CPS:C9	4:D:5009:CPS:C10	2.55	0.85
1:E:215:GLN:HB3	5:E:6005:RXP:H18	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:5007:CPS:C10	4:B:5007:CPS:C9	2.54	0.85
4:B:5002:CPS:C10	4:B:5002:CPS:C6	2.54	0.84
4:B:5002:CPS:C10	4:B:5002:CPS:C9	2.54	0.84
1:B:138:LEU:HD13	1:B:221:PHE:CD2	2.12	0.84
4:D:5004:CPS:C10	4:D:5004:CPS:C6	2.56	0.84
4:F:5011:CPS:C9	4:F:5011:CPS:C10	2.56	0.84
4:D:5004:CPS:C10	4:D:5004:CPS:C9	2.55	0.84
4:A:5006:CPS:C6	4:A:5006:CPS:C10	2.56	0.83
4:C:5008:CPS:C9	4:C:5008:CPS:C10	2.56	0.83
1:A:165:ARG:HH11	1:A:165:ARG:HB2	1.44	0.83
4:F:5091:CPS:C18	4:F:5091:CPS:C3	2.56	0.83
1:C:245:TYR:HB3	6:C:6183:HOH:O	1.76	0.83
1:D:245:TYR:O	1:D:246:PRO:C	2.04	0.83
1:D:101:MET:O	1:D:112:THR:HG23	1.78	0.83
4:A:5001:CPS:C10	4:A:5001:CPS:C9	2.55	0.82
4:E:5005:CPS:C6	4:E:5005:CPS:C10	2.56	0.82
4:E:5010:CPS:C10	4:E:5010:CPS:C6	2.56	0.82
1:A:236:LEU:HD22	1:A:249:LEU:HD23	1.59	0.82
4:A:5001:CPS:C10	4:A:5001:CPS:C6	2.57	0.82
4:B:5007:CPS:C10	4:B:5007:CPS:C4	2.57	0.82
1:A:165:ARG:HH11	1:A:165:ARG:CB	1.91	0.82
4:E:5010:CPS:C10	4:E:5010:CPS:C9	2.57	0.82
1:F:240:PHE:CE2	4:F:5091:CPS:H29B	2.14	0.82
4:E:5005:CPS:C10	4:E:5005:CPS:C9	2.57	0.82
1:A:114:LEU:HD21	6:A:6118:HOH:O	1.80	0.82
1:B:251:PRO:O	1:B:255:ARG:HG3	1.79	0.81
4:F:5091:CPS:H25	6:F:493:HOH:O	1.78	0.81
1:B:189:THR:CG2	6:B:6013:HOH:O	1.90	0.81
4:D:5004:CPS:C10	4:D:5004:CPS:C4	2.58	0.81
4:C:5003:CPS:C10	4:C:5003:CPS:C6	2.58	0.81
4:E:5010:CPS:C4	4:E:5010:CPS:C10	2.58	0.81
4:D:5009:CPS:C10	4:D:5009:CPS:C6	2.58	0.81
4:B:5007:CPS:C10	4:B:5007:CPS:C6	2.58	0.81
1:F:180:ILE:HG13	6:F:1080:HOH:O	1.81	0.81
4:C:5008:CPS:C4	4:C:5008:CPS:C10	2.58	0.81
1:A:215:GLN:HE22	1:A:244:ARG:H	1.26	0.81
1:F:138:LEU:HD13	1:F:221:PHE:CD2	2.17	0.80
1:F:246:PRO:HB2	6:F:1638:HOH:O	1.82	0.80
4:F:5011:CPS:C10	4:F:5011:CPS:C6	2.59	0.80
4:A:5001:CPS:C10	4:A:5001:CPS:C4	2.60	0.79
1:E:166:TYR:C	1:E:167:TRP:CA	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5009:CPS:C4	4:D:5009:CPS:C10	2.59	0.79
5:E:6005:RXP:C36	6:E:6013:HOH:O	2.30	0.78
4:F:5011:CPS:C4	4:F:5011:CPS:C10	2.61	0.78
1:B:245:TYR:O	1:B:247:LEU:N	2.16	0.78
1:F:165:ARG:O	1:F:166:TYR:C	2.19	0.78
4:E:5005:CPS:C4	4:E:5005:CPS:C10	2.60	0.78
1:A:165:ARG:NH1	1:A:165:ARG:HB2	1.97	0.78
1:E:209:GLN:HA	1:E:209:GLN:HE21	1.47	0.77
1:C:114:LEU:HD21	6:C:6273:HOH:O	1.84	0.77
4:B:5002:CPS:C4	4:B:5002:CPS:C10	2.63	0.77
1:B:180:ILE:HD13	5:B:6002:RXP:H7	1.67	0.77
4:A:5006:CPS:C10	4:A:5006:CPS:C4	2.63	0.77
1:B:236:LEU:HG	6:B:6080:HOH:O	1.85	0.76
4:C:5003:CPS:C4	4:C:5003:CPS:C10	2.63	0.76
1:A:115:THR:HG23	1:C:101:MET:CE	2.15	0.76
1:C:113:ASP:OD1	1:C:148:THR:HG21	1.85	0.75
1:D:236:LEU:HD22	1:D:249:LEU:HD12	1.67	0.75
1:A:111:LYS:HG2	1:C:111:LYS:HG2	1.68	0.75
1:E:213:LEU:HD23	6:E:6302:HOH:O	1.85	0.74
1:A:186:PHE:CE2	4:A:5006:CPS:H16	2.23	0.74
1:B:138:LEU:HB3	6:B:6229:HOH:O	1.86	0.74
1:B:128:GLU:HA	6:B:6038:HOH:O	1.87	0.74
4:F:5091:CPS:H29A	6:F:1547:HOH:O	1.59	0.74
1:E:183:HIS:HB3	6:E:6342:HOH:O	1.88	0.73
1:D:257:ILE:CG1	6:D:660:HOH:O	2.37	0.73
1:A:215:GLN:NE2	1:A:244:ARG:H	1.87	0.73
1:F:101:MET:HA	1:F:112:THR:OG1	1.88	0.73
1:B:222:GLY:CA	1:B:237:MET:HE1	2.16	0.73
1:B:213:LEU:HD12	6:B:6277:HOH:O	1.90	0.72
1:E:236:LEU:CD2	1:E:249:LEU:HD23	2.18	0.72
4:F:5091:CPS:C4	4:F:5091:CPS:C10	2.68	0.72
1:C:246:PRO:HD3	6:C:6183:HOH:O	1.89	0.71
1:A:115:THR:HG23	1:C:101:MET:HE2	1.70	0.71
4:F:5091:CPS:C17	4:F:5091:CPS:C19	2.66	0.71
1:A:104:LEU:HG	6:A:6189:HOH:O	1.91	0.71
1:D:215:GLN:HB3	5:D:6004:RXP:H18	1.71	0.70
1:D:214:LEU:HD11	6:D:937:HOH:O	1.91	0.70
1:B:189:THR:HG23	1:B:190:HIS:CD2	2.26	0.70
1:C:236:LEU:HD22	1:C:249:LEU:HD23	1.73	0.70
1:F:125:LEU:O	6:F:750:HOH:O	2.09	0.69
4:F:5091:CPS:C10	4:F:5091:CPS:C6	2.69	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:MET:CG	1:F:102:PHE:H	2.06	0.69
4:F:5091:CPS:H261	6:F:1762:HOH:O	1.92	0.69
1:C:245:TYR:O	1:C:247:LEU:N	2.26	0.68
4:F:5091:CPS:H271	6:F:1260:HOH:O	1.93	0.68
1:B:207:ASP:OD2	1:B:209:GLN:HG3	1.94	0.68
1:A:138:LEU:HD13	1:A:221:PHE:CD2	2.29	0.68
1:C:211:THR:HG23	6:C:6251:HOH:O	1.93	0.68
1:B:166:TYR:HB3	1:B:167:TRP:HE3	1.58	0.67
1:F:248:SER:HA	6:F:581:HOH:O	1.95	0.67
1:B:262:GLY:HA3	6:B:6177:HOH:O	1.93	0.67
1:B:235:ALA:HB1	6:B:6151:HOH:O	1.93	0.66
1:B:110:GLU:HG2	6:B:6134:HOH:O	1.95	0.66
1:F:168:HIS:N	1:F:168:HIS:ND1	2.44	0.66
1:C:205:ILE:O	1:C:205:ILE:HD12	1.95	0.65
1:F:112:THR:HG22	6:F:997:HOH:O	1.95	0.65
1:B:165:ARG:HD2	1:B:200:ASP:OD1	1.97	0.65
4:F:5091:CPS:C10	4:F:5091:CPS:C9	2.70	0.65
1:C:102:PHE:CE1	6:C:6013:HOH:O	2.49	0.65
1:D:189:THR:HG22	1:D:189:THR:O	1.96	0.65
1:B:238:SER:HB2	6:B:6149:HOH:O	1.96	0.65
1:A:137:ALA:HA	6:A:6115:HOH:O	1.96	0.64
1:B:215:GLN:HB3	5:B:6002:RXP:H18	1.79	0.64
1:A:228:GLN:HG2	6:A:6229:HOH:O	1.97	0.64
1:F:209:GLN:HA	1:F:209:GLN:HE21	1.63	0.64
1:E:167:TRP:CB	1:E:167:TRP:N	2.58	0.63
1:F:101:MET:HG3	1:F:112:THR:N	2.06	0.63
1:E:131:ARG:HD3	6:E:6198:HOH:O	1.98	0.63
1:A:127:ARG:HB2	6:A:6337:HOH:O	1.97	0.63
1:C:102:PHE:CD1	6:C:6013:HOH:O	2.51	0.63
1:D:148:THR:HG22	6:D:448:HOH:O	1.97	0.63
1:E:265:GLN:CD	1:E:265:GLN:N	2.52	0.62
1:F:101:MET:CG	1:F:102:PHE:N	2.63	0.62
1:C:219:HIS:HA	6:C:6357:HOH:O	1.99	0.62
1:B:259:HIS:O	1:B:259:HIS:ND1	2.33	0.62
1:A:197:PHE:CE1	6:A:6365:HOH:O	2.45	0.62
1:C:215:GLN:HB3	5:C:6003:RXP:H18	1.81	0.61
1:A:137:ALA:O	1:A:140:VAL:HG12	2.00	0.61
1:E:139:GLN:O	1:E:143:GLU:HG3	2.00	0.61
1:A:139:GLN:O	1:A:143:GLU:HG3	2.00	0.61
1:C:247:LEU:HA	6:C:6136:HOH:O	1.99	0.61
1:A:218:ALA:HB2	6:A:6115:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HG	6:C:6122:HOH:O	2.00	0.60
1:D:234:LYS:HD3	6:D:1691:HOH:O	2.00	0.60
1:A:127:ARG:HD3	6:A:6017:HOH:O	2.00	0.60
1:E:214:LEU:HD13	1:E:247:LEU:HD22	1.83	0.60
1:B:113:ASP:OD1	1:B:148:THR:HG21	2.00	0.60
1:D:103:VAL:HB	6:D:835:HOH:O	2.00	0.60
1:D:138:LEU:HD13	1:D:221:PHE:CD2	2.37	0.60
4:F:5091:CPS:O1	6:F:493:HOH:O	2.16	0.60
1:A:113:ASP:HB2	6:A:6299:HOH:O	2.02	0.60
1:E:165:ARG:NH2	1:E:166:TYR:HE1	1.99	0.60
1:F:245:TYR:O	1:F:246:PRO:C	2.30	0.60
1:F:245:TYR:O	1:F:247:LEU:N	2.35	0.60
1:B:209:GLN:CD	1:B:210:GLY:N	2.54	0.60
1:A:165:ARG:NH1	1:A:200:ASP:OD2	2.35	0.60
1:E:145:THR:HB	1:E:146:PRO:CD	2.32	0.60
1:D:236:LEU:CD2	1:D:249:LEU:HD12	2.32	0.60
1:C:204:THR:HB	1:C:207:ASP:HB3	1.84	0.59
1:E:219:HIS:CD2	5:E:6005:RXP:H392	2.37	0.59
1:C:113:ASP:HA	1:C:148:THR:CG2	2.26	0.59
1:A:128:GLU:HG2	6:A:6137:HOH:O	2.01	0.59
1:B:149:PHE:HB2	6:B:6229:HOH:O	2.01	0.59
1:B:109:TRP:HZ3	6:B:6180:HOH:O	1.85	0.59
1:F:188:LYS:HB2	6:F:876:HOH:O	2.02	0.59
1:E:228:GLN:NE2	4:E:5005:CPS:O2	2.35	0.58
1:F:101:MET:CG	1:F:112:THR:H	2.11	0.58
1:B:233:ALA:HA	6:B:6203:HOH:O	2.03	0.58
1:E:244:ARG:HD2	6:E:6246:HOH:O	2.02	0.58
1:A:115:THR:HG22	1:C:101:MET:N	2.18	0.58
1:A:115:THR:CG2	1:C:101:MET:N	2.66	0.58
1:E:167:TRP:HA	1:E:167:TRP:N	2.03	0.58
1:B:236:LEU:HD11	1:B:247:LEU:CD1	2.34	0.58
1:A:245:TYR:O	6:A:6051:HOH:O	2.17	0.58
1:A:128:GLU:HG2	6:A:6251:HOH:O	2.03	0.57
1:F:126:VAL:CG2	1:F:129:GLN:HG3	2.34	0.57
1:B:131:ARG:NH1	6:B:6037:HOH:O	2.36	0.57
1:D:227:LEU:N	1:D:227:LEU:HD12	2.20	0.57
1:B:101:MET:HE2	6:D:1978:HOH:O	2.04	0.57
1:F:240:PHE:CE2	4:F:5091:CPS:H28A	2.40	0.57
1:B:255:ARG:HG2	6:B:6255:HOH:O	2.04	0.57
1:F:215:GLN:NE2	6:F:585:HOH:O	1.79	0.57
1:E:138:LEU:HD13	1:E:221:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:5091:CPS:H32	6:F:1237:HOH:O	2.06	0.56
1:F:172:LEU:HB3	1:F:183:HIS:CE1	2.40	0.56
4:F:5091:CPS:C19	4:F:5091:CPS:C6	2.77	0.56
1:A:236:LEU:HD22	1:A:249:LEU:CD2	2.35	0.56
1:B:131:ARG:HD2	6:B:6038:HOH:O	2.05	0.56
1:D:118:ILE:HG13	6:D:1833:HOH:O	2.05	0.56
1:A:170:ASP:O	1:A:171:ASN:HB2	2.06	0.56
1:D:172:LEU:HD12	6:D:1632:HOH:O	2.06	0.56
