Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 07:56 AM EDT

PDB ID	:	3UNF
Title	:	Mouse 20S immunoproteasome in complex with PR-957
Authors	:	Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on	:	2011-11-15
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

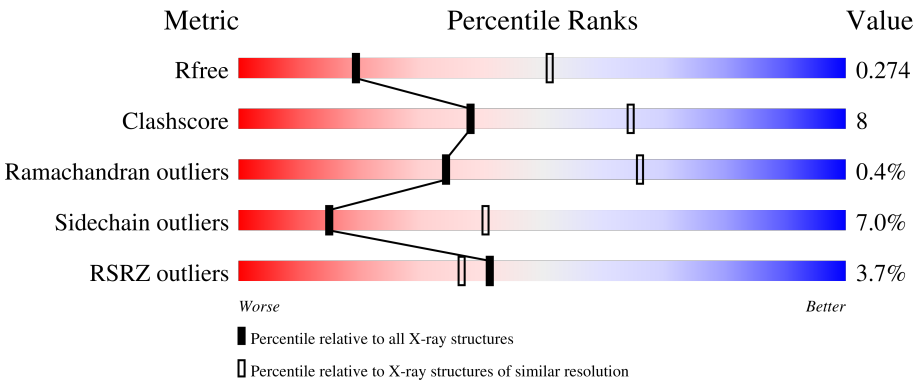
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	234	5% 73% 24% • •
1	O	234	2% 75% 21% • •
2	B	261	6% 75% 18% • 5%
2	P	261	5% 76% 17% • 5%
3	C	248	12% 67% 25% • •

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Mol	Chain	Length	Quality of chain
3	Q	248	11% 68% 25%
4	D	241	7% 80% 16%
4	R	241	5% 80% 16%
5	E	263	4% 76% 13% 10%
5	S	263	3% 76% 13% 10%
6	F	255	2% 77% 18%
6	T	255	4% 77% 17%
7	G	246	5% 80% 16%
7	U	246	7% 79% 18%
8	H	234	3% 70% 21% 6%
8	V	234	3% 68% 22% 6%
9	I	205	2% 72% 25%
9	W	205	% 71% 25%
10	J	201	% 82% 13%
10	X	201	82% 13%
11	K	204	% 69% 25%
11	Y	204	2% 70% 25%
12	L	213	% 83% 16%
12	Z	213	81% 18%
13	M	219	84% 14%
13	a	219	93% 5%
14	N	199	% 81% 16%
14	b	199	94% 6%

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
16	K	L	303	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49805 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1801	1150	308	337	6	0	0	0
1	O	230	1801	1150	308	337	6	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	1950	1232	335	373	10	0	0	0
2	P	248	1950	1232	335	373	10	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	238	1876	1179	331	361	5	0	0	0
3	Q	238	1876	1179	331	361	5	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	233	1778	1116	294	357	11	0	0	0
4	R	233	1778	1116	294	357	11	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	238	1872	1171	336	354	11	0	0	0
5	S	238	1872	1171	336	354	11	0	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	1903	1206	325	361	11	0	0	0
6	T	244	1903	1206	325	361	11	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	243	1890	1199	315	363	13	0	0	0
7	U	243	1890	1199	315	363	13	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	219	1619	1010	294	307	8	0	0	0
8	V	219	1619	1010	294	307	8	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1592	1013	265	295	19	0	0	0
9	W	204	1592	1013	265	295	19	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	196	1570	1006	267	288	9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	196	1570	1006	267	288	9	0	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	201	1566	981	268	302	15	0	0	0
11	Y	201	1566	981	268	302	15	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	213	1654	1047	284	313	10	0	0	0
12	Z	213	1654	1047	284	313	10	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	216	1685	1063	291	319	12	0	0	0
13	a	216	1685	1063	291	319	12	0	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	199	1498	947	254	289	8	0	0	0
14	b	199	1498	947	254	289	8	0	0	0

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
15	A	3	3	3	0	0
15	D	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
15	E	1	1	1	0	0
15	H	1	1	1	0	0
15	I	1	1	1	0	0
15	J	1	1	1	0	0
15	L	2	2	2	0	0
15	M	4	4	4	0	0
15	N	1	1	1	0	0
15	O	2	2	2	0	0
15	P	1	1	1	0	0
15	Q	4	4	4	0	0
15	R	3	3	3	0	0
15	S	2	2	2	0	0
15	U	1	1	1	0	0
15	V	4	4	4	0	0
15	W	1	1	1	0	0
15	X	3	3	3	0	0
15	Z	1	1	1	0	0
15	a	4	4	4	0	0

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
16	B	1	1	1	0	0

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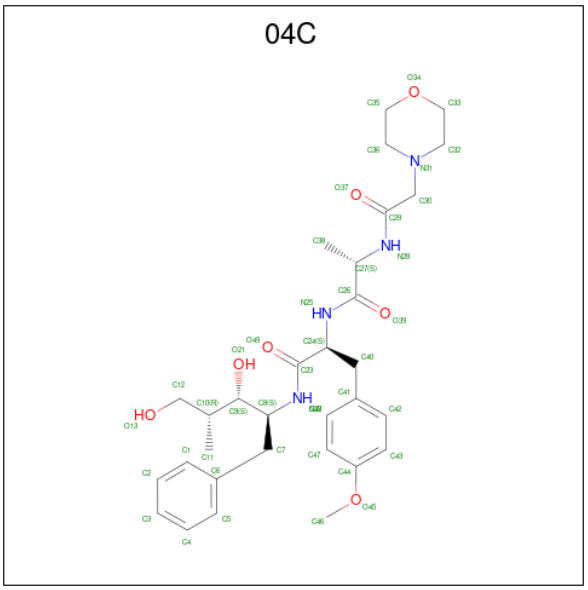
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total K 1 1	0	0
16	I	1	Total K 1 1	0	0
16	K	1	Total K 1 1	0	0
16	L	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0
16	S	1	Total K 1 1	0	0
16	X	1	Total K 1 1	0	0
16	Z	3	Total K 3 3	0	0
16	a	1	Total K 1 1	0	0
16	b	1	Total K 1 1	0	0

- Molecule 17 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: $C_{31}H_{44}N_4O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O 42 31 4 7	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	K	1	42	31	4	7	0	0
17	N	1	42	31	4	7	0	0
17	V	1	42	31	4	7	0	0
17	Y	1	42	31	4	7	0	0
17	b	1	42	31	4	7	0	0

- Molecule 18 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
18	H	1	1	1	0	0
18	K	1	1	1	0	0
18	N	1	1	1	0	0
18	V	1	1	1	0	0
18	Y	1	1	1	0	0
18	b	1	1	1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	43	43	43	0	0
19	B	42	42	42	0	0
19	C	29	29	29	0	0
19	D	24	24	24	0	0
19	E	39	39	39	0	0
19	F	37	37	37	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	G	44	Total O 44 44	0	0
19	H	40	Total O 40 40	0	0
19	I	25	Total O 25 25	0	0
19	J	28	Total O 28 28	0	0
19	K	32	Total O 32 32	0	0
19	L	43	Total O 43 43	0	0
19	M	50	Total O 50 50	0	0
19	N	29	Total O 29 29	0	0
19	O	44	Total O 44 44	0	0
19	P	38	Total O 38 38	0	0
19	Q	13	Total O 13 13	0	0
19	R	24	Total O 24 24	0	0
19	S	40	Total O 40 40	0	0
19	T	32	Total O 32 32	0	0
19	U	38	Total O 38 38	0	0
19	V	39	Total O 39 39	0	0
19	W	39	Total O 39 39	0	0
19	X	20	Total O 20 20	0	0
19	Y	36	Total O 36 36	0	0
19	Z	49	Total O 49 49	0	0
19	a	35	Total O 35 35	0	0

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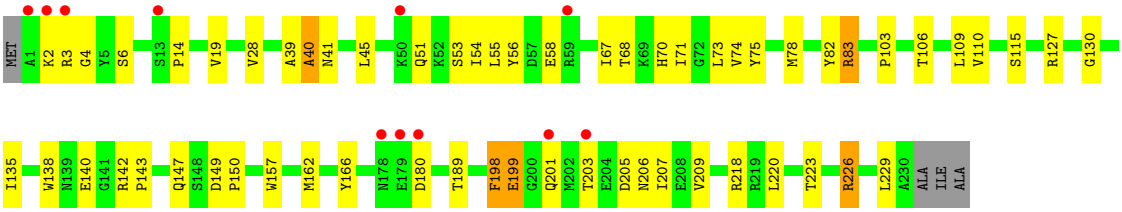
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	b	33	33	33	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

