Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:34 PM GMT

PDB ID	:	3RG1
Title	:	Crystal structure of the RP105/MD-1 complex
Authors	:	Yoon, S.I.; Hong, M.; Wilson, I.A.
Deposited on	:	2011-04-07
Resolution	:	2.91 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:

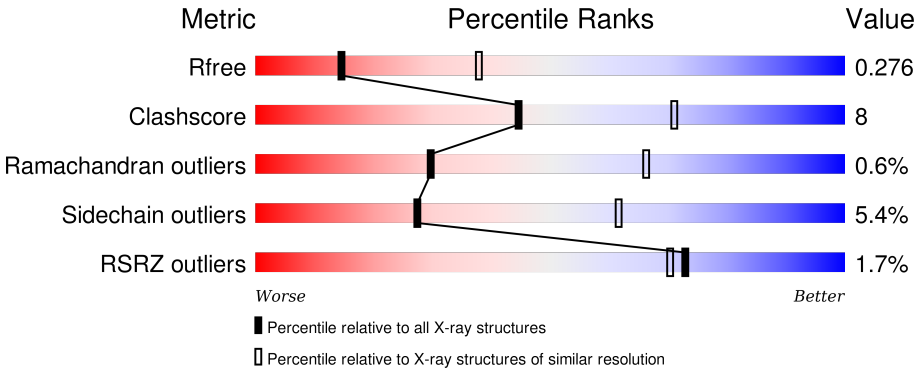
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.91 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	612	2% 79% 16%
1	B	612	79% 17%
1	E	612	3% 78% 17%
1	F	612	% 78% 18%
1	I	612	2% 55% 9% 35%

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Mol	Chain	Length	Quality of chain
1	J	612	3% 79% 18%
1	M	612	% 76% 19%
1	N	612	% 77% 19%
2	C	147	% 78% 15% 6%
2	D	147	% 76% 16% 7%
2	G	147	% 79% 14% 6%
2	H	147	% 77% 16% 6%
2	K	147	3% 79% 12% 7%
2	L	147	% 80% 13% 6%
2	O	147	% 77% 14% 6%
2	P	147	3% 80% 12% 8%

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	MAN	A	908	-	-	-	X
4	MAN	F	908	-	-	-	X
4	MAN	I	908	-	-	-	X
4	MAN	M	908	-	-	-	X
5	PGT	D	201	-	-	-	X
5	PGT	H	201	-	-	-	X
5	PGT	L	201	-	-	-	X
5	PGT	P	201	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43795 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 CD180 molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4450	2805	766	860	19			
1	E	592	Total	C	N	O	S	0	0	0
			4381	2763	750	849	19			
1	I	397	Total	C	N	O	S	0	0	0
			2931	1862	489	570	10			
1	M	593	Total	C	N	O	S	0	0	0
			4447	2806	763	859	19			
1	B	599	Total	C	N	O	S	0	0	0
			4616	2921	788	885	22			
1	F	599	Total	C	N	O	S	0	0	0
			4493	2833	768	870	22			
1	J	599	Total	C	N	O	S	0	0	0
			4458	2816	756	865	21			
1	N	599	Total	C	N	O	S	0	0	0
			4591	2909	783	877	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
A	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
A	627	THR	-	EXPRESSION TAG	UNP A6QNK7
A	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
A	629	MET	-	EXPRESSION TAG	UNP A6QNK7
A	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
A	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
A	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
A	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
E	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
E	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
E	627	THR	-	EXPRESSION TAG	UNP A6QNK7
E	628	HIS	-	EXPRESSION TAG	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	629	MET	-	EXPRESSION TAG	UNP A6QNK7
E	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
E	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
E	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
E	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
I	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
I	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
I	627	THR	-	EXPRESSION TAG	UNP A6QNK7
I	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
I	629	MET	-	EXPRESSION TAG	UNP A6QNK7
I	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
I	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
I	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
I	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
M	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
M	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
M	627	THR	-	EXPRESSION TAG	UNP A6QNK7
M	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
M	629	MET	-	EXPRESSION TAG	UNP A6QNK7
M	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
M	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
M	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
M	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
B	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
B	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
B	627	THR	-	EXPRESSION TAG	UNP A6QNK7
B	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
B	629	MET	-	EXPRESSION TAG	UNP A6QNK7
B	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
B	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
B	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
B	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
F	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
F	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
F	627	THR	-	EXPRESSION TAG	UNP A6QNK7
F	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
F	629	MET	-	EXPRESSION TAG	UNP A6QNK7
F	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
F	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
F	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
F	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
J	22	ALA	-	EXPRESSION TAG	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
J	627	THR	-	EXPRESSION TAG	UNP A6QNK7
J	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
J	629	MET	-	EXPRESSION TAG	UNP A6QNK7
J	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
J	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
J	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
J	633	ARG	-	EXPRESSION TAG	UNP A6QNK7
N	22	ALA	-	EXPRESSION TAG	UNP A6QNK7
N	23	GLY	-	EXPRESSION TAG	UNP A6QNK7
N	627	THR	-	EXPRESSION TAG	UNP A6QNK7
N	628	HIS	-	EXPRESSION TAG	UNP A6QNK7
N	629	MET	-	EXPRESSION TAG	UNP A6QNK7
N	630	LEU	-	EXPRESSION TAG	UNP A6QNK7
N	631	VAL	-	EXPRESSION TAG	UNP A6QNK7
N	632	PRO	-	EXPRESSION TAG	UNP A6QNK7
N	633	ARG	-	EXPRESSION TAG	UNP A6QNK7

- Molecule 2 is a protein called LY86 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1026	656	170	193	7			
2	D	136	Total	C	N	O	S	0	0	0
			1022	656	167	192	7			
2	G	138	Total	C	N	O	S	0	0	0
			1031	664	170	190	7			
2	H	138	Total	C	N	O	S	0	0	0
			1046	667	176	196	7			
2	K	136	Total	C	N	O	S	0	0	0
			1003	640	167	189	7			
2	L	138	Total	C	N	O	S	0	0	0
			1046	667	172	200	7			
2	O	138	Total	C	N	O	S	0	0	0
			1028	658	169	194	7			
2	P	135	Total	C	N	O	S	0	0	0
			1001	640	166	188	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	EXPRESSION TAG	UNP A4IFT3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
C	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
C	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
C	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
C	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
C	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
C	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
D	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
D	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
D	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
D	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
D	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
D	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
D	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
D	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
G	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
G	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
G	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
G	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
G	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
G	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
G	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
G	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
H	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
H	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
H	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
H	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
H	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
H	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
H	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
H	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
K	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
K	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
K	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
K	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
K	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
K	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
K	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
K	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
L	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
L	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
L	161	ARG	-	EXPRESSION TAG	UNP A4IFT3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
L	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
L	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
L	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
L	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
O	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
O	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
O	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
O	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
O	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
O	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
O	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
O	166	ARG	-	EXPRESSION TAG	UNP A4IFT3
P	20	ALA	-	EXPRESSION TAG	UNP A4IFT3
P	160	ALA	-	EXPRESSION TAG	UNP A4IFT3
P	161	ARG	-	EXPRESSION TAG	UNP A4IFT3
P	162	GLY	-	EXPRESSION TAG	UNP A4IFT3
P	163	LEU	-	EXPRESSION TAG	UNP A4IFT3
P	164	VAL	-	EXPRESSION TAG	UNP A4IFT3
P	165	PRO	-	EXPRESSION TAG	UNP A4IFT3
P	166	ARG	-	EXPRESSION TAG	UNP A4IFT3

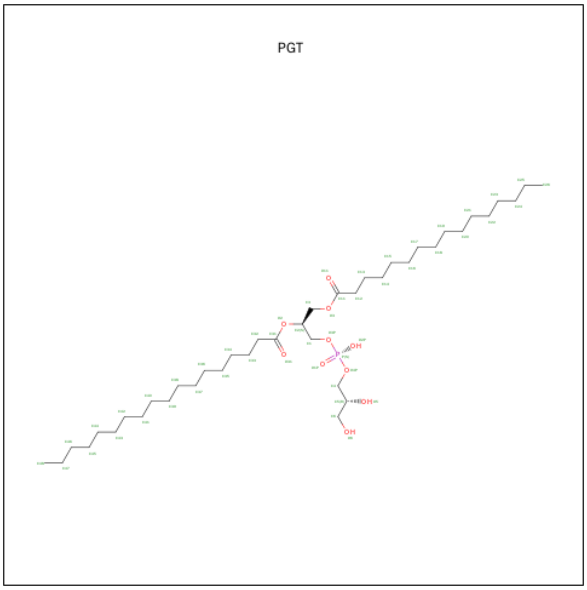
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	8	Total	C	N	O	0	0
			94	52	2	40		
4	E	8	Total	C	N	O	0	0
			94	52	2	40		
4	I	8	Total	C	N	O	0	0
			94	52	2	40		
4	M	8	Total	C	N	O	0	0
			94	52	2	40		
4	B	8	Total	C	N	O	0	0
			94	52	2	40		
4	F	8	Total	C	N	O	0	0
			94	52	2	40		
4	J	8	Total	C	N	O	0	0
			94	52	2	40		
4	N	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 5 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			31	27	4		
5	H	1	Total	C	O	0	0
			31	27	4		
5	L	1	Total	C	O	0	0
			31	27	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total C O 31 27 4	0	0

- Molecule 6 is water.

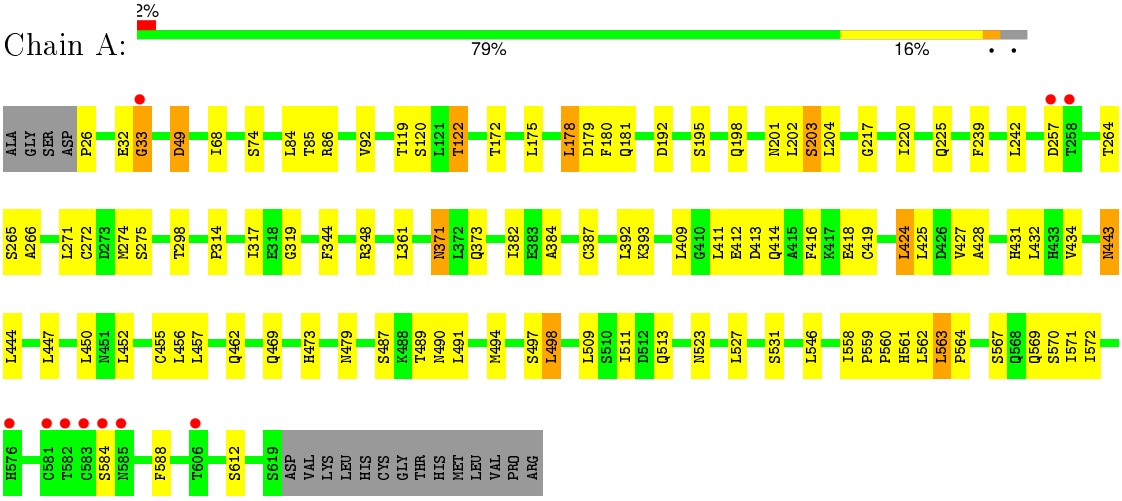
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	E	2	Total O 2 2	0	0
6	I	1	Total O 1 1	0	0
6	M	5	Total O 5 5	0	0
6	B	9	Total O 9 9	0	0
6	F	1	Total O 1 1	0	0
6	J	1	Total O 1 1	0	0
6	N	6	Total O 6 6	0	0
6	C	1	Total O 1 1	0	0
6	D	3	Total O 3 3	0	0
6	G	1	Total O 1 1	0	0
6	L	1	Total O 1 1	0	0

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.

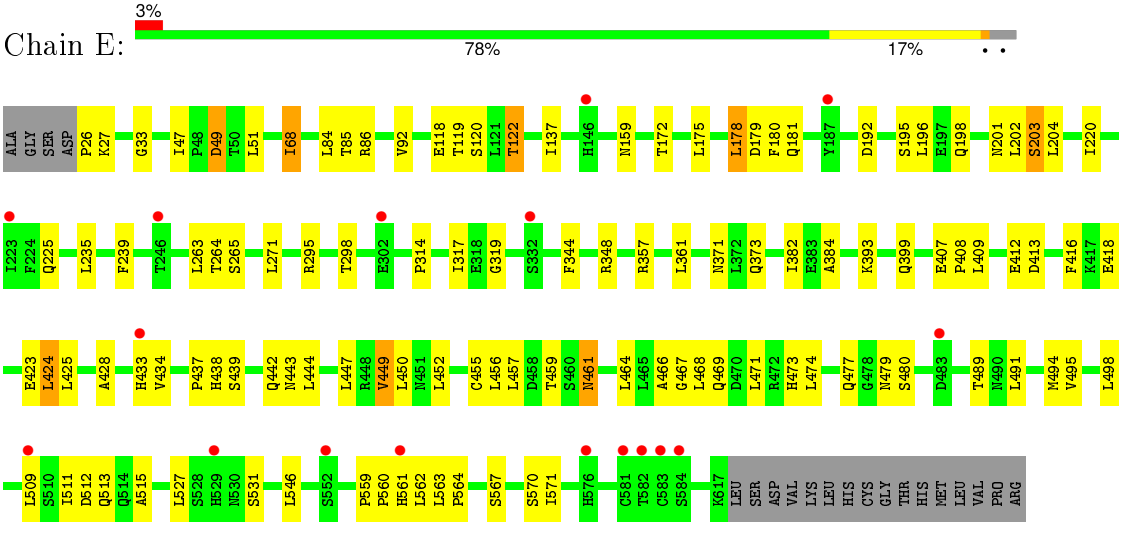
- Molecule 1: CD180 molecule

Chain A:



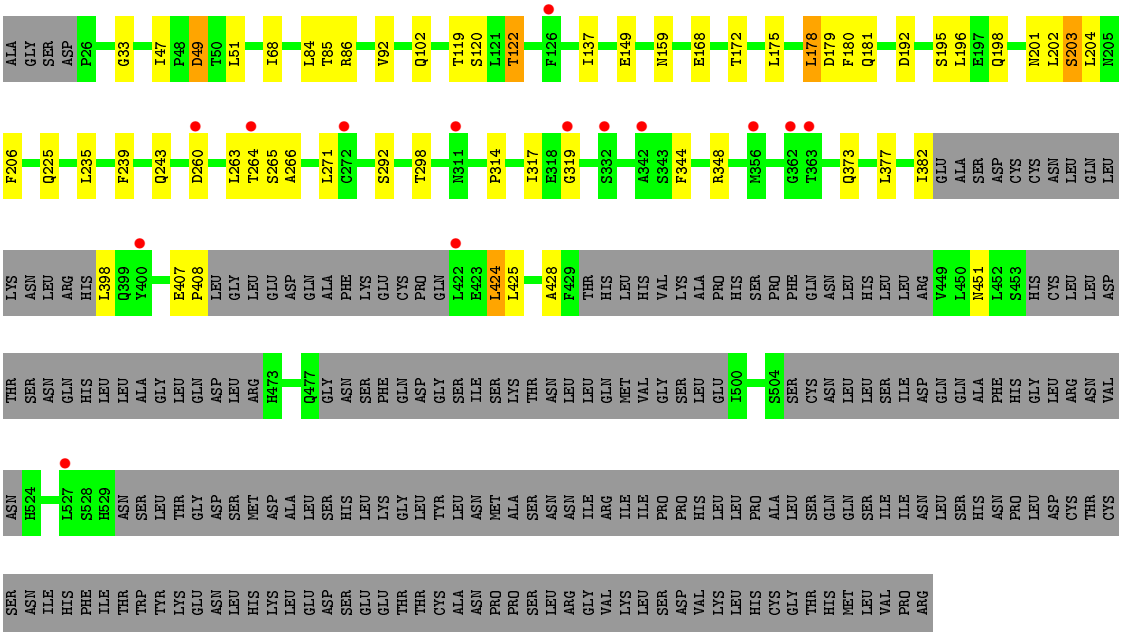
- Molecule 1: CD180 molecule

Chain E:



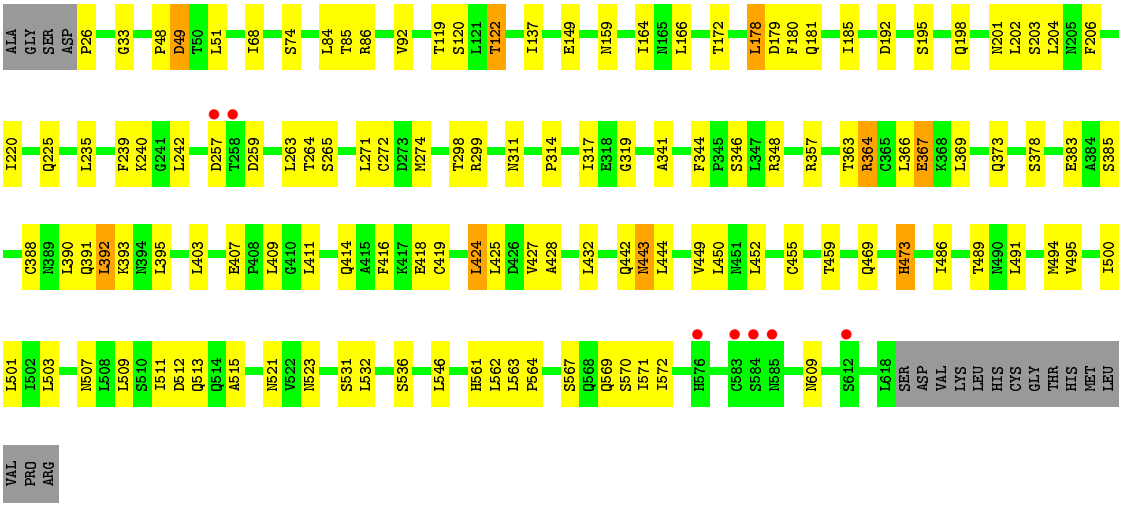
- Molecule 1: CD180 molecule

Chain I:



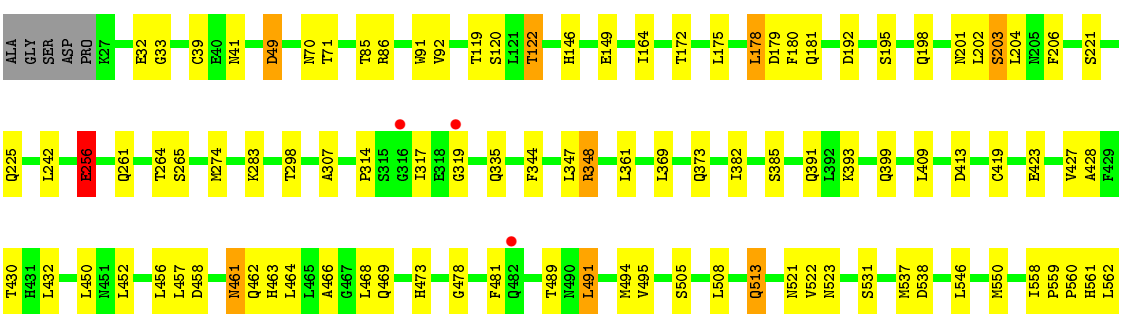
• Molecule 1: CD180 molecule

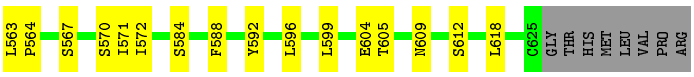
Chain M:



• Molecule 1: CD180 molecule

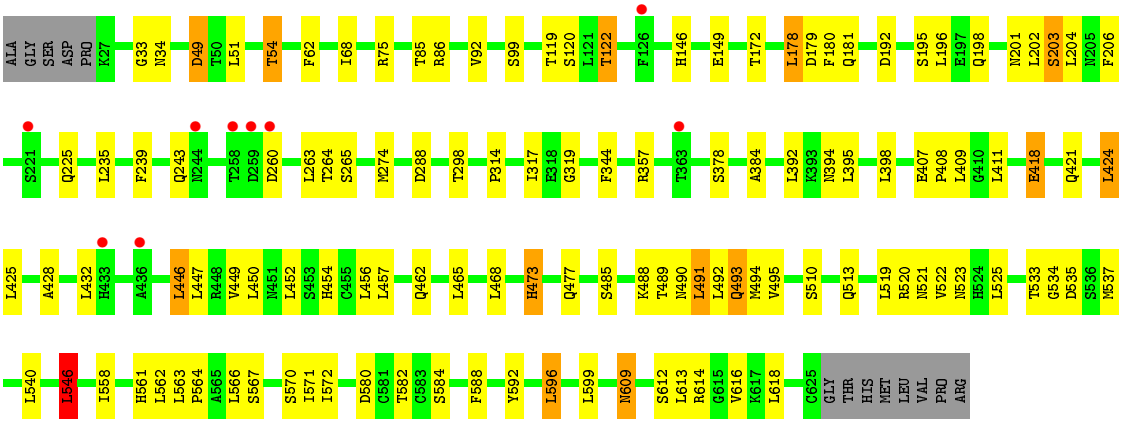
Chain B:





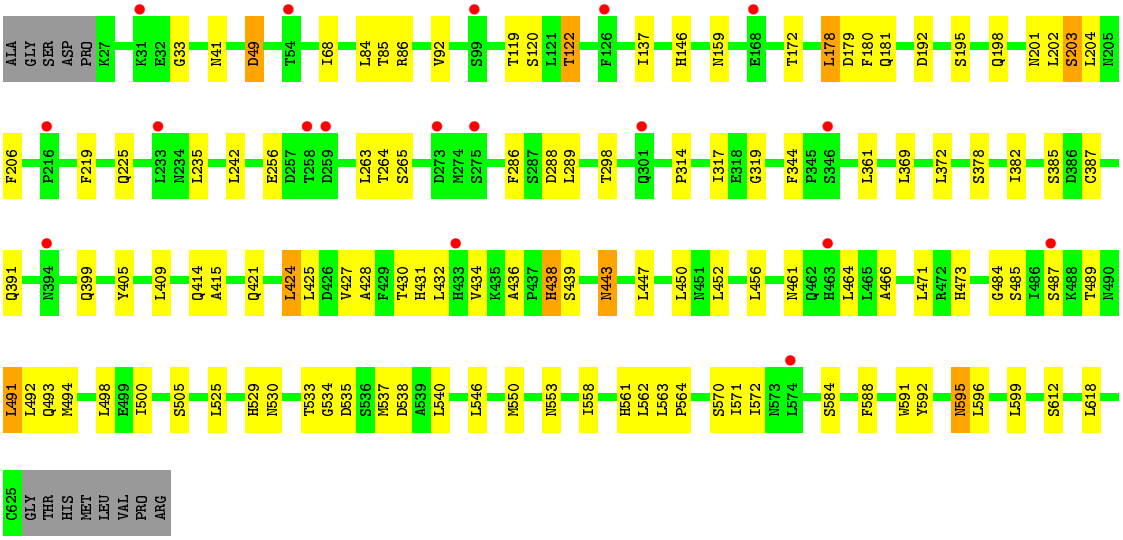
• Molecule 1: CD180 molecule

Chain F:



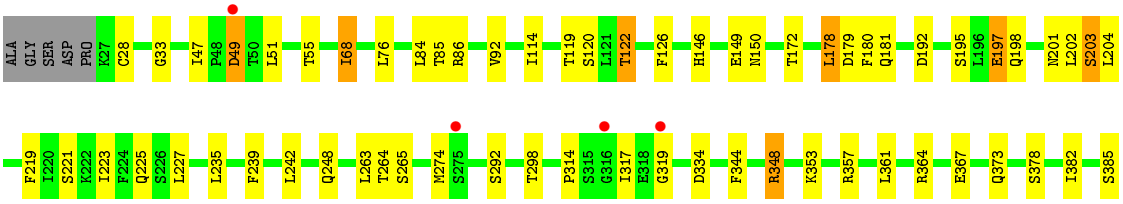
• Molecule 1: CD180 molecule

Chain J:



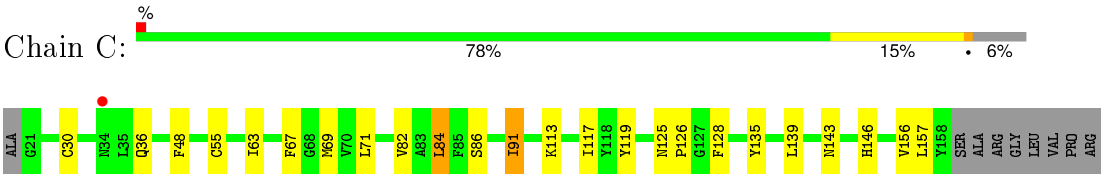
• Molecule 1: CD180 molecule

Chain N:



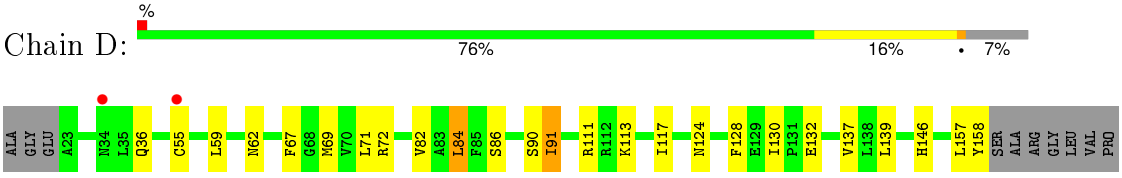
• Molecule 2: LY86 protein

Chain C:



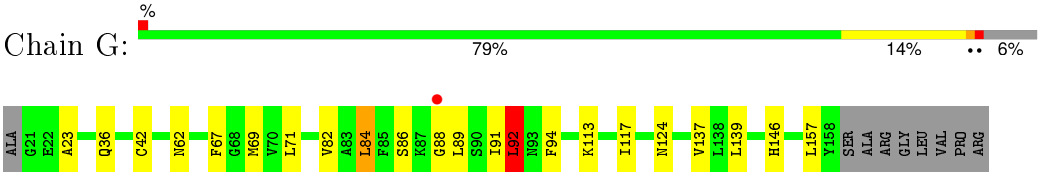
• Molecule 2: LY86 protein

Chain D:



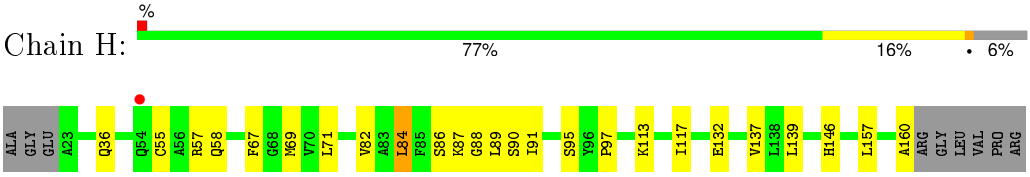
• Molecule 2: LY86 protein

Chain G:



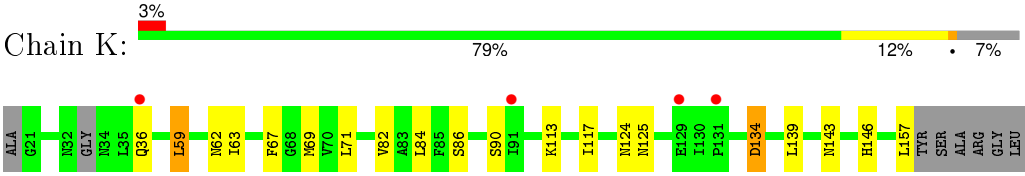
• Molecule 2: LY86 protein

Chain H:



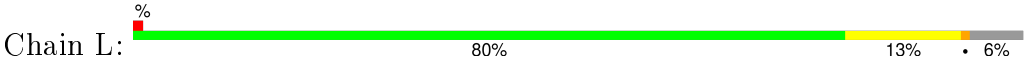
• Molecule 2: LY86 protein

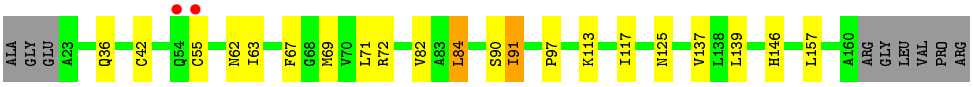
Chain K:



• Molecule 2: LY86 protein

Chain L:



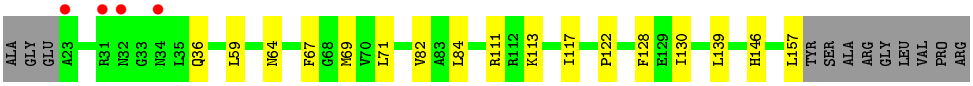


• Molecule 2: LY86 protein

Chain O:

• Molecule 2: LY86 protein

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	101.51Å 141.58Å 141.95Å 94.00° 91.66° 91.37°	Depositor
Resolution (Å)	20.00 – 2.91 20.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-2.91) 91.0 (20.00-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.238 , 0.276 0.240 , 0.276	Depositor DCC
R_{free} test set	8028 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.0	EDS
Estimated twinning fraction	0.048 for h,-k,-l 0.013 for -h,l,k 0.022 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 160097 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	43795	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: PGT, BMA, NAG, MAN

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	0.63	0/4537	0.67	0/6190
1	B	0.70	3/4708 (0.1%)	0.74	0/6409
1	E	0.50	0/4467	0.60	0/6104
1	F	0.50	0/4581	0.62	1/6256 (0.0%)
1	I	0.49	0/2980	0.58	0/4064
1	J	0.50	0/4546	0.62	0/6213
1	M	0.63	1/4534 (0.0%)	0.68	0/6189
1	N	0.65	1/4682 (0.0%)	0.69	1/6377 (0.0%)
2	C	0.70	1/1051 (0.1%)	0.69	1/1436 (0.1%)
2	D	0.73	0/1048	0.73	2/1432 (0.1%)
2	G	0.61	0/1057	0.69	1/1443 (0.1%)
2	H	0.68	0/1072	0.71	0/1463
2	K	0.52	0/1026	0.63	1/1401 (0.1%)
2	L	0.63	0/1072	0.67	0/1464
2	O	0.71	0/1054	0.70	1/1440 (0.1%)
2	P	0.70	0/1026	0.71	1/1402 (0.1%)
All	All	0.60	6/43441 (0.0%)	0.66	9/59283 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	28	CYS	CB-SG	5.89	1.92	1.82
1	B	256	GLU	CG-CD	5.68	1.60	1.51
1	B	39	CYS	CB-SG	-5.64	1.72	1.81
1	M	419	CYS	CB-SG	-5.39	1.73	1.81
2	C	30	CYS	CB-SG	-5.21	1.73	1.81
1	B	419	CYS	CB-SG	-5.13	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	111	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	G	92	LEU	CA-CB-CG	6.03	129.17	115.30
2	K	59	LEU	CA-CB-CG	5.48	127.91	115.30
2	D	111	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	C	55	CYS	CA-CB-SG	-5.29	104.48	114.00
1	N	556	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	D	55	CYS	CA-CB-SG	-5.08	104.86	114.00
2	O	55	CYS	CA-CB-SG	-5.05	104.91	114.00
1	F	546	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4450	0	4175	61	0
1	B	4616	0	4440	75	0
1	E	4381	0	4045	84	0
1	F	4493	0	4211	76	0
1	I	2931	0	2684	37	0
1	J	4458	0	4137	73	0
1	M	4447	0	4175	73	0
1	N	4591	0	4415	84	0
2	C	1026	0	929	17	0
2	D	1022	0	927	16	0
2	G	1031	0	946	13	0
2	H	1046	0	953	15	0
2	K	1003	0	895	9	0
2	L	1046	0	947	12	0
2	O	1028	0	923	15	0
2	P	1001	0	898	9	0
3	A	39	0	34	1	0
3	B	39	0	34	2	0
3	E	39	0	34	1	0
3	F	39	0	34	2	0
3	I	39	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	39	0	34	2	0
3	M	39	0	34	1	0
3	N	39	0	34	1	0
4	A	94	0	79	0	0
4	B	94	0	79	1	0
4	E	94	0	79	1	0
4	F	94	0	79	4	0
4	I	94	0	79	2	0
4	J	94	0	79	3	0
4	M	94	0	79	1	0
4	N	94	0	79	1	0
5	D	31	0	44	1	0
5	H	31	0	44	1	0
5	L	31	0	44	1	0
5	P	31	0	44	1	0
6	A	6	0	0	0	0
6	B	9	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
6	M	5	0	0	0	0
6	N	6	0	0	0	0
All	All	43795	0	40780	671	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 8.