1:D:242:THR:HG23	6:D:842:HOH:O	2.06	0.56
1:E:170:ASP:O	1:E:171:ASN:HB2	2.06	0.56
1:C:137:ALA:O	1:C:140:VAL:HG12	2.06	0.56
1:B:187:PRO:HG3	1:B:194:ASP:OD1	2.06	0.55
1:C:245:TYR:HD2	6:C:6183:HOH:O	1.88	0.55
1:E:245:TYR:O	1:E:247:LEU:N	2.40	0.55
1:A:162:ASP:O	1:A:196:HIS:HA	2.05	0.55
6:A:6260:HOH:O	1:C:191:ARG:HD2	2.07	0.55
1:E:205:ILE:HD11	6:E:6302:HOH:O	2.05	0.55
1:F:101:MET:HG2	1:F:102:PHE:N	2.22	0.55
1:C:246:PRO:CD	6:C:6183:HOH:O	2.50	0.55
1:C:205:ILE:HA	6:C:6107:HOH:O	2.07	0.55
1:F:137:ALA:O	1:F:140:VAL:HG13	2.06	0.55
1:A:165:ARG:N	6:A:6022:HOH:O	2.39	0.55
1:F:167:TRP:CE3	6:F:514:HOH:O	2.53	0.55
1:C:208:ASN:HD22	1:C:208:ASN:C	2.10	0.55
1:C:208:ASN:HD22	1:C:209:GLN:N	2.05	0.55
1:F:240:PHE:HD2	4:F:5091:CPS:C29	2.03	0.55
1:B:245:TYR:O	1:B:246:PRO:C	2.30	0.55
1:E:236:LEU:HD22	1:E:249:LEU:HD23	1.89	0.55
5:E:6005:RXP:H17	6:E:6090:HOH:O	2.06	0.54
1:D:215:GLN:HE22	1:D:243:PHE:HA	1.73	0.54
1:F:143:GLU:HG2	6:F:1686:HOH:O	2.08	0.54
1:B:133:THR:OG1	1:B:205:ILE:HD12	2.07	0.54
1:E:229:HIS:ND1	4:E:5005:CPS:H14	2.23	0.54
1:E:221:PHE:HA	1:E:224:VAL:HG12	1.90	0.54
1:D:108:ARG:HH11	1:D:108:ARG:HG3	1.71	0.54
1:D:257:ILE:HG12	6:D:660:HOH:O	2.06	0.53
1:E:138:LEU:HD13	1:E:221:PHE:CE2	2.43	0.53
1:F:145:THR:HB	1:F:146:PRO:HD2	1.91	0.53
1:B:237:MET:HB2	6:B:6151:HOH:O	2.07	0.53
1:A:111:LYS:HB2	1:C:111:LYS:HE2	1.90	0.53
1:B:249:LEU:HB3	1:B:253:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LYS:H	1:E:111:LYS:HD2	1.74	0.53
1:D:189:THR:CG2	1:D:189:THR:O	2.58	0.53
1:B:101:MET:N	6:B:6043:HOH:O	2.42	0.53
1:D:129:GLN:HG2	6:D:466:HOH:O	2.07	0.52
1:D:124:GLN:H	1:D:124:GLN:NE2	2.07	0.52
1:D:121:PHE:HB3	6:D:774:HOH:O	2.08	0.52
1:A:111:LYS:CG	1:C:111:LYS:HG2	2.37	0.52
1:F:101:MET:HG3	1:F:102:PHE:H	1.75	0.52
1:D:132:GLN:HG2	6:D:1413:HOH:O	2.10	0.52
1:C:116:TYR:CZ	1:C:151:GLU:HB2	2.44	0.52
1:D:208:ASN:H	1:D:208:ASN:ND2	2.07	0.52
1:F:103:VAL:HB	6:F:997:HOH:O	2.09	0.52
1:F:138:LEU:HD13	1:F:221:PHE:CE2	2.44	0.52
1:E:254:ARG:HD2	6:E:6202:HOH:O	2.10	0.52
1:E:228:GLN:HE21	1:E:228:GLN:HA	1.74	0.52
6:A:6072:HOH:O	1:C:102:PHE:CZ	2.41	0.52
1:E:121:PHE:HB3	6:E:6039:HOH:O	2.09	0.52
1:C:202:THR:HB	6:C:6293:HOH:O	2.10	0.52
1:C:138:LEU:HD13	1:C:221:PHE:CD2	2.45	0.52
1:A:215:GLN:HE22	1:A:244:ARG:N	2.04	0.52
1:F:209:GLN:HA	1:F:209:GLN:NE2	2.23	0.52
1:E:126:VAL:HG12	6:E:6136:HOH:O	2.09	0.52
1:E:165:ARG:NH2	1:E:166:TYR:CE1	2.78	0.52
1:E:264:PRO:HB3	6:E:6356:HOH:O	2.10	0.52
1:E:127:ARG:HD3	6:E:6138:HOH:O	2.10	0.51
1:E:228:GLN:NE2	1:E:228:GLN:HA	2.25	0.51
1:D:247:LEU:HB3	6:D:937:HOH:O	2.11	0.51
1:E:137:ALA:O	1:E:140:VAL:HG12	2.10	0.51
1:B:232:ALA:HB3	1:B:235:ALA:HB2	1.91	0.51
1:D:233:ALA:O	1:D:234:LYS:HB2	2.11	0.51
1:A:122:PRO:HD3	1:A:163:PHE:CE2	2.46	0.51
1:C:236:LEU:HD22	1:C:249:LEU:CD2	2.39	0.51
1:F:139:GLN:O	1:F:143:GLU:HG3	2.11	0.51
1:E:108:ARG:HG3	1:E:108:ARG:HH11	1.75	0.51
1:B:113:ASP:OD1	1:B:148:THR:CG2	2.59	0.51
1:E:254:ARG:HB3	6:E:6202:HOH:O	2.09	0.50
1:F:121:PHE:HB3	1:F:122:PRO:HD2	1.94	0.50
1:B:116:TYR:CZ	1:B:151:GLU:HB2	2.46	0.50
1:A:165:ARG:NH1	1:A:165:ARG:CB	2.63	0.50
1:F:244:ARG:HD3	6:F:607:HOH:O	2.11	0.50
1:A:115:THR:HG23	1:C:101:MET:HE3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PRO:HD3	1:D:163:PHE:CE2	2.46	0.50
1:F:261:TYR:O	1:F:262:GLY:O	2.29	0.50
1:C:186:PHE:CE2	4:C:5008:CPS:H16	2.47	0.50
1:A:129:GLN:NE2	6:A:6139:HOH:O	2.44	0.50
1:F:167:TRP:HE3	6:F:514:HOH:O	1.90	0.50
1:B:260:LEU:HD21	6:B:6188:HOH:O	2.11	0.50
1:E:166:TYR:O	1:E:168:HIS:CE1	2.62	0.50
1:B:255:ARG:HB3	6:B:6164:HOH:O	2.12	0.50
1:E:146:PRO:HB3	1:E:265:GLN:OE1	2.12	0.49
1:D:156:ARG:NH1	1:D:192:GLU:OE1	2.45	0.49
1:E:246:PRO:HD2	6:E:6093:HOH:O	2.12	0.49
1:D:145:THR:HG21	6:D:1611:HOH:O	2.12	0.49
1:A:215:GLN:HB3	5:A:6001:RXP:H18	1.94	0.49
1:B:180:ILE:HD12	5:B:6002:RXP:O5	2.13	0.49
1:E:245:TYR:O	1:E:246:PRO:C	2.37	0.49
1:D:112:THR:HG21	6:D:835:HOH:O	2.12	0.49
1:D:146:PRO:HD3	6:D:1854:HOH:O	2.12	0.49
1:A:145:THR:HB	1:A:146:PRO:HD2	1.93	0.49
1:B:189:THR:HG23	1:B:190:HIS:HD2	1.74	0.49
1:E:219:HIS:CE1	1:E:238:SER:O	2.65	0.49
1:F:103:VAL:HG23	1:F:112:THR:HG21	1.95	0.49
1:D:117:ARG:HD2	6:D:625:HOH:O	2.12	0.48
1:A:214:LEU:HD22	6:A:6115:HOH:O	2.13	0.48
4:E:5005:CPS:H18	4:E:5005:CPS:H10A	1.94	0.48
1:B:236:LEU:HD11	1:B:247:LEU:HD11	1.94	0.48
1:C:154:GLU:HB2	6:C:6014:HOH:O	2.13	0.48
5:E:6005:RXP:C37	6:E:6013:HOH:O	2.59	0.47
1:E:130:VAL:HA	6:E:6302:HOH:O	2.13	0.47
1:C:215:GLN:OE1	1:C:242:THR:O	2.33	0.47
1:E:233:ALA:C	1:E:234:LYS:HG2	2.35	0.47
1:E:108:ARG:NH1	6:E:6082:HOH:O	2.39	0.47
1:F:254:ARG:HD2	6:F:1396:HOH:O	2.14	0.47
4:B:5002:CPS:H12	6:B:6300:HOH:O	2.14	0.47
1:E:180:ILE:CG2	6:E:6342:HOH:O	2.62	0.47
1:D:117:ARG:HG3	1:D:118:ILE:N	2.27	0.47
1:F:124:GLN:CD	1:F:124:GLN:H	2.17	0.47
1:F:248:SER:HB2	6:F:587:HOH:O	2.15	0.47
1:D:172:LEU:HB2	6:D:1632:HOH:O	2.14	0.47
1:B:229:HIS:ND1	4:B:5002:CPS:H14	2.29	0.47
1:D:208:ASN:HD22	1:D:208:ASN:N	2.12	0.47
1:E:108:ARG:HG3	1:E:108:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HB	6:A:6165:HOH:O	2.15	0.47
1:A:210:GLY:O	6:A:6043:HOH:O	2.21	0.47
4:F:5011:CPS:C8	4:F:5011:CPS:C10	2.93	0.47
1:B:113:ASP:HA	1:B:148:THR:HG23	1.96	0.47
1:F:111:LYS:HG2	6:F:794:HOH:O	2.15	0.47
1:E:113:ASP:OD2	1:E:148:THR:OG1	2.33	0.47
1:A:191:ARG:HD3	6:C:6161:HOH:O	2.15	0.46
1:B:103:VAL:CG2	1:B:112:THR:CG2	2.93	0.46
1:D:111:LYS:HA	6:D:885:HOH:O	2.15	0.46
1:B:244:ARG:HB2	6:B:6233:HOH:O	2.15	0.46
1:D:101:MET:HA	1:D:112:THR:OG1	2.16	0.46
1:E:130:VAL:O	1:E:134:VAL:HG23	2.15	0.46
1:F:165:ARG:HB2	6:F:1074:HOH:O	2.13	0.46
1:C:230:THR:HB	6:C:6317:HOH:O	2.15	0.46
1:B:236:LEU:HD11	1:B:247:LEU:HD12	1.97	0.46
1:E:231:THR:HG23	6:E:6272:HOH:O	2.14	0.46
1:A:186:PHE:HE2	4:A:5006:CPS:H16	1.79	0.46
1:C:245:TYR:O	1:C:246:PRO:C	2.45	0.46
1:B:116:TYR:HA	1:B:159:ILE:O	2.16	0.46
1:B:139:GLN:HA	1:B:142:SER:OG	2.15	0.46
1:D:126:VAL:HG13	6:D:789:HOH:O	2.14	0.46
1:A:126:VAL:HG21	6:A:6251:HOH:O	2.16	0.46
1:A:256:GLY:HA2	6:A:6333:HOH:O	2.15	0.46
4:E:5005:CPS:C10	4:E:5005:CPS:H18	2.46	0.46
1:A:255:ARG:HD3	1:E:123:TRP:CD2	2.51	0.46
1:F:255:ARG:HB3	6:F:568:HOH:O	2.15	0.46
1:B:223:HIS:CE1	6:B:6144:HOH:O	2.68	0.46
1:F:214:LEU:HD13	1:F:247:LEU:HD12	1.98	0.46
1:B:111:LYS:HB3	6:D:1612:HOH:O	2.15	0.46
1:A:167:TRP:HA	6:A:6026:HOH:O	2.15	0.46
1:C:148:THR:HB	6:C:6346:HOH:O	2.15	0.45
1:E:240:PHE:CD1	1:E:240:PHE:N	2.84	0.45
1:D:208:ASN:H	1:D:208:ASN:HD22	1.64	0.45
1:E:251:PRO:HA	6:E:6202:HOH:O	2.16	0.45
1:F:234:LYS:HA	1:F:244:ARG:CZ	2.47	0.45
1:E:215:GLN:HE22	1:E:243:PHE:HA	1.82	0.45
1:E:127:ARG:HD2	6:E:6209:HOH:O	2.16	0.45
4:B:5002:CPS:H18	4:B:5002:CPS:H10A	1.99	0.45
1:B:138:LEU:HD13	1:B:221:PHE:CE2	2.51	0.45
1:B:205:ILE:HG12	1:B:205:ILE:O	2.16	0.45
1:D:108:ARG:NH1	1:D:108:ARG:HG3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LYS:HD3	6:C:6343:HOH:O	2.16	0.45
4:E:5010:CPS:C10	4:E:5010:CPS:C8	2.94	0.45
1:A:197:PHE:HZ	6:A:6365:HOH:O	1.76	0.45
4:C:5008:CPS:H10A	4:C:5008:CPS:H18	1.99	0.45
4:E:5010:CPS:C10	4:E:5010:CPS:C7	2.94	0.45
1:D:120:ARG:HB2	1:D:162:ASP:OD1	2.17	0.45
4:F:5011:CPS:C7	4:F:5011:CPS:C10	2.95	0.44
1:C:184:ALA:HA	1:C:194:ASP:O	2.17	0.44
1:E:238:SER:O	5:E:6005:RXP:H15	2.17	0.44
1:D:227:LEU:CD1	1:D:227:LEU:N	2.81	0.44
1:F:257:ILE:HA	1:F:257:ILE:HD13	1.87	0.44
5:E:6005:RXP:H17	6:E:6088:HOH:O	2.17	0.44
5:E:6005:RXP:H26	6:E:6218:HOH:O	2.16	0.44
1:F:180:ILE:HD13	5:F:6006:RXP:H7	1.99	0.44
1:B:246:PRO:HD2	6:B:6086:HOH:O	2.15	0.44
1:B:176:GLY:HA2	1:B:200:ASP:OD2	2.17	0.44
1:F:126:VAL:HG23	1:F:129:GLN:HG3	1.99	0.44
1:C:139:GLN:O	1:C:143:GLU:HG3	2.17	0.44
1:A:180:ILE:HD13	5:A:6001:RXP:H7	1.99	0.44
1:B:180:ILE:CD1	5:B:6002:RXP:H7	2.44	0.44
1:A:247:LEU:HG	6:A:6115:HOH:O	2.16	0.44