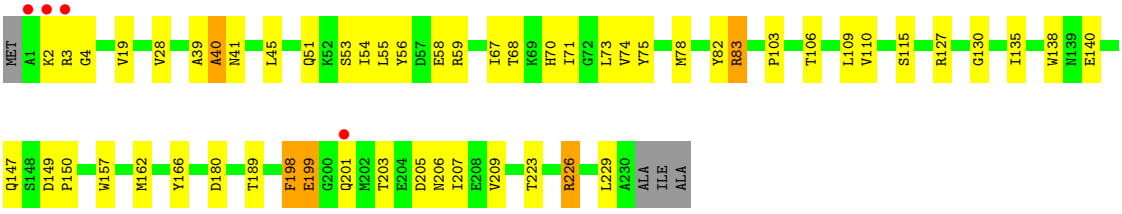
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



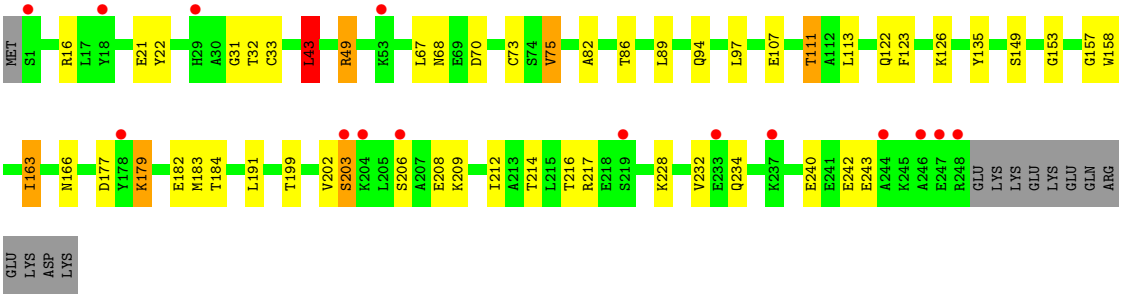
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



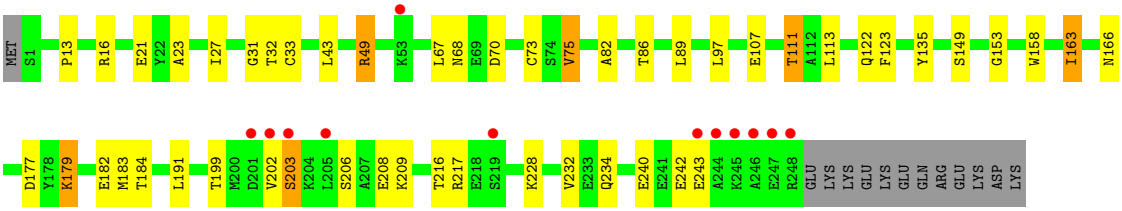
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



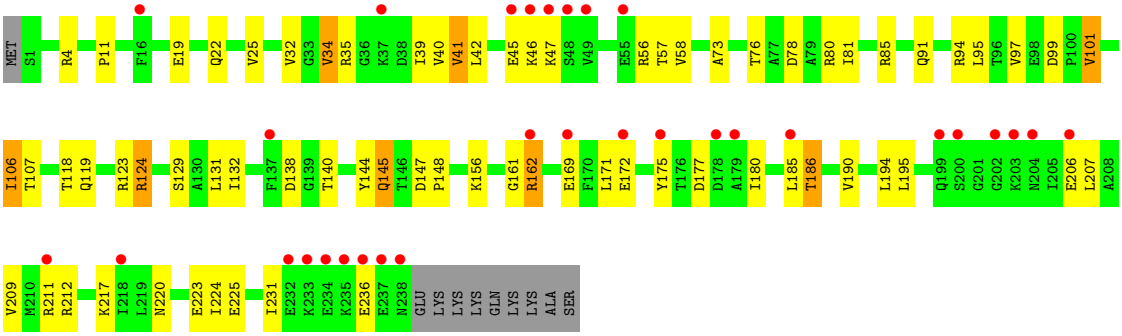
• Molecule 2: Proteasome subunit alpha type-4

Chain P:



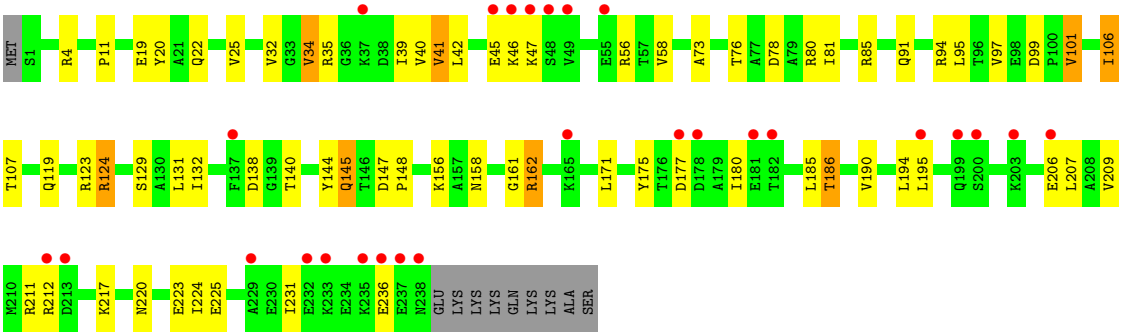
- Molecule 3: Proteasome subunit alpha type-7

Chain C:



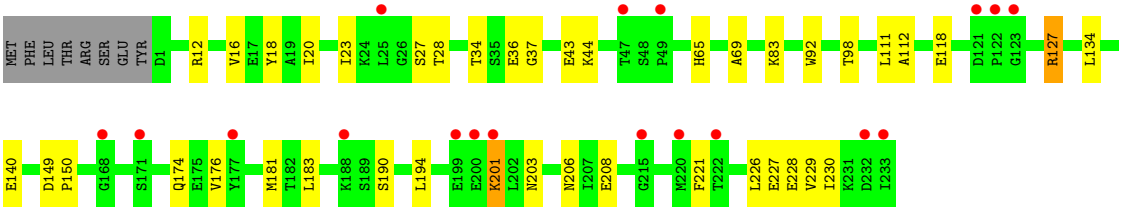
- Molecule 3: Proteasome subunit alpha type-7

Chain Q:



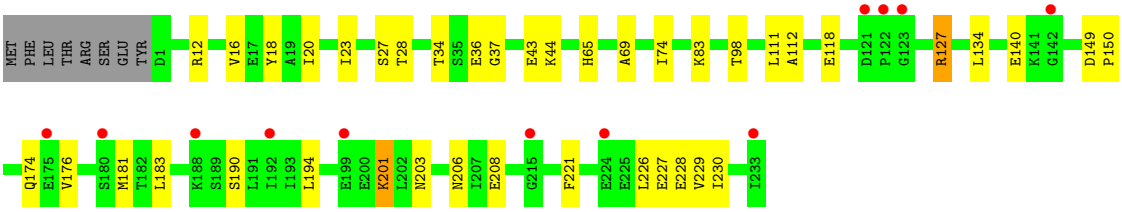
- Molecule 4: Proteasome subunit alpha type-5

Chain D:



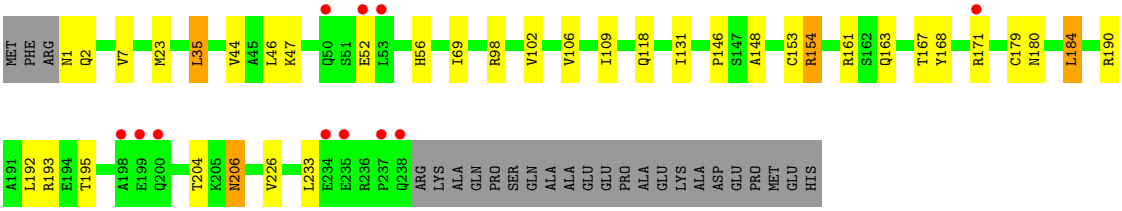
- Molecule 4: Proteasome subunit alpha type-5