All (671) 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)
1:J:450:LEU:HD11	1:J:452:LEU:HD21	1.48	0.95
2:H:82:VAL:HG22	2:H:139:LEU:HD23	1.49	0.93
1:M:242:LEU:HB2	1:M:274:MET:HE1	1.52	0.92
1:N:523:ASN:C	1:N:523:ASN:HD22	1.75	0.90
2:D:62:ASN:HD22	2:D:124:ASN:HA	1.38	0.89
1:E:468:LEU:O	1:E:495:VAL:HG12	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:ILE:HD12	1:F:588:PHE:CE1	2.11	0.85
1:E:384:ALA:HB3	1:E:409:LEU:CD2	2.06	0.85
2:P:82:VAL:HG22	2:P:139:LEU:HD23	1.58	0.84
2:L:82:VAL:HG22	2:L:139:LEU:HD23	1.59	0.84
2:C:82:VAL:HG22	2:C:139:LEU:HD23	1.61	0.83
1:N:348:ARG:HG3	1:N:373:GLN:HE21	1.42	0.82
1:E:384:ALA:HB3	1:E:409:LEU:HD23	1.60	0.82
1:F:558:ILE:HD12	1:F:588:PHE:CD1	2.15	0.82
2:G:82:VAL:HG22	2:G:139:LEU:HD23	1.60	0.81
1:F:488:LYS:O	1:F:493:GLN:NE2	2.14	0.81
2:K:82:VAL:HG22	2:K:139:LEU:HD23	1.63	0.80
1:E:461:ASN:HD22	1:E:464:LEU:HD12	1.45	0.79
2:O:82:VAL:HG22	2:O:139:LEU:HD23	1.66	0.78
1:B:348:ARG:HG3	1:B:373:GLN:HE21	1.49	0.77
1:F:447:LEU:HD21	1:F:450:LEU:HD13	1.67	0.77
2:D:82:VAL:HG22	2:D:139:LEU:HD23	1.66	0.77
1:A:178:LEU:HD22	1:A:180:PHE:CE2	2.21	0.76
2:C:84:LEU:HD23	2:C:91:ILE:HG13	1.67	0.76
1:E:416:PHE:HB2	1:E:444:LEU:HD21	1.68	0.76
1:E:434:VAL:HG21	1:E:464:LEU:HD11	1.66	0.76
1:J:592:TYR:CE1	1:J:599:LEU:HD13	2.21	0.76
1:F:452:LEU:HD13	1:F:457:LEU:HD11	1.67	0.75
2:L:71:LEU:HD11	2:L:117:ILE:HD11	1.68	0.75
1:E:361:LEU:HD21	1:E:382:ILE:HD13	1.68	0.75
1:A:561:HIS:NE2	1:A:562:LEU:HD23	2.02	0.74
2:D:71:LEU:HD11	2:D:117:ILE:HD11	1.70	0.74
2:K:71:LEU:HD11	2:K:117:ILE:HD11	1.69	0.74
2:D:62:ASN:ND2	2:D:124:ASN:HA	2.03	0.73
2:G:84:LEU:HD23	2:G:91:ILE:HB	1.70	0.73
1:A:432:LEU:HD12	1:A:455:CYS:HB3	1.69	0.73
1:E:450:LEU:HG	1:E:452:LEU:HD11	1.70	0.73
1:J:178:LEU:HD22	1:J:180:PHE:CE2	2.24	0.73
2:O:86:SER:HB3	2:O:91:ILE:HD11	1.70	0.72
2:H:84:LEU:HD23	2:H:91:ILE:HB	1.69	0.72
2:G:71:LEU:HD11	2:G:117:ILE:HD11	1.70	0.72
1:F:384:ALA:HB3	1:F:409:LEU:HD23	1.72	0.72
1:B:592:TYR:CE1	1:B:599:LEU:HD13	2.24	0.72
1:N:178:LEU:HD22	1:N:180:PHE:CE2	2.25	0.72
1:B:452:LEU:HD12	1:B:457:LEU:HD11	1.72	0.71
1:N:179:ASP:CG	1:N:181:GLN:HE21	1.94	0.71
1:I:348:ARG:HG3	1:I:373:GLN:HE21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:558:ILE:HD12	1:J:588:PHE:CD1	2.25	0.71
1:E:457:LEU:HD22	1:E:464:LEU:HD21	1.71	0.71
1:F:570:SER:O	1:F:571:ILE:HD13	1.90	0.71
1:B:452:LEU:CD1	1:B:457:LEU:HD11	2.20	0.70
2:P:71:LEU:HD11	2:P:117:ILE:HD11	1.71	0.70
1:E:561:HIS:NE2	1:E:562:LEU:HD23	2.06	0.70
1:F:519:LEU:HB3	1:F:522:VAL:HG23	1.73	0.70
1:J:558:ILE:HD12	1:J:588:PHE:CE1	2.27	0.70
1:B:179:ASP:CG	1:B:181:GLN:HE21	1.95	0.69
2:O:84:LEU:HD23	2:O:91:ILE:HB	1.74	0.69
1:J:450:LEU:HD11	1:J:452:LEU:CD2	2.22	0.69
1:N:605:THR:HG22	1:N:618:LEU:HD13	1.74	0.69
1:A:179:ASP:CG	1:A:181:GLN:HE21	1.96	0.68
1:N:523:ASN:C	1:N:523:ASN:ND2	2.46	0.68
1:M:393:LYS:HA	1:M:418:GLU:HG2	1.74	0.68
1:A:371:ASN:HD22	1:A:371:ASN:N	1.92	0.68
1:F:537:MET:HE2	1:F:566:LEU:HD21	1.75	0.68
2:D:59:LEU:HD23	2:D:128:PHE:CZ	2.28	0.68
1:B:537:MET:CE	1:B:550:MET:HE3	2.24	0.67
1:E:179:ASP:CG	1:E:181:GLN:HE21	1.98	0.67
1:A:384:ALA:HB3	1:A:409:LEU:HD22	1.77	0.67
1:J:561:HIS:NE2	1:J:562:LEU:HD23	2.08	0.67
1:A:570:SER:O	1:A:571:ILE:HD13	1.94	0.67
1:E:178:LEU:HD22	1:E:180:PHE:CE2	2.31	0.66
2:O:125:ASN:ND2	2:O:126:PRO:O	2.28	0.66
1:J:570:SER:O	1:J:571:ILE:HD13	1.96	0.66
1:F:178:LEU:HD22	1:F:180:PHE:CE2	2.30	0.66
1:M:178:LEU:HD22	1:M:180:PHE:CE2	2.30	0.66
1:M:561:HIS:NE2	1:M:562:LEU:HD23	2.10	0.66
1:N:561:HIS:NE2	1:N:562:LEU:HD23	2.11	0.66
1:N:592:TYR:CE1	1:N:599:LEU:HD13	2.31	0.65
1:B:558:ILE:HD12	1:B:588:PHE:CD1	2.32	0.65
1:I:179:ASP:CG	1:I:181:GLN:HE21	1.98	0.65
1:F:561:HIS:NE2	1:F:562:LEU:HD23	2.11	0.64
1:I:92:VAL:HG12	1:I:120:SER:HB2	1.80	0.64
2:O:71:LEU:HD11	2:O:117:ILE:HD11	1.79	0.64
1:B:558:ILE:HD12	1:B:588:PHE:CE1	2.33	0.64
1:M:179:ASP:CG	1:M:181:GLN:HE21	2.00	0.64
1:N:468:LEU:HB2	1:N:495:VAL:HG12	1.79	0.63
1:F:179:ASP:CG	1:F:181:GLN:HE21	2.02	0.63
1:J:428:ALA:HB3	3:J:801:NAG:H82	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ASN:O	1:F:54:THR:OG1	2.15	0.63
1:F:411:LEU:HD12	1:F:432:LEU:HD13	1.80	0.63
1:B:561:HIS:NE2	1:B:562:LEU:HD23	2.14	0.63
1:F:446:LEU:O	1:F:446:LEU:HD13	1.97	0.63
1:B:178:LEU:HD22	1:B:180:PHE:CE2	2.34	0.63
2:C:71:LEU:HD11	2:C:117:ILE:HD11	1.81	0.63
1:F:462:GLN:HE22	1:F:490:ASN:HA	1.63	0.62
1:E:450:LEU:HG	1:E:452:LEU:CD1	2.28	0.62
1:I:239:PHE:CE1	1:I:271:LEU:HD13	2.34	0.62
2:H:71:LEU:HD11	2:H:117:ILE:HD11	1.80	0.61
1:N:572:ILE:N	1:N:572:ILE:HD12	2.15	0.61
1:M:383:GLU:OE2	1:M:407:GLU:HB3	2.01	0.61
1:E:393:LYS:HA	1:E:418:GLU:HG2	1.82	0.61
1:E:416:PHE:CB	1:E:444:LEU:HD21	2.31	0.61
1:E:26:PRO:O	1:E:27:LYS:HG2	2.01	0.61
1:A:411:LEU:CD1	1:A:432:LEU:HD22	2.30	0.61
1:E:424:LEU:HD13	1:E:449:VAL:HB	1.83	0.61
2:P:59:LEU:HD22	2:P:128:PHE:CZ	2.36	0.61
2:G:67:PHE:HE2	2:G:69:MET:HE2	1.65	0.61
1:I:178:LEU:HD22	1:I:180:PHE:CE2	2.36	0.61
1:B:537:MET:CE	1:B:550:MET:CE	2.80	0.60
1:A:447:LEU:HD21	1:A:450:LEU:HD13	1.83	0.60
1:F:92:VAL:HG12	1:F:120:SER:HB2	1.83	0.60
1:J:92:VAL:HG12	1:J:120:SER:HB2	1.84	0.60
1:N:92:VAL:HG12	1:N:120:SER:HB2	1.83	0.60
1:F:317:ILE:HG22	1:F:319:GLY:H	1.67	0.59
2:G:92:LEU:HD11	2:G:94:PHE:HD1	1.67	0.59
1:M:569:GLN:HB2	1:M:572:ILE:HD11	1.83	0.59
1:N:570:SER:O	1:N:571:ILE:HD13	2.03	0.59
1:B:570:SER:O	1:B:571:ILE:HD13	2.03	0.59
1:E:348:ARG:HG3	1:E:373:GLN:HE21	1.68	0.59
1:B:537:MET:HG3	1:B:550:MET:HE1	1.83	0.59
2:G:92:LEU:HD11	2:G:94:PHE:CD1	2.38	0.59
1:M:92:VAL:HG12	1:M:120:SER:HB2	1.83	0.59
1:E:570:SER:O	1:E:571:ILE:HD13	2.02	0.59
1:I:428:ALA:HB3	3:I:801:NAG:H82	1.83	0.59
1:A:424:LEU:HD12	1:A:425:LEU:N	2.18	0.58
1:M:450:LEU:HD11	1:M:452:LEU:HD21	1.85	0.58
1:M:119:THR:HA	1:M:122:THR:HG23	1.85	0.58
1:B:391:GLN:OE1	1:B:391:GLN:N	2.34	0.58
5:D:201:PGT:H122	5:D:201:PGT:H322	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:597:HIS:CE1	1:N:598:LYS:HG3	2.38	0.58
1:E:461:ASN:HD22	1:E:464:LEU:CD1	2.14	0.58
1:B:427:VAL:HG21	1:B:432:LEU:HD11	1.85	0.58
1:B:202:LEU:HG	1:B:204:LEU:CD1	2.33	0.58
1:B:537:MET:HE3	1:B:550:MET:HE3	1.85	0.58
2:D:67:PHE:HE2	2:D:69:MET:HE2	1.68	0.58
2:D:84:LEU:HD23	2:D:91:ILE:HD12	1.86	0.58
1:E:92:VAL:HG12	1:E:120:SER:HB2	1.85	0.58
1:B:495:VAL:HG23	1:B:495:VAL:O	2.03	0.58
1:M:348:ARG:HG3	1:M:373:GLN:HE21	1.68	0.58
1:F:609:ASN:OD1	1:F:609:ASN:N	2.36	0.58
1:A:314:PRO:HG2	1:A:317:ILE:HD11	1.86	0.58
1:B:348:ARG:CG	1:B:373:GLN:HE21	2.15	0.58
1:B:314:PRO:HG2	1:B:317:ILE:HD11	1.86	0.57
1:F:519:LEU:HB3	1:F:522:VAL:CG2	2.34	0.57
2:K:63:ILE:HG22	2:K:125:ASN:OD1	2.04	0.57
1:N:537:MET:HG3	1:N:550:MET:HE1	1.86	0.57
2:P:59:LEU:HD22	2:P:128:PHE:CE2	2.39	0.57
1:E:459:THR:CB	1:E:491:LEU:HD11	2.34	0.57
1:M:570:SER:O	1:M:571:ILE:HD13	2.03	0.57
2:L:67:PHE:HE2	2:L:69:MET:HE2	1.68	0.57
1:J:202:LEU:HG	1:J:204:LEU:CD1	2.34	0.57
1:B:361:LEU:HD21	1:B:382:ILE:HD13	1.86	0.57
1:E:434:VAL:HG11	1:E:464:LEU:HD12	1.86	0.57
1:B:537:MET:HE2	1:B:550:MET:CE	2.34	0.57
2:P:67:PHE:HE2	2:P:69:MET:HE2	1.70	0.56
1:N:558:ILE:HD12	1:N:588:PHE:CD1	2.40	0.56
1:F:202:LEU:HG	1:F:204:LEU:CD1	2.36	0.56
2:C:84:LEU:HD23	2:C:91:ILE:CG1	2.33	0.56
2:C:84:LEU:CD2	2:C:91:ILE:HD12	2.36	0.56
2:H:67:PHE:HE2	2:H:69:MET:HE2	1.71	0.56
1:J:179:ASP:CG	1:J:181:GLN:HE21	2.07	0.56
2:P:59:LEU:CD2	2:P:128:PHE:CZ	2.89	0.56
1:B:537:MET:HE2	1:B:550:MET:HE3	1.87	0.56
1:J:436:ALA:HB2	1:J:461:ASN:HB2	1.87	0.56
1:E:202:LEU:HG	1:E:204:LEU:CD1	2.35	0.56
1:M:563:LEU:N	1:M:564:PRO:HD2	2.21	0.56
1:A:92:VAL:HG12	1:A:120:SER:HB2	1.86	0.56
1:E:467:GLY:C	1:E:469:GLN:HE22	2.07	0.56
1:J:439:SER:CB	1:J:466:ALA:HB3	2.35	0.56
1:M:202:LEU:HG	1:M:204:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:VAL:HG11	1:E:464:LEU:CD1	2.36	0.55
1:F:317:ILE:HG22	1:F:319:GLY:N	2.21	0.55
1:J:41:ASN:OD1	2:L:72:ARG:NH1	2.39	0.55
1:M:459:THR:HG22	1:M:491:LEU:CD2	2.36	0.55
1:N:179:ASP:OD1	1:N:181:GLN:NE2	2.38	0.55
1:I:85:THR:HG22	1:I:86:ARG:HB2	1.87	0.55
1:E:450:LEU:CG	1:E:452:LEU:HD11	2.36	0.55
1:N:537:MET:HE2	1:N:566:LEU:HD21	1.89	0.55
1:A:257:ASP:HB3	2:C:119:TYR:OH	2.07	0.55
2:H:36:GLN:HE21	2:H:157:LEU:HD12	1.72	0.55
1:M:411:LEU:HD11	1:M:432:LEU:HD22	1.89	0.55
1:A:424:LEU:HD12	1:A:424:LEU:C	2.26	0.55
1:J:85:THR:HG22	1:J:86:ARG:HB2	1.88	0.55
1:F:537:MET:HE1	1:F:566:LEU:HD11	1.89	0.55
2:G:67:PHE:CE2	2:G:69:MET:HE2	2.41	0.55
1:N:202:LEU:HG	1:N:204:LEU:CD1	2.37	0.55
2:K:67:PHE:HE2	2:K:69:MET:HE2	1.72	0.55
1:E:409:LEU:O	1:E:433:HIS:N	2.39	0.55
1:B:452:LEU:HD13	1:B:457:LEU:HD21	1.89	0.55
1:E:459:THR:HB	1:E:491:LEU:HD11	1.87	0.55
1:N:317:ILE:HG22	1:N:319:GLY:H	1.72	0.55
1:B:572:ILE:HB	1:B:599:LEU:HD23	1.89	0.55
1:E:449:VAL:HG13	1:E:473:HIS:HB3	1.89	0.55
1:N:537:MET:CE	1:N:550:MET:HE2	2.37	0.55
1:B:537:MET:CG	1:B:550:MET:HE1	2.37	0.54
1:N:558:ILE:HD12	1:N:588:PHE:CE1	2.43	0.54
5:H:201:PGT:H322	5:H:201:PGT:H122	1.88	0.54
2:G:86:SER:HB3	2:G:91:ILE:HD11	1.88	0.54
1:B:179:ASP:OD1	1:B:181:GLN:NE2	2.40	0.54
1:E:459:THR:HA	1:E:491:LEU:HD21	1.90	0.54
1:J:537:MET:HB2	1:J:562:LEU:HD13	1.88	0.54
1:M:264:THR:HG22	1:M:265:SER:N	2.23	0.54
1:A:563:LEU:N	1:A:564:PRO:HD2	2.22	0.54
5:P:201:PGT:H122	5:P:201:PGT:H322	1.89	0.54
1:B:592:TYR:CZ	1:B:599:LEU:HD13	2.43	0.53
2:P:36:GLN:HE21	2:P:157:LEU:HD12	1.73	0.53
1:I:202:LEU:HG	1:I:204:LEU:CD1	2.38	0.53
1:A:348:ARG:HG3	1:A:373:GLN:HE21	1.73	0.53
2:G:36:GLN:HE21	2:G:157:LEU:HD12	1.73	0.53
1:N:334:ASP:OD2	1:N:357:ARG:HD2	2.08	0.53
1:J:533:THR:O	1:J:535:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:LEU:HD13	1:I:202:LEU:HD21	1.90	0.53
1:M:424:LEU:HD12	1:M:425:LEU:N	2.24	0.53
1:A:457:LEU:HG	1:A:479:ASN:OD1	2.08	0.53
1:M:317:ILE:HG22	1:M:319:GLY:H	1.74	0.53
1:A:414:GLN:HB3	1:A:443:ASN:HD21	1.74	0.53
1:A:411:LEU:HD11	1:A:432:LEU:HD22	1.91	0.53
1:F:492:LEU:C	1:F:494:MET:H	2.10	0.53
1:J:439:SER:HB3	1:J:466:ALA:HB3	1.91	0.53
1:A:511:ILE:HD11	1:A:527:LEU:HD22	1.90	0.53
1:B:92:VAL:HG12	1:B:120:SER:HB2	1.91	0.53
1:I:377:LEU:HB3	1:I:382:ILE:CD1	2.38	0.53
1:N:317:ILE:HG22	1:N:319:GLY:N	2.24	0.53
1:J:525:LEU:HD23	1:J:540:LEU:HD21	1.91	0.53
1:I:317:ILE:HG22	1:I:319:GLY:H	1.74	0.53
1:B:466:ALA:HA	1:B:494:MET:CG	2.39	0.53
1:B:605:THR:HG22	1:B:618:LEU:HD13	1.90	0.53
5:L:201:PGT:H322	5:L:201:PGT:H122	1.91	0.53
2:D:67:PHE:CE2	2:D:69:MET:HE2	2.44	0.53
1:N:537:MET:HG3	1:N:550:MET:CE	2.39	0.53
1:I:373:GLN:C	1:I:398:LEU:HD12	2.29	0.52
1:B:203:SER:C	1:B:204:LEU:HD12	2.29	0.52
1:M:314:PRO:HG2	1:M:317:ILE:HD11	1.92	0.52
1:A:264:THR:HG22	1:A:265:SER:N	2.24	0.52
1:A:317:ILE:HG22	1:A:319:GLY:H	1.74	0.52
1:J:414:GLN:HB3	1:J:443:ASN:ND2	2.24	0.52
1:E:179:ASP:OD1	1:E:181:GLN:NE2	2.42	0.52
1:N:264:THR:HG22	1:N:265:SER:N	2.24	0.52
2:O:67:PHE:HE2	2:O:69:MET:HE2	1.75	0.52
1:N:197:GLU:OE2	1:N:221:SER:OG	2.27	0.52
1:A:202:LEU:HG	1:A:204:LEU:CD1	2.40	0.52
1:I:317:ILE:HG22	1:I:319:GLY:N	2.25	0.52
1:E:563:LEU:N	1:E:564:PRO:HD2	2.25	0.52
1:J:201:ASN:HD22	1:J:225:GLN:HB2	1.75	0.52
1:N:378:SER:HB2	4:N:901:NAG:H62	1.92	0.52
1:N:314:PRO:HG2	1:N:317:ILE:HD11	1.91	0.52
1:M:364:ARG:O	1:M:367:GLU:HB3	2.10	0.52
1:M:366:LEU:HB3	1:M:369:LEU:HD12	1.91	0.52
2:O:36:GLN:HE21	2:O:157:LEU:HD12	1.75	0.52
2:C:36:GLN:HE21	2:C:157:LEU:HD12	1.74	0.52
1:F:428:ALA:HB3	3:F:801:NAG:H82	1.91	0.52
2:C:67:PHE:HE2	2:C:69:MET:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:LEU:CD1	1:F:432:LEU:HD13	2.39	0.51
1:B:466:ALA:HA	1:B:494:MET:HG2	1.90	0.51
1:A:203:SER:C	1:A:204:LEU:HD12	2.30	0.51
1:B:409:LEU:HD12	1:B:430:THR:HG21	1.93	0.51
1:E:424:LEU:HD12	1:E:425:LEU:N	2.25	0.51
1:A:239:PHE:CE1	1:A:271:LEU:HD13	2.45	0.51
1:N:471:LEU:O	1:N:498:LEU:HD23	2.10	0.51
1:J:203:SER:C	1:J:204:LEU:HD12	2.30	0.51
1:E:442:GLN:HA	1:E:467:GLY:HA3	1.92	0.51
1:M:317:ILE:HG22	1:M:319:GLY:N	2.25	0.51
1:A:317:ILE:HG22	1:A:319:GLY:N	2.25	0.51
2:K:36:GLN:HE21	2:K:157:LEU:HD12	1.75	0.51
1:A:119:THR:HA	1:A:122:THR:HG23	1.93	0.51
1:E:428:ALA:HB3	3:E:801:NAG:H82	1.92	0.51
1:B:85:THR:HG22	1:B:86:ARG:HB2	1.92	0.51
1:N:393:LYS:HA	1:N:418:GLU:HG2	1.93	0.51
1:J:317:ILE:HG22	1:J:319:GLY:H	1.76	0.51
1:E:314:PRO:HG2	1:E:317:ILE:HD11	1.92	0.51
2:O:127:GLY:O	2:O:128:PHE:HB3	2.11	0.51
1:F:85:THR:HG22	1:F:86:ARG:HB2	1.93	0.51
1:B:317:ILE:HG22	1:B:319:GLY:N	2.26	0.51
1:I:119:THR:HA	1:I:122:THR:HG23	1.92	0.51
1:J:119:THR:HA	1:J:122:THR:HG23	1.92	0.51
1:N:477:GLN:HG3	1:N:504:SER:OG	2.11	0.51
1:F:525:LEU:HD23	1:F:540:LEU:HD21	1.93	0.51
1:B:122:THR:HG21	1:B:146:HIS:CD2	2.46	0.51
1:A:201:ASN:HD22	1:A:225:GLN:HB2	1.74	0.51
1:J:563:LEU:N	1:J:564:PRO:HD2	2.26	0.51
1:I:373:GLN:HA	1:I:398:LEU:HA	1.93	0.50
1:N:585:ASN:OD1	1:N:588:PHE:HB3	2.11	0.50
1:J:427:VAL:HG21	1:J:432:LEU:HD11	1.93	0.50
1:J:447:LEU:HD21	1:J:450:LEU:HB2	1.93	0.50
2:P:67:PHE:CE2	2:P:69:MET:HE2	2.46	0.50
1:F:314:PRO:HG2	1:F:317:ILE:HD11	1.94	0.50
1:N:563:LEU:N	1:N:564:PRO:HD2	2.27	0.50
2:H:82:VAL:HG22	2:H:139:LEU:CD2	2.33	0.50
1:A:371:ASN:ND2	1:A:371:ASN:N	2.59	0.50
1:N:596:LEU:HA	1:N:599:LEU:HD12	1.94	0.50
1:M:311:ASN:HD22	2:H:160:ALA:H	1.59	0.50
2:C:84:LEU:HD21	2:C:91:ILE:HD12	1.93	0.50
1:A:192:ASP:O	1:A:195:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:192:ASP:O	1:N:195:SER:HB3	2.12	0.50
1:E:511:ILE:HG22	1:E:512:ASP:O	2.11	0.50
1:J:537:MET:HG2	1:J:550:MET:HE2	1.94	0.50
1:E:317:ILE:HG22	1:E:319:GLY:N	2.26	0.50
1:J:595:ASN:N	1:J:595:ASN:OD1	2.43	0.50
1:F:122:THR:HG21	1:F:146:HIS:CD2	2.46	0.50
1:J:409:LEU:CD1	1:J:430:THR:HG21	2.42	0.50
1:B:428:ALA:HB3	3:B:801:NAG:H82	1.93	0.50
1:N:85:THR:HG22	1:N:86:ARG:HB2	1.92	0.50
1:N:427:VAL:HG21	1:N:432:LEU:HD11	1.94	0.50
1:F:392:LEU:HB3	1:F:395:LEU:HD12	1.94	0.50
1:F:119:THR:HA	1:F:122:THR:HG23	1.93	0.49
1:F:563:LEU:N	1:F:564:PRO:HD2	2.27	0.49
1:M:85:THR:HG22	1:M:86:ARG:HB2	1.92	0.49
1:E:447:LEU:HD23	1:E:471:LEU:HD13	1.93	0.49
1:I:314:PRO:HG2	1:I:317:ILE:HD11	1.93	0.49
1:J:314:PRO:HG2	1:J:317:ILE:HD11	1.93	0.49
1:E:85:THR:HG22	1:E:86:ARG:HB2	1.93	0.49
1:M:424:LEU:C	1:M:424:LEU:HD12	2.33	0.49
1:M:532:LEU:HD22	1:M:536:SER:OG	2.13	0.49
1:M:512:ASP:OD2	1:M:513:GLN:N	2.45	0.49
1:J:592:TYR:CZ	1:J:599:LEU:HD13	2.47	0.49
1:N:119:THR:HA	1:N:122:THR:HG23	1.94	0.49
1:N:580:ASP:HB3	1:N:585:ASN:HD22	1.78	0.49
1:N:514:GLN:HG2	1:N:517:HIS:CE1	2.48	0.49
1:M:363:THR:HG22	1:M:390:LEU:HB3	1.94	0.49
1:E:413:ASP:HB2	1:E:438:HIS:CD2	2.48	0.49
1:E:317:ILE:HG22	1:E:319:GLY:H	1.78	0.49
1:N:203:SER:C	1:N:204:LEU:HD12	2.33	0.48
1:N:114:ILE:HA	2:O:116:GLN:NE2	2.28	0.48
1:A:179:ASP:OD1	1:A:181:GLN:NE2	2.45	0.48
1:M:201:ASN:HD22	1:M:225:GLN:HB2	1.76	0.48
1:A:85:THR:HG22	1:A:86:ARG:HB2	1.94	0.48
1:J:286:PHE:CD1	1:J:289:LEU:HD13	2.47	0.48
1:J:471:LEU:HD23	1:J:498:LEU:HD21	1.95	0.48
4:F:908:MAN:H2	2:H:97:PRO:CG	2.44	0.48
1:M:414:GLN:OE1	1:M:443:ASN:ND2	2.47	0.48
1:A:393:LYS:HA	1:A:418:GLU:HG2	1.94	0.48
2:D:86:SER:CB	2:D:91:ILE:HD11	2.44	0.48
2:D:132:GLU:HG3	2:D:158:TYR:CB	2.43	0.48
1:M:388:CYS:HB3	1:M:392:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:486:ILE:HB	1:M:511:ILE:HG23	1.94	0.48
1:N:540:LEU:HD13	1:N:548:LEU:HD13	1.95	0.48
1:I:451:ASN:CB	3:I:801:NAG:C1	2.92	0.48
1:E:49:ASP:OD1	1:E:49:ASP:N	2.46	0.48
2:L:36:GLN:HE21	2:L:157:LEU:HD12	1.78	0.48
1:E:264:THR:HG22	1:E:265:SER:N	2.28	0.48
1:F:398:LEU:O	1:F:421:GLN:CB	2.62	0.48
1:A:569:GLN:HB2	1:A:572:ILE:HD11	1.94	0.48
1:F:424:LEU:HD12	1:F:425:LEU:N	2.28	0.48