1:A:147:LEU:HD21	4:A:5006:CPS:H10B	2.00	0.44
1:C:170:ASP:O	1:C:171:ASN:HB2	2.17	0.44
1:C:148:THR:HG23	6:C:6091:HOH:O	2.16	0.44
1:F:234:LYS:HA	1:F:244:ARG:NH2	2.32	0.44
1:A:187:PRO:HD2	1:A:192:GLU:O	2.18	0.44
1:E:147:LEU:HD21	1:E:261:TYR:CD2	2.52	0.44
4:A:5006:CPS:C8	4:A:5006:CPS:C10	2.96	0.44
1:E:147:LEU:HD21	1:E:261:TYR:CE2	2.53	0.44
1:A:184:ALA:HA	1:A:194:ASP:O	2.18	0.44
1:E:263:ARG:HH11	1:E:263:ARG:HG3	1.83	0.44
1:E:108:ARG:HA	6:E:6310:HOH:O	2.17	0.44
1:C:234:LYS:HE3	6:C:6227:HOH:O	2.18	0.44
1:C:251:PRO:HD3	6:C:6150:HOH:O	2.18	0.44
1:B:147:LEU:HD22	6:B:6264:HOH:O	2.18	0.43
1:B:244:ARG:HD2	6:B:6234:HOH:O	2.18	0.43
1:B:121:PHE:HB3	1:B:122:PRO:HD2	2.00	0.43
1:B:242:THR:HG22	6:B:6295:HOH:O	2.17	0.43
1:E:209:GLN:CA	1:E:209:GLN:HE21	2.25	0.43
1:E:243:PHE:HB2	6:E:6326:HOH:O	2.18	0.43
1:F:111:LYS:HB2	6:F:2103:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:O	1:A:168:HIS:ND1	2.51	0.43
1:B:213:LEU:HA	6:B:6277:HOH:O	2.18	0.43
1:E:111:LYS:N	1:E:111:LYS:HD2	2.32	0.43
1:D:191:ARG:HG2	1:D:191:ARG:H	1.49	0.43
1:D:242:THR:HG21	6:D:1584:HOH:O	2.19	0.43
1:A:182:ALA:O	5:A:6001:RXP:H211	2.18	0.43
1:E:229:HIS:HD1	4:E:5005:CPS:H14	1.82	0.43
1:D:208:ASN:ND2	1:D:208:ASN:N	2.67	0.43
1:E:120:ARG:HG2	6:E:6166:HOH:O	2.18	0.43
1:C:156:ARG:NH1	1:C:192:GLU:OE1	2.52	0.43
1:B:216:VAL:O	1:B:220:GLU:HG2	2.19	0.43
1:A:138:LEU:HD13	1:A:221:PHE:CG	2.53	0.43
1:F:215:GLN:HG2	6:F:585:HOH:O	2.17	0.43
1:E:263:ARG:HG3	1:E:263:ARG:NH1	2.33	0.43
1:C:229:HIS:ND1	4:C:5003:CPS:H14	2.34	0.43
1:C:113:ASP:OD1	1:C:148:THR:CG2	2.60	0.43
1:D:257:ILE:HB	6:D:660:HOH:O	2.18	0.43
1:D:137:ALA:O	1:D:140:VAL:HG12	2.18	0.43
1:F:216:VAL:O	1:F:220:GLU:HG2	2.19	0.43
4:B:5007:CPS:C10	4:B:5007:CPS:C8	2.97	0.43
1:F:101:MET:O	1:F:102:PHE:HB2	2.18	0.43
1:C:245:TYR:CB	6:C:6183:HOH:O	2.48	0.43
1:A:209:GLN:HB2	6:A:6347:HOH:O	2.18	0.43
1:B:139:GLN:O	1:B:143:GLU:HG3	2.18	0.42
4:B:5007:CPS:H14	4:B:5007:CPS:H19	1.99	0.42
4:F:5011:CPS:C8	4:F:5011:CPS:H10	2.50	0.42
1:B:129:GLN:HG2	1:B:205:ILE:HD13	2.02	0.42
1:C:245:TYR:O	1:C:245:TYR:CG	2.69	0.42
1:F:242:THR:HG22	6:F:613:HOH:O	2.20	0.42
4:A:5001:CPS:H4	5:A:6001:RXP:O5	2.19	0.42
1:C:214:LEU:HB2	6:C:6107:HOH:O	2.18	0.42
1:F:114:LEU:N	1:F:114:LEU:HD23	2.34	0.42
1:C:222:GLY:O	1:C:227:LEU:HD23	2.19	0.42
4:C:5008:CPS:C7	4:C:5008:CPS:C10	2.97	0.42
1:C:165:ARG:O	1:C:174:PHE:HB2	2.19	0.42
1:A:168:HIS:ND1	1:A:168:HIS:N	2.67	0.42
4:A:5001:CPS:H18	4:A:5001:CPS:H10A	2.01	0.42
1:C:208:ASN:ND2	1:C:208:ASN:C	2.73	0.42
1:C:231:THR:O	1:C:231:THR:HG22	2.19	0.42
1:C:215:GLN:HE22	1:C:244:ARG:H	1.67	0.42
1:C:188:LYS:HG2	6:C:6274:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:PHE:CD1	1:E:197:PHE:HB2	2.55	0.42
1:D:101:MET:HB2	6:D:885:HOH:O	2.19	0.42
1:C:191:ARG:HG2	1:C:191:ARG:H	1.66	0.42
1:B:127:ARG:HD2	6:B:6147:HOH:O	2.20	0.42
5:A:6001:RXP:H26	6:A:6035:HOH:O	2.20	0.41
1:A:220:GLU:HB2	6:A:6365:HOH:O	2.20	0.41
1:C:247:LEU:HD12	6:C:6136:HOH:O	2.18	0.41
1:A:111:LYS:CB	1:C:111:LYS:HG2	2.49	0.41
1:F:226:GLY:HA3	1:F:260:LEU:HD21	2.02	0.41
1:E:116:TYR:CZ	1:E:151:GLU:HB2	2.55	0.41
1:C:257:ILE:HA	1:C:257:ILE:HD13	1.84	0.41
4:C:5008:CPS:C8	4:C:5008:CPS:C10	2.99	0.41
1:E:165:ARG:CZ	1:E:166:TYR:HE1	2.33	0.41
1:C:188:LYS:HA	6:C:6274:HOH:O	2.21	0.41
1:E:191:ARG:H	1:E:191:ARG:HG2	1.75	0.41
4:A:5006:CPS:C10	4:A:5006:CPS:C7	2.97	0.41
1:A:111:LYS:HG2	1:C:111:LYS:CG	2.45	0.41
1:D:257:ILE:HG13	6:D:660:HOH:O	2.15	0.41
1:D:145:THR:HB	1:D:146:PRO:HD2	2.02	0.41
1:B:165:ARG:O	1:B:168:HIS:ND1	2.52	0.41
1:A:245:TYR:N	6:A:6051:HOH:O	2.44	0.41
1:B:103:VAL:CG2	1:B:112:THR:HG22	2.50	0.41
1:C:149:PHE:HB2	6:C:6185:HOH:O	2.20	0.41
1:E:176:GLY:HA2	1:E:200:ASP:OD2	2.20	0.41
4:B:5002:CPS:C10	4:B:5002:CPS:H18	2.50	0.41
1:B:185:PHE:O	1:B:187:PRO:HD3	2.21	0.41
1:B:191:ARG:H	1:B:191:ARG:HG2	1.68	0.41
1:E:166:TYR:N	1:E:174:PHE:HB2	2.35	0.41
1:B:257:ILE:HD12	1:B:257:ILE:HA	1.88	0.41
4:B:5007:CPS:C10	4:B:5007:CPS:C7	2.99	0.41
1:F:209:GLN:CA	1:F:209:GLN:HE21	2.27	0.41
4:D:5004:CPS:C10	4:D:5004:CPS:C8	2.99	0.41
4:A:5001:CPS:C10	4:A:5001:CPS:H18	2.51	0.41
1:E:174:PHE:HA	6:E:6291:HOH:O	2.20	0.41
1:C:205:ILE:O	1:C:205:ILE:CD1	2.66	0.41
1:E:121:PHE:HB3	1:E:122:PRO:HD2	2.03	0.41
1:E:225:LEU:HA	1:E:225:LEU:HD23	1.91	0.41
1:A:227:LEU:HD11	1:A:257:ILE:HD13	2.02	0.41
1:F:191:ARG:HA	6:F:520:HOH:O	2.20	0.41
1:E:139:GLN:O	1:E:139:GLN:HG2	2.21	0.41
1:C:204:THR:CB	1:C:207:ASP:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:LYS:HE3	1:E:244:ARG:NH2	2.36	0.41
1:E:166:TYR:H	1:E:174:PHE:HB2	1.85	0.40
5:F:6006:RXP:H37	6:F:498:HOH:O	2.20	0.40
1:D:198:ASP:HB3	1:D:201:GLU:HG2	2.01	0.40
4:C:5003:CPS:C8	4:C:5003:CPS:C10	2.99	0.40
1:C:215:GLN:HG2	6:C:6109:HOH:O	2.20	0.40
1:F:188:LYS:HE2	6:F:876:HOH:O	2.21	0.40
1:F:126:VAL:HG22	1:F:129:GLN:HG3	2.02	0.40
1:A:101:MET:HG2	1:A:102:PHE:N	2.37	0.40
4:E:5005:CPS:H12	6:E:6108:HOH:O	2.21	0.40
1:F:108:ARG:HG3	1:F:108:ARG:NH1	2.37	0.40
1:E:188:LYS:HB2	6:E:6226:HOH:O	2.21	0.40
1:F:240:PHE:CZ	4:F:5091:CPS:H28A	2.55	0.40
6:A:6089:HOH:O	1:E:165:ARG:N	2.54	0.40
1:F:214:LEU:HG	6:F:532:HOH:O	2.21	0.40
1:D:257:ILE:CB	6:D:660:HOH:O	2.67	0.40
4:C:5008:CPS:H18	4:C:5008:CPS:C10	2.51	0.40
1:D:225:LEU:HD13	6:D:1611:HOH:O	2.20	0.40
1:D:116:TYR:CZ	1:D:151:GLU:HB2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:MET:CE	6:E:6062:HOH:O[2_665]	1.33	0.87

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	160/165 (97%)	155 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	162/165 (98%)	148 (91%)	12 (7%)	2 (1%)	16 33
1	C	160/165 (97%)	151 (94%)	9 (6%)	0	100 100
1	D	160/165 (97%)	151 (94%)	7 (4%)	2 (1%)	15 30
1	E	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	30 56
1	F	160/165 (97%)	153 (96%)	7 (4%)	0	100 100
All	All	965/990 (98%)	910 (94%)	50 (5%)	5 (0%)	34 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	LYS
1	B	189	THR
1	D	167	TRP
1	E	167	TRP
1	D	245	TYR

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	137/140 (98%)	132 (96%)	5 (4%)	42 71
1	B	139/140 (99%)	126 (91%)	13 (9%)	11 20
1	C	137/140 (98%)	131 (96%)	6 (4%)	35 63
1	D	137/140 (98%)	125 (91%)	12 (9%)	12 24
1	E	140/140 (100%)	127 (91%)	13 (9%)	11 21
1	F	137/140 (98%)	125 (91%)	12 (9%)	12 24
All	All	827/840 (98%)	766 (93%)	61 (7%)	17 34

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	165	ARG
1	A	187	PRO
1	A	191	ARG
1	A	214	LEU
1	B	104	LEU
1	B	117	ARG
1	B	138	LEU
1	B	148	THR
1	B	209	GLN
1	B	214	LEU
1	B	225	LEU
1	B	227	LEU
1	B	228	GLN
1	B	236	LEU
1	B	245	TYR
1	B	252	ASP
1	B	259	HIS
1	C	101	MET
1	C	138	LEU
1	C	165	ARG
1	C	208	ASN
1	C	214	LEU
1	C	255	ARG
1	D	124	GLN
1	D	126	VAL
1	D	138	LEU
1	D	165	ARG
1	D	170	ASP
1	D	191	ARG
1	D	208	ASN
1	D	214	LEU
1	D	245	TYR
1	D	247	LEU
1	D	249	LEU
1	D	255	ARG
1	E	111	LYS
1	E	126	VAL
1	E	138	LEU
1	E	165	ARG
1	E	209	GLN
1	E	214	LEU
1	E	227	LEU

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Mol	Chain	Res	Type
1	E	230	THR
1	E	234	LYS
1	E	236	LEU
1	E	244	ARG
1	E	245	TYR
1	E	265	GLN
1	F	105	SER
1	F	114	LEU
1	F	117	ARG
1	F	124	GLN
1	F	138	LEU
1	F	165	ARG
1	F	172	LEU
1	F	209	GLN
1	F	214	LEU
1	F	244	ARG
1	F	247	LEU
1	F	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	215	GLN
1	A	258	GLN
1	B	129	GLN
1	B	190	HIS
1	B	258	GLN
1	C	129	GLN
1	C	208	ASN
1	C	215	GLN
1	D	124	GLN
1	D	129	GLN
1	D	132	GLN
1	D	208	ASN
1	D	215	GLN
1	D	258	GLN
1	E	129	GLN
1	E	190	HIS
1	E	209	GLN
1	E	215	GLN
1	E	228	GLN

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Mol	Chain	Res	Type
1	E	259	HIS
1	F	258	GLN

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

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 for Mogul analysis.