Chain R:



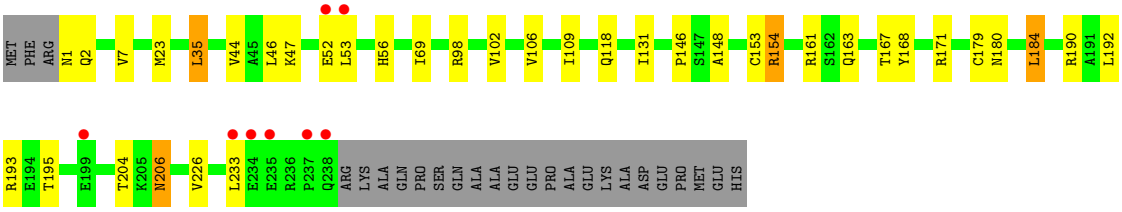
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



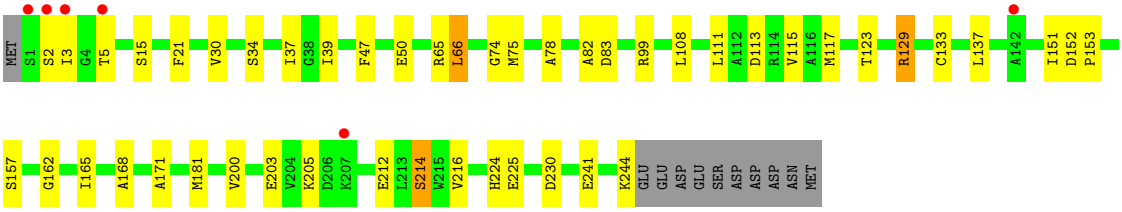
• Molecule 5: Proteasome subunit alpha type-1

Chain S:



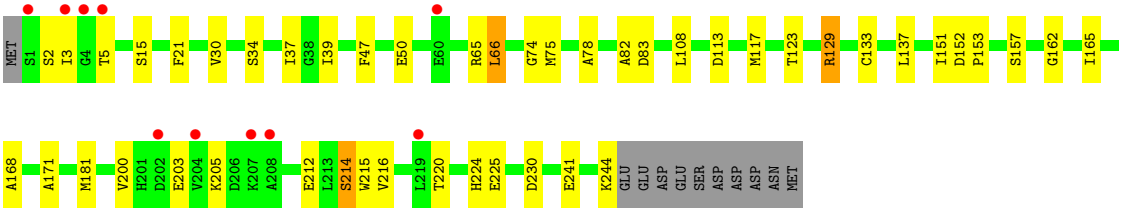
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



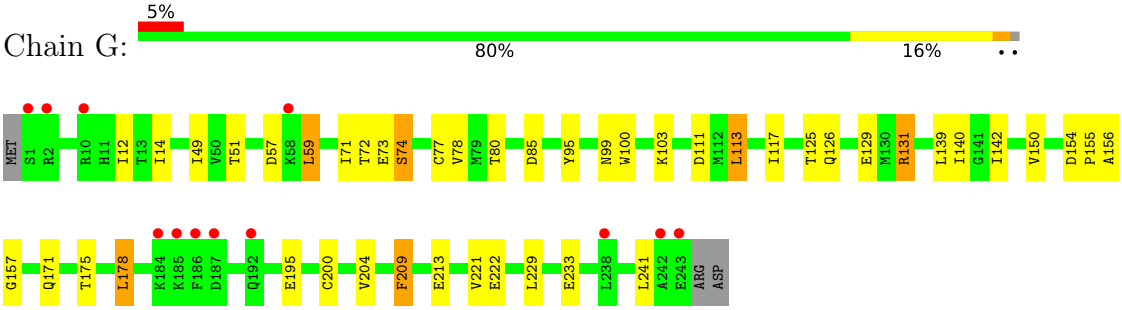
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



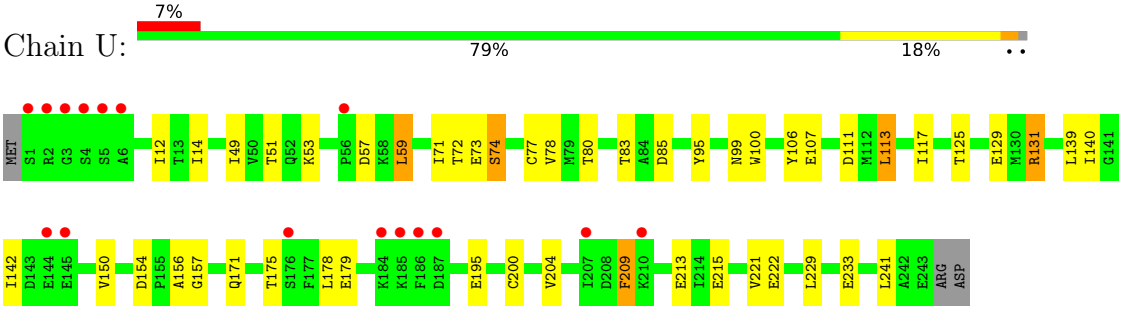
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



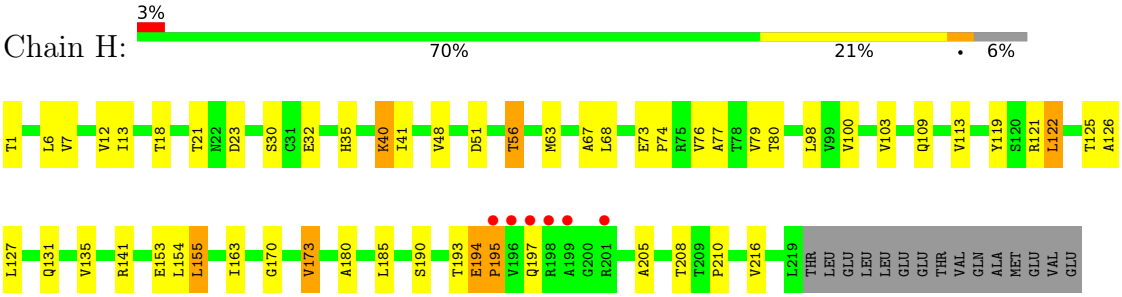
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



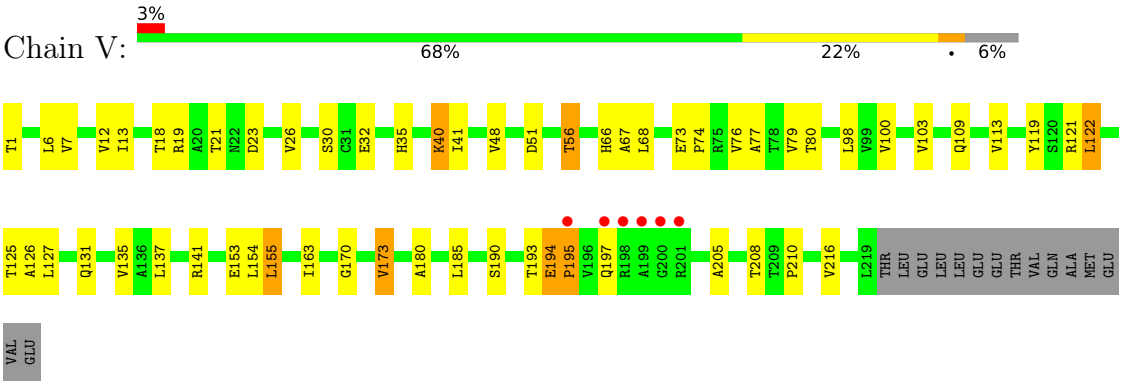
• Molecule 8: Proteasome subunit beta type-10

Chain H:



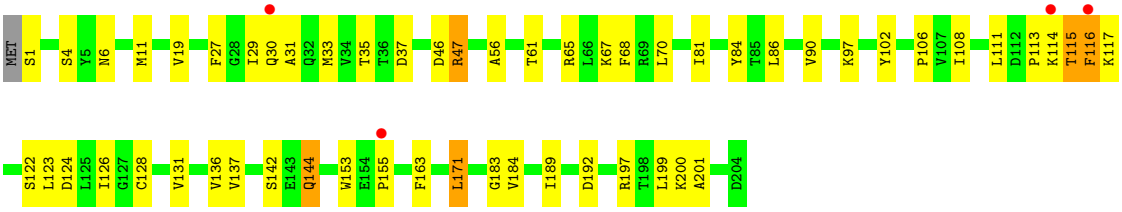
• Molecule 8: Proteasome subunit beta type-10