1:M:392:LEU:HB3	1:M:395:LEU:HD12	1.96	0.48
1:F:51:LEU:O	1:F:75:ARG:NE	2.46	0.48
3:B:802:NAG:HO6	4:B:901:NAG:HO3	1.61	0.48
1:B:119:THR:HA	1:B:122:THR:HG23	1.95	0.47
1:E:119:THR:HA	1:E:122:THR:HG23	1.94	0.47
1:B:458:ASP:C	1:B:458:ASP:OD2	2.51	0.47
1:E:469:GLN:N	1:E:469:GLN:CD	2.67	0.47
1:J:378:SER:HB2	4:J:901:NAG:H62	1.96	0.47
1:B:49:ASP:N	1:B:49:ASP:OD1	2.46	0.47
1:F:447:LEU:CD2	1:F:450:LEU:HD13	2.42	0.47
1:F:179:ASP:OD1	1:F:181:GLN:NE2	2.47	0.47
2:K:67:PHE:CE2	2:K:69:MET:HE2	2.50	0.47
2:K:62:ASN:HD22	2:K:124:ASN:HA	1.78	0.47
1:N:442:GLN:HA	1:N:467:GLY:HA3	1.96	0.47
1:E:452:LEU:HA	1:E:455:CYS:SG	2.54	0.47
2:G:92:LEU:HD13	2:G:92:LEU:C	2.35	0.47
1:J:317:ILE:HG22	1:J:319:GLY:N	2.28	0.47
1:M:311:ASN:ND2	2:H:160:ALA:H	2.12	0.47
1:A:509:LEU:HD23	1:A:531:SER:HB2	1.95	0.47
1:I:424:LEU:HD12	1:I:425:LEU:N	2.30	0.47
1:J:434:VAL:HG13	1:J:438:HIS:HB2	1.97	0.47
1:J:202:LEU:HG	1:J:204:LEU:HD11	1.96	0.47
1:J:447:LEU:HD23	1:J:471:LEU:CD1	2.45	0.47
1:N:537:MET:CE	1:N:550:MET:CE	2.92	0.47
1:N:424:LEU:HD12	1:N:425:LEU:N	2.29	0.47
1:N:225:GLN:HG3	1:N:248:GLN:HE21	1.80	0.47
1:M:495:VAL:HG23	1:M:495:VAL:O	2.13	0.47
1:N:495:VAL:HG23	1:N:495:VAL:O	2.14	0.47
1:B:563:LEU:N	1:B:564:PRO:HD2	2.30	0.47
1:M:179:ASP:OD1	1:M:181:GLN:NE2	2.48	0.47
1:N:415:ALA:HB3	1:N:416:PHE:CD1	2.50	0.47
1:N:364:ARG:O	1:N:367:GLU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:GLN:HE21	2:D:157:LEU:HD12	1.79	0.47
1:B:256:GLU:HG2	1:B:283:LYS:NZ	2.30	0.47
1:B:283:LYS:HA	1:B:307:ALA:O	2.15	0.47
1:N:201:ASN:HD22	1:N:225:GLN:HB2	1.80	0.47
1:E:399:GLN:NE2	1:E:423:GLU:OE2	2.46	0.47
1:I:179:ASP:OD1	1:I:181:GLN:NE2	2.47	0.46
2:L:67:PHE:CE2	2:L:69:MET:HE2	2.48	0.46
1:B:317:ILE:HG22	1:B:319:GLY:H	1.79	0.46
1:E:459:THR:HG22	1:E:491:LEU:HD11	1.96	0.46
2:L:63:ILE:HG22	2:L:125:ASN:OD1	2.16	0.46
1:F:592:TYR:CE1	1:F:599:LEU:HD13	2.50	0.46
1:M:391:GLN:N	1:M:391:GLN:OE1	2.43	0.46
1:F:462:GLN:O	1:F:494:MET:HE2	2.16	0.46
1:N:537:MET:HE2	1:N:550:MET:HE2	1.96	0.46
1:N:563:LEU:HD21	1:N:591:TRP:HB2	1.96	0.46
1:N:225:GLN:CG	1:N:248:GLN:HE21	2.28	0.46
1:F:537:MET:HA	1:F:540:LEU:HD12	1.98	0.46
1:B:201:ASN:HD22	1:B:225:GLN:HB2	1.79	0.46
1:E:192:ASP:O	1:E:195:SER:HB3	2.15	0.46
1:F:378:SER:HB2	4:F:901:NAG:H62	1.98	0.46
2:C:135:TYR:HB2	2:C:156:VAL:HB	1.97	0.46
1:B:41:ASN:OD1	2:D:72:ARG:NH1	2.48	0.46
1:J:592:TYR:CD1	1:J:599:LEU:HD13	2.51	0.46
1:N:235:LEU:HD12	1:N:263:LEU:HD21	1.98	0.46
2:C:84:LEU:CD2	2:C:91:ILE:CD1	2.94	0.46
2:C:67:PHE:CE2	2:C:69:MET:HE2	2.51	0.46
1:N:564:PRO:HA	1:N:567:SER:OG	2.16	0.46
1:F:264:THR:HG22	1:F:265:SER:N	2.30	0.46
1:E:201:ASN:HD22	1:E:225:GLN:HB2	1.80	0.46
1:I:68:ILE:HD11	1:I:84:LEU:HD13	1.97	0.46
1:F:491:LEU:HD12	1:F:492:LEU:N	2.30	0.46
1:I:264:THR:HG22	1:I:265:SER:N	2.31	0.46
2:L:84:LEU:HD12	2:L:137:VAL:HG22	1.98	0.46
1:J:192:ASP:O	1:J:195:SER:HB3	2.16	0.46
1:J:491:LEU:HD13	1:J:492:LEU:HD23	1.98	0.46
1:F:201:ASN:HD22	1:F:225:GLN:HB2	1.81	0.46
1:N:202:LEU:HG	1:N:204:LEU:HD11	1.98	0.46
1:A:431:HIS:CE1	1:A:456:LEU:HD22	2.51	0.46
1:N:172:THR:OG1	1:N:198:GLN:HB2	2.16	0.46
1:M:257:ASP:N	1:M:257:ASP:OD2	2.49	0.46
1:F:572:ILE:HD12	1:F:572:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASP:O	1:B:195:SER:HB3	2.16	0.46
1:N:592:TYR:CZ	1:N:599:LEU:HD13	2.51	0.45
2:L:84:LEU:HD23	2:L:91:ILE:HB	1.98	0.45
4:E:905:MAN:C1	4:E:908:MAN:O2	2.64	0.45
1:B:202:LEU:HG	1:B:204:LEU:HD11	1.97	0.45
2:C:63:ILE:HG22	2:C:125:ASN:OD1	2.17	0.45
1:B:264:THR:HG22	1:B:265:SER:N	2.32	0.45
1:N:485:SER:HB2	1:N:510:SER:OG	2.17	0.45
1:B:450:LEU:HD11	1:B:452:LEU:HD21	1.99	0.45
1:F:537:MET:HB2	1:F:562:LEU:HD13	1.99	0.45
1:E:469:GLN:H	1:E:469:GLN:NE2	2.14	0.45
1:E:511:ILE:HD11	1:E:527:LEU:HD13	1.99	0.45
1:A:68:ILE:HD11	1:A:84:LEU:HD13	1.98	0.45
1:J:450:LEU:CD1	1:J:452:LEU:HD21	2.31	0.45
2:C:84:LEU:HD23	2:C:91:ILE:CD1	2.46	0.45
1:F:533:THR:O	1:F:534:GLY:C	2.54	0.45
1:E:203:SER:C	1:E:204:LEU:HD12	2.37	0.45
1:M:459:THR:HG22	1:M:491:LEU:HD21	1.98	0.45
1:A:257:ASP:OD2	1:A:257:ASP:N	2.46	0.45
1:N:122:THR:HG21	1:N:146:HIS:CD2	2.52	0.45
1:N:68:ILE:HD11	1:N:84:LEU:HD13	1.99	0.45
1:J:447:LEU:HD23	1:J:471:LEU:HD13	1.99	0.45
1:M:571:ILE:C	1:M:572:ILE:HD12	2.36	0.45
1:F:204:LEU:HD23	1:F:206:PHE:CZ	2.52	0.45
1:M:68:ILE:HD11	1:M:84:LEU:HD13	1.98	0.45
1:J:172:THR:OG1	1:J:198:GLN:HB2	2.16	0.45
2:H:87:LYS:O	2:H:89:LEU:N	2.46	0.45
2:H:67:PHE:CE2	2:H:69:MET:HE2	2.50	0.45
2:D:84:LEU:HD12	2:D:137:VAL:HG22	1.99	0.45
1:J:439:SER:OG	1:J:466:ALA:HB3	2.16	0.45
1:J:387:CYS:O	1:J:415:ALA:HB1	2.15	0.45
1:N:239:PHE:O	1:N:274:MET:HE1	2.17	0.45
1:F:613:LEU:O	1:F:616:VAL:HG23	2.16	0.45
1:N:537:MET:CG	1:N:550:MET:HE1	2.46	0.45
2:P:64:ASN:HD22	2:P:122:PRO:HA	1.82	0.45
1:A:427:VAL:HG22	1:A:452:LEU:HD23	2.00	0.44
1:F:580:ASP:OD2	1:F:609:ASN:ND2	2.51	0.44
1:B:347:LEU:HB3	1:B:369:LEU:HD22	1.99	0.44
1:I:49:ASP:OD1	1:I:49:ASP:N	2.47	0.44
1:J:530:ASN:O	1:J:553:ASN:HA	2.17	0.44
1:B:537:MET:CG	1:B:550:MET:CE	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:413:ASP:HB2	1:N:438:HIS:CD2	2.52	0.44
1:M:192:ASP:O	1:M:195:SER:HB3	2.18	0.44
1:B:513:GLN:HG3	1:B:538:ASP:OD2	2.17	0.44
1:B:172:THR:OG1	1:B:198:GLN:HB2	2.17	0.44
1:M:242:LEU:HB2	1:M:274:MET:CE	2.34	0.44
1:N:593:LYS:HE2	1:N:619:SER:O	2.17	0.44
4:J:905:MAN:C1	4:J:908:MAN:O2	2.65	0.44
1:N:122:THR:CG2	1:N:146:HIS:CD2	3.01	0.44
1:N:540:LEU:HD13	1:N:548:LEU:CD1	2.47	0.44
1:M:428:ALA:HB3	3:M:801:NAG:H82	1.99	0.44
1:F:49:ASP:N	1:F:49:ASP:OD1	2.50	0.44
1:I:175:LEU:HA	1:I:175:LEU:HD12	1.85	0.44
1:A:202:LEU:HG	1:A:204:LEU:HD11	1.99	0.44
1:A:416:PHE:HB2	1:A:444:LEU:HD21	2.00	0.44
1:J:137:ILE:O	1:J:159:ASN:HB3	2.18	0.44
2:K:134:ASP:N	2:K:134:ASP:OD1	2.49	0.44
1:F:452:LEU:CD1	1:F:457:LEU:HD11	2.42	0.44
1:N:424:LEU:HD12	1:N:424:LEU:C	2.38	0.44
1:E:437:PRO:HA	1:E:461:ASN:OD1	2.18	0.44
1:B:452:LEU:HD13	1:B:457:LEU:HD11	1.99	0.44
1:A:348:ARG:CG	1:A:373:GLN:HE21	2.31	0.44
1:M:427:VAL:HG23	1:M:455:CYS:SG	2.58	0.44
1:E:196:LEU:HD23	1:E:196:LEU:N	2.32	0.44
3:F:802:NAG:HO6	4:F:901:NAG:HO3	1.64	0.43
1:A:32:GLU:HG3	1:A:33:GLY:N	2.33	0.43
2:G:62:ASN:HD22	2:G:124:ASN:HA	1.83	0.43
1:M:348:ARG:CG	1:M:373:GLN:HE21	2.32	0.43
1:E:202:LEU:HG	1:E:204:LEU:HD11	1.99	0.43
1:A:563:LEU:HD21	1:A:588:PHE:HA	2.00	0.43
1:F:122:THR:CG2	1:F:146:HIS:CD2	3.00	0.43
1:F:468:LEU:HB2	1:F:495:VAL:HG12	2.00	0.43
1:A:172:THR:OG1	1:A:198:GLN:HB2	2.18	0.43
1:F:582:THR:HG1	1:F:584:SER:HG	1.66	0.43
1:E:235:LEU:HD12	1:E:263:LEU:HD21	2.00	0.43
1:N:55:THR:HB	1:N:76:LEU:HD22	2.00	0.43
3:I:801:NAG:O4	4:I:901:NAG:H83	2.18	0.43
1:M:459:THR:HB	1:M:491:LEU:HD23	2.00	0.43
1:F:465:LEU:HB3	1:F:495:VAL:HG13	1.99	0.43
1:J:505:SER:HA	1:J:529:HIS:O	2.18	0.43
4:I:905:MAN:C1	4:I:908:MAN:O2	2.66	0.43
1:E:424:LEU:C	1:E:424:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:491:LEU:C	1:M:491:LEU:HD12	2.39	0.43
1:A:428:ALA:HB3	3:A:801:NAG:H82	2.00	0.43
1:F:454:HIS:CE1	1:F:477:GLN:HG2	2.52	0.43
1:B:461:ASN:O	1:B:463:HIS:N	2.51	0.43
1:N:571:ILE:C	1:N:572:ILE:HD12	2.38	0.43
1:N:242:LEU:HB2	1:N:274:MET:HE1	1.99	0.43
1:F:172:THR:OG1	1:F:198:GLN:HB2	2.18	0.43
4:F:905:MAN:O3	2:H:95:SER:O	2.16	0.43
1:A:217:GLY:O	1:A:220:ILE:HG13	2.18	0.43
1:J:49:ASP:N	1:J:49:ASP:OD1	2.51	0.43
1:I:348:ARG:CG	1:I:373:GLN:HE21	2.26	0.43
1:E:459:THR:CG2	1:E:491:LEU:HD11	2.48	0.43
1:I:203:SER:C	1:I:204:LEU:HD12	2.39	0.43
1:N:49:ASP:OD1	1:N:49:ASP:N	2.51	0.43
1:E:434:VAL:CG2	1:E:464:LEU:HD11	2.42	0.43
1:B:204:LEU:HD23	1:B:206:PHE:CZ	2.53	0.43
1:F:394:ASN:H	1:F:418:GLU:HG2	1.84	0.43
1:E:137:ILE:O	1:E:159:ASN:HB3	2.19	0.43
1:F:519:LEU:O	1:F:521:ASN:N	2.52	0.43
1:F:62:PHE:CE2	1:F:86:ARG:HG2	2.54	0.43
1:N:68:ILE:HD13	1:N:68:ILE:HG21	1.71	0.43
1:J:385:SER:O	1:J:387:CYS:N	2.44	0.43
1:A:559:PRO:HA	1:A:560:PRO:HD3	1.93	0.43
1:I:172:THR:OG1	1:I:198:GLN:HB2	2.19	0.43
2:D:59:LEU:HD23	2:D:128:PHE:CE2	2.54	0.43
1:J:179:ASP:OD1	1:J:181:GLN:NE2	2.52	0.43
1:I:204:LEU:HD23	1:I:206:PHE:CZ	2.53	0.43
1:E:461:ASN:ND2	1:E:464:LEU:HD12	2.23	0.42
1:F:192:ASP:O	1:F:195:SER:HB3	2.19	0.42
1:I:192:ASP:O	1:I:195:SER:HB3	2.18	0.42
1:I:47:ILE:HG23	1:I:51:LEU:HD12	2.00	0.42
1:A:427:VAL:HG23	1:A:455:CYS:SG	2.59	0.42
1:E:450:LEU:HB3	1:E:471:LEU:HD21	2.00	0.42
1:E:495:VAL:HG23	1:E:495:VAL:O	2.19	0.42
1:A:558:ILE:HG22	1:A:563:LEU:HD13	2.02	0.42
1:M:203:SER:C	1:M:204:LEU:HD12	2.40	0.42
1:A:264:THR:HG22	1:A:266:ALA:H	1.82	0.42
1:B:122:THR:HG22	1:B:146:HIS:HB3	2.02	0.42
1:M:388:CYS:HB3	1:M:392:LEU:HD12	2.01	0.42
1:B:91:TRP:CH2	2:C:48:PHE:HA	2.55	0.42
1:M:119:THR:CA	1:M:122:THR:HG23	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:537:MET:HE3	1:N:550:MET:HE2	2.01	0.42
1:A:413:ASP:O	1:A:414:GLN:C	2.58	0.42
2:H:57:ARG:NE	2:H:132:GLU:HG3	2.35	0.42
1:M:311:ASN:CB	2:H:132:GLU:HB3	2.50	0.42
1:M:164:ILE:CG2	1:M:185:ILE:HD13	2.50	0.42
1:A:462:GLN:OE1	1:A:490:ASN:C	2.57	0.42
2:H:84:LEU:HD12	2:H:137:VAL:HG22	2.01	0.42
1:B:564:PRO:HA	1:B:567:SER:OG	2.20	0.42
1:I:235:LEU:HD12	1:I:263:LEU:HD21	2.01	0.42
1:M:403:LEU:HD13	1:M:409:LEU:HD11	2.01	0.42
1:M:473:HIS:CD2	1:M:500:ILE:HD12	2.55	0.42
1:M:501:LEU:HD21	1:M:503:LEU:HD11	2.01	0.42
1:E:172:THR:OG1	1:E:198:GLN:HB2	2.18	0.42
1:A:497:SER:O	1:A:498:LEU:C	2.58	0.42
1:A:564:PRO:HA	1:A:567:SER:OG	2.20	0.42
1:J:473:HIS:CD2	1:J:500:ILE:HD12	2.55	0.42
1:J:264:THR:HG22	1:J:265:SER:N	2.34	0.42
1:M:49:ASP:OD1	1:M:49:ASP:N	2.51	0.42
1:B:537:MET:HB2	1:B:562:LEU:HD13	2.02	0.42
1:M:202:LEU:HG	1:M:204:LEU:HD11	2.02	0.42
1:J:122:THR:HG21	1:J:146:HIS:CD2	2.54	0.42
1:E:512:ASP:OD1	1:E:513:GLN:N	2.52	0.42
1:I:68:ILE:HG21	1:I:68:ILE:HD13	1.77	0.42
2:K:143:ASN:C	2:K:143:ASN:OD1	2.58	0.42
1:J:204:LEU:HD23	1:J:206:PHE:CZ	2.55	0.42
1:E:474:LEU:HB2	1:E:498:LEU:HD21	2.01	0.42
1:B:559:PRO:HA	1:B:560:PRO:HD3	1.93	0.42
1:M:137:ILE:O	1:M:159:ASN:HB3	2.20	0.42
1:A:49:ASP:N	1:A:49:ASP:OD1	2.53	0.42
1:F:449:VAL:HG22	1:F:473:HIS:HB3	2.02	0.41
2:O:59:LEU:HA	2:O:59:LEU:HD12	1.84	0.41
1:N:126:PHE:HA	1:N:150:ASN:HD22	1.85	0.41
2:O:64:ASN:HD22	2:O:122:PRO:HA	1.85	0.41
1:J:405:TYR:HE2	3:J:801:NAG:H81	1.84	0.41
2:D:84:LEU:HD23	2:D:91:ILE:CD1	2.50	0.41
1:E:459:THR:OG1	1:E:480:SER:O	2.28	0.41
1:I:201:ASN:HD22	1:I:225:GLN:HB2	1.85	0.41
1:E:47:ILE:HG23	1:E:51:LEU:HD12	2.02	0.41
1:B:399:GLN:NE2	1:B:423:GLU:OE2	2.52	0.41
1:N:449:VAL:HG22	1:N:473:HIS:HB3	2.01	0.41
1:M:48:PRO:HD2	1:M:51:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:391:GLN:OE1	1:J:391:GLN:N	2.51	0.41
1:M:564:PRO:HA	1:M:567:SER:OG	2.20	0.41
1:J:591:TRP:NE1	1:J:595:ASN:ND2	2.69	0.41
1:F:394:ASN:N	1:F:418:GLU:HG2	2.34	0.41
1:N:428:ALA:HB3	3:N:801:NAG:H82	2.02	0.41
1:J:431:HIS:CD2	1:J:456:LEU:HD13	2.55	0.41
1:N:447:LEU:HD21	1:N:450:LEU:HD13	2.01	0.41
1:J:424:LEU:HD12	1:J:425:LEU:N	2.34	0.41
1:A:392:LEU:HD13	1:A:419:CYS:SG	2.60	0.41
1:E:384:ALA:HB3	1:E:409:LEU:HD21	1.98	0.41
2:O:86:SER:CB	2:O:91:ILE:HD11	2.47	0.41
1:M:204:LEU:HD23	1:M:206:PHE:CZ	2.56	0.41
1:E:511:ILE:CG2	1:E:515:ALA:HB3	2.50	0.41
1:E:235:LEU:HD12	1:E:263:LEU:CD2	2.50	0.41
1:J:473:HIS:CD2	1:J:500:ILE:CD1	3.04	0.41
1:J:235:LEU:HD12	1:J:263:LEU:HD21	2.02	0.41
1:E:564:PRO:HA	1:E:567:SER:OG	2.21	0.41
1:B:481:PHE:CD1	1:B:508:LEU:HD21	2.55	0.41
1:E:477:GLN:O	1:E:479:ASN:ND2	2.54	0.41
1:F:407:GLU:HB3	1:F:408:PRO:HD2	2.03	0.41
1:E:175:LEU:HD12	1:E:175:LEU:HA	1.85	0.41
1:J:537:MET:HG2	1:J:550:MET:CE	2.50	0.41
1:F:203:SER:C	1:F:204:LEU:HD12	2.41	0.41
1:I:202:LEU:HG	1:I:204:LEU:HD11	2.02	0.41
1:B:466:ALA:CA	1:B:494:MET:HG2	2.51	0.41
1:J:443:ASN:OD1	1:J:443:ASN:N	2.54	0.41
1:N:47:ILE:HG23	1:N:51:LEU:HD12	2.03	0.41
1:B:468:LEU:HB2	1:B:495:VAL:HG12	2.02	0.41
1:M:341:ALA:HB1	1:M:369:LEU:HD21	2.03	0.41
1:M:449:VAL:HG22	1:M:473:HIS:HB3	2.01	0.41
1:F:523:ASN:HA	1:F:546:LEU:HB3	2.03	0.41
1:F:537:MET:CE	1:F:566:LEU:HD11	2.50	0.41
1:F:537:MET:CE	1:F:566:LEU:HD21	2.47	0.41
1:M:572:ILE:HD12	1:M:572:ILE:N	2.36	0.41
1:F:596:LEU:HA	1:F:599:LEU:HD12	2.02	0.41
1:J:572:ILE:HB	1:J:599:LEU:HD23	2.03	0.41
2:D:86:SER:HB2	2:D:91:ILE:HD11	2.02	0.41
2:C:69:MET:HB3	2:C:69:MET:HE2	1.94	0.41
1:B:122:THR:CG2	1:B:146:HIS:CD2	3.04	0.41
1:N:514:GLN:HA	1:N:517:HIS:CD2	2.56	0.41
1:M:511:ILE:HG22	1:M:515:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:84:LEU:HD23	2:L:91:ILE:CG2	2.50	0.41
4:J:908:MAN:H2	2:L:97:PRO:CG	2.51	0.41
1:F:235:LEU:HD12	1:F:263:LEU:HD21	2.03	0.41
1:B:478:GLY:HA2	1:B:505:SER:O	2.21	0.41
1:J:68:ILE:HD11	1:J:84:LEU:HD13	2.02	0.41
1:A:361:LEU:HD21	1:A:382:ILE:HD13	2.02	0.41
1:B:464:LEU:HD23	1:B:491:LEU:HD23	2.03	0.41
1:A:175:LEU:HA	1:A:175:LEU:HD12	1.90	0.41
1:E:509:LEU:HD23	1:E:531:SER:HB2	2.03	0.41
2:G:84:LEU:HD12	2:G:137:VAL:HG22	2.03	0.41
1:I:264:THR:HG22	1:I:266:ALA:H	1.86	0.41
1:M:416:PHE:HB2	1:M:444:LEU:HD21	2.03	0.41
1:I:137:ILE:O	1:I:159:ASN:HB3	2.21	0.41
1:J:369:LEU:HD13	1:J:372:LEU:HD13	2.03	0.41
2:O:67:PHE:CE2	2:O:69:MET:HE2	2.55	0.40
1:M:166:LEU:HB2	1:M:195:SER:OG	2.20	0.40
1:E:239:PHE:CE1	1:E:271:LEU:HD13	2.56	0.40
1:A:242:LEU:HB2	1:A:274:MET:CE	2.51	0.40
1:B:242:LEU:HB2	1:B:274:MET:HE1	2.03	0.40
1:M:172:THR:OG1	1:M:198:GLN:HB2	2.21	0.40
1:E:407:GLU:HB3	1:E:408:PRO:HD2	2.03	0.40
1:F:68:ILE:HD13	1:F:68:ILE:HG21	1.75	0.40
1:A:572:ILE:HD12	1:A:572:ILE:N	2.37	0.40
1:M:378:SER:HB2	4:M:901:NAG:H62	2.04	0.40
1:J:464:LEU:HD12	1:J:464:LEU:HA	1.60	0.40
2:O:84:LEU:HD12	2:O:137:VAL:HG22	2.02	0.40
1:B:537:MET:HG2	1:B:550:MET:CE	2.51	0.40
1:B:164:ILE:HG21	1:B:206:PHE:HE1	1.87	0.40
1:F:564:PRO:HA	1:F:567:SER:OG	2.21	0.40
1:I:235:LEU:HD12	1:I:263:LEU:CD2	2.51	0.40
1:F:239:PHE:HA	1:F:274:MET:HE1	2.02	0.40
1:I:407:GLU:HB3	1:I:408:PRO:HD2	2.04	0.40
1:E:68:ILE:HD11	1:E:84:LEU:HD13	2.02	0.40
1:N:361:LEU:HD21	1:N:382:ILE:HD13	2.02	0.40
1:N:478:GLY:HA2	1:N:505:SER:O	2.21	0.40
2:L:82:VAL:HG22	2:L:139:LEU:CD2	2.43	0.40
2:G:82:VAL:HG22	2:G:139:LEU:CD2	2.43	0.40
1:J:361:LEU:HD21	1:J:382:ILE:HD13	2.03	0.40
1:J:219:PHE:CD1	1:J:242:LEU:HD23	2.56	0.40
1:E:439:SER:HB3	1:E:466:ALA:HB3	2.03	0.40
1:E:371:ASN:N	1:E:371:ASN:ND2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.92	0.40
1:B:70:ASN:OD1	1:B:71:THR:HG23	2.21	0.40
1:F:424:LEU:HD12	1:F:424:LEU:C	2.40	0.40
1:N:219:PHE:CD2	1:N:227:LEU:HD11	2.57	0.40
1:E:559:PRO:HA	1:E:560:PRO:HD3	1.93	0.40
2:O:27:HIS:HB2	2:O:39:TYR:CE1	2.56	0.40
2:C:143:ASN:C	2:C:143:ASN:OD1	2.60	0.40
1:M:235:LEU:HD12	1:M:263:LEU:HD21	2.03	0.40
1:M:239:PHE:CE1	1:M:271:LEU:HD13	2.56	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	592/612 (97%)	552 (93%)	36 (6%)	4 (1%)	26 62
1	B	597/612 (98%)	556 (93%)	38 (6%)	3 (0%)	34 70
1	E	590/612 (96%)	544 (92%)	43 (7%)	3 (0%)	34 70
1	F	597/612 (98%)	557 (93%)	37 (6%)	3 (0%)	34 70
1	I	383/612 (63%)	361 (94%)	21 (6%)	1 (0%)	46 78
1	J	597/612 (98%)	553 (93%)	39 (6%)	5 (1%)	24 58
1	M	591/612 (97%)	546 (92%)	43 (7%)	2 (0%)	46 78
1	N	597/612 (98%)	560 (94%)	35 (6%)	2 (0%)	46 78
2	C	136/147 (92%)	125 (92%)	8 (6%)	3 (2%)	8 30
2	D	134/147 (91%)	125 (93%)	8 (6%)	1 (1%)	26 62
2	G	136/147 (92%)	127 (93%)	6 (4%)	3 (2%)	8 30
2	H	136/147 (92%)	126 (93%)	9 (7%)	1 (1%)	26 62
2	K	132/147 (90%)	125 (95%)	6 (4%)	1 (1%)	24 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	136/147 (92%)	127 (93%)	8 (6%)	1 (1%)	26	62
2	O	136/147 (92%)	129 (95%)	6 (4%)	1 (1%)	26	62
2	P	133/147 (90%)	123 (92%)	9 (7%)	1 (1%)	24	58
All	All	5623/6072 (93%)	5236 (93%)	352 (6%)	35 (1%)	30	66