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	$\#\|Z\| > 2$
4	CPS	A	5001	-	29,29,45	4.86	17 (58%)	47,47,70	4.05	27 (57%)
4	CPS	A	5006	-	29,29,45	4.67	17 (58%)	47,47,70	3.99	24 (51%)
5	RXP	A	6001	2	49,54,54	5.07	38 (77%)	52,73,73	2.53	22 (42%)
4	CPS	B	5002	-	29,29,45	4.76	16 (55%)	47,47,70	3.92	28 (59%)
4	CPS	B	5007	-	29,29,45	4.78	17 (58%)	47,47,70	3.91	27 (57%)
5	RXP	B	6002	2	49,54,54	6.04	36 (73%)	52,73,73	2.81	17 (32%)
4	CPS	C	5003	-	29,29,45	4.71	14 (48%)	47,47,70	4.05	29 (61%)
4	CPS	C	5008	-	29,29,45	4.80	17 (58%)	47,47,70	3.93	24 (51%)
5	RXP	C	6003	2	49,54,54	4.98	36 (73%)	52,73,73	2.77	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CPS	D	5004	-	29,29,45	4.76	16 (55%)	47,47,70	3.93	28 (59%)
4	CPS	D	5009	-	29,29,45	4.94	16 (55%)	47,47,70	3.88	27 (57%)
5	RXP	D	6004	2	49,54,54	5.10	34 (69%)	52,73,73	2.51	19 (36%)
4	CPS	E	5005	-	29,29,45	4.76	15 (51%)	47,47,70	4.13	28 (59%)
4	CPS	E	5010	-	29,29,45	4.81	16 (55%)	47,47,70	3.92	25 (53%)
5	RXP	E	6005	2	49,54,54	5.02	32 (65%)	52,73,73	2.30	19 (36%)
4	CPS	F	5011	-	29,29,45	4.85	17 (58%)	47,47,70	3.82	26 (55%)
4	CPS	F	5091	-	44,45,45	4.67	23 (52%)	67,70,70	3.27	32 (47%)
5	RXP	F	6006	2	49,54,54	5.02	32 (65%)	52,73,73	2.30	18 (34%)

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
4	CPS	A	5001	-	-	0/6/71/90	0/4/4/4
4	CPS	A	5006	-	-	0/6/71/90	0/4/4/4
5	RXP	A	6001	2	-	0/39/46/46	0/5/5/5
4	CPS	B	5002	-	-	0/6/71/90	0/4/4/4
4	CPS	B	5007	-	-	0/6/71/90	0/4/4/4
5	RXP	B	6002	2	-	0/39/46/46	0/5/5/5
4	CPS	C	5003	-	-	0/6/71/90	0/4/4/4
4	CPS	C	5008	-	-	0/6/71/90	0/4/4/4
5	RXP	C	6003	2	-	0/39/46/46	0/5/5/5
4	CPS	D	5004	-	-	0/6/71/90	0/4/4/4
4	CPS	D	5009	-	-	0/6/71/90	0/4/4/4
5	RXP	D	6004	2	-	0/39/46/46	0/5/5/5
4	CPS	E	5005	-	-	0/6/71/90	0/4/4/4
4	CPS	E	5010	-	-	0/6/71/90	0/4/4/4
5	RXP	E	6005	2	-	0/39/46/46	0/5/5/5
4	CPS	F	5011	-	-	0/6/71/90	0/4/4/4
4	CPS	F	5091	-	-	1/25/90/90	0/4/4/4
5	RXP	F	6006	2	-	0/39/46/46	0/5/5/5

All (409) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5009	CPS	O4-C4	-13.15	1.21	1.43
4	D	5004	CPS	O4-C4	-13.02	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	CPS	O4-C4	-12.34	1.22	1.43
4	E	5010	CPS	O4-C4	-12.16	1.22	1.43
4	B	5007	CPS	O4-C4	-11.78	1.23	1.43
4	B	5002	CPS	O4-C4	-11.63	1.23	1.43
4	C	5008	CPS	O4-C4	-11.56	1.23	1.43
4	C	5003	CPS	O4-C4	-11.53	1.23	1.43
4	F	5011	CPS	O4-C4	-11.50	1.24	1.43
4	E	5005	CPS	O4-C4	-11.02	1.24	1.43
4	A	5006	CPS	O4-C4	-10.84	1.25	1.43
5	A	6001	RXP	P-O1P	-10.04	1.31	1.49
4	F	5091	CPS	O4-C4	-9.81	1.26	1.43
4	C	5008	CPS	C5-C9	-7.19	1.42	1.55
5	D	6004	RXP	P-O1P	-7.17	1.36	1.49
4	A	5001	CPS	C5-C9	-7.00	1.43	1.55
4	B	5007	CPS	C5-C9	-6.87	1.43	1.55
4	A	5006	CPS	C5-C9	-6.84	1.43	1.55
4	D	5004	CPS	C5-C9	-6.80	1.43	1.55
4	B	5002	CPS	C5-C9	-6.77	1.43	1.55
4	E	5010	CPS	C5-C9	-6.75	1.43	1.55
4	F	5011	CPS	C5-C9	-6.57	1.44	1.55
4	D	5009	CPS	C5-C9	-6.55	1.44	1.55
4	C	5003	CPS	C5-C9	-6.08	1.44	1.55
4	E	5005	CPS	C5-C9	-5.89	1.45	1.55
5	E	6005	RXP	P-O1P	-5.84	1.38	1.49
5	F	6006	RXP	P-O1P	-5.80	1.39	1.49
5	D	6004	RXP	C23-C24	-5.77	1.37	1.51
4	A	5001	CPS	O3-C17	-5.73	1.30	1.43
4	C	5003	CPS	O3-C17	-5.73	1.30	1.43
4	B	5007	CPS	O3-C17	-5.67	1.30	1.43
4	F	5091	CPS	O3-C17	-5.51	1.31	1.43
4	E	5010	CPS	O3-C17	-5.41	1.31	1.43
4	B	5002	CPS	O3-C17	-4.85	1.32	1.43
4	E	5005	CPS	O3-C17	-4.84	1.32	1.43
4	D	5004	CPS	O3-C17	-4.76	1.32	1.43
4	C	5008	CPS	C5-C4	-4.42	1.47	1.54
4	A	5006	CPS	O3-C17	-4.42	1.33	1.43
5	B	6002	RXP	P-O1P	-4.41	1.41	1.49
5	E	6005	RXP	C23-C24	-4.29	1.40	1.51
5	F	6006	RXP	C23-C24	-4.28	1.40	1.51
4	A	5006	CPS	C16-C15	-4.10	1.46	1.53
4	D	5009	CPS	C16-C15	-4.07	1.46	1.53
4	C	5003	CPS	C16-C15	-4.02	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5091	CPS	C5-C9	-3.99	1.48	1.55
4	C	5008	CPS	C16-C15	-3.83	1.47	1.53
4	C	5008	CPS	O3-C17	-3.83	1.34	1.43
4	E	5010	CPS	C5-C4	-3.74	1.48	1.54
4	D	5009	CPS	C5-C4	-3.71	1.48	1.54
4	A	5001	CPS	C16-C15	-3.70	1.47	1.53
5	C	6003	RXP	C23-C24	-3.69	1.42	1.51
5	A	6001	RXP	P-C21	-3.64	1.76	1.79
4	D	5009	CPS	O3-C17	-3.63	1.35	1.43
4	F	5011	CPS	O3-C17	-3.58	1.35	1.43
5	A	6001	RXP	O2-C12	-3.52	1.16	1.23
5	C	6003	RXP	C22-N4	-3.52	1.42	1.46
4	D	5004	CPS	C16-C15	-3.47	1.47	1.53
4	B	5007	CPS	C5-C4	-3.45	1.49	1.54
4	F	5011	CPS	C16-C15	-3.43	1.47	1.53
4	F	5011	CPS	C5-C4	-3.29	1.49	1.54
5	C	6003	RXP	O1-C11	-3.19	1.17	1.23
4	B	5002	CPS	C16-C15	-3.06	1.48	1.53
4	E	5010	CPS	C16-C15	-2.97	1.48	1.53
4	A	5001	CPS	C5-C4	-2.94	1.49	1.54
4	B	5007	CPS	C16-C15	-2.86	1.48	1.53
4	B	5007	CPS	C3-C19	-2.85	1.49	1.53
4	D	5004	CPS	C5-C4	-2.82	1.50	1.54
5	A	6001	RXP	C23-C24	-2.80	1.44	1.51
4	E	5005	CPS	C16-C15	-2.77	1.49	1.53
5	D	6004	RXP	O2-C12	-2.74	1.18	1.23
5	B	6002	RXP	O1-C11	-2.46	1.19	1.23
4	F	5091	CPS	C5-C6	-2.44	1.51	1.55
5	B	6002	RXP	O2-C12	-2.41	1.18	1.23
5	C	6003	RXP	P-O1P	-2.28	1.45	1.49
4	C	5008	CPS	C7-C6	-2.23	1.49	1.54
4	A	5006	CPS	C3-C19	-2.18	1.50	1.53
4	A	5001	CPS	C7-C6	-2.17	1.49	1.54
4	B	5002	CPS	C5-C6	-2.15	1.51	1.55
5	A	6001	RXP	C39-C14	-2.14	1.45	1.51
4	A	5006	CPS	C5-C4	-2.00	1.51	1.54
5	A	6001	RXP	C11-N1	2.02	1.36	1.32
5	B	6002	RXP	C1-N2	2.10	1.50	1.45
5	D	6004	RXP	C15-C14	2.10	1.43	1.38
5	C	6003	RXP	C5-N3	2.11	1.40	1.36
5	E	6005	RXP	C1-C11	2.16	1.56	1.52
5	F	6006	RXP	C1-C11	2.17	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5003	CPS	C14-C13	2.20	1.56	1.51
4	F	5091	CPS	C1-C2	2.24	1.58	1.54
4	F	5091	CPS	C29-N2	2.34	1.56	1.50
5	D	6004	RXP	C18-C17	2.36	1.44	1.38
4	B	5002	CPS	C20-C9	2.38	1.58	1.54
4	D	5004	CPS	C20-C9	2.46	1.59	1.54
4	F	5091	CPS	O2-C13	2.49	1.51	1.43
4	A	5001	CPS	O2-C13	2.53	1.51	1.43
5	A	6001	RXP	C18-C17	2.55	1.44	1.38
4	C	5008	CPS	C11-C2	2.57	1.59	1.54
5	D	6004	RXP	O6-C31	2.58	1.51	1.45
4	F	5091	CPS	O3S-S	2.64	1.53	1.45
4	C	5008	CPS	C14-C13	2.66	1.56	1.51
5	C	6003	RXP	C8-C6	2.67	1.46	1.41
4	F	5091	CPS	O2S-S	2.68	1.53	1.46
4	F	5011	CPS	C2-C19	2.68	1.61	1.56
4	A	5006	CPS	C20-C9	2.70	1.59	1.54
4	D	5009	CPS	C14-C13	2.76	1.57	1.51
4	E	5005	CPS	C14-C15	2.77	1.58	1.53
4	B	5002	CPS	C14-C13	2.77	1.57	1.51
4	D	5004	CPS	C14-C15	2.83	1.58	1.53
4	F	5091	CPS	C21-C20	2.83	1.60	1.53
4	B	5007	CPS	C11-C2	2.84	1.59	1.54
5	D	6004	RXP	C5-C3	2.85	1.44	1.38
5	A	6001	RXP	C15-C14	2.85	1.44	1.38
4	F	5011	CPS	C20-C9	2.86	1.59	1.54
4	E	5005	CPS	C14-C13	2.89	1.57	1.51
4	F	5011	CPS	C11-C2	2.90	1.59	1.54
4	B	5007	CPS	O2-C13	2.91	1.52	1.43
4	E	5005	CPS	C20-C9	2.93	1.59	1.54
4	A	5006	CPS	C11-C2	2.96	1.59	1.54
4	A	5001	CPS	C20-C9	2.97	1.60	1.54
4	C	5008	CPS	C20-C9	2.97	1.60	1.54
5	D	6004	RXP	C18-C19	2.97	1.45	1.38
4	C	5003	CPS	C20-C9	2.98	1.60	1.54
5	E	6005	RXP	O5-C30	3.01	1.27	1.21
5	F	6006	RXP	C17-C16	3.01	1.45	1.38
5	E	6005	RXP	C17-C16	3.02	1.45	1.38
5	F	6006	RXP	O5-C30	3.02	1.27	1.21
4	E	5010	CPS	C11-C2	3.02	1.60	1.54
4	E	5010	CPS	C20-C9	3.09	1.60	1.54
4	D	5009	CPS	C11-C2	3.13	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5009	CPS	C20-C9	3.14	1.60	1.54
5	B	6002	RXP	C5-N3	3.14	1.43	1.36
4	F	5091	CPS	C18-C6	3.16	1.60	1.53
4	B	5002	CPS	C11-C2	3.16	1.60	1.54
5	D	6004	RXP	C30-N4	3.20	1.43	1.34
5	F	6006	RXP	C30-N4	3.21	1.43	1.34
5	E	6005	RXP	C30-N4	3.21	1.43	1.34
5	A	6001	RXP	C17-C16	3.21	1.46	1.38
4	E	5010	CPS	C14-C13	3.23	1.58	1.51
5	C	6003	RXP	C15-C14	3.24	1.45	1.38
4	B	5007	CPS	C20-C9	3.25	1.60	1.54
4	B	5002	CPS	C14-C15	3.25	1.59	1.53
4	D	5009	CPS	C14-C15	3.26	1.59	1.53
5	D	6004	RXP	C1-C11	3.26	1.58	1.52
4	A	5001	CPS	C14-C15	3.26	1.59	1.53
4	A	5006	CPS	O2-C13	3.28	1.53	1.43
5	B	6002	RXP	C15-C14	3.29	1.45	1.38
5	A	6001	RXP	C20-C12	3.29	1.57	1.51
4	A	5006	CPS	C14-C13	3.30	1.58	1.51
5	A	6001	RXP	C8-C6	3.31	1.47	1.41
5	A	6001	RXP	C5-C3	3.32	1.44	1.38
5	A	6001	RXP	C30-N4	3.33	1.43	1.34
4	C	5003	CPS	C11-C2	3.35	1.60	1.54
4	B	5007	CPS	C14-C13	3.36	1.58	1.51
4	A	5001	CPS	C14-C13	3.36	1.58	1.51
4	C	5008	CPS	C14-C15	3.37	1.59	1.53
4	C	5003	CPS	O2-C13	3.38	1.53	1.43
4	F	5091	CPS	O1S-S	3.41	1.55	1.45
4	A	5006	CPS	C14-C15	3.45	1.59	1.53
5	A	6001	RXP	C7-C4	3.45	1.49	1.42
4	A	5001	CPS	C8-C7	3.45	1.63	1.54
5	C	6003	RXP	C5-C3	3.46	1.45	1.38
4	E	5005	CPS	O2-C13	3.47	1.53	1.43
5	C	6003	RXP	C18-C17	3.49	1.47	1.38
4	D	5004	CPS	C14-C13	3.51	1.58	1.51