Chain V:



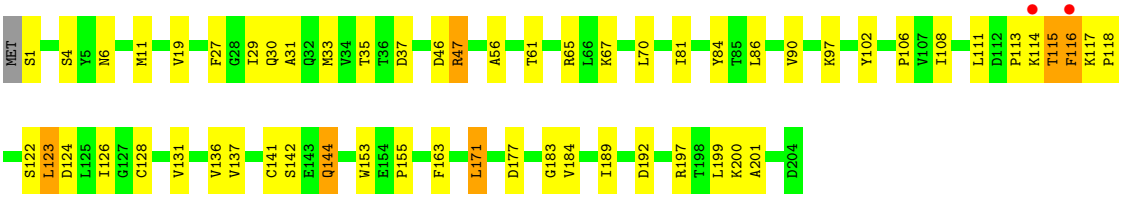
• Molecule 9: Proteasome subunit beta type-3

Chain I:



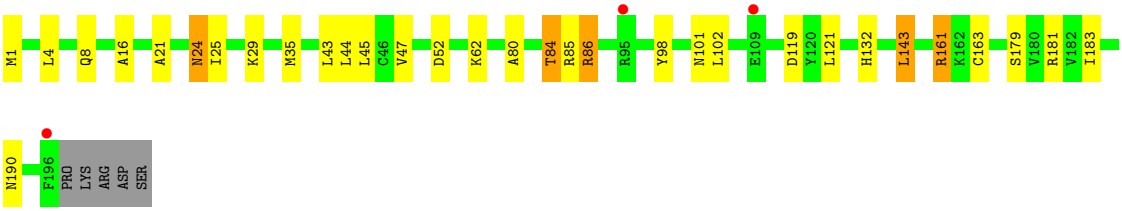
• Molecule 9: Proteasome subunit beta type-3

Chain W:



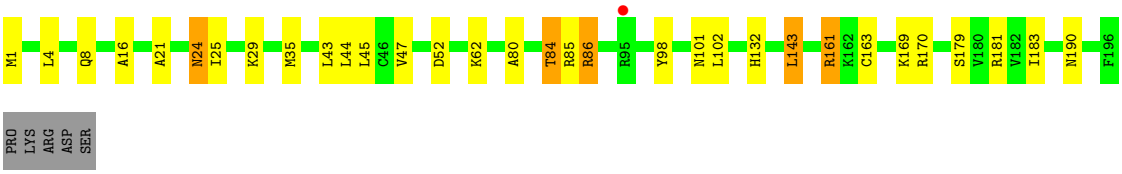
• Molecule 10: Proteasome subunit beta type-2

Chain J:



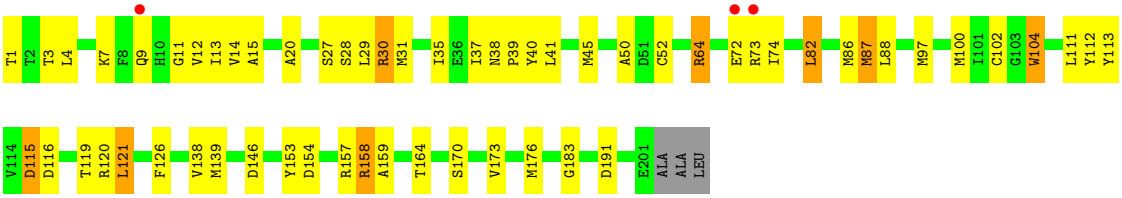
• Molecule 10: Proteasome subunit beta type-2

Chain X:



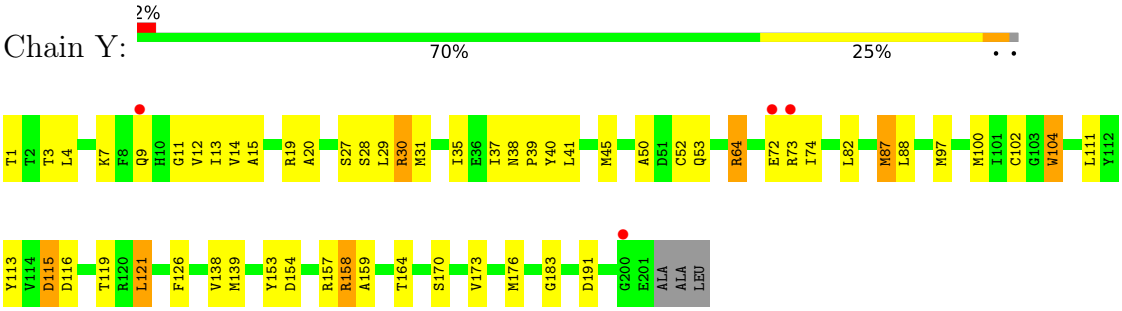
• Molecule 11: Proteasome subunit beta type-8

Chain K:



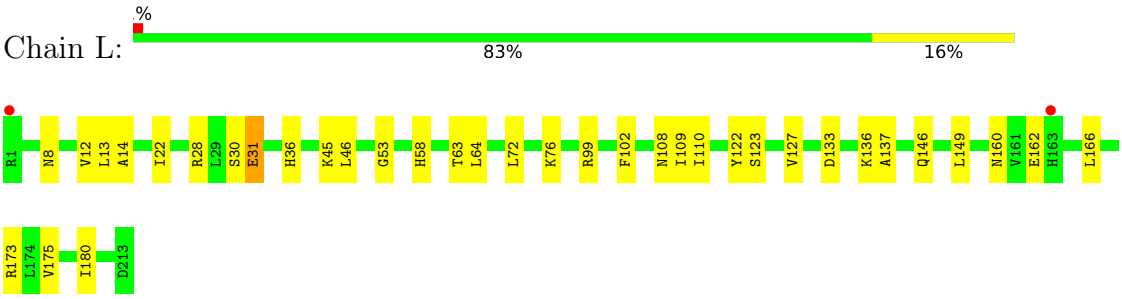
• Molecule 11: Proteasome subunit beta type-8

Chain Y:



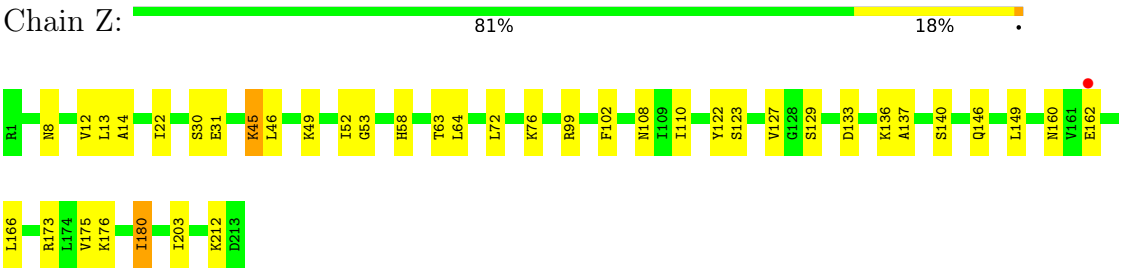
• Molecule 12: Proteasome subunit beta type-1

Chain L:



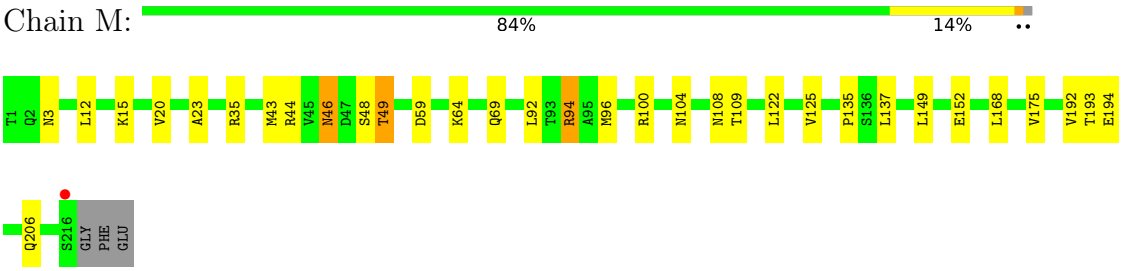
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