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	494	MET
1	J	438	HIS
1	J	534	GLY
1	N	494	MET
2	C	128	PHE
2	O	128	PHE
1	A	494	MET
1	A	498	LEU
1	J	484	GLY
2	G	88	GLY
1	A	33	GLY
1	E	461	ASN
1	B	461	ASN
1	B	462	GLN
1	J	493	GLN
1	A	412	GLU
1	E	412	GLU
1	B	33	GLY
1	F	520	ARG
2	D	91	ILE
2	G	23	ALA
1	F	493	GLN
1	J	33	GLY
2	C	86	SER
2	G	89	LEU
2	K	86	SER
2	L	91	ILE
1	E	33	GLY
1	I	33	GLY
1	M	33	GLY
2	C	126	PRO
2	P	130	ILE
1	F	33	GLY

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Mol	Chain	Res	Type
1	N	33	GLY
2	H	88	GLY

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	481/561 (86%)	455 (95%)	26 (5%)	27	61
1	B	516/561 (92%)	484 (94%)	32 (6%)	23	54
1	E	463/561 (82%)	445 (96%)	18 (4%)	39	74
1	F	488/561 (87%)	457 (94%)	31 (6%)	22	53
1	I	304/561 (54%)	291 (96%)	13 (4%)	35	71
1	J	478/561 (85%)	454 (95%)	24 (5%)	30	65
1	M	481/561 (86%)	449 (93%)	32 (7%)	20	50
1	N	511/561 (91%)	484 (95%)	27 (5%)	28	62
2	C	102/125 (82%)	98 (96%)	4 (4%)	39	74
2	D	103/125 (82%)	98 (95%)	5 (5%)	31	66
2	G	103/125 (82%)	98 (95%)	5 (5%)	31	66
2	H	105/125 (84%)	98 (93%)	7 (7%)	20	50
2	K	98/125 (78%)	92 (94%)	6 (6%)	23	55
2	L	106/125 (85%)	99 (93%)	7 (7%)	21	50
2	O	102/125 (82%)	96 (94%)	6 (6%)	24	57
2	P	99/125 (79%)	96 (97%)	3 (3%)	48	82
All	All	4540/5488 (83%)	4294 (95%)	246 (5%)	27	61

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	49	ASP

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Mol	Chain	Res	Type
1	A	74	SER
1	A	122	THR
1	A	178	LEU
1	A	203	SER
1	A	272	CYS
1	A	275	SER
1	A	298	THR
1	A	344	PHE
1	A	371	ASN
1	A	387	CYS
1	A	424	LEU
1	A	434	VAL
1	A	443	ASN
1	A	469	GLN
1	A	473	HIS
1	A	487	SER
1	A	489	THR
1	A	491	LEU
1	A	513	GLN
1	A	523	ASN
1	A	546	LEU
1	A	563	LEU
1	A	584	SER
1	A	612	SER
1	E	49	ASP
1	E	68	ILE
1	E	118	GLU
1	E	122	THR
1	E	178	LEU
1	E	203	SER
1	E	220	ILE
1	E	295	ARG
1	E	298	THR
1	E	344	PHE
1	E	357	ARG
1	E	424	LEU
1	E	443	ASN
1	E	449	VAL
1	E	456	LEU
1	E	489	THR
1	E	494	MET
1	E	546	LEU

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Mol	Chain	Res	Type
1	I	49	ASP
1	I	102	GLN
1	I	122	THR
1	I	149	GLU
1	I	168	GLU
1	I	178	LEU
1	I	203	SER
1	I	243	GLN
1	I	260	ASP
1	I	292	SER
1	I	298	THR
1	I	344	PHE
1	I	424	LEU
1	M	26	PRO
1	M	49	ASP
1	M	74	SER
1	M	122	THR
1	M	149	GLU
1	M	178	LEU
1	M	220	ILE
1	M	240	LYS
1	M	259	ASP
1	M	272	CYS
1	M	298	THR
1	M	299	ARG
1	M	344	PHE
1	M	346	SER
1	M	357	ARG
1	M	364	ARG
1	M	367	GLU
1	M	385	SER
1	M	392	LEU
1	M	424	LEU
1	M	442	GLN
1	M	443	ASN
1	M	469	GLN
1	M	473	HIS
1	M	489	THR
1	M	507	ASN
1	M	509	LEU
1	M	521	ASN
1	M	523	ASN