4	A	5001	CPS	C11-C2	3.51	1.60	1.54
5	E	6005	RXP	C20-C12	3.55	1.57	1.51
5	A	6001	RXP	C27-C25	3.55	1.46	1.38
5	F	6006	RXP	C20-C12	3.56	1.57	1.51
4	F	5011	CPS	C14-C13	3.56	1.58	1.51
4	C	5003	CPS	C8-C7	3.59	1.64	1.54
4	F	5011	CPS	C8-C7	3.60	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5010	CPS	O2-C13	3.64	1.54	1.43
4	D	5004	CPS	O2-C13	3.65	1.54	1.43
4	D	5004	CPS	C8-C7	3.66	1.64	1.54
5	A	6001	RXP	C1-C11	3.69	1.58	1.52
5	D	6004	RXP	O6-C30	3.70	1.42	1.35
4	E	5010	CPS	C14-C15	3.73	1.60	1.53
4	C	5008	CPS	O2-C13	3.74	1.54	1.43
4	D	5004	CPS	C11-C2	3.77	1.61	1.54
4	C	5008	CPS	C8-C7	3.78	1.64	1.54
4	E	5005	CPS	C11-C2	3.83	1.61	1.54
4	A	5006	CPS	C8-C7	3.85	1.64	1.54
5	B	6002	RXP	C31-C32	3.87	1.59	1.50
5	B	6002	RXP	C18-C17	3.90	1.48	1.38
4	B	5002	CPS	C8-C7	3.98	1.65	1.54
5	C	6003	RXP	C20-C12	3.99	1.58	1.51
5	F	6006	RXP	C15-C14	4.07	1.47	1.38
5	E	6005	RXP	C15-C14	4.08	1.47	1.38
5	A	6001	RXP	C29-C27	4.11	1.48	1.38
5	F	6006	RXP	C18-C17	4.12	1.48	1.38
5	E	6005	RXP	C18-C17	4.12	1.48	1.38
5	F	6006	RXP	C19-C14	4.13	1.47	1.38
5	E	6005	RXP	C19-C14	4.17	1.47	1.38
5	E	6005	RXP	C4-C6	4.18	1.53	1.42
4	E	5010	CPS	C8-C7	4.19	1.65	1.54
4	D	5009	CPS	O2-C13	4.19	1.56	1.43
5	F	6006	RXP	C4-C6	4.20	1.53	1.42
5	A	6001	RXP	C31-C32	4.20	1.60	1.50
5	B	6002	RXP	O6-C30	4.21	1.43	1.35
5	C	6003	RXP	C16-C15	4.26	1.47	1.38
4	B	5007	CPS	C14-C15	4.26	1.61	1.53
4	B	5002	CPS	O2-C13	4.26	1.56	1.43
4	F	5011	CPS	C14-C15	4.28	1.61	1.53
4	F	5091	CPS	C14-C15	4.29	1.61	1.53
4	B	5002	CPS	C3-C4	4.31	1.61	1.53
5	D	6004	RXP	C20-C12	4.33	1.59	1.51
5	B	6002	RXP	C5-C3	4.34	1.46	1.38
4	F	5091	CPS	C2-C15	4.35	1.62	1.55
4	F	5091	CPS	C8-C7	4.39	1.66	1.54
5	C	6003	RXP	C26-C24	4.40	1.48	1.38
5	A	6001	RXP	C16-C15	4.41	1.48	1.38
4	B	5007	CPS	C8-C7	4.41	1.66	1.54
5	B	6002	RXP	O6-C31	4.42	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	6003	RXP	C4-C6	4.44	1.54	1.42
4	C	5008	CPS	C8-C9	4.44	1.64	1.54
4	E	5005	CPS	C8-C7	4.48	1.66	1.54
4	F	5091	CPS	C8-C9	4.54	1.64	1.54
4	A	5001	CPS	C8-C9	4.58	1.64	1.54
5	C	6003	RXP	C7-C4	4.64	1.51	1.42
4	F	5011	CPS	O2-C13	4.64	1.57	1.43
4	E	5010	CPS	C8-C9	4.67	1.65	1.54
4	A	5006	CPS	C8-C9	4.72	1.65	1.54
4	F	5091	CPS	C14-C13	4.76	1.60	1.51
5	A	6001	RXP	C18-C19	4.77	1.48	1.38
4	B	5007	CPS	C8-C9	4.80	1.65	1.54
5	C	6003	RXP	C17-C16	4.80	1.50	1.38
4	D	5009	CPS	C8-C7	4.83	1.67	1.54
5	C	6003	RXP	O6-C30	4.84	1.45	1.35
4	E	5005	CPS	C8-C9	4.89	1.65	1.54
5	C	6003	RXP	C30-N4	4.90	1.48	1.34
5	F	6006	RXP	C27-C25	4.97	1.49	1.38
5	C	6003	RXP	C27-C25	4.98	1.49	1.38
5	C	6003	RXP	C29-C27	4.99	1.50	1.38
5	E	6005	RXP	C27-C25	5.01	1.49	1.38
4	F	5011	CPS	C8-C9	5.02	1.66	1.54
5	A	6001	RXP	C4-C6	5.06	1.56	1.42
4	D	5004	CPS	C8-C9	5.08	1.66	1.54
4	B	5002	CPS	C8-C9	5.08	1.66	1.54
5	F	6006	RXP	C26-C24	5.09	1.49	1.38
5	E	6005	RXP	C26-C24	5.10	1.49	1.38
5	D	6004	RXP	C8-C6	5.16	1.51	1.41
4	C	5003	CPS	C8-C9	5.17	1.66	1.54
5	D	6004	RXP	O5-C30	5.26	1.31	1.21
5	D	6004	RXP	C16-C15	5.26	1.49	1.38
4	D	5004	CPS	C3-C4	5.31	1.63	1.53
4	C	5008	CPS	C3-C4	5.33	1.63	1.53
5	A	6001	RXP	C26-C24	5.34	1.50	1.38
5	D	6004	RXP	C17-C16	5.36	1.51	1.38
5	B	6002	RXP	C20-C12	5.38	1.60	1.51
4	F	5091	CPS	C11-C2	5.40	1.64	1.54
5	D	6004	RXP	C4-C6	5.49	1.57	1.42
5	A	6001	RXP	O6-C31	5.50	1.57	1.45
5	B	6002	RXP	C17-C16	5.52	1.52	1.38
5	A	6001	RXP	C28-C26	5.59	1.50	1.38
5	F	6006	RXP	C16-C15	5.62	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C16-C15	5.62	1.50	1.38
5	D	6004	RXP	C9-C7	5.67	1.49	1.36
5	F	6006	RXP	C29-C28	5.68	1.52	1.38
5	E	6005	RXP	C29-C28	5.69	1.52	1.38
4	B	5007	CPS	C3-C4	5.70	1.63	1.53
5	D	6004	RXP	C19-C14	5.73	1.51	1.38
5	B	6002	RXP	C8-C6	5.74	1.52	1.41
5	F	6006	RXP	C7-C4	5.76	1.53	1.42
5	E	6005	RXP	C7-C4	5.77	1.53	1.42
5	D	6004	RXP	C33-C32	5.77	1.51	1.38
5	C	6003	RXP	C28-C26	5.79	1.50	1.38
5	B	6002	RXP	C30-N4	5.85	1.50	1.34
5	C	6003	RXP	C10-C9	5.90	1.53	1.38
5	A	6001	RXP	C29-C28	5.90	1.53	1.38
4	C	5003	CPS	C18-C17	5.91	1.63	1.53
4	D	5004	CPS	C18-C17	5.95	1.63	1.53
5	C	6003	RXP	C25-C24	5.99	1.51	1.38
5	C	6003	RXP	C29-C28	5.99	1.53	1.38
5	E	6005	RXP	C29-C27	6.04	1.53	1.38
4	D	5009	CPS	C3-C4	6.07	1.64	1.53
5	F	6006	RXP	C29-C27	6.08	1.53	1.38
5	B	6002	RXP	C9-C7	6.11	1.50	1.36
5	C	6003	RXP	C31-C32	6.11	1.64	1.50
4	E	5010	CPS	C3-C4	6.18	1.64	1.53
5	B	6002	RXP	C7-C4	6.19	1.54	1.42
4	E	5010	CPS	C18-C17	6.19	1.63	1.53
4	F	5011	CPS	C3-C4	6.20	1.64	1.53
5	F	6006	RXP	C37-C32	6.20	1.52	1.38
5	E	6005	RXP	C37-C32	6.25	1.52	1.38
4	D	5009	CPS	C8-C9	6.26	1.68	1.54
5	A	6001	RXP	C9-C7	6.26	1.51	1.36
4	A	5006	CPS	C3-C4	6.28	1.64	1.53
5	D	6004	RXP	C27-C25	6.30	1.51	1.38
5	C	6003	RXP	C9-C7	6.34	1.51	1.36
5	F	6006	RXP	O6-C30	6.34	1.48	1.35
5	E	6005	RXP	O6-C30	6.35	1.48	1.35
5	C	6003	RXP	C18-C19	6.38	1.52	1.38
4	E	5005	CPS	C3-C4	6.42	1.65	1.53
5	B	6002	RXP	C27-C25	6.43	1.52	1.38
5	D	6004	RXP	C36-C35	6.44	1.54	1.38
5	A	6001	RXP	C10-C8	6.46	1.51	1.36
5	F	6006	RXP	C9-C7	6.49	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C9-C7	6.50	1.51	1.36
4	A	5001	CPS	C3-C4	6.53	1.65	1.53
5	B	6002	RXP	C4-C6	6.54	1.60	1.42
4	F	5091	CPS	C20-C9	6.54	1.66	1.54
5	B	6002	RXP	C18-C19	6.59	1.52	1.38
4	A	5001	CPS	C18-C17	6.60	1.64	1.53
5	C	6003	RXP	C19-C14	6.66	1.53	1.38
4	C	5003	CPS	C3-C4	6.67	1.65	1.53
5	D	6004	RXP	C29-C28	6.67	1.55	1.38
5	F	6006	RXP	C8-C6	6.72	1.54	1.41
5	E	6005	RXP	C8-C6	6.76	1.54	1.41
4	F	5091	CPS	C3-C4	6.76	1.65	1.53
4	B	5007	CPS	C18-C17	6.79	1.64	1.53
5	C	6003	RXP	O6-C31	6.80	1.60	1.45
4	F	5011	CPS	C18-C17	6.83	1.64	1.53
5	F	6006	RXP	C18-C19	6.85	1.53	1.38
5	D	6004	RXP	C29-C27	6.87	1.55	1.38
4	F	5091	CPS	C18-C17	6.87	1.64	1.53
5	E	6005	RXP	C18-C19	6.88	1.53	1.38
5	B	6002	RXP	C10-C9	6.91	1.55	1.38
5	B	6002	RXP	C19-C14	6.92	1.53	1.38
5	A	6001	RXP	C19-C14	6.99	1.53	1.38
5	D	6004	RXP	C7-C4	7.00	1.56	1.42
5	E	6005	RXP	C33-C32	7.03	1.53	1.38
5	F	6006	RXP	C33-C32	7.06	1.53	1.38
5	C	6003	RXP	C36-C35	7.08	1.56	1.38
5	A	6001	RXP	C36-C35	7.13	1.56	1.38
5	A	6001	RXP	O6-C30	7.16	1.49	1.35
4	B	5002	CPS	C18-C17	7.17	1.65	1.53
5	B	6002	RXP	C26-C24	7.18	1.54	1.38
5	D	6004	RXP	C37-C32	7.27	1.54	1.38
5	C	6003	RXP	C10-C8	7.27	1.53	1.36
4	C	5008	CPS	C18-C19	7.27	1.68	1.53
5	B	6002	RXP	C16-C15	7.27	1.53	1.38
5	A	6001	RXP	C35-C34	7.31	1.56	1.38
4	A	5006	CPS	C18-C17	7.32	1.65	1.53
5	C	6003	RXP	O5-C30	7.32	1.35	1.21
4	D	5009	CPS	C18-C19	7.38	1.68	1.53
5	F	6006	RXP	C10-C9	7.41	1.57	1.38
5	B	6002	RXP	C10-C8	7.42	1.53	1.36
5	E	6005	RXP	C10-C9	7.42	1.57	1.38
5	D	6004	RXP	C35-C34	7.46	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	6003	RXP	C33-C32	7.50	1.54	1.38
5	D	6004	RXP	C10-C9	7.51	1.57	1.38
5	D	6004	RXP	C26-C24	7.54	1.54	1.38
5	E	6005	RXP	C25-C24	7.56	1.54	1.38
5	F	6006	RXP	C25-C24	7.56	1.54	1.38
5	A	6001	RXP	C10-C9	7.60	1.57	1.38
5	F	6006	RXP	C34-C33	7.63	1.54	1.38
5	B	6002	RXP	O5-C30	7.65	1.36	1.21
4	E	5005	CPS	C18-C17	7.66	1.66	1.53
5	E	6005	RXP	C34-C33	7.67	1.54	1.38
5	A	6001	RXP	C33-C32	7.69	1.55	1.38
4	A	5001	CPS	C18-C19	7.74	1.69	1.53
5	B	6002	RXP	C36-C35	7.78	1.58	1.38
4	A	5006	CPS	C18-C19	7.78	1.69	1.53
5	E	6005	RXP	C36-C35	7.84	1.58	1.38
5	F	6006	RXP	C36-C35	7.85	1.58	1.38
5	E	6005	RXP	C28-C26	7.85	1.55	1.38
5	F	6006	RXP	C28-C26	7.86	1.55	1.38
5	F	6006	RXP	C10-C8	7.88	1.54	1.36
5	E	6005	RXP	C10-C8	7.89	1.54	1.36
5	F	6006	RXP	O6-C31	7.90	1.63	1.45
5	A	6001	RXP	C25-C24	7.91	1.55	1.38
5	E	6005	RXP	O6-C31	7.92	1.63	1.45
5	D	6004	RXP	C25-C24	7.97	1.55	1.38
4	B	5007	CPS	C18-C19	8.16	1.70	1.53
5	A	6001	RXP	C34-C33	8.23	1.55	1.38
5	A	6001	RXP	O5-C30	8.24	1.37	1.21
4	D	5004	CPS	C18-C19	8.26	1.70	1.53
5	B	6002	RXP	C29-C27	8.28	1.59	1.38
5	B	6002	RXP	C29-C28	8.32	1.59	1.38
4	E	5010	CPS	C18-C19	8.39	1.70	1.53
4	C	5003	CPS	C18-C19	8.42	1.70	1.53
5	C	6003	RXP	C36-C37	8.46	1.56	1.38
5	C	6003	RXP	C35-C34	8.48	1.59	1.38
5	F	6006	RXP	C35-C34	8.49	1.59	1.38
5	E	6005	RXP	C35-C34	8.51	1.59	1.38
4	D	5009	CPS	C18-C17	8.52	1.67	1.53
4	F	5011	CPS	C18-C19	8.54	1.70	1.53
4	E	5005	CPS	C18-C19	8.57	1.70	1.53
5	B	6002	RXP	C28-C26	8.81	1.57	1.38
5	A	6001	RXP	C37-C32	8.85	1.57	1.38
5	D	6004	RXP	C36-C37	8.87	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	6004	RXP	C10-C8	8.93	1.57	1.36