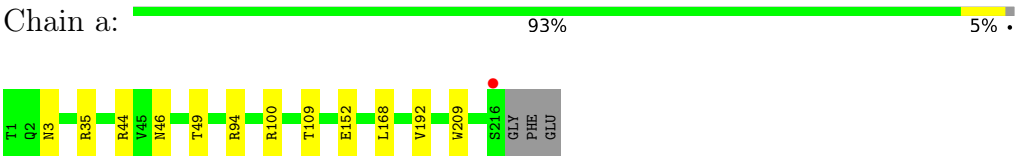
• Molecule 13: Proteasome subunit beta type-4

Chain M:



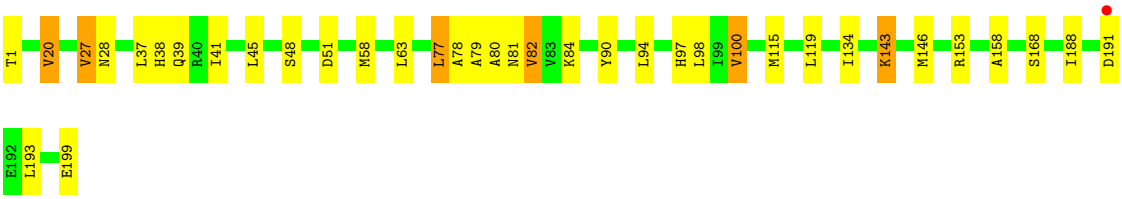
• Molecule 13: Proteasome subunit beta type-4

Chain a:



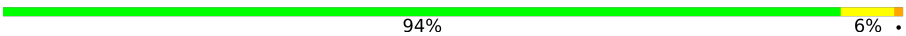
• Molecule 14: Proteasome subunit beta type-9

Chain N:



- Molecule 14: Proteasome subunit beta type-9

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.30Å 194.60Å 157.70Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-2.90) 97.2 (29.79-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.235 , 0.275 0.234 , 0.274	Depositor DCC
R_{free} test set	7255 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	49805	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, CL, 04C

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	0.39	1/1840 (0.1%)	0.50	0/2491
1	O	0.39	1/1840 (0.1%)	0.50	0/2491
2	B	0.37	1/1980 (0.1%)	0.51	1/2667 (0.0%)
2	P	0.37	1/1980 (0.1%)	0.51	0/2667
3	C	0.34	0/1903	0.51	0/2569
3	Q	0.34	0/1903	0.51	0/2569
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	0/1805	0.47	0/2437
5	E	0.38	0/1907	0.51	0/2578
5	S	0.37	0/1907	0.51	0/2578
6	F	0.38	0/1938	0.49	0/2608
6	T	0.38	0/1938	0.49	0/2608
7	G	0.37	1/1924 (0.1%)	0.49	0/2600
7	U	0.37	1/1924 (0.1%)	0.49	0/2600
8	H	0.36	1/1645 (0.1%)	0.53	0/2235
8	V	0.37	1/1645 (0.1%)	0.53	0/2235
9	I	0.34	0/1621	0.50	0/2185
9	W	0.34	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.50	0/2167
10	X	0.33	0/1602	0.49	0/2167
11	K	0.43	1/1597 (0.1%)	0.55	0/2151
11	Y	0.43	1/1597 (0.1%)	0.55	0/2151
12	L	0.32	0/1685	0.49	0/2271
12	Z	0.32	0/1685	0.50	0/2271
13	M	0.40	0/1718	0.50	0/2325
13	a	0.40	1/1718 (0.1%)	0.50	0/2325
14	N	0.37	0/1526	0.51	0/2071
14	b	0.37	0/1526	0.51	1/2071 (0.0%)
All	All	0.37	12/49382 (0.0%)	0.50	2/66710 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
14	N	0	2
14	b	0	1
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	1	THR	C-N	5.77	1.47	1.34
8	H	1	THR	C-N	5.51	1.46	1.34
11	Y	104	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.04	1.47	1.41
1	A	138	TRP	CD2-CE2	5.04	1.47	1.41
11	K	104	TRP	CD2-CE2	5.03	1.47	1.41
7	G	100	TRP	CD2-CE2	5.03	1.47	1.41
1	O	138	TRP	CD2-CE2	5.03	1.47	1.41
2	P	158	TRP	CD2-CE2	5.02	1.47	1.41
4	D	92	TRP	CD2-CE2	5.01	1.47	1.41
13	a	209	TRP	CD2-CE2	5.00	1.47	1.41
2	B	158	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1	THR	C-N-CA	5.78	136.14	121.70
2	B	43	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
14	N	1	THR	Mainchain,Peptide
11	Y	1	THR	Peptide
14	b	1	THR	Peptide