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Mol	Chain	Res	Type
1	M	531	SER
1	M	546	LEU
1	M	609	ASN
1	B	32	GLU
1	B	49	ASP
1	B	122	THR
1	B	149	GLU
1	B	178	LEU
1	B	203	SER
1	B	221	SER
1	B	256	GLU
1	B	261	GLN
1	B	298	THR
1	B	335	GLN
1	B	344	PHE
1	B	348	ARG
1	B	385	SER
1	B	393	LYS
1	B	413	ASP
1	B	456	LEU
1	B	469	GLN
1	B	473	HIS
1	B	489	THR
1	B	491	LEU
1	B	513	GLN
1	B	521	ASN
1	B	522	VAL
1	B	523	ASN
1	B	531	SER
1	B	546	LEU
1	B	584	SER
1	B	596	LEU
1	B	604	GLU
1	B	609	ASN
1	B	612	SER
1	F	49	ASP
1	F	54	THR
1	F	99	SER
1	F	122	THR
1	F	149	GLU
1	F	178	LEU
1	F	196	LEU

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Mol	Chain	Res	Type
1	F	203	SER
1	F	243	GLN
1	F	260	ASP
1	F	288	ASP
1	F	298	THR
1	F	344	PHE
1	F	357	ARG
1	F	418	GLU
1	F	424	LEU
1	F	446	LEU
1	F	456	LEU
1	F	473	HIS
1	F	485	SER
1	F	489	THR
1	F	491	LEU
1	F	510	SER
1	F	513	GLN
1	F	535	ASP
1	F	546	LEU
1	F	596	LEU
1	F	609	ASN
1	F	612	SER
1	F	614	ARG
1	F	618	LEU
1	J	49	ASP
1	J	122	THR
1	J	178	LEU
1	J	203	SER
1	J	256	GLU
1	J	288	ASP
1	J	298	THR
1	J	344	PHE
1	J	399	GLN
1	J	421	GLN
1	J	424	LEU
1	J	443	ASN
1	J	485	SER
1	J	487	SER
1	J	489	THR
1	J	491	LEU
1	J	494	MET
1	J	538	ASP

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Mol	Chain	Res	Type
1	J	546	LEU
1	J	584	SER
1	J	595	ASN
1	J	596	LEU
1	J	612	SER
1	J	618	LEU
1	N	49	ASP
1	N	68	ILE
1	N	122	THR
1	N	149	GLU
1	N	178	LEU
1	N	197	GLU
1	N	203	SER
1	N	223	ILE
1	N	292	SER
1	N	298	THR
1	N	344	PHE
1	N	348	ARG
1	N	353	LYS
1	N	385	SER
1	N	393	LYS
1	N	419	CYS
1	N	424	LEU
1	N	473	HIS
1	N	482	GLN
1	N	483	ASP
1	N	489	THR
1	N	491	LEU
1	N	513	GLN
1	N	523	ASN
1	N	546	LEU
1	N	596	LEU
1	N	612	SER
2	C	84	LEU
2	C	91	ILE
2	C	113	LYS
2	C	146	HIS
2	D	84	LEU
2	D	90	SER
2	D	113	LYS
2	D	130	ILE
2	D	146	HIS

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Mol	Chain	Res	Type
2	G	42	CYS
2	G	84	LEU
2	G	92	LEU
2	G	113	LYS
2	G	146	HIS
2	H	55	CYS
2	H	58	GLN
2	H	84	LEU
2	H	86	SER
2	H	90	SER
2	H	113	LYS
2	H	146	HIS
2	K	59	LEU
2	K	84	LEU
2	K	90	SER
2	K	113	LYS
2	K	134	ASP
2	K	146	HIS
2	L	42	CYS
2	L	55	CYS
2	L	62	ASN
2	L	84	LEU
2	L	90	SER
2	L	113	LYS
2	L	146	HIS
2	O	59	LEU
2	O	84	LEU
2	O	113	LYS
2	O	125	ASN
2	O	128	PHE
2	O	146	HIS
2	P	84	LEU
2	P	113	LYS
2	P	146	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	102	GLN
1	A	104	ASN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	201	ASN
1	A	225	GLN
1	A	311	ASN
1	A	371	ASN
1	A	373	GLN
1	A	431	HIS
1	A	443	ASN
1	A	469	GLN
1	A	482	GLN
1	A	523	ASN
1	E	34	ASN
1	E	104	ASN
1	E	181	GLN
1	E	201	ASN
1	E	225	GLN
1	E	248	GLN
1	E	311	ASN
1	E	371	ASN
1	E	373	GLN
1	E	433	HIS
1	E	438	HIS
1	E	461	ASN
1	E	469	GLN
1	E	477	GLN
1	I	102	GLN
1	I	104	ASN
1	I	146	HIS
1	I	181	GLN
1	I	201	ASN
1	I	225	GLN
1	I	243	GLN
1	I	311	ASN
1	I	373	GLN
1	M	101	HIS
1	M	104	ASN
1	M	181	GLN
1	M	201	ASN
1	M	225	GLN
1	M	311	ASN
1	M	371	ASN
1	M	373	GLN
1	M	414	GLN

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Mol	Chain	Res	Type
1	M	421	GLN
1	M	443	ASN
1	M	517	HIS
1	M	523	ASN
1	M	529	HIS
1	B	104	ASN
1	B	146	HIS
1	B	150	ASN
1	B	181	GLN
1	B	201	ASN
1	B	225	GLN
1	B	261	GLN
1	B	311	ASN
1	B	373	GLN
1	B	445	HIS
1	B	469	GLN
1	B	514	GLN
1	B	517	HIS
1	B	523	ASN
1	B	609	ASN
1	F	104	ASN
1	F	146	HIS
1	F	150	ASN
1	F	181	GLN
1	F	201	ASN
1	F	225	GLN
1	F	311	ASN
1	F	462	GLN
1	F	477	GLN
1	F	493	GLN
1	F	568	GLN
1	F	597	HIS
1	J	104	ASN
1	J	146	HIS
1	J	150	ASN
1	J	181	GLN
1	J	201	ASN
1	J	225	GLN
1	J	311	ASN
1	J	462	GLN
1	J	477	GLN
1	J	597	HIS

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Mol	Chain	Res	Type
1	J	609	ASN
1	N	104	ASN
1	N	146	HIS
1	N	150	ASN
1	N	181	GLN
1	N	186	HIS
1	N	201	ASN
1	N	225	GLN
1	N	248	GLN
1	N	261	GLN
1	N	311	ASN
1	N	373	GLN
1	N	477	GLN
1	N	493	GLN
1	N	517	HIS
1	N	523	ASN
2	C	62	ASN
2	C	64	ASN
2	D	36	GLN
2	D	62	ASN
2	D	64	ASN
2	G	36	GLN
2	G	62	ASN
2	G	64	ASN
2	H	62	ASN
2	H	64	ASN
2	K	36	GLN
2	K	62	ASN
2	K	64	ASN
2	L	36	GLN
2	L	62	ASN
2	L	64	ASN
2	L	124	ASN
2	O	36	GLN
2	O	62	ASN
2	O	64	ASN
2	P	36	GLN
2	P	64	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

88 carbohydrates 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	$\#\|Z\| > 2$
3	NAG	A	801	1,3	14,14,15	0.76	0	15,19,21	1.12	1 (6%)
3	NAG	A	802	3	14,14,15	0.75	0	15,19,21	1.80	3 (20%)
3	BMA	A	803	3	11,11,12	1.02	0	14,15,17	1.30	1 (7%)
4	NAG	A	901	1,4	14,14,15	0.49	0	15,19,21	1.16	1 (6%)
4	NAG	A	902	4	14,14,15	0.64	0	15,19,21	1.00	1 (6%)
4	BMA	A	903	4	11,11,12	0.77	0	14,15,17	1.63	2 (14%)
4	MAN	A	904	4	11,11,12	0.72	0	14,15,17	1.26	3 (21%)
4	MAN	A	905	4	11,11,12	0.64	0	14,15,17	2.22	4 (28%)
4	MAN	A	906	4	11,11,12	0.75	0	14,15,17	1.06	0
4	MAN	A	907	4	11,11,12	0.84	0	14,15,17	2.36	6 (42%)
4	MAN	A	908	4	11,11,12	0.79	0	14,15,17	3.13	5 (35%)
3	NAG	B	801	1,3	14,14,15	1.09	2 (14%)	15,19,21	1.16	2 (13%)
3	NAG	B	802	3	14,14,15	0.84	0	15,19,21	1.51	3 (20%)
3	BMA	B	803	3	11,11,12	0.89	0	14,15,17	1.24	2 (14%)
4	NAG	B	901	1,4	14,14,15	0.91	2 (14%)	15,19,21	1.13	1 (6%)
4	NAG	B	902	4	14,14,15	1.06	1 (7%)	15,19,21	1.12	2 (13%)
4	BMA	B	903	4	11,11,12	0.64	0	14,15,17	1.61	3 (21%)
4	MAN	B	904	4	11,11,12	1.05	1 (9%)	14,15,17	1.48	2 (14%)
4	MAN	B	905	4	11,11,12	1.22	1 (9%)	14,15,17	2.34	4 (28%)
4	MAN	B	906	4	11,11,12	1.21	1 (9%)	14,15,17	1.60	3 (21%)
4	MAN	B	907	4	11,11,12	0.75	0	14,15,17	2.14	7 (50%)
4	MAN	B	908	4	11,11,12	1.05	1 (9%)	14,15,17	2.67	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	801	1,3	14,14,15	0.76	0	15,19,21	0.89	1 (6%)
3	NAG	E	802	3	14,14,15	0.76	0	15,19,21	1.73	4 (26%)
3	BMA	E	803	3	11,11,12	1.34	0	14,15,17	1.30	2 (14%)
4	NAG	E	901	1,4	14,14,15	0.56	0	15,19,21	0.73	0
4	NAG	E	902	4	14,14,15	0.88	0	15,19,21	1.01	0
4	BMA	E	903	4	11,11,12	1.18	2 (18%)	14,15,17	1.33	2 (14%)
4	MAN	E	904	4	11,11,12	0.55	0	14,15,17	1.04	1 (7%)
4	MAN	E	905	4	11,11,12	0.67	0	14,15,17	2.55	4 (28%)
4	MAN	E	906	4	11,11,12	0.87	0	14,15,17	1.36	2 (14%)
4	MAN	E	907	4	11,11,12	0.87	0	14,15,17	2.31	7 (50%)
4	MAN	E	908	4	11,11,12	0.64	0	14,15,17	2.86	7 (50%)
3	NAG	F	801	1,3	14,14,15	0.58	0	15,19,21	1.24	2 (13%)
3	NAG	F	802	3	14,14,15	0.59	0	15,19,21	2.29	4 (26%)
3	BMA	F	803	3	11,11,12	1.09	0	14,15,17	1.15	1 (7%)
4	NAG	F	901	1,4	14,14,15	0.50	0	15,19,21	0.64	0
4	NAG	F	902	4	14,14,15	0.64	0	15,19,21	0.99	1 (6%)
4	BMA	F	903	4	11,11,12	0.82	0	14,15,17	1.29	2 (14%)
4	MAN	F	904	4	11,11,12	0.52	0	14,15,17	1.09	1 (7%)
4	MAN	F	905	4	11,11,12	0.89	0	14,15,17	2.32	4 (28%)
4	MAN	F	906	4	11,11,12	0.78	0	14,15,17	1.22	1 (7%)
4	MAN	F	907	4	11,11,12	0.93	0	14,15,17	2.43	8 (57%)
4	MAN	F	908	4	11,11,12	0.81	0	14,15,17	2.93	6 (42%)
3	NAG	I	801	3	14,14,15	0.74	0	15,19,21	1.17	2 (13%)
3	NAG	I	802	3	14,14,15	0.44	0	15,19,21	2.03	3 (20%)
3	BMA	I	803	3	11,11,12	1.25	1 (9%)	14,15,17	0.98	1 (7%)
4	NAG	I	901	1,4	14,14,15	0.69	0	15,19,21	0.93	1 (6%)
4	NAG	I	902	4	14,14,15	0.66	0	15,19,21	1.06	0
4	BMA	I	903	4	11,11,12	1.16	1 (9%)	14,15,17	1.40	2 (14%)
4	MAN	I	904	4	11,11,12	0.61	0	14,15,17	1.31	2 (14%)
4	MAN	I	905	4	11,11,12	0.87	1 (9%)	14,15,17	2.67	6 (42%)
4	MAN	I	906	4	11,11,12	0.80	0	14,15,17	1.34	3 (21%)
4	MAN	I	907	4	11,11,12	0.62	0	14,15,17	2.12	6 (42%)
4	MAN	I	908	4	11,11,12	0.73	0	14,15,17	2.77	5 (35%)
3	NAG	J	801	1,3	14,14,15	0.71	0	15,19,21	1.44	1 (6%)
3	NAG	J	802	3	14,14,15	0.57	0	15,19,21	2.00	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	J	803	3	11,11,12	1.07	0	14,15,17	1.21	2 (14%)
4	NAG	J	901	1,4	14,14,15	0.35	0	15,19,21	1.00	0
4	NAG	J	902	4	14,14,15	0.81	0	15,19,21	0.98	1 (6%)
4	BMA	J	903	4	11,11,12	0.83	0	14,15,17	1.42	2 (14%)
4	MAN	J	904	4	11,11,12	0.63	0	14,15,17	0.99	1 (7%)
4	MAN	J	905	4	11,11,12	0.94	0	14,15,17	2.31	5 (35%)
4	MAN	J	906	4	11,11,12	0.84	0	14,15,17	1.28	2 (14%)
4	MAN	J	907	4	11,11,12	0.86	0	14,15,17	1.97	4 (28%)
4	MAN	J	908	4	11,11,12	0.65	0	14,15,17	2.91	6 (42%)
3	NAG	M	801	1,3	14,14,15	0.82	1 (7%)	15,19,21	1.10	2 (13%)
3	NAG	M	802	3	14,14,15	0.79	0	15,19,21	1.52	3 (20%)
3	BMA	M	803	3	11,11,12	1.01	1 (9%)	14,15,17	1.20	1 (7%)
4	NAG	M	901	1,4	14,14,15	0.53	0	15,19,21	1.25	1 (6%)
4	NAG	M	902	4	14,14,15	0.77	0	15,19,21	1.03	2 (13%)
4	BMA	M	903	4	11,11,12	0.80	0	14,15,17	1.32	1 (7%)
4	MAN	M	904	4	11,11,12	0.85	0	14,15,17	0.94	0
4	MAN	M	905	4	11,11,12	0.64	0	14,15,17	2.17	4 (28%)
4	MAN	M	906	4	11,11,12	0.61	0	14,15,17	1.06	1 (7%)
4	MAN	M	907	4	11,11,12	0.86	0	14,15,17	2.11	6 (42%)
4	MAN	M	908	4	11,11,12	0.75	0	14,15,17	2.82	5 (35%)
3	NAG	N	801	1,3	14,14,15	0.82	0	15,19,21	1.15	2 (13%)
3	NAG	N	802	3	14,14,15	0.74	0	15,19,21	1.47	4 (26%)
3	BMA	N	803	3	11,11,12	1.06	0	14,15,17	1.13	1 (7%)
4	NAG	N	901	1,4	14,14,15	0.69	0	15,19,21	1.31	2 (13%)
4	NAG	N	902	4	14,14,15	0.85	1 (7%)	15,19,21	1.08	1 (6%)
4	BMA	N	903	4	11,11,12	0.74	0	14,15,17	1.49	2 (14%)
4	MAN	N	904	4	11,11,12	0.75	0	14,15,17	1.20	1 (7%)
4	MAN	N	905	4	11,11,12	0.96	0	14,15,17	2.26	2 (14%)
4	MAN	N	906	4	11,11,12	1.05	1 (9%)	14,15,17	1.44	1 (7%)
4	MAN	N	907	4	11,11,12	0.67	0	14,15,17	2.20	7 (50%)
4	MAN	N	908	4	11,11,12	0.98	0	14,15,17	2.96	5 (35%)