4	C	5008	CPS	C18-C17	9.12	1.68	1.53
4	B	5002	CPS	C18-C19	9.15	1.71	1.53
5	D	6004	RXP	C34-C33	9.34	1.58	1.38
5	B	6002	RXP	C33-C32	9.37	1.58	1.38
5	B	6002	RXP	C35-C34	9.39	1.62	1.38
5	D	6004	RXP	C28-C26	9.65	1.58	1.38
5	C	6003	RXP	C34-C33	9.76	1.59	1.38
5	C	6003	RXP	C37-C32	9.91	1.59	1.38
5	A	6001	RXP	C36-C37	10.07	1.59	1.38
5	B	6002	RXP	C25-C24	10.29	1.60	1.38
5	E	6005	RXP	C36-C37	10.72	1.61	1.38
5	F	6006	RXP	C36-C37	10.73	1.61	1.38
4	F	5091	CPS	C18-C19	10.86	1.75	1.53
5	B	6002	RXP	C34-C33	11.49	1.62	1.38
5	B	6002	RXP	C36-C37	11.78	1.63	1.38
4	B	5007	CPS	C10-C5	12.54	1.74	1.54
4	D	5009	CPS	C10-C5	12.58	1.75	1.54
5	B	6002	RXP	C37-C32	12.60	1.65	1.38
4	D	5004	CPS	C10-C5	12.65	1.75	1.54
4	E	5010	CPS	C10-C5	12.85	1.75	1.54
4	A	5006	CPS	C10-C5	13.02	1.75	1.54
4	C	5008	CPS	C10-C5	13.11	1.75	1.54
4	B	5002	CPS	C10-C5	13.41	1.76	1.54
4	C	5003	CPS	C10-C5	13.50	1.76	1.54
4	A	5001	CPS	C10-C5	13.65	1.76	1.54
4	E	5005	CPS	C10-C5	13.69	1.76	1.54
4	F	5011	CPS	C10-C5	13.72	1.76	1.54
4	F	5091	CPS	C10-C5	18.43	1.84	1.54

All (438) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5011	CPS	C19-C18-C17	-10.00	100.11	111.92
4	D	5009	CPS	C19-C18-C17	-9.09	101.18	111.92
4	C	5003	CPS	C19-C18-C17	-9.03	101.25	111.92
4	E	5010	CPS	C19-C18-C17	-8.85	101.47	111.92
4	A	5006	CPS	C19-C18-C17	-8.84	101.48	111.92
4	B	5007	CPS	C19-C18-C17	-8.67	101.68	111.92
4	D	5004	CPS	C19-C18-C17	-8.41	101.98	111.92
4	A	5001	CPS	C19-C18-C17	-8.33	102.08	111.92
4	B	5002	CPS	C19-C18-C17	-8.27	102.15	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	5005	CPS	C19-C18-C17	-8.20	102.23	111.92
4	C	5008	CPS	C19-C18-C17	-7.67	102.86	111.92
4	F	5091	CPS	C19-C18-C17	-7.37	103.21	111.92
5	C	6003	RXP	O5-C30-N4	-7.12	112.43	124.86
5	D	6004	RXP	C39-C14-C15	-6.86	103.88	121.25
5	D	6004	RXP	C1-C11-N1	-6.76	105.69	116.60
4	A	5001	CPS	C7-C6-C18	-6.54	108.82	118.32
4	F	5091	CPS	C7-C6-C18	-6.45	108.95	118.32
4	F	5011	CPS	C7-C6-C18	-6.36	109.08	118.32
4	C	5003	CPS	C7-C6-C18	-6.30	109.17	118.32
4	C	5008	CPS	C7-C6-C18	-6.29	109.18	118.32
4	E	5005	CPS	C10-C5-C6	-6.28	101.31	111.22
5	A	6001	RXP	C39-C14-C15	-6.28	105.36	121.25
4	C	5008	CPS	C10-C5-C6	-6.27	101.33	111.22
4	F	5091	CPS	C3-C19-C18	-6.22	101.88	110.73
4	F	5091	CPS	C21-C20-C22	-6.21	100.00	110.35
4	A	5006	CPS	C3-C19-C18	-6.18	101.93	110.73
4	B	5002	CPS	C10-C5-C6	-6.11	101.59	111.22
4	C	5003	CPS	C3-C19-C18	-6.08	102.07	110.73
4	D	5004	CPS	C7-C6-C18	-6.08	109.49	118.32
4	D	5009	CPS	C3-C19-C18	-6.08	102.08	110.73
4	E	5005	CPS	C7-C6-C18	-6.08	109.50	118.32
4	F	5011	CPS	C3-C19-C18	-6.03	102.16	110.73
4	C	5008	CPS	C3-C19-C18	-6.03	102.16	110.73
4	E	5010	CPS	C3-C19-C18	-6.01	102.18	110.73
4	B	5007	CPS	C3-C19-C18	-6.01	102.18	110.73
4	E	5005	CPS	C3-C19-C18	-6.00	102.19	110.73
4	A	5006	CPS	C7-C6-C18	-6.00	109.61	118.32
4	F	5091	CPS	O1S-S-C32	-5.95	101.83	106.91
4	A	5001	CPS	C3-C19-C18	-5.92	102.30	110.73
4	E	5010	CPS	C7-C6-C18	-5.92	109.73	118.32
5	B	6002	RXP	O2-C12-C20	-5.91	114.45	122.12
4	B	5007	CPS	C7-C6-C18	-5.76	109.96	118.32
4	D	5004	CPS	C3-C19-C18	-5.73	102.58	110.73
5	C	6003	RXP	C39-C14-C15	-5.68	106.87	121.25
4	B	5002	CPS	C7-C6-C18	-5.66	110.10	118.32
4	A	5006	CPS	C10-C5-C6	-5.62	102.35	111.22
4	A	5001	CPS	C10-C5-C6	-5.60	102.38	111.22
5	C	6003	RXP	O1-C11-C1	-5.50	112.73	120.31
5	B	6002	RXP	C39-C14-C15	-5.48	107.38	121.25
4	B	5002	CPS	C3-C19-C18	-5.46	102.96	110.73
4	D	5004	CPS	C10-C5-C6	-5.46	102.61	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	6006	RXP	C39-C14-C15	-5.44	107.49	121.25
5	E	6005	RXP	C39-C14-C15	-5.41	107.55	121.25
4	D	5009	CPS	C10-C5-C6	-5.37	102.74	111.22
4	E	5010	CPS	C10-C5-C6	-5.36	102.77	111.22
5	E	6005	RXP	C1-C11-N1	-5.30	108.05	116.60
5	F	6006	RXP	C1-C11-N1	-5.29	108.06	116.60
4	C	5003	CPS	C10-C5-C6	-5.28	102.89	111.22
4	F	5091	CPS	C15-C14-C13	-5.18	105.21	112.91
4	D	5009	CPS	C7-C6-C18	-5.14	110.85	118.32
5	C	6003	RXP	P-C22-N4	-5.06	96.34	108.93
4	D	5009	CPS	O4-C4-C5	-4.80	103.32	111.11
4	F	5011	CPS	C10-C5-C6	-4.71	103.79	111.22
4	E	5005	CPS	C10-C5-C4	-4.68	104.53	109.09
4	B	5007	CPS	C10-C5-C6	-4.67	103.85	111.22
4	C	5008	CPS	O4-C4-C5	-4.29	104.15	111.11
4	A	5006	CPS	C10-C5-C9	-4.29	104.44	111.22
4	C	5003	CPS	C10-C5-C9	-4.28	104.46	111.22
5	A	6001	RXP	O5-C30-N4	-4.26	117.42	124.86
4	E	5010	CPS	O4-C4-C5	-4.25	104.22	111.11
5	D	6004	RXP	O6-C30-N4	-4.20	101.22	110.54
4	F	5091	CPS	C10-C5-C4	-4.09	105.10	109.09
4	F	5011	CPS	O4-C4-C5	-4.05	104.55	111.11
4	B	5007	CPS	C10-C5-C4	-3.88	105.30	109.09
4	D	5004	CPS	C10-C5-C4	-3.87	105.31	109.09
4	F	5091	CPS	O3-C17-C18	-3.86	100.75	109.26
5	A	6001	RXP	O1-C11-C1	-3.81	115.06	120.31
4	A	5001	CPS	C10-C5-C4	-3.80	105.39	109.09
4	D	5004	CPS	O4-C4-C5	-3.75	105.03	111.11
4	E	5010	CPS	C10-C5-C4	-3.74	105.45	109.09
4	B	5002	CPS	C10-C5-C9	-3.71	105.37	111.22
5	D	6004	RXP	C16-C15-C14	-3.71	114.75	120.65
5	A	6001	RXP	C35-C36-C37	-3.68	114.81	120.19
5	F	6006	RXP	O2-C12-C20	-3.61	117.43	122.12
5	E	6005	RXP	O2-C12-C20	-3.60	117.45	122.12
4	A	5001	CPS	C15-C14-C13	-3.60	107.56	112.91
4	A	5001	CPS	C10-C5-C9	-3.59	105.56	111.22
4	F	5091	CPS	C16-C15-C14	-3.58	107.05	111.05
4	A	5001	CPS	O4-C4-C5	-3.56	105.34	111.11
4	F	5091	CPS	C11-C2-C19	-3.56	105.84	111.18
5	A	6001	RXP	C18-C19-C14	-3.55	115.00	120.65
4	E	5005	CPS	C15-C14-C13	-3.53	107.66	112.91
5	C	6003	RXP	C31-O6-C30	-3.49	107.59	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	6001	RXP	O2P-P-O1P	-3.47	108.39	113.72
5	C	6003	RXP	C35-C36-C37	-3.46	115.12	120.19
4	B	5007	CPS	O4-C4-C5	-3.45	105.52	111.11
4	A	5006	CPS	O4-C4-C5	-3.42	105.57	111.11
4	E	5005	CPS	C10-C5-C9	-3.41	105.84	111.22
4	C	5003	CPS	C15-C14-C13	-3.40	107.85	112.91
4	F	5011	CPS	C10-C5-C9	-3.39	105.87	111.22
4	E	5010	CPS	C15-C14-C13	-3.39	107.88	112.91
5	F	6006	RXP	O5-C30-N4	-3.38	118.95	124.86
4	B	5002	CPS	C19-C2-C15	-3.37	103.69	108.67
5	E	6005	RXP	O5-C30-N4	-3.36	118.99	124.86
4	B	5002	CPS	C10-C5-C4	-3.36	105.81	109.09
4	F	5011	CPS	C19-C2-C15	-3.35	103.72	108.67
4	B	5007	CPS	C10-C5-C9	-3.32	105.98	111.22
4	C	5003	CPS	O4-C4-C5	-3.27	105.81	111.11
4	D	5009	CPS	C10-C5-C9	-3.24	106.11	111.22
4	D	5009	CPS	C15-C14-C13	-3.20	108.15	112.91
4	C	5003	CPS	C8-C9-C20	-3.19	106.36	112.05
4	C	5008	CPS	C19-C2-C15	-3.18	103.97	108.67
4	D	5004	CPS	C15-C14-C13	-3.17	108.20	112.91
4	C	5008	CPS	C8-C9-C20	-3.16	106.42	112.05
4	A	5006	CPS	C8-C9-C20	-3.16	106.42	112.05
4	B	5007	CPS	O3-C17-C18	-3.13	102.35	109.26
4	E	5010	CPS	C19-C2-C15	-3.10	104.09	108.67
4	B	5007	CPS	C19-C2-C15	-3.09	104.10	108.67
4	D	5004	CPS	C10-C5-C9	-3.06	106.39	111.22
4	C	5008	CPS	C10-C5-C4	-3.06	106.11	109.09
4	B	5007	CPS	C15-C14-C13	-3.05	108.37	112.91
4	D	5009	CPS	O4-C4-C3	-3.05	102.82	109.06
4	A	5006	CPS	C15-C14-C13	-3.01	108.44	112.91
4	F	5091	CPS	C26-C25-N1	-3.00	103.41	112.19
4	B	5002	CPS	C8-C9-C20	-2.99	106.72	112.05
4	A	5001	CPS	O3-C17-C18	-2.98	102.68	109.26
4	F	5091	CPS	C10-C5-C6	-2.98	106.51	111.22
4	B	5002	CPS	O4-C4-C3	-2.98	102.96	109.06
5	F	6006	RXP	C9-C7-C4	-2.96	116.69	120.88
4	E	5005	CPS	O4-C4-C5	-2.96	106.31	111.11
4	E	5005	CPS	C8-C9-C20	-2.95	106.79	112.05
4	F	5011	CPS	C8-C9-C20	-2.94	106.80	112.05
4	A	5006	CPS	C16-C15-C14	-2.94	107.76	111.05
4	F	5091	CPS	C30-N2-C27	-2.94	97.77	111.11
4	F	5091	CPS	C25-N1-C24	-2.94	117.02	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5011	CPS	O3-C17-C18	-2.93	102.80	109.26
4	C	5003	CPS	C16-C15-C14	-2.92	107.79	111.05
5	E	6005	RXP	C9-C7-C4	-2.91	116.77	120.88
4	A	5001	CPS	C11-C2-C19	-2.88	106.86	111.18
4	A	5001	CPS	C8-C9-C20	-2.88	106.92	112.05
5	A	6001	RXP	C29-C27-C25	-2.88	115.98	120.19
4	B	5002	CPS	C16-C15-C14	-2.87	107.84	111.05
4	E	5010	CPS	O3-C17-C18	-2.87	102.94	109.26
4	D	5004	CPS	O3-C17-C18	-2.85	102.97	109.26
5	C	6003	RXP	C37-C32-C33	-2.82	113.61	118.13
4	C	5003	CPS	O3-C17-C18	-2.79	103.10	109.26
4	F	5011	CPS	C10-C5-C4	-2.78	106.37	109.09
4	A	5006	CPS	O3-C17-C18	-2.78	103.13	109.26
4	D	5004	CPS	C19-C2-C15	-2.74	104.61	108.67
4	D	5009	CPS	C10-C5-C4	-2.73	106.43	109.09
4	B	5002	CPS	C15-C14-C13	-2.73	108.86	112.91
4	F	5091	CPS	C23-C24-N1	-2.72	111.74	116.46