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	1801	0	1800	41	0
1	O	1801	0	1800	35	0
2	B	1950	0	1973	29	0
2	P	1950	0	1973	24	0
3	C	1876	0	1902	45	0
3	Q	1876	0	1902	43	0
4	D	1778	0	1767	25	0
4	R	1778	0	1767	27	0
5	E	1872	0	1859	24	0
5	S	1872	0	1859	24	0
6	F	1903	0	1894	30	0
6	T	1903	0	1894	29	0
7	G	1890	0	1900	28	0
7	U	1890	0	1900	31	0
8	H	1619	0	1640	27	0
8	V	1619	0	1640	30	0
9	I	1592	0	1612	32	0
9	W	1592	0	1612	32	0
10	J	1570	0	1573	19	0
10	X	1570	0	1573	18	0
11	K	1566	0	1516	41	1
11	Y	1566	0	1515	40	0
12	L	1654	0	1652	20	0
12	Z	1654	0	1651	25	0
13	M	1685	0	1664	17	1
13	a	1685	0	1664	0	0
14	N	1498	0	1476	20	0
14	b	1498	0	1476	0	0
15	A	3	0	0	0	0
15	D	1	0	0	0	0
15	E	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	L	2	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	2	0	0	0	0
15	P	1	0	0	0	0
15	Q	4	0	0	0	0
15	R	3	0	0	0	0
15	S	2	0	0	0	0
15	U	1	0	0	0	0
15	V	4	0	0	0	0
15	W	1	0	0	0	0
15	X	3	0	0	0	0
15	Z	1	0	0	0	0
15	a	4	0	0	0	0
16	B	1	0	0	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	S	1	0	0	0	0
16	X	1	0	0	0	0
16	Z	3	0	0	0	0
16	a	1	0	0	0	0
16	b	1	0	0	0	0
17	H	42	0	42	0	0
17	K	42	0	42	3	0
17	N	42	0	42	3	0
17	V	42	0	42	1	0
17	Y	42	0	42	3	0
17	b	42	0	42	0	0
18	H	1	0	0	0	0
18	K	1	0	0	1	0
18	N	1	0	0	0	0
18	V	1	0	0	1	0
18	Y	1	0	0	0	0
18	b	1	0	0	0	0
19	A	43	0	0	2	0
19	B	42	0	0	4	0
19	C	29	0	0	0	0
19	D	24	0	0	0	0
19	E	39	0	0	0	0
19	F	37	0	0	0	0
19	G	44	0	0	1	0
19	H	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	25	0	0	0	0
19	J	28	0	0	0	0
19	K	32	0	0	3	0
19	L	43	0	0	3	0
19	M	50	0	0	1	0
19	N	29	0	0	2	0
19	O	44	0	0	0	0
19	P	38	0	0	0	0
19	Q	13	0	0	0	0
19	R	24	0	0	0	0
19	S	40	0	0	0	0
19	T	32	0	0	0	0
19	U	38	0	0	3	0
19	V	39	0	0	0	0
19	W	39	0	0	0	0
19	X	20	0	0	0	0
19	Y	36	0	0	0	0
19	Z	49	0	0	5	0
19	a	35	0	0	0	0
19	b	33	0	0	0	0
All	All	49805	0	48706	700	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:154:ARG:HG2	5:S:154:ARG:HH11	1.26	0.98
11:Y:31:MET:HG2	17:Y:301:04C:H42	1.45	0.98
5:E:154:ARG:HG2	5:E:154:ARG:HH11	1.27	0.96
5:E:2:GLN:HE22	6:F:5:THR:HA	1.29	0.96
3:C:162:ARG:HG2	3:C:162:ARG:HH11	1.31	0.95
3:Q:35:ARG:HH21	3:Q:156:LYS:HG3	1.32	0.93
3:Q:162:ARG:HG2	3:Q:162:ARG:HH11	1.31	0.93
3:C:35:ARG:HH21	3:C:156:LYS:HG3	1.32	0.92
12:Z:110:ILE:HA	19:Z:426:HOH:O	1.67	0.92
12:Z:49:LYS:HB3	19:Z:415:HOH:O	1.72	0.89
8:H:194:GLU:H	8:H:195:PRO:HD3	1.37	0.88
8:V:194:GLU:H	8:V:195:PRO:HD3	1.37	0.87
4:R:201:LYS:HE2	4:R:201:LYS:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:MET:HG2	17:K:301:04C:H42	1.57	0.84
12:Z:52:ILE:HA	19:Z:426:HOH:O	1.76	0.84
4:D:201:LYS:HE2	4:D:201:LYS:H	1.44	0.81
8:H:40:LYS:HE2	8:H:73:GLU:HG3	1.63	0.81
11:Y:53:GLN:OE1	12:Z:129:SER:HA	1.82	0.79
8:V:40:LYS:HE2	8:V:73:GLU:HG3	1.65	0.77
5:E:2:GLN:NE2	6:F:5:THR:HA	2.00	0.76
9:W:124:ASP:HB2	9:W:128:CYS:H	1.50	0.76
3:C:41:VAL:HB	3:C:209:VAL:HG12	1.68	0.75
3:C:162:ARG:HG2	3:C:162:ARG:NH1	1.95	0.75
5:S:2:GLN:HE22	6:T:5:THR:HA	1.51	0.75
3:Q:41:VAL:HB	3:Q:209:VAL:HG12	1.68	0.74
5:S:47:LYS:HB3	5:S:56:HIS:HB3	1.69	0.74
12:L:13:LEU:HD11	12:L:149:LEU:HD11	1.70	0.74
9:I:124:ASP:HB2	9:I:128:CYS:H	1.50	0.74
5:E:47:LYS:HB3	5:E:56:HIS:HB3	1.69	0.73
2:P:68:ASN:HD22	2:P:70:ASP:H	1.37	0.73
6:T:151:ILE:HG12	6:T:157:SER:HB3	1.70	0.73
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.70	0.73
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.70	0.72
2:B:68:ASN:HD22	2:B:70:ASP:H	1.37	0.72
6:F:151:ILE:HG12	6:F:157:SER:HB3	1.71	0.72
5:S:154:ARG:HG2	5:S:154:ARG:NH1	2.02	0.71
3:Q:162:ARG:HG2	3:Q:162:ARG:NH1	1.95	0.71
8:V:131:GLN:O	8:V:135:VAL:HG23	1.90	0.71
8:H:131:GLN:O	8:H:135:VAL:HG23	1.91	0.70
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.73	0.70
1:O:83:ARG:HH11	1:O:83:ARG:HG2	1.56	0.69
2:P:166:ASN:HB2	2:P:199:THR:HG23	1.73	0.69
9:W:115:THR:O	9:W:116:PHE:CD2	2.46	0.69
9:I:115:THR:O	9:I:116:PHE:CD2	2.46	0.69
11:Y:138:VAL:HG21	11:Y:159:ALA:HA	1.75	0.69
11:Y:64:ARG:HG3	11:Y:64:ARG:HH11	1.57	0.68
2:B:212:ILE:HG22	19:B:434:HOH:O	1.92	0.68
1:O:45:LEU:HB3	1:O:74:VAL:HG21	1.76	0.68
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.76	0.68
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.57	0.68
2:B:166:ASN:HB2	2:B:199:THR:HG23	1.73	0.68
4:D:221:PHE:HB3	4:D:226:LEU:CD1	2.24	0.68
4:R:221:PHE:HB3	4:R:226:LEU:CD1	2.25	0.67
8:H:194:GLU:N	8:H:195:PRO:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:138:VAL:HG21	11:K:159:ALA:HA	1.75	0.67
1:A:127:ARG:HH21	7:G:125:THR:HG22	1.58	0.67
5:E:2:GLN:HE22	6:F:5:THR:CA	2.06	0.66
12:Z:110:ILE:HG12	19:Z:426:HOH:O	1.93	0.66
8:V:194:GLU:N	8:V:195:PRO:HD3	2.09	0.66
10:J:52:ASP:HB3	10:J:98:TYR:HD2	1.61	0.66
5:E:148:ALA:HB3	6:F:82:ALA:HB1	1.77	0.66
5:E:154:ARG:HG2	5:E:154:ARG:NH1	2.03	0.66
11:Y:41:LEU:HB2	11:Y:73:ARG:HH22	1.60	0.66
8:V:40:LYS:H	8:V:40:LYS:HD3	1.61	0.66
6:T:39:ILE:HG22	6:T:162:GLY:HA2	1.77	0.65
5:S:148:ALA:HB3	6:T:82:ALA:HB1	1.77	0.65
11:K:41:LEU:HB2	11:K:73:ARG:HH22	1.60	0.65
1:O:203:THR:H	1:O:206:ASN:HD22	1.43	0.65
1:A:203:THR:H	1:A:206:ASN:HD22	1.43	0.65
4:R:176:VAL:O	4:R:176:VAL:HG12	1.96	0.65
4:R:34:THR:HG22	4:R:36:GLU:H	1.62	0.65
10:X:52:ASP:HB3	10:X:98:TYR:HD2	1.61	0.65