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
3	NAG	A	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	802	3	-	0/6/23/26	0/1/1/1
3	BMA	A	803	3	-	0/2/19/22	0/1/1/1
4	NAG	A	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	902	4	-	0/6/23/26	0/1/1/1
4	BMA	A	903	4	-	0/2/19/22	0/1/1/1
4	MAN	A	904	4	-	0/2/19/22	0/1/1/1
4	MAN	A	905	4	-	0/2/19/22	0/1/1/1
4	MAN	A	906	4	-	0/2/19/22	0/1/1/1
4	MAN	A	907	4	-	0/2/19/22	0/1/1/1
4	MAN	A	908	4	-	0/2/19/22	1/1/1/1
3	NAG	B	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	802	3	-	0/6/23/26	0/1/1/1
3	BMA	B	803	3	-	0/2/19/22	0/1/1/1
4	NAG	B	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	902	4	-	0/6/23/26	0/1/1/1
4	BMA	B	903	4	-	0/2/19/22	0/1/1/1
4	MAN	B	904	4	-	0/2/19/22	0/1/1/1
4	MAN	B	905	4	-	0/2/19/22	0/1/1/1
4	MAN	B	906	4	-	0/2/19/22	0/1/1/1
4	MAN	B	907	4	-	0/2/19/22	0/1/1/1
4	MAN	B	908	4	-	0/2/19/22	1/1/1/1
3	NAG	E	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	802	3	-	0/6/23/26	0/1/1/1
3	BMA	E	803	3	-	0/2/19/22	0/1/1/1
4	NAG	E	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	902	4	-	0/6/23/26	0/1/1/1
4	BMA	E	903	4	-	0/2/19/22	0/1/1/1
4	MAN	E	904	4	-	0/2/19/22	0/1/1/1
4	MAN	E	905	4	-	0/2/19/22	0/1/1/1
4	MAN	E	906	4	-	0/2/19/22	0/1/1/1
4	MAN	E	907	4	-	0/2/19/22	0/1/1/1
4	MAN	E	908	4	-	0/2/19/22	1/1/1/1
3	NAG	F	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	802	3	-	0/6/23/26	0/1/1/1
3	BMA	F	803	3	-	0/2/19/22	0/1/1/1
4	NAG	F	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	902	4	-	0/6/23/26	0/1/1/1
4	BMA	F	903	4	-	0/2/19/22	0/1/1/1
4	MAN	F	904	4	-	0/2/19/22	0/1/1/1
4	MAN	F	905	4	-	0/2/19/22	0/1/1/1
4	MAN	F	906	4	-	0/2/19/22	0/1/1/1
4	MAN	F	907	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	908	4	-	0/2/19/22	1/1/1/1
3	NAG	I	801	3	-	0/6/23/26	0/1/1/1
3	NAG	I	802	3	-	0/6/23/26	0/1/1/1
3	BMA	I	803	3	-	0/2/19/22	0/1/1/1
4	NAG	I	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	902	4	-	0/6/23/26	0/1/1/1
4	BMA	I	903	4	-	0/2/19/22	0/1/1/1
4	MAN	I	904	4	-	0/2/19/22	0/1/1/1
4	MAN	I	905	4	-	0/2/19/22	0/1/1/1
4	MAN	I	906	4	-	0/2/19/22	0/1/1/1
4	MAN	I	907	4	-	0/2/19/22	0/1/1/1
4	MAN	I	908	4	-	0/2/19/22	1/1/1/1
3	NAG	J	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	802	3	-	0/6/23/26	0/1/1/1
3	BMA	J	803	3	-	0/2/19/22	0/1/1/1
4	NAG	J	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	902	4	-	0/6/23/26	0/1/1/1
4	BMA	J	903	4	-	0/2/19/22	0/1/1/1
4	MAN	J	904	4	-	0/2/19/22	0/1/1/1
4	MAN	J	905	4	-	0/2/19/22	0/1/1/1
4	MAN	J	906	4	-	0/2/19/22	0/1/1/1
4	MAN	J	907	4	-	0/2/19/22	0/1/1/1
4	MAN	J	908	4	-	0/2/19/22	1/1/1/1
3	NAG	M	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	802	3	-	0/6/23/26	0/1/1/1
3	BMA	M	803	3	-	0/2/19/22	0/1/1/1
4	NAG	M	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	902	4	-	0/6/23/26	0/1/1/1
4	BMA	M	903	4	-	0/2/19/22	0/1/1/1
4	MAN	M	904	4	-	0/2/19/22	0/1/1/1
4	MAN	M	905	4	-	0/2/19/22	0/1/1/1
4	MAN	M	906	4	-	0/2/19/22	0/1/1/1
4	MAN	M	907	4	-	0/2/19/22	0/1/1/1
4	MAN	M	908	4	-	0/2/19/22	1/1/1/1
3	NAG	N	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	802	3	-	0/6/23/26	0/1/1/1
3	BMA	N	803	3	-	0/2/19/22	0/1/1/1
4	NAG	N	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	902	4	-	0/6/23/26	0/1/1/1
4	BMA	N	903	4	-	0/2/19/22	0/1/1/1
4	MAN	N	904	4	-	0/2/19/22	0/1/1/1
4	MAN	N	905	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	N	906	4	-	0/2/19/22	0/1/1/1
4	MAN	N	907	4	-	0/2/19/22	0/1/1/1
4	MAN	N	908	4	-	0/2/19/22	1/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	906	MAN	O5-C5	-2.77	1.37	1.43
4	B	902	NAG	O5-C1	-2.67	1.39	1.43
3	B	801	NAG	O5-C1	-2.58	1.39	1.43
4	B	904	MAN	O5-C1	-2.57	1.39	1.43
3	B	801	NAG	O5-C5	-2.56	1.37	1.43
4	N	902	NAG	O5-C1	-2.51	1.39	1.43
4	B	906	MAN	O5-C5	-2.33	1.38	1.43
4	B	908	MAN	O2-C2	-2.21	1.38	1.43
4	B	905	MAN	O4-C4	-2.21	1.37	1.43
4	B	901	NAG	O5-C5	-2.20	1.38	1.43
4	B	901	NAG	O5-C1	-2.02	1.40	1.43
4	E	903	BMA	C1-C2	2.02	1.57	1.52
4	I	903	BMA	C1-C2	2.04	1.57	1.52
3	M	801	NAG	C1-C2	2.04	1.55	1.52
3	I	803	BMA	O3-C3	2.05	1.47	1.43
3	M	803	BMA	O3-C3	2.05	1.47	1.43
4	I	905	MAN	C1-C2	2.14	1.57	1.52
4	E	903	BMA	O5-C1	2.16	1.47	1.43

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	802	NAG	C1-O5-C5	-6.82	103.59	112.25
4	M	908	MAN	C1-O5-C5	-6.28	104.28	112.25
4	A	908	MAN	C1-O5-C5	-5.93	104.73	112.25
4	J	908	MAN	C1-O5-C5	-5.82	104.86	112.25
4	N	908	MAN	O2-C2-C3	-5.75	98.56	110.12
4	I	908	MAN	C2-C3-C4	-5.59	101.54	111.04
3	J	802	NAG	C1-O5-C5	-5.57	105.18	112.25
4	E	908	MAN	C2-C3-C4	-5.54	101.64	111.04
4	E	908	MAN	C1-O5-C5	-5.30	105.52	112.25
4	I	908	MAN	C1-O5-C5	-5.27	105.56	112.25
4	A	908	MAN	C2-C3-C4	-5.13	102.33	111.04
4	F	908	MAN	O5-C1-C2	-5.10	102.58	110.86
4	F	908	MAN	C1-O5-C5	-5.09	105.78	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	908	MAN	C2-C3-C4	-5.06	102.44	111.04
4	N	908	MAN	C1-O5-C5	-5.04	105.86	112.25
3	I	802	NAG	C1-O5-C5	-5.00	105.91	112.25
3	A	802	NAG	C1-O5-C5	-4.90	106.02	112.25
4	M	908	MAN	C2-C3-C4	-4.90	102.72	111.04
4	F	908	MAN	C2-C3-C4	-4.88	102.75	111.04
4	A	908	MAN	O5-C1-C2	-4.73	103.18	110.86
4	J	908	MAN	O5-C1-C2	-4.73	103.18	110.86
4	J	908	MAN	C2-C3-C4	-4.72	103.02	111.04
4	N	908	MAN	C2-C3-C4	-4.64	103.16	111.04
4	A	908	MAN	C3-C4-C5	-4.52	102.32	110.20
4	N	908	MAN	O5-C1-C2	-4.48	103.59	110.86
4	B	908	MAN	C1-O5-C5	-4.48	106.57	112.25
3	I	802	NAG	C2-N2-C7	-4.39	117.41	123.04
4	J	908	MAN	C3-C4-C5	-4.38	102.56	110.20
4	A	908	MAN	O2-C2-C3	-4.20	101.68	110.12
4	F	908	MAN	C3-C4-C5	-4.19	102.90	110.20
4	E	908	MAN	O5-C1-C2	-4.11	104.20	110.86
4	B	908	MAN	C3-C4-C5	-4.05	103.13	110.20
4	F	908	MAN	O2-C2-C3	-4.04	102.00	110.12
4	M	908	MAN	O5-C1-C2	-4.02	104.33	110.86
4	A	907	MAN	C1-O5-C5	-4.01	107.17	112.25
4	E	907	MAN	C1-O5-C5	-3.98	107.20	112.25
4	I	908	MAN	O2-C2-C3	-3.97	102.13	110.12
4	E	905	MAN	O2-C2-C3	-3.96	102.15	110.12
4	E	908	MAN	C3-C4-C5	-3.93	103.35	110.20
4	F	907	MAN	O3-C3-C2	-3.91	102.93	110.00
4	N	908	MAN	C3-C4-C5	-3.89	103.42	110.20
4	N	905	MAN	O2-C2-C3	-3.88	102.32	110.12
3	M	802	NAG	C1-O5-C5	-3.79	107.44	112.25
4	B	908	MAN	O2-C2-C3	-3.77	102.54	110.12
4	I	907	MAN	C1-O5-C5	-3.71	107.54	112.25
4	I	905	MAN	O2-C2-C3	-3.65	102.78	110.12
4	M	908	MAN	C3-C4-C5	-3.61	103.90	110.20
4	F	905	MAN	O2-C2-C3	-3.56	102.95	110.12
4	M	905	MAN	O2-C2-C3	-3.53	103.02	110.12
3	E	802	NAG	C2-N2-C7	-3.50	118.54	123.04
4	B	906	MAN	O5-C1-C2	-3.50	105.17	110.86
3	E	802	NAG	C1-O5-C5	-3.48	107.83	112.25
4	A	907	MAN	O3-C3-C2	-3.43	103.81	110.00
4	N	906	MAN	C1-C2-C3	-3.42	105.50	109.54
3	F	802	NAG	C2-N2-C7	-3.35	118.73	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	905	MAN	O2-C2-C3	-3.35	103.38	110.12
4	I	908	MAN	C3-C4-C5	-3.34	104.37	110.20
4	F	905	MAN	C2-C3-C4	-3.32	105.41	111.04
4	B	908	MAN	O5-C1-C2	-3.27	105.55	110.86
4	M	906	MAN	O5-C1-C2	-3.26	105.56	110.86
4	B	903	BMA	O2-C2-C3	-3.21	103.66	110.12
4	N	903	BMA	O2-C2-C3	-3.14	103.79	110.12
4	A	903	BMA	O2-C2-C3	-3.14	103.81	110.12
4	B	907	MAN	C1-O5-C5	-3.11	108.30	112.25
4	B	906	MAN	C1-C2-C3	-3.10	105.88	109.54
4	M	908	MAN	O2-C2-C3	-3.10	103.89	110.12
4	N	907	MAN	O3-C3-C4	-3.07	103.42	110.34
3	B	802	NAG	C2-N2-C7	-3.03	119.14	123.04
4	J	905	MAN	C3-C4-C5	-3.03	104.92	110.20
3	F	801	NAG	O4-C4-C5	-2.99	101.33	109.24
4	B	905	MAN	O2-C2-C3	-2.98	104.12	110.12
4	B	907	MAN	O3-C3-C2	-2.98	104.61	110.00
4	J	908	MAN	O2-C2-C3	-2.94	104.20	110.12
4	M	907	MAN	O3-C3-C4	-2.93	103.73	110.34
4	F	906	MAN	C1-C2-C3	-2.91	106.09	109.54
3	N	802	NAG	C1-O5-C5	-2.91	108.55	112.25
4	I	908	MAN	O5-C1-C2	-2.90	106.16	110.86
4	F	907	MAN	O2-C2-C3	-2.86	104.36	110.12
4	M	907	MAN	C1-O5-C5	-2.86	108.62	112.25
3	J	801	NAG	O4-C4-C5	-2.82	101.76	109.24
4	B	907	MAN	O5-C1-C2	-2.81	106.29	110.86
4	I	906	MAN	O5-C1-C2	-2.80	106.32	110.86
4	I	905	MAN	O3-C3-C4	-2.79	104.05	110.34
4	J	906	MAN	O5-C1-C2	-2.77	106.37	110.86
4	E	906	MAN	O5-C1-C2	-2.77	106.37	110.86
3	J	802	NAG	C2-N2-C7	-2.76	119.50	123.04
4	N	901	NAG	O7-C7-C8	-2.74	117.03	122.06
3	B	802	NAG	O4-C4-C3	-2.72	104.22	110.34
3	M	801	NAG	O4-C4-C5	-2.69	102.10	109.24
4	J	903	BMA	O2-C2-C3	-2.68	104.72	110.12
4	N	907	MAN	C1-O5-C5	-2.66	108.87	112.25
4	A	905	MAN	C1-C2-C3	-2.66	106.39	109.54
3	N	802	NAG	C2-N2-C7	-2.66	119.62	123.04
4	B	902	NAG	O7-C7-C8	-2.65	117.19	122.06
4	J	905	MAN	O2-C2-C3	-2.65	104.80	110.12
3	A	801	NAG	O4-C4-C5	-2.54	102.51	109.24
3	A	802	NAG	C2-N2-C7	-2.54	119.78	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	905	MAN	C1-C2-C3	-2.51	106.58	109.54
4	F	907	MAN	C1-O5-C5	-2.50	109.08	112.25
4	J	905	MAN	O3-C3-C4	-2.46	104.81	110.34
4	E	905	MAN	C1-C2-C3	-2.45	106.64	109.54
4	E	908	MAN	O2-C2-C3	-2.44	105.20	110.12
4	N	907	MAN	O5-C1-C2	-2.44	106.89	110.86
4	J	907	MAN	O3-C3-C2	-2.42	105.63	110.00
4	I	905	MAN	C1-C2-C3	-2.42	106.68	109.54
3	M	802	NAG	C2-N2-C7	-2.40	119.95	123.04
3	B	801	NAG	O4-C4-C5	-2.38	102.93	109.24
4	I	903	BMA	O2-C2-C3	-2.38	105.34	110.12
3	E	802	NAG	O4-C4-C3	-2.36	105.01	110.34
3	N	801	NAG	O4-C4-C5	-2.36	103.00	109.24
4	J	906	MAN	C1-C2-C3	-2.35	106.76	109.54
4	B	906	MAN	O4-C4-C3	-2.35	105.05	110.34
4	F	908	MAN	O6-C6-C5	-2.32	103.66	111.33
4	B	905	MAN	C2-C3-C4	-2.29	107.14	111.04
4	I	904	MAN	O2-C2-C1	-2.27	104.66	109.21
4	F	905	MAN	C1-O5-C5	-2.26	109.38	112.25
4	I	907	MAN	O3-C3-C2	-2.26	105.92	110.00
4	F	903	BMA	O2-C2-C3	-2.24	105.62	110.12
4	F	907	MAN	O5-C1-C2	-2.18	107.31	110.86
4	J	908	MAN	O2-C2-C1	-2.17	104.86	109.21
3	M	801	NAG	O7-C7-C8	-2.16	118.10	122.06
4	I	906	MAN	C1-C2-C3	-2.16	106.99	109.54
3	N	802	NAG	O4-C4-C3	-2.16	105.48	110.34
4	J	905	MAN	C1-C2-C3	-2.13	107.03	109.54
4	E	906	MAN	C1-C2-C3	-2.12	107.03	109.54
4	B	908	MAN	O6-C6-C5	-2.12	104.34	111.33
4	M	902	NAG	O7-C7-C8	-2.11	118.19	122.06
4	M	905	MAN	C3-C4-C5	-2.10	106.53	110.20
4	I	905	MAN	C3-C4-C5	-2.09	106.55	110.20
3	E	801	NAG	O4-C4-C5	-2.09	103.70	109.24
4	E	907	MAN	O3-C3-C2	-2.08	106.24	110.00
4	E	907	MAN	O5-C1-C2	-2.06	107.52	110.86
3	I	801	NAG	O4-C4-C5	-2.06	103.79	109.24
4	E	905	MAN	O3-C3-C2	-2.04	106.31	110.00
3	F	802	NAG	O4-C4-C3	-2.01	105.81	110.34
4	E	903	BMA	O2-C2-C3	-2.01	106.08	110.12
3	J	803	BMA	C1-O5-C5	-2.00	109.71	112.25
4	E	908	MAN	O4-C4-C5	2.01	114.55	109.24
4	M	902	NAG	C4-C3-C2	2.03	114.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	801	NAG	O3-C3-C2	2.03	113.14	109.11
3	J	802	NAG	O3-C3-C4	2.04	114.94	110.34
4	I	905	MAN	O5-C1-C2	2.08	114.23	110.86
3	E	803	BMA	C3-C4-C5	2.09	113.83	110.20
4	N	902	NAG	C4-C3-C2	2.10	114.49	111.23
4	B	901	NAG	C2-N2-C7	2.10	125.74	123.04
3	F	803	BMA	C3-C4-C5	2.13	113.91	110.20
4	B	904	MAN	O5-C5-C6	2.13	111.97	107.35
4	I	901	NAG	O4-C4-C3	2.13	115.14	110.34
4	I	907	MAN	O2-C2-C1	2.14	113.50	109.21
3	I	803	BMA	C3-C4-C5	2.15	113.94	110.20
4	A	904	MAN	O5-C5-C6	2.16	112.02	107.35
3	N	801	NAG	O3-C3-C2	2.16	113.40	109.11
4	F	904	MAN	C1-O5-C5	2.18	115.01	112.25
3	M	803	BMA	C3-C4-C5	2.18	114.00	110.20
3	J	803	BMA	C3-C4-C5	2.18	114.00	110.20
4	J	902	NAG	C4-C3-C2	2.19	114.63	111.23
4	E	904	MAN	C1-O5-C5	2.20	115.03	112.25
4	J	904	MAN	C1-O5-C5	2.20	115.04	112.25
4	N	907	MAN	C3-C4-C5	2.20	114.04	110.20
4	M	905	MAN	O5-C1-C2	2.21	114.44	110.86
3	B	803	BMA	O2-C2-C1	2.21	113.63	109.21
4	A	901	NAG	O5-C5-C6	2.21	112.13	107.35
3	N	803	BMA	C3-C4-C5	2.21	114.05	110.20
4	I	904	MAN	O3-C3-C2	2.22	114.01	110.00
4	B	902	NAG	C4-C3-C2	2.24	114.72	111.23
4	A	904	MAN	C1-O5-C5	2.27	115.12	112.25
4	I	906	MAN	O2-C2-C1	2.31	113.84	109.21
4	B	907	MAN	O2-C2-C1	2.33	113.89	109.21
4	I	907	MAN	C3-C4-C5	2.37	114.33	110.20
4	E	908	MAN	O3-C3-C2	2.40	114.33	110.00
4	M	907	MAN	O5-C5-C6	2.41	112.57	107.35
4	M	907	MAN	C3-C4-C5	2.41	114.40	110.20
4	N	904	MAN	C1-O5-C5	2.42	115.32	112.25
4	J	907	MAN	O5-C5-C6	2.47	112.70	107.35
4	F	907	MAN	C1-C2-C3	2.48	112.48	109.54
4	J	907	MAN	O2-C2-C1	2.51	114.24	109.21
4	A	905	MAN	O5-C1-C2	2.52	114.94	110.86
4	B	907	MAN	O5-C5-C6	2.52	112.80	107.35
4	M	901	NAG	O4-C4-C3	2.52	116.01	110.34
4	N	907	MAN	O2-C2-C1	2.53	114.28	109.21
3	I	802	NAG	O5-C5-C6	2.53	112.83	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	802	NAG	O5-C5-C6	2.54	112.84	107.35
4	A	907	MAN	O5-C5-C6	2.55	112.87	107.35
4	A	904	MAN	C1-C2-C3	2.57	112.58	109.54
4	E	907	MAN	O5-C5-C6	2.57	112.92	107.35
4	A	902	NAG	C4-C3-C2	2.60	115.27	111.23
4	N	907	MAN	O5-C5-C6	2.60	112.97	107.35
4	M	907	MAN	O2-C2-C1	2.60	114.42	109.21
4	N	901	NAG	O7-C7-N2	2.62	127.21	121.86
3	E	803	BMA	O2-C2-C1	2.64	114.50	109.21
3	N	802	NAG	O5-C5-C6	2.69	113.16	107.35
4	B	907	MAN	C3-C4-C5	2.69	114.89	110.20
3	A	803	BMA	O3-C3-C4	2.71	116.44	110.34
4	F	902	NAG	C4-C3-C2	2.72	115.45	111.23
4	B	903	BMA	C1-O5-C5	2.72	115.70	112.25
3	B	803	BMA	C3-C4-C5	2.72	114.94	110.20
3	I	801	NAG	O5-C5-C6	2.77	113.34	107.35
3	J	802	NAG	O5-C5-C6	2.79	113.38	107.35
4	I	907	MAN	O5-C5-C6	2.80	113.40	107.35
4	A	907	MAN	C3-C4-C5	2.80	115.08	110.20
3	E	802	NAG	O5-C5-C6	2.84	113.49	107.35
4	F	907	MAN	C3-C4-C5	2.84	115.14	110.20
3	A	802	NAG	O5-C5-C6	2.95	113.72	107.35
4	E	907	MAN	C3-C4-C5	3.17	115.72	110.20
3	F	802	NAG	O5-C5-C6	3.21	114.30	107.35
3	B	802	NAG	O5-C5-C6	3.26	114.41	107.35
4	E	907	MAN	O2-C2-C1	3.28	115.77	109.21
4	F	907	MAN	O2-C2-C1	3.31	115.83	109.21
4	B	907	MAN	C2-C3-C4	3.31	116.66	111.04
4	A	907	MAN	C2-C3-C4	3.50	116.99	111.04
3	B	801	NAG	C1-O5-C5	3.54	116.74	112.25
4	I	907	MAN	C2-C3-C4	3.55	117.06	111.04
4	E	907	MAN	C2-C3-C4	3.55	117.07	111.04
4	B	903	BMA	C1-C2-C3	3.55	113.74	109.54
4	J	903	BMA	C1-C2-C3	3.55	113.75	109.54
4	F	903	BMA	C1-C2-C3	3.59	113.78	109.54
4	I	903	BMA	C1-C2-C3	3.65	113.86	109.54
4	F	907	MAN	C2-C3-C4	3.72	117.36	111.04
4	A	907	MAN	O2-C2-C1	3.78	116.78	109.21
4	N	903	BMA	C1-C2-C3	4.00	114.28	109.54
4	M	903	BMA	C1-C2-C3	4.01	114.29	109.54
4	M	907	MAN	C2-C3-C4	4.04	117.90	111.04
4	E	903	BMA	C1-C2-C3	4.05	114.33	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	907	MAN	C2-C3-C4	4.11	118.02	111.04
4	A	903	BMA	C1-C2-C3	4.22	114.54	109.54
4	J	907	MAN	C2-C3-C4	4.58	118.83	111.04
4	B	904	MAN	C1-O5-C5	4.63	118.13	112.25
4	M	905	MAN	O2-C2-C1	5.86	120.96	109.21
4	J	905	MAN	O2-C2-C1	6.09	121.42	109.21
4	F	905	MAN	O2-C2-C1	6.14	121.52	109.21
4	A	905	MAN	O2-C2-C1	6.22	121.67	109.21
4	N	905	MAN	O2-C2-C1	6.46	122.16	109.21
4	B	905	MAN	O2-C2-C1	6.75	122.75	109.21
4	E	905	MAN	O2-C2-C1	7.40	124.04	109.21
4	I	905	MAN	O2-C2-C1	7.55	124.34	109.21

There are no chirality outliers.