4	C	5003	CPS	O4-C4-C3	-2.70	103.53	109.06
4	E	5005	CPS	O3-C17-C18	-2.69	103.32	109.26
4	D	5004	CPS	C11-C2-C19	-2.66	107.18	111.18
4	F	5011	CPS	C15-C14-C13	-2.66	108.96	112.91
4	C	5008	CPS	C10-C5-C9	-2.65	107.04	111.22
4	E	5010	CPS	C10-C5-C9	-2.63	107.08	111.22
4	C	5003	CPS	C19-C2-C15	-2.62	104.80	108.67
4	B	5002	CPS	O3-C17-C18	-2.60	103.54	109.26
4	F	5091	CPS	C19-C2-C15	-2.58	104.86	108.67
4	A	5006	CPS	C19-C2-C15	-2.57	104.88	108.67
4	E	5005	CPS	C19-C2-C15	-2.56	104.89	108.67
5	B	6002	RXP	C23-C24-C26	-2.56	115.55	120.90
4	D	5004	CPS	C8-C9-C20	-2.55	107.50	112.05
4	C	5003	CPS	C10-C5-C4	-2.54	106.61	109.09
4	D	5004	CPS	O4-C4-C3	-2.54	103.86	109.06
4	C	5008	CPS	C15-C14-C13	-2.53	109.15	112.91
4	E	5005	CPS	C16-C15-C14	-2.53	108.22	111.05
4	C	5003	CPS	C11-C2-C19	-2.50	107.43	111.18
5	F	6006	RXP	C35-C36-C37	-2.50	116.53	120.19
4	A	5006	CPS	O4-C4-C3	-2.50	103.95	109.06
5	E	6005	RXP	C35-C36-C37	-2.49	116.54	120.19
5	A	6001	RXP	C10-C8-C6	-2.49	116.08	120.06
4	A	5001	CPS	C19-C2-C15	-2.48	105.00	108.67
5	B	6002	RXP	C36-C35-C34	-2.47	115.60	119.93
4	C	5008	CPS	C16-C15-C14	-2.45	108.31	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5009	CPS	C16-C15-C14	-2.44	108.32	111.05
5	A	6001	RXP	O2-C12-N2	-2.41	118.21	122.93
5	B	6002	RXP	O6-C30-O5	-2.40	119.27	124.22
4	D	5009	CPS	C19-C2-C15	-2.40	105.13	108.67
5	C	6003	RXP	O2-C12-C20	-2.38	119.03	122.12
4	B	5002	CPS	O4-C4-C5	-2.37	107.27	111.11
5	A	6001	RXP	C9-C7-C4	-2.35	117.55	120.88
4	B	5007	CPS	C8-C9-C20	-2.35	107.87	112.05
4	A	5001	CPS	C16-C15-C14	-2.35	108.42	111.05
4	D	5004	CPS	C16-C15-C14	-2.34	108.43	111.05
5	A	6001	RXP	C13-C20-C21	-2.33	101.72	109.91
4	E	5010	CPS	C8-C9-C20	-2.32	107.91	112.05
5	C	6003	RXP	C18-C19-C14	-2.25	117.06	120.65
5	E	6005	RXP	C31-C32-C37	-2.23	115.30	120.66
5	F	6006	RXP	C31-C32-C37	-2.22	115.33	120.66
4	B	5007	CPS	O4-C4-C3	-2.20	104.55	109.06
4	B	5007	CPS	C16-C15-C14	-2.20	108.58	111.05
5	B	6002	RXP	C31-C32-C37	-2.19	115.40	120.66
5	D	6004	RXP	C27-C25-C24	-2.16	117.22	120.65
4	D	5009	CPS	C8-C9-C20	-2.12	108.26	112.05
4	B	5002	CPS	C11-C2-C19	-2.11	108.01	111.18
4	B	5002	CPS	C3-C19-C2	-2.10	111.61	113.79
5	F	6006	RXP	C18-C19-C14	-2.07	117.36	120.65
5	E	6005	RXP	C18-C19-C14	-2.06	117.36	120.65
5	B	6002	RXP	C34-C33-C32	-2.04	117.40	120.65
4	F	5011	CPS	C3-C4-C5	-2.03	109.14	111.20
5	E	6005	RXP	C35-C34-C33	-2.02	117.24	120.19
4	E	5005	CPS	O4-C4-C3	-2.00	104.97	109.06
5	D	6004	RXP	C17-C16-C15	2.01	123.13	120.19
5	A	6001	RXP	C28-C29-C27	2.01	123.46	119.93
5	D	6004	RXP	C29-C27-C25	2.03	123.16	120.19
4	D	5009	CPS	C1-C12-C13	2.06	113.78	110.43
4	D	5009	CPS	C14-C15-C2	2.07	114.93	112.66
4	E	5005	CPS	C14-C15-C2	2.11	114.98	112.66
5	C	6003	RXP	C2-C1-N2	2.12	115.24	110.80
4	F	5091	CPS	C1-C2-C19	2.16	114.93	111.45
4	C	5003	CPS	C6-C5-C4	2.17	109.33	107.39
5	A	6001	RXP	C17-C18-C19	2.17	123.37	120.19
4	F	5091	CPS	C28-N2-C30	2.22	115.07	109.43
4	B	5002	CPS	C11-C2-C1	2.31	112.08	108.20
5	A	6001	RXP	C36-C37-C32	2.34	124.37	120.65
4	B	5007	CPS	C11-C2-C1	2.35	112.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5009	CPS	C16-C17-C18	2.36	113.97	111.47
4	F	5011	CPS	C1-C12-C13	2.38	114.30	110.43
4	A	5001	CPS	C1-C12-C13	2.39	114.32	110.43
5	B	6002	RXP	C2-C3-C5	2.39	130.92	127.97
5	D	6004	RXP	O1-C11-C1	2.40	123.63	120.31
4	E	5005	CPS	C1-C12-C13	2.43	114.37	110.43
4	B	5007	CPS	C1-C12-C13	2.47	114.44	110.43
5	E	6005	RXP	C10-C9-C7	2.47	124.05	120.45
5	B	6002	RXP	C38-C39-C14	2.48	123.13	113.71
4	C	5003	CPS	C1-C12-C13	2.48	114.45	110.43
5	F	6006	RXP	C10-C9-C7	2.48	124.06	120.45
4	D	5004	CPS	C1-C12-C13	2.50	114.48	110.43
4	F	5091	CPS	C22-C20-C9	2.53	115.55	110.24
4	F	5091	CPS	C9-C5-C6	2.53	102.61	100.05
4	C	5003	CPS	C5-C9-C20	2.54	122.59	119.50
4	A	5001	CPS	C11-C2-C1	2.55	112.49	108.20
5	D	6004	RXP	C1-N2-C12	2.55	127.34	121.62
4	E	5005	CPS	C11-C2-C1	2.55	112.50	108.20
5	E	6005	RXP	C34-C33-C32	2.57	124.72	120.65
4	E	5010	CPS	C11-C2-C1	2.57	112.53	108.20
5	F	6006	RXP	C34-C33-C32	2.58	124.74	120.65
5	A	6001	RXP	C1-N2-C12	2.58	127.41	121.62
4	B	5002	CPS	C1-C12-C13	2.60	114.65	110.43
5	A	6001	RXP	C19-C14-C15	2.65	122.38	118.13
4	A	5001	CPS	C6-C5-C4	2.65	109.77	107.39
5	C	6003	RXP	C19-C14-C15	2.66	122.39	118.13
4	D	5004	CPS	C11-C2-C1	2.66	112.68	108.20
4	E	5005	CPS	C5-C9-C20	2.67	122.75	119.50
4	F	5011	CPS	C11-C2-C1	2.68	112.70	108.20
5	A	6001	RXP	C20-C12-N2	2.69	120.56	116.30
4	D	5009	CPS	C5-C9-C20	2.70	122.78	119.50
4	F	5011	CPS	C16-C17-C18	2.70	114.33	111.47
5	C	6003	RXP	C2-C1-C11	2.71	119.61	111.09
4	D	5009	CPS	C6-C5-C4	2.73	109.83	107.39
4	C	5003	CPS	C14-C15-C2	2.75	115.68	112.66
4	B	5007	CPS	C6-C5-C4	2.77	109.87	107.39
5	D	6004	RXP	C19-C14-C15	2.78	122.59	118.13
4	C	5008	CPS	C6-C5-C4	2.80	109.89	107.39
4	C	5008	CPS	C16-C17-C18	2.80	114.44	111.47
4	D	5004	CPS	C5-C9-C20	2.80	122.91	119.50
5	F	6006	RXP	O1-C11-N1	2.82	127.26	123.08
5	E	6005	RXP	O1-C11-N1	2.84	127.30	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	6005	RXP	C31-C32-C33	2.84	127.48	120.66
5	F	6006	RXP	C31-C32-C33	2.85	127.50	120.66
5	B	6002	RXP	C31-C32-C33	2.86	127.54	120.66
4	C	5003	CPS	C11-C2-C1	2.88	113.04	108.20
5	D	6004	RXP	C26-C24-C25	2.89	122.76	118.13
4	F	5091	CPS	O3S-S-C32	2.91	109.38	106.91
4	E	5010	CPS	C1-C12-C13	2.93	115.18	110.43
4	D	5009	CPS	C11-C2-C1	2.94	113.16	108.20
5	F	6006	RXP	O6-C30-N4	2.98	117.14	110.54
5	E	6005	RXP	O6-C30-N4	3.00	117.18	110.54
4	A	5006	CPS	C11-C2-C1	3.00	113.25	108.20
5	D	6004	RXP	C31-O6-C30	3.07	123.23	115.91
4	E	5005	CPS	C21-C20-C9	3.11	118.14	112.96
4	A	5001	CPS	C5-C9-C20	3.12	123.30	119.50
5	D	6004	RXP	C2-C3-C5	3.12	131.82	127.97
4	D	5004	CPS	C16-C17-C18	3.15	114.82	111.47
4	E	5005	CPS	C6-C5-C4	3.17	110.22	107.39
5	B	6002	RXP	C1-N2-C12	3.19	128.76	121.62
4	A	5006	CPS	C21-C20-C9	3.19	118.28	112.96
4	A	5001	CPS	C21-C20-C9	3.21	118.31	112.96
4	C	5003	CPS	C21-C20-C9	3.23	118.35	112.96
4	F	5011	CPS	C6-C5-C4	3.28	110.33	107.39
5	D	6004	RXP	C38-C39-C14	3.31	126.29	113.71
4	B	5002	CPS	C16-C17-C18	3.31	114.98	111.47
4	C	5008	CPS	C21-C20-C9	3.37	118.57	112.96
4	B	5007	CPS	C21-C20-C9	3.40	118.61	112.96
4	D	5004	CPS	C21-C20-C9	3.41	118.63	112.96
5	A	6001	RXP	C2-C1-C11	3.42	121.83	111.09
4	E	5010	CPS	C21-C20-C9	3.43	118.67	112.96
4	F	5011	CPS	C21-C20-C9	3.43	118.68	112.96
4	C	5008	CPS	C11-C2-C1	3.44	113.99	108.20
4	E	5005	CPS	C5-C6-C18	3.46	119.21	114.75
4	D	5009	CPS	C21-C20-C9	3.52	118.82	112.96
4	B	5007	CPS	C5-C9-C20	3.53	123.80	119.50
4	D	5004	CPS	C6-C5-C4	3.55	110.57	107.39
4	C	5003	CPS	C16-C17-C18	3.57	115.26	111.47
4	E	5010	CPS	C6-C5-C4	3.60	110.62	107.39
5	C	6003	RXP	C39-C14-C19	3.61	130.38	121.25
4	B	5002	CPS	C5-C6-C18	3.66	119.47	114.75
5	D	6004	RXP	O6-C30-O5	3.67	131.77	124.22
4	F	5091	CPS	C14-C13-C12	3.68	115.21	110.52
4	E	5010	CPS	C7-C6-C5	3.71	107.28	103.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	5005	CPS	C16-C17-C18	3.71	115.41	111.47
5	F	6006	RXP	C38-C39-C14	3.73	127.89	113.71
5	E	6005	RXP	C38-C39-C14	3.74	127.95	113.71
4	F	5011	CPS	C15-C16-C17	3.74	118.61	114.44
5	B	6002	RXP	C31-O6-C30	3.75	124.85	115.91
4	A	5006	CPS	C5-C9-C20	3.79	124.12	119.50
5	A	6001	RXP	O6-C31-C32	3.80	118.92	109.36
4	F	5011	CPS	C7-C6-C5	3.82	107.39	103.60
4	B	5002	CPS	C21-C20-C9	3.85	119.37	112.96
4	D	5009	CPS	C15-C16-C17	3.90	118.79	114.44
4	B	5002	CPS	C6-C5-C4	3.93	110.91	107.39
4	B	5007	CPS	C7-C6-C5	3.96	107.54	103.60
4	E	5010	CPS	C5-C9-C20	4.03	124.41	119.50
4	E	5010	CPS	C16-C17-C18	4.08	115.80	111.47
4	C	5008	CPS	C5-C9-C20	4.08	124.47	119.50
5	B	6002	RXP	C39-C14-C19	4.13	131.71	121.25
4	F	5091	CPS	C31-C30-N2	4.14	124.51	115.57
5	D	6004	RXP	C2-C1-C11	4.14	124.09	111.09
4	A	5001	CPS	C16-C17-C18	4.15	115.87	111.47
4	A	5001	CPS	C5-C6-C18	4.16	120.12	114.75
4	F	5011	CPS	C5-C9-C20	4.17	124.58	119.50
5	E	6005	RXP	C39-C14-C19	4.20	131.88	121.25
4	A	5006	CPS	C16-C17-C18	4.20	115.93	111.47
5	F	6006	RXP	C39-C14-C19	4.21	131.91	121.25
5	F	6006	RXP	C31-O6-C30	4.21	125.95	115.91
5	E	6005	RXP	C31-O6-C30	4.23	126.00	115.91
4	E	5005	CPS	C7-C6-C5	4.28	107.86	103.60
5	A	6001	RXP	C39-C14-C19	4.35	132.26	121.25