4:D:176:VAL:HG12	4:D:176:VAL:O	1.96	0.65
3:Q:101:VAL:HG11	3:Q:106:ILE:HG12	1.80	0.64
6:F:39:ILE:HG22	6:F:162:GLY:HA2	1.78	0.64
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.45	0.64
8:H:40:LYS:H	8:H:40:LYS:HD3	1.61	0.64
2:B:135:TYR:HE1	2:B:149:SER:HB2	1.63	0.64
9:W:144:GLN:H	9:W:144:GLN:HE21	1.46	0.64
8:V:205:ALA:O	8:V:208:THR:HG23	1.97	0.64
4:D:227:GLU:HA	4:D:230:ILE:HG22	1.79	0.63
13:M:59:ASP:HB3	13:M:108:ASN:HD21	1.62	0.63
1:O:149:ASP:HB2	1:O:150:PRO:HD2	1.80	0.63
3:C:101:VAL:HG11	3:C:106:ILE:HG12	1.80	0.63
2:P:135:TYR:HE1	2:P:149:SER:HB2	1.63	0.63
9:I:144:GLN:H	9:I:144:GLN:HE21	1.47	0.63
11:K:30:ARG:O	11:K:30:ARG:HG2	1.99	0.63
4:D:34:THR:HG22	4:D:36:GLU:H	1.62	0.63
12:L:8:ASN:HD22	12:L:58:HIS:H	1.45	0.63
8:H:205:ALA:O	8:H:208:THR:HG23	1.98	0.62
8:H:13:ILE:HG12	8:H:155:LEU:HD22	1.80	0.62
14:N:20:VAL:CG2	14:N:27:VAL:HG22	2.28	0.62
1:O:67:ILE:HD11	1:O:73:LEU:HD12	1.81	0.62
11:K:7:LYS:HB3	11:K:12:VAL:HG22	1.81	0.62
1:A:149:ASP:HB2	1:A:150:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:ARG:HH11	3:C:162:ARG:CG	2.10	0.62
4:R:227:GLU:HA	4:R:230:ILE:HG22	1.80	0.62
12:Z:12:VAL:HG21	12:Z:53:GLY:HA3	1.82	0.61
1:A:67:ILE:HD11	1:A:73:LEU:HD12	1.81	0.61
11:Y:7:LYS:HB3	11:Y:12:VAL:HG22	1.81	0.61
11:Y:30:ARG:O	11:Y:30:ARG:HG2	2.00	0.61
4:R:221:PHE:HB3	4:R:226:LEU:HD12	1.83	0.61
9:I:86:LEU:O	9:I:90:VAL:HG23	2.01	0.61
12:L:14:ALA:HA	12:L:22:ILE:O	2.01	0.60
9:W:86:LEU:O	9:W:90:VAL:HG23	2.01	0.60
3:C:41:VAL:HG22	3:C:190:VAL:HG21	1.83	0.60
11:K:64:ARG:HG2	11:K:64:ARG:HH11	1.66	0.60
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.01	0.60
3:C:35:ARG:NH2	3:C:156:LYS:HG3	2.11	0.60
1:O:4:GLY:HA2	7:U:129:GLU:HG2	1.82	0.60
1:O:127:ARG:HH21	7:U:125:THR:HG22	1.67	0.60
3:Q:41:VAL:HG22	3:Q:190:VAL:HG21	1.83	0.59
4:D:221:PHE:HB3	4:D:226:LEU:HD12	1.83	0.59
3:Q:162:ARG:HH11	3:Q:162:ARG:CG	2.10	0.59
6:T:168:ALA:HB3	6:T:200:VAL:HG13	1.84	0.59
6:F:47:PHE:HB2	6:F:214:SER:HB2	1.85	0.59
1:A:45:LEU:HD13	1:A:74:VAL:HG23	1.85	0.59
12:L:12:VAL:HG21	12:L:53:GLY:HA3	1.84	0.59
10:J:86:ARG:HE	10:J:86:ARG:HA	1.67	0.58
4:D:44:LYS:HE2	4:D:208:GLU:HG3	1.85	0.58
6:F:66:LEU:HD22	6:F:212:GLU:HB3	1.85	0.58
1:O:45:LEU:HD13	1:O:74:VAL:HG23	1.85	0.58
10:X:86:ARG:HE	10:X:86:ARG:HA	1.67	0.58
14:N:80:ALA:HB1	14:N:119:LEU:HD11	1.85	0.58
6:T:47:PHE:HB2	6:T:214:SER:HB2	1.85	0.58
6:T:66:LEU:HD22	6:T:212:GLU:HB3	1.85	0.58
11:K:73:ARG:HD2	11:K:74:ILE:H	1.69	0.58
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.84	0.58
4:R:44:LYS:HE2	4:R:208:GLU:HG3	1.85	0.58
8:V:13:ILE:HG12	8:V:155:LEU:HD22	1.86	0.57
3:Q:35:ARG:NH2	3:Q:156:LYS:HG3	2.11	0.57
3:Q:39:ILE:HG22	3:Q:211:ARG:HA	1.87	0.57
8:V:41:ILE:HG21	8:V:79:VAL:HG21	1.87	0.57
11:Y:38:ASN:HB2	11:Y:73:ARG:NH2	2.20	0.57
11:Y:73:ARG:HD2	11:Y:74:ILE:H	1.70	0.57
1:A:45:LEU:HB3	1:A:74:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:HB2	11:K:73:ARG:NH2	2.19	0.56
3:C:39:ILE:HG22	3:C:211:ARG:HA	1.87	0.56
3:C:45:GLU:OE2	3:C:194:LEU:HB3	2.06	0.56
3:Q:45:GLU:OE2	3:Q:194:LEU:HB3	2.06	0.56
5:S:2:GLN:NE2	6:T:5:THR:HA	2.19	0.56
1:A:218:ARG:HG3	19:A:430:HOH:O	2.04	0.56
8:H:41:ILE:HG21	8:H:79:VAL:HG21	1.88	0.56
8:V:141:ARG:HB2	8:V:154:LEU:HD13	1.87	0.56
9:I:184:VAL:HB	9:I:199:LEU:HD12	1.88	0.56
13:M:92:LEU:O	13:M:96:MET:HG2	2.06	0.56
2:P:135:TYR:CE1	2:P:149:SER:HB2	2.41	0.56
5:E:161:ARG:HD2	5:E:195:THR:O	2.06	0.56
9:W:184:VAL:HB	9:W:199:LEU:HD12	1.88	0.56
1:O:45:LEU:HB3	1:O:74:VAL:CG2	2.35	0.55
5:S:161:ARG:HD2	5:S:195:THR:O	2.07	0.55
11:Y:3:THR:HG22	11:Y:100:MET:CE	2.36	0.55
11:K:37:ILE:HG22	11:K:38:ASN:HD22	1.72	0.55
14:N:98:LEU:HD21	19:N:310:HOH:O	2.05	0.55
17:N:201:04C:H8	17:N:201:04C:H22	1.88	0.55
11:Y:37:ILE:HG22	11:Y:38:ASN:HD22	1.71	0.55
3:C:25:VAL:HG21	3:C:129:SER:HB2	1.87	0.55
11:K:3:THR:HG22	11:K:100:MET:CE	2.36	0.55
8:V:109:GLN:HG2	8:V:121:ARG:HH11	1.71	0.55
2:B:135:TYR:CE1	2:B:149:SER:HB2	2.41	0.55
4:R:174:GLN:HE21	5:S:52:GLU:HG2	1.72	0.55
8:H:141:ARG:HB2	8:H:154:LEU:HD13	1.88	0.55
8:H:194:GLU:N	8:H:195:PRO:CD	2.70	0.55
2:P:153:GLY:O	3:Q:80:ARG:NH2	2.34	0.55
3:Q:25:VAL:HG21	3:Q:129:SER:HB2	1.87	0.55
5:E:44:VAL:HG12	5:E:192:LEU:HD22	1.89	0.55
8:H:109:GLN:HG2	8:H:121:ARG:HH11	1.70	0.55
7:U:57:ASP:OD2	7:U:59:LEU:HB2	2.06	0.55
2:B:75:VAL:HG21	2:B:82:ALA:HB1	1.89	0.54
8:V:35:HIS:CG	8:V:56:THR:HG21	2.42	0.54
7:G:57:ASP:OD2	7:G:59:LEU:HB2	2.07	0.54
5:S:193:ARG:HH22	5:S:233:LEU:HD12	1.73	0.54
3:Q:32:VAL:HG12	3:Q:194:LEU:HD21	1.88	0.54
1:A:39:ALA:O	1:A:41:ASN:N	2.36	0.54
3:C:32:VAL:HG12	3:C:194:LEU:HD21	1.87	0.54
11:K:112:TYR:HB3	19:K:406:HOH:O	2.06	0.54
3:C:58:VAL:HG12	3:C:58:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:40:LYS:HD3	8:V:40:LYS:N	2.23	0.54
2:P:75:VAL:HG21	2:P:82:ALA:HB1	1.90	0.54
7:U:95:TYR:O	7:U:99:ASN:HB2	2.08	0.54
3:C:19:GLU:HA	3:C:22:GLN:HE21	1.72	0.54
5:E:193:ARG:HH22	5:E:233:LEU:HD12	1.73	0.54
7:G:95:TYR:O	7:G:99:ASN:HB2	2.08	0.54
6:T:152:ASP:HB2	6:T:153:PRO:HD2	1.90	0.54
8:V:98:LEU:HB2	8:V:113:VAL:HG13	1.90	0.54
3:Q:58:VAL:O	3:Q:58:VAL:HG12	2.07	0.53
2:B:212:ILE:CG2	19:B:434:HOH:O	2.53	0.53
13:M:15:LYS:HB3	13:M:20:VAL:HG22	1.88	0.53
3:Q:19:GLU:HA	3:Q:22:GLN:HE21	1.72	0.53