There are no torsion outliers.

All (8) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	908	MAN	C1-C2-C3-C4-C5-O5
4	J	908	MAN	C1-C2-C3-C4-C5-O5
4	A	908	MAN	C1-C2-C3-C4-C5-O5
4	N	908	MAN	C1-C2-C3-C4-C5-O5
4	F	908	MAN	C1-C2-C3-C4-C5-O5
4	E	908	MAN	C1-C2-C3-C4-C5-O5
4	I	908	MAN	C1-C2-C3-C4-C5-O5
4	B	908	MAN	C1-C2-C3-C4-C5-O5

24 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	NAG	1	0
3	B	801	NAG	1	0
3	B	802	NAG	1	0
4	B	901	NAG	1	0
3	E	801	NAG	1	0
4	E	905	MAN	1	0
4	E	908	MAN	1	0
3	F	801	NAG	1	0
3	F	802	NAG	1	0
4	F	901	NAG	2	0
4	F	905	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	908	MAN	1	0
3	I	801	NAG	3	0
4	I	901	NAG	1	0
4	I	905	MAN	1	0
4	I	908	MAN	1	0
3	J	801	NAG	2	0
4	J	901	NAG	1	0
4	J	905	MAN	1	0
4	J	908	MAN	2	0
3	M	801	NAG	1	0
4	M	901	NAG	1	0
3	N	801	NAG	1	0
4	N	901	NAG	1	0

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
5	PGT	D	201	-	30,30,50	0.99	2 (6%)	31,31,56	1.11	4 (12%)
5	PGT	H	201	-	30,30,50	1.08	2 (6%)	31,31,56	1.15	3 (9%)
5	PGT	L	201	-	30,30,50	1.06	3 (10%)	31,31,56	1.04	3 (9%)
5	PGT	P	201	-	30,30,50	1.04	3 (10%)	31,31,56	1.16	3 (9%)

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
5	PGT	D	201	-	-	0/30/30/55	0/0/0/0
5	PGT	H	201	-	-	0/30/30/55	0/0/0/0
5	PGT	L	201	-	-	0/30/30/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGT	P	201	-	-	0/30/30/55	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	201	PGT	C32-C31	2.03	1.56	1.50
5	P	201	PGT	C12-C11	2.05	1.56	1.50
5	L	201	PGT	O3-C11	2.07	1.39	1.33
5	D	201	PGT	C12-C11	2.09	1.56	1.50
5	L	201	PGT	C12-C11	2.12	1.57	1.50
5	P	201	PGT	C32-C31	2.16	1.57	1.50
5	H	201	PGT	C32-C31	2.20	1.57	1.50
5	P	201	PGT	O3-C11	2.20	1.39	1.33
5	H	201	PGT	O3-C11	2.22	1.40	1.33
5	L	201	PGT	C32-C31	2.25	1.57	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	201	PGT	O2-C31-O31	-2.43	117.22	123.49
5	P	201	PGT	O2-C31-O31	-2.39	117.33	123.49
5	H	201	PGT	O2-C31-O31	-2.30	117.55	123.49
5	L	201	PGT	O2-C31-O31	-2.06	118.17	123.49
5	D	201	PGT	O3-C3-C2	2.02	114.52	108.54
5	D	201	PGT	O3-C11-C12	2.66	120.01	111.90
5	L	201	PGT	O3-C11-C12	2.69	120.10	111.90
5	L	201	PGT	O2-C31-C32	2.88	120.67	111.90
5	P	201	PGT	O3-C11-C12	2.96	120.93	111.90
5	H	201	PGT	O2-C31-C32	3.00	121.06	111.90
5	P	201	PGT	O2-C31-C32	3.07	121.25	111.90
5	D	201	PGT	O2-C31-C32	3.10	121.36	111.90
5	H	201	PGT	O3-C11-C12	3.25	121.79	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	PGT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	201	PGT	1	0
5	L	201	PGT	1	0
5	P	201	PGT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	594/612 (97%)	-0.08	10 (1%) 73 70	47, 67, 96, 120	0
1	B	599/612 (97%)	-0.22	3 (0%) 91 90	41, 59, 76, 85	0
1	E	592/612 (96%)	0.10	17 (2%) 55 49	55, 94, 128, 161	0
1	F	599/612 (97%)	-0.03	9 (1%) 76 74	57, 85, 118, 134	0
1	I	397/612 (64%)	0.15	14 (3%) 48 41	55, 94, 136, 151	0
1	J	599/612 (97%)	0.06	18 (3%) 54 47	65, 89, 114, 127	0
1	M	593/612 (96%)	-0.08	7 (1%) 81 78	47, 71, 98, 124	0
1	N	599/612 (97%)	-0.22	4 (0%) 89 88	46, 63, 88, 104	0
2	C	138/147 (93%)	-0.25	1 (0%) 89 88	46, 61, 98, 108	0
2	D	136/147 (92%)	-0.18	2 (1%) 76 74	43, 59, 108, 125	0
2	G	138/147 (93%)	-0.16	1 (0%) 89 88	54, 72, 104, 112	0
2	H	138/147 (93%)	-0.21	1 (0%) 89 88	54, 65, 82, 86	0
2	K	136/147 (92%)	0.17	4 (2%) 55 49	59, 84, 139, 159	0
2	L	138/147 (93%)	-0.16	2 (1%) 78 76	57, 68, 85, 93	0
2	O	138/147 (93%)	-0.28	1 (0%) 89 88	45, 59, 100, 117	0
2	P	135/147 (91%)	-0.03	4 (2%) 54 47	45, 64, 112, 131	0
All	All	5669/6072 (93%)	-0.07	98 (1%) 73 70	41, 74, 116, 161	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	258	THR	5.1
1	E	584	SER	5.0
1	I	311	ASN	5.0
1	E	552	SER	4.9
1	E	583	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	394	ASN	4.1
1	J	273	ASP	4.1
1	A	583	CYS	4.0
1	E	582	THR	4.0
1	M	576	HIS	3.8
2	L	54	GLN	3.8
2	P	32	ASN	3.7
1	J	259	ASP	3.7
1	F	126	PHE	3.7
1	I	319	GLY	3.6
1	I	363	THR	3.6
1	J	275	SER	3.6
1	N	316	GLY	3.6
1	I	332	SER	3.5
1	F	259	ASP	3.5
2	D	34	ASN	3.5
1	M	258	THR	3.5
1	E	483	ASP	3.5
1	J	31	LYS	3.5
1	J	233	LEU	3.4
1	B	319	GLY	3.4
2	P	23	ALA	3.3
1	I	362	GLY	3.3
1	I	342	ALA	3.3
1	E	576	HIS	3.2
1	F	363	THR	3.1
2	C	34	ASN	3.1
1	A	585	ASN	3.0
1	A	258	THR	3.0
2	L	55	CYS	3.0
2	P	31	ARG	3.0
2	H	54	GLN	2.9
2	K	129	GLU	2.9
1	A	582	THR	2.9
2	K	131	PRO	2.8
1	I	260	ASP	2.8
1	A	606	THR	2.7
1	I	356	MET	2.7
1	N	319	GLY	2.7
1	A	576	HIS	2.7
1	J	433	HIS	2.6
1	A	581	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	258	THR	2.6
1	J	346	SER	2.6
1	E	223	ILE	2.6
1	M	583	CYS	2.6
1	E	581	CYS	2.5
1	E	433	HIS	2.5
1	M	584	SER	2.5
1	I	422	LEU	2.5
1	I	272	CYS	2.4
1	J	301	GLN	2.4
1	I	264	THR	2.4
1	J	216	PRO	2.4
1	F	260	ASP	2.4
2	D	55	CYS	2.4
2	K	91	ILE	2.3
1	E	561	HIS	2.3
1	E	302	GLU	2.3
1	E	187	TYR	2.3
1	B	482	GLN	2.3
1	B	316	GLY	2.3
1	A	257	ASP	2.2
1	A	584	SER	2.2
2	O	34	ASN	2.2
1	A	33	GLY	2.2
1	M	612	SER	2.2
1	M	257	ASP	2.2
1	F	244	ASN	2.2
1	N	49	ASP	2.2
1	J	54	THR	2.2
1	E	529	HIS	2.2
1	I	126	PHE	2.2
1	E	509	LEU	2.1
1	I	527	LEU	2.1
1	J	574	LEU	2.1
2	P	34	ASN	2.1
1	J	487	SER	2.1
1	I	400	TYR	2.1
1	J	126	PHE	2.1
1	F	436	ALA	2.1
1	E	246	THR	2.1
1	J	168	GLU	2.1
2	K	36	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	221	SER	2.0
1	J	99	SER	2.0
1	N	275	SER	2.0
1	E	332	SER	2.0
2	G	88	GLY	2.0
1	E	146	HIS	2.0
1	M	585	ASN	2.0
1	F	433	HIS	2.0
1	J	463	HIS	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)

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
4	MAN	M	908	11/12	0.93	0.30	8.13	47,48,53,56	0
4	MAN	I	908	11/12	0.91	0.33	3.39	47,48,53,56	0
4	MAN	A	908	11/12	0.89	0.29	3.17	47,48,53,56	0
4	MAN	F	908	11/12	0.93	0.22	2.23	47,48,53,56	0
4	MAN	J	908	11/12	0.93	0.20	0.59	47,48,53,56	0
4	NAG	M	901	14/15	0.95	0.20	0.53	45,48,51,52	0
4	BMA	A	903	11/12	0.94	0.23	0.41	46,47,48,49	0
4	MAN	B	908	11/12	0.94	0.17	0.12	46,48,53,56	0
4	MAN	E	908	11/12	0.94	0.18	0.08	47,48,53,56	0
4	NAG	N	901	14/15	0.93	0.19	0.00	45,47,51,52	0
4	BMA	J	903	11/12	0.94	0.21	-0.07	46,47,48,49	0
4	BMA	M	903	11/12	0.94	0.20	-0.32	46,47,47,49	0
4	NAG	B	901	14/15	0.97	0.18	-0.35	45,47,51,52	0
4	MAN	N	908	11/12	0.94	0.17	-0.37	47,48,53,56	0
4	BMA	I	903	11/12	0.92	0.21	-0.68	46,47,48,49	0
3	NAG	I	801	14/15	0.92	0.15	-0.88	44,46,50,51	0
3	NAG	E	801	14/15	0.95	0.15	-1.06	44,46,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	M	801	14/15	0.95	0.18	-1.07	44,46,49,51	0
4	NAG	A	901	14/15	0.95	0.17	-1.24	45,47,51,52	0
4	NAG	J	901	14/15	0.93	0.17	-1.35	45,48,51,52	0
4	NAG	E	901	14/15	0.93	0.17	-1.59	45,48,51,52	0
4	BMA	N	903	11/12	0.95	0.13	-1.62	46,46,47,49	0
3	NAG	N	801	14/15	0.97	0.13	-1.80	43,46,49,51	0
3	NAG	J	801	14/15	0.94	0.14	-1.96	43,46,49,51	0
4	NAG	F	901	14/15	0.94	0.15	-2.10	45,48,51,52	0
3	NAG	B	801	14/15	0.96	0.14	-2.56	43,46,49,51	0
4	NAG	I	901	14/15	0.93	0.13	-2.73	45,48,51,52	0
3	NAG	A	801	14/15	0.96	0.13	-2.74	44,46,50,51	0
3	NAG	F	801	14/15	0.96	0.13	-2.80	44,46,50,51	0
4	MAN	N	904	11/12	0.96	0.10	-2.82	46,47,48,48	0
4	MAN	J	904	11/12	0.97	0.10	-3.22	46,47,48,48	0
4	MAN	B	904	11/12	0.95	0.15	-	46,46,48,48	0
4	MAN	I	905	11/12	0.94	0.34	-	46,47,49,50	0
4	MAN	A	905	11/12	0.95	0.22	-	46,47,48,49	0
3	BMA	B	803	11/12	0.88	0.29	-	51,54,56,58	0
4	MAN	B	907	11/12	0.92	0.24	-	51,51,54,55	0
4	MAN	I	907	11/12	0.86	0.35	-	51,51,54,55	0
4	NAG	F	902	14/15	0.97	0.21	-	47,48,50,50	0
4	MAN	B	906	11/12	0.92	0.17	-	47,49,49,52	0
4	NAG	I	902	14/15	0.91	0.26	-	46,48,50,50	0
4	NAG	M	902	14/15	0.91	0.22	-	46,48,50,51	0
4	MAN	F	905	11/12	0.95	0.17	-	46,47,48,49	0
4	NAG	N	902	14/15	0.96	0.17	-	46,47,50,50	0
4	MAN	M	905	11/12	0.97	0.23	-	46,47,48,49	0
4	NAG	A	902	14/15	0.97	0.14	-	47,48,50,50	0
3	BMA	I	803	11/12	0.84	0.38	-	51,54,56,58	0
4	MAN	E	907	11/12	0.92	0.39	-	51,51,54,55	0
3	NAG	N	802	14/15	0.97	0.13	-	47,49,52,56	0
4	MAN	J	906	11/12	0.86	0.21	-	47,49,49,53	0
4	MAN	N	907	11/12	0.91	0.29	-	51,51,54,55	0
4	MAN	E	906	11/12	0.91	0.36	-	47,49,50,52	0
4	NAG	B	902	14/15	0.94	0.18	-	46,48,50,50	0
4	MAN	F	904	11/12	0.96	0.11	-	46,47,48,49	0
3	BMA	A	803	11/12	0.91	0.40	-	51,54,56,58	0
3	NAG	J	802	14/15	0.92	0.23	-	47,50,52,56	0
4	BMA	F	903	11/12	0.94	0.15	-	46,47,48,49	0
4	MAN	I	906	11/12	0.88	0.38	-	47,49,50,52	0
4	BMA	E	903	11/12	0.91	0.25	-	46,47,48,49	0
3	BMA	M	803	11/12	0.89	0.42	-	52,54,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	E	902	14/15	0.88	0.32	-	47,48,50,51	0
4	MAN	E	905	11/12	0.91	0.25	-	47,47,48,50	0
4	MAN	M	907	11/12	0.92	0.34	-	51,51,54,55	0
3	NAG	E	802	14/15	0.90	0.23	-	47,50,53,56	0
4	MAN	M	906	11/12	0.91	0.25	-	47,49,49,52	0
4	MAN	E	904	11/12	0.95	0.18	-	46,47,48,49	0
3	BMA	N	803	11/12	0.85	0.26	-	51,54,56,57	0
3	BMA	F	803	11/12	0.87	0.38	-	51,54,56,58	0
3	BMA	E	803	11/12	0.82	0.40	-	51,54,56,58	0
3	NAG	M	802	14/15	0.93	0.26	-	47,50,52,56	0
4	NAG	J	902	14/15	0.96	0.27	-	47,48,50,50	0
4	MAN	B	905	11/12	0.97	0.16	-	46,47,48,49	0
3	BMA	J	803	11/12	0.87	0.26	-	51,54,56,58	0
3	NAG	I	802	14/15	0.88	0.27	-	48,50,52,56	0
3	NAG	F	802	14/15	0.93	0.23	-	47,50,52,56	0
4	MAN	A	904	11/12	0.96	0.16	-	46,47,48,49	0
4	MAN	N	906	11/12	0.92	0.15	-	47,49,49,52	0
4	MAN	I	904	11/12	0.93	0.28	-	46,47,48,49	0
4	MAN	A	907	11/12	0.89	0.28	-	51,51,54,55	0
4	MAN	J	905	11/12	0.95	0.14	-	46,47,49,49	0
4	BMA	B	903	11/12	0.94	0.15	-	46,46,47,49	0
4	MAN	A	906	11/12	0.92	0.18	-	47,49,50,52	0
4	MAN	J	907	11/12	0.83	0.30	-	51,51,54,55	0
4	MAN	F	907	11/12	0.87	0.24	-	51,51,54,55	0
3	NAG	B	802	14/15	0.96	0.14	-	47,49,52,56	0
4	MAN	M	904	11/12	0.96	0.17	-	46,47,48,49	0
4	MAN	F	906	11/12	0.90	0.18	-	47,49,49,52	0
4	MAN	N	905	11/12	0.97	0.18	-	46,47,48,49	0
3	NAG	A	802	14/15	0.91	0.28	-	47,50,52,56	0

6.4 Ligands

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	PGT	D	201	31/51	0.70	0.39	5.22	71,78,92,93	0
5	PGT	L	201	31/51	0.56	0.47	5.12	71,78,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PGT	H	201	31/51	0.65	0.40	5.00	71,79,92,93	0
5	PGT	P	201	31/51	0.74	0.34	3.39	71,78,92,93	0

6.5 Other polymers (i)

There are no such residues in this entry.