5	B	6002	RXP	C35-C34-C33	4.37	126.58	120.19
4	C	5008	CPS	C5-C6-C18	4.39	120.41	114.75
4	D	5009	CPS	C5-C6-C18	4.39	120.41	114.75
5	F	6006	RXP	C13-C38-C39	4.39	124.30	112.56
5	E	6005	RXP	C13-C38-C39	4.41	124.34	112.56
4	F	5091	CPS	C21-C20-C9	4.42	120.31	112.96
4	A	5006	CPS	C5-C6-C18	4.43	120.46	114.75
5	A	6001	RXP	O1-C11-N1	4.43	129.65	123.08
4	C	5008	CPS	C7-C6-C5	4.49	108.06	103.60
5	C	6003	RXP	O6-C30-N4	4.51	120.55	110.54
4	F	5091	CPS	C9-C5-C4	4.51	121.68	117.68
4	F	5011	CPS	C9-C5-C6	4.52	104.62	100.05
5	C	6003	RXP	C36-C37-C32	4.56	127.90	120.65
4	D	5009	CPS	C7-C6-C5	4.56	108.14	103.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5006	CPS	C7-C6-C5	4.59	108.17	103.60
4	A	5001	CPS	C7-C6-C5	4.74	108.31	103.60
4	F	5091	CPS	C7-C6-C5	4.78	108.35	103.60
4	B	5007	CPS	C15-C16-C17	4.79	119.78	114.44
5	D	6004	RXP	C39-C14-C19	4.82	133.45	121.25
4	F	5091	CPS	C19-C3-C4	4.84	120.47	114.36
5	D	6004	RXP	C13-C38-C39	4.87	125.57	112.56
4	C	5003	CPS	C5-C6-C18	4.88	121.04	114.75
4	D	5004	CPS	C5-C6-C18	4.94	121.12	114.75
4	B	5007	CPS	C5-C6-C18	4.95	121.13	114.75
4	D	5004	CPS	C7-C6-C5	4.95	108.53	103.60
4	E	5005	CPS	C15-C16-C17	5.02	120.03	114.44
4	B	5002	CPS	C15-C16-C17	5.06	120.08	114.44
5	F	6006	RXP	O6-C31-C32	5.07	122.12	109.36
5	E	6005	RXP	O6-C31-C32	5.07	122.12	109.36
4	C	5003	CPS	C7-C6-C5	5.08	108.65	103.60
5	B	6002	RXP	C13-C38-C39	5.09	126.16	112.56
4	C	5008	CPS	C15-C16-C17	5.10	120.12	114.44
5	C	6003	RXP	O1-C11-N1	5.10	130.64	123.08
4	F	5091	CPS	C6-C5-C4	5.11	111.97	107.39
4	C	5003	CPS	C15-C16-C17	5.11	120.14	114.44
5	D	6004	RXP	O1-C11-N1	5.12	130.68	123.08
4	A	5006	CPS	C15-C16-C17	5.19	120.22	114.44
4	E	5010	CPS	C5-C6-C18	5.20	121.45	114.75
4	B	5007	CPS	C16-C17-C18	5.23	117.02	111.47
4	A	5001	CPS	C15-C16-C17	5.28	120.33	114.44
5	C	6003	RXP	C13-C38-C39	5.33	126.81	112.56
4	F	5011	CPS	C2-C19-C18	5.40	117.81	111.88
4	F	5091	CPS	C15-C16-C17	5.41	120.47	114.44
4	D	5004	CPS	C15-C16-C17	5.48	120.54	114.44
4	F	5091	CPS	C16-C17-C18	5.52	117.33	111.47
4	B	5002	CPS	C7-C6-C5	5.53	109.09	103.60
4	E	5010	CPS	C15-C16-C17	5.57	120.65	114.44
4	F	5011	CPS	C5-C6-C18	5.70	122.09	114.75
4	E	5010	CPS	C9-C5-C6	5.71	105.82	100.05
5	C	6003	RXP	O6-C31-C32	5.79	123.94	109.36
4	D	5004	CPS	C9-C5-C6	5.88	105.99	100.05
4	C	5003	CPS	C9-C5-C6	6.02	106.14	100.05
4	C	5008	CPS	C9-C5-C4	6.11	123.09	117.68
4	D	5009	CPS	C9-C5-C4	6.12	123.11	117.68
4	E	5010	CPS	C2-C19-C18	6.17	118.65	111.88
4	E	5010	CPS	C9-C5-C4	6.29	123.26	117.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	5002	CPS	C9-C5-C4	6.33	123.29	117.68
4	B	5007	CPS	C2-C19-C18	6.34	118.84	111.88
4	B	5007	CPS	C9-C5-C6	6.34	106.46	100.05
5	B	6002	RXP	C20-C12-N2	6.36	126.35	116.30
4	D	5004	CPS	C2-C19-C18	6.49	119.00	111.88
4	F	5091	CPS	C6-C18-C17	6.50	120.75	111.74
4	D	5009	CPS	C9-C5-C6	6.63	106.76	100.05
4	F	5091	CPS	C2-C19-C18	6.66	119.19	111.88
4	B	5007	CPS	C9-C5-C4	6.75	123.66	117.68
4	C	5003	CPS	C2-C19-C18	6.78	119.33	111.88
4	A	5006	CPS	C2-C19-C18	6.80	119.34	111.88
4	A	5001	CPS	C9-C5-C6	6.80	106.92	100.05
4	A	5006	CPS	C9-C5-C6	6.93	107.05	100.05
4	A	5001	CPS	C2-C19-C18	6.97	119.53	111.88
4	D	5004	CPS	C9-C5-C4	7.05	123.93	117.68
4	C	5008	CPS	C9-C5-C6	7.08	107.21	100.05
4	C	5008	CPS	C2-C19-C18	7.10	119.67	111.88
4	B	5002	CPS	C2-C19-C18	7.10	119.67	111.88
5	A	6001	RXP	C13-C38-C39	7.14	131.64	112.56
4	F	5011	CPS	C9-C5-C4	7.24	124.10	117.68
4	B	5002	CPS	C9-C5-C6	7.44	107.57	100.05
4	D	5009	CPS	C2-C19-C18	7.53	120.15	111.88
4	E	5005	CPS	C9-C5-C6	7.60	107.73	100.05
4	F	5011	CPS	C19-C3-C4	7.74	124.14	114.36
4	A	5001	CPS	C9-C5-C4	7.79	124.59	117.68
4	E	5005	CPS	C9-C5-C4	7.82	124.61	117.68
4	A	5006	CPS	C9-C5-C4	7.82	124.61	117.68
4	E	5005	CPS	C2-C19-C18	7.94	120.59	111.88
4	C	5003	CPS	C9-C5-C4	8.50	125.21	117.68
4	E	5010	CPS	C19-C3-C4	8.61	125.24	114.36
4	B	5002	CPS	C19-C3-C4	8.92	125.62	114.36
4	B	5007	CPS	C19-C3-C4	8.92	125.63	114.36
4	A	5006	CPS	C19-C3-C4	8.94	125.65	114.36
4	D	5004	CPS	C19-C3-C4	9.00	125.73	114.36
4	C	5003	CPS	C19-C3-C4	9.11	125.87	114.36
4	C	5008	CPS	C19-C3-C4	9.29	126.09	114.36
4	A	5001	CPS	C19-C3-C4	9.45	126.30	114.36
4	D	5009	CPS	C19-C3-C4	9.57	126.45	114.36
4	B	5002	CPS	C6-C18-C17	10.06	125.69	111.74
4	F	5011	CPS	C6-C18-C17	10.07	125.70	111.74
4	C	5003	CPS	C6-C18-C17	10.09	125.73	111.74
4	D	5009	CPS	C6-C18-C17	10.12	125.77	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5004	CPS	C6-C18-C17	10.14	125.80	111.74
4	E	5005	CPS	C19-C3-C4	10.16	127.20	114.36
4	A	5006	CPS	C6-C18-C17	10.17	125.84	111.74
4	A	5001	CPS	C6-C18-C17	10.45	126.23	111.74
4	E	5010	CPS	C6-C18-C17	10.58	126.41	111.74
4	B	5007	CPS	C6-C18-C17	10.66	126.53	111.74
4	C	5008	CPS	C6-C18-C17	10.70	126.58	111.74
4	E	5005	CPS	C6-C18-C17	10.89	126.85	111.74
5	B	6002	RXP	O6-C31-C32	11.19	137.51	109.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	5091	CPS	C32-C31-C30-N2

There are no ring outliers.

18 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5001	CPS	7	0
4	A	5006	CPS	9	0
5	A	6001	RXP	5	0
4	B	5002	CPS	8	0
4	B	5007	CPS	7	0
5	B	6002	RXP	4	0
4	C	5003	CPS	6	0
4	C	5008	CPS	9	0
5	C	6003	RXP	1	0
4	D	5004	CPS	5	0
4	D	5009	CPS	4	0
5	D	6004	RXP	1	0
4	E	5005	CPS	10	0
4	E	5010	CPS	6	0
5	E	6005	RXP	9	0
4	F	5011	CPS	7	0
4	F	5091	CPS	23	0
5	F	6006	RXP	2	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	162/165 (98%)	-0.48	2 (1%)	81 77	15, 26, 38, 50	0
1	B	164/165 (99%)	-0.15	9 (5%)	29 21	20, 36, 53, 60	0
1	C	162/165 (98%)	-0.39	3 (1%)	70 64	19, 30, 44, 53	0
1	D	162/165 (98%)	-0.36	3 (1%)	70 64	16, 29, 45, 55	0
1	E	165/165 (100%)	-0.30	3 (1%)	71 66	14, 31, 48, 56	0
1	F	162/165 (98%)	-0.31	5 (3%)	52 45	17, 31, 43, 56	0
All	All	977/990 (98%)	-0.33	25 (2%)	59 53	14, 30, 47, 60	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	6.7
1	C	245	TYR	4.8
1	E	233	ALA	4.6
1	F	245	TYR	4.5
1	F	233	ALA	4.5
1	C	233	ALA	3.9
1	F	189	THR	3.5
1	E	265	GLN	3.4
1	D	233	ALA	3.4
1	B	188	LYS	3.2
1	A	101	MET	2.9
1	D	101	MET	2.8
1	F	101	MET	2.8
1	F	188	LYS	2.8
1	C	189	THR	2.7
1	B	255	ARG	2.6
1	B	171	ASN	2.6
1	B	231	THR	2.6
1	B	209	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	232	ALA	2.4
1	D	106	GLY	2.3
1	E	232	ALA	2.2
1	B	252	ASP	2.2
1	B	166	TYR	2.1
1	A	188	LYS	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	RXP	E	6005	50/50	0.81	0.32	7.62	32,41,62,62	0
4	CPS	E	5005	26/42	0.85	0.33	7.43	46,48,49,50	4
4	CPS	F	5091	42/42	0.69	0.35	4.91	17,17,17,17	0
5	RXP	C	6003	50/50	0.91	0.21	3.63	25,34,53,54	0
5	RXP	A	6001	50/50	0.90	0.22	3.48	22,29,50,51	0
4	CPS	B	5002	26/42	0.85	0.29	2.78	50,51,52,53	4
5	RXP	B	6002	50/50	0.88	0.26	2.55	36,44,63,64	0
5	RXP	D	6004	50/50	0.94	0.18	2.25	21,27,42,43	0
5	RXP	F	6006	50/50	0.94	0.18	2.03	20,25,52,53	0
4	CPS	D	5004	26/42	0.86	0.20	1.63	35,37,38,39	4
4	CPS	C	5008	26/42	0.82	0.20	1.25	48,49,50,50	4
4	CPS	F	5011	26/42	0.82	0.24	1.03	53,54,55,55	4
4	CPS	D	5009	26/42	0.85	0.19	0.79	58,59,59,60	4
4	CPS	C	5003	26/42	0.87	0.20	0.65	34,36,38,38	4
4	CPS	A	5006	26/42	0.86	0.18	0.52	49,50,51,51	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CPS	A	5001	26/42	0.91	0.16	0.37	34,36,37,39	4
4	CPS	E	5010	26/42	0.94	0.14	-0.26	30,32,34,34	4
4	CPS	B	5007	26/42	0.94	0.13	-0.30	33,34,35,37	4
3	CA	D	5512	1/1	0.97	0.11	-0.31	15,15,15,15	0
3	CA	F	5518	1/1	0.98	0.06	-1.96	18,18,18,18	0
3	CA	B	5506	1/1	0.96	0.06	-2.10	26,26,26,26	0
2	ZN	C	5507	1/1	0.99	0.09	-2.27	23,23,23,23	0
2	ZN	A	5501	1/1	0.98	0.07	-2.49	24,24,24,24	0
2	ZN	A	5502	1/1	0.99	0.07	-2.98	19,19,19,19	0
2	ZN	B	5504	1/1	0.99	0.09	-3.05	25,25,25,25	0
2	ZN	F	5516	1/1	0.99	0.09	-3.28	26,26,26,26	0
3	CA	A	5503	1/1	0.98	0.05	-3.29	18,18,18,18	0
2	ZN	D	5510	1/1	0.99	0.08	-3.44	22,22,22,22	0
3	CA	E	5515	1/1	0.98	0.04	-3.74	28,28,28,28	0
2	ZN	F	5517	1/1	1.00	0.07	-4.27	23,23,23,23	0
2	ZN	B	5505	1/1	0.98	0.06	-4.62	26,26,26,26	0
2	ZN	E	5513	1/1	0.99	0.06	-4.66	24,24,24,24	0
2	ZN	C	5508	1/1	1.00	0.05	-4.68	16,16,16,16	0
3	CA	C	5509	1/1	0.98	0.04	-4.73	24,24,24,24	0
2	ZN	D	5511	1/1	0.99	0.08	-4.86	18,18,18,18	0
2	ZN	E	5514	1/1	0.99	0.04	-9.68	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.