4:D:221:PHE:HB3	4:D:226:LEU:HD11	1.89	0.53
11:K:153:TYR:O	11:K:157:ARG:HB2	2.09	0.53
8:V:194:GLU:N	8:V:195:PRO:CD	2.70	0.53
14:N:45:LEU:HD23	17:N:201:04C:H44	1.89	0.53
6:T:34:SER:HB2	6:T:50:GLU:HG3	1.90	0.53
5:S:44:VAL:HG12	5:S:192:LEU:HD22	1.89	0.53
12:L:109:ILE:HB	19:L:442:HOH:O	2.08	0.53
4:R:221:PHE:HB3	4:R:226:LEU:HD11	1.90	0.53
6:F:152:ASP:HB2	6:F:153:PRO:HD2	1.90	0.53
8:H:35:HIS:CG	8:H:56:THR:HG21	2.44	0.53
4:D:203:ASN:HB3	4:D:206:ASN:HB2	1.91	0.53
3:Q:81:ILE:O	3:Q:85:ARG:HG2	2.09	0.53
13:M:15:LYS:HE2	13:M:135:PRO:HA	1.91	0.53
14:N:20:VAL:HG23	14:N:27:VAL:HG22	1.91	0.53
3:C:95:LEU:HG	10:J:62:LYS:HG2	1.89	0.53
9:I:171:LEU:HD21	9:I:199:LEU:HD13	1.91	0.53
11:Y:153:TYR:O	11:Y:157:ARG:HB2	2.09	0.52
3:C:81:ILE:O	3:C:85:ARG:HG2	2.09	0.52
6:F:34:SER:HB2	6:F:50:GLU:HG3	1.90	0.52
3:Q:180:ILE:HA	3:Q:186:THR:HG23	1.91	0.52
4:R:16:VAL:O	4:R:20:ILE:HG12	2.09	0.52
10:X:35:MET:HG2	10:X:45:LEU:HD22	1.92	0.52
9:I:11:MET:HG3	9:I:137:VAL:HG12	1.91	0.52
4:D:16:VAL:O	4:D:20:ILE:HG12	2.09	0.52
11:Y:3:THR:HG22	11:Y:100:MET:HE1	1.90	0.52
11:Y:97:MET:H	11:Y:116:ASP:HB3	1.74	0.52
12:L:99:ARG:HD2	12:L:102:PHE:O	2.10	0.52
4:D:27:SER:HB2	4:D:43:GLU:HG3	1.91	0.52
2:P:31:GLY:HA2	2:P:49:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:11:MET:HG3	9:W:137:VAL:HG12	1.91	0.52
9:W:171:LEU:HD21	9:W:199:LEU:HD13	1.91	0.52
7:G:77:CYS:HB3	7:G:139:LEU:HD23	1.92	0.52
11:K:40:TYR:HB3	11:K:183:GLY:HA2	1.91	0.52
11:K:40:TYR:HE1	11:K:73:ARG:HG2	1.75	0.52
11:Y:38:ASN:HB2	11:Y:73:ARG:CZ	2.39	0.52
2:B:31:GLY:HA2	2:B:49:ARG:NH1	2.25	0.52
14:N:84:LYS:HG3	14:N:119:LEU:HB2	1.92	0.52
8:V:210:PRO:HB2	9:W:200:LYS:HB3	1.92	0.52
6:F:123:THR:O	7:G:131:ARG:NH1	2.43	0.52
7:U:77:CYS:HB3	7:U:139:LEU:HD23	1.92	0.52
6:F:78:ALA:HB3	6:F:165:ILE:HD12	1.92	0.52
8:H:40:LYS:HD3	8:H:40:LYS:N	2.23	0.52
8:H:98:LEU:HB2	8:H:113:VAL:HG13	1.92	0.52
11:K:138:VAL:CG2	11:K:159:ALA:HA	2.40	0.52
10:X:21:ALA:HB3	10:X:29:LYS:HB2	1.92	0.52
11:Y:40:TYR:HB3	11:Y:183:GLY:HA2	1.91	0.52
11:K:74:ILE:HD11	19:K:422:HOH:O	2.10	0.51
4:R:203:ASN:HB3	4:R:206:ASN:HB2	1.91	0.51
11:K:97:MET:H	11:K:116:ASP:HB3	1.74	0.51
11:K:115:ASP:HB2	11:K:119:THR:HB	1.92	0.51
3:Q:78:ASP:OD1	3:Q:124:ARG:NH2	2.43	0.51
12:Z:99:ARG:HD2	12:Z:102:PHE:O	2.10	0.51
2:B:153:GLY:O	3:C:80:ARG:NH2	2.36	0.51
3:C:78:ASP:OD1	3:C:124:ARG:NH2	2.44	0.51
1:O:198:PHE:O	1:O:199:GLU:CB	2.59	0.51
8:V:103:VAL:HG11	8:V:180:ALA:HA	1.91	0.51
10:J:35:MET:HG2	10:J:45:LEU:HD22	1.92	0.51
11:K:38:ASN:HB2	11:K:73:ARG:CZ	2.41	0.51
11:K:100:MET:SD	11:K:126:PHE:HB2	2.51	0.51
4:R:174:GLN:HA	5:S:53:LEU:HD21	1.92	0.51
11:Y:115:ASP:HB2	11:Y:119:THR:HB	1.92	0.51
11:Y:138:VAL:CG2	11:Y:159:ALA:HA	2.41	0.51
12:Z:110:ILE:HB	12:Z:122:TYR:HB2	1.92	0.51
3:C:180:ILE:HA	3:C:186:THR:HG23	1.91	0.51
11:Y:40:TYR:HE1	11:Y:73:ARG:HG2	1.76	0.51
2:B:67:LEU:HD11	2:B:73:CYS:HB3	1.93	0.51
1:O:39:ALA:O	1:O:41:ASN:N	2.36	0.51
6:T:78:ALA:HB3	6:T:165:ILE:HD12	1.92	0.51
11:Y:100:MET:SD	11:Y:126:PHE:HB2	2.51	0.51
8:H:103:VAL:HG11	8:H:180:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLN:HE21	9:I:68:PHE:HA	1.76	0.51
6:F:241:GLU:HA	6:F:244:LYS:NZ	2.25	0.50
8:H:67:ALA:HB2	8:H:74:PRO:HG3	1.93	0.50
13:M:92:LEU:HD23	13:M:125:VAL:HG21	1.93	0.50
4:R:27:SER:HB2	4:R:43:GLU:HG3	1.91	0.50
1:A:51:GLN:HG2	1:A:56:TYR:CD2	2.46	0.50
1:A:198:PHE:O	1:A:199:GLU:CB	2.59	0.50
9:W:47:ARG:HG2	9:W:111:LEU:HB2	1.94	0.50
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.94	0.50
12:L:8:ASN:ND2	12:L:58:HIS:H	2.09	0.50
3:Q:95:LEU:HG	10:X:62:LYS:HG2	1.93	0.50
10:X:101:ASN:HB3	10:X:132:HIS:CE1	2.46	0.50
11:Y:87:MET:HG3	11:Y:116:ASP:HA	1.93	0.50
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.93	0.50
9:I:46:ASP:O	9:I:47:ARG:CB	2.59	0.50
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.46	0.50
2:P:31:GLY:HA2	2:P:49:ARG:HH11	1.77	0.50
2:P:206:SER:HB3	2:P:209:LYS:HD2	1.94	0.49
10:J:21:ALA:HB3	10:J:29:LYS:HB2	1.93	0.49
11:K:72:GLU:HG2	11:K:72:GLU:O	2.12	0.49
2:P:67:LEU:HD11	2:P:73:CYS:HB3	1.93	0.49
4:R:34:THR:HB	4:R:37:GLY:O	2.12	0.49
9:W:46:ASP:O	9:W:47:ARG:CB	2.59	0.49
4:D:34:THR:HB	4:D:37:GLY:O	2.12	0.49
8:V:67:ALA:HB2	8:V:74:PRO:HG3	1.94	0.49
11:Y:40:TYR:CE1	11:Y:73:ARG:HG2	2.47	0.49
3:C:35:ARG:HA	3:C:40:VAL:HG13	1.95	0.49
14:N:63:LEU:HD21	14:N:79:ALA:HA	1.93	0.49
11:Y:31:MET:CG	17:Y:301:04C:H42	2.32	0.49
1:A:220:LEU:HD23	19:A:430:HOH:O	2.12	0.49
7:G:171:GLN:O	7:G:175:THR:HG23	2.12	0.49
1:A:106:THR:O	1:A:110:VAL:HG23	2.13	0.49
2:B:206:SER:HB3	2:B:209:LYS:HD2	1.94	0.49
12:L:22:ILE:HG21	12:L:175:VAL:HG21	1.95	0.49
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.48	0.49
9:I:47:ARG:HG2	9:I:111:LEU:HB2	1.94	0.49
2:P:13:PRO:HA	3:Q:20:TYR:CE2	2.46	0.49
9:I:124:ASP:HB3	9:I:126:ILE:H	1.78	0.49
12:L:8:ASN:HA	12:L:30:SER:O	2.13	0.49
3:Q:35:ARG:HA	3:Q:40:VAL:HG13	1.95	0.49
7:U:171:GLN:O	7:U:175:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:LEU:HD23	3:C:145:GLN:HB3	1.95	0.48
11:K:40:TYR:CE1	11:K:73:ARG:HG2	2.47	0.48
11:K:87:MET:HG3	11:K:116:ASP:HA	1.94	0.48
1:O:106:THR:O	1:O:110:VAL:HG23	2.13	0.48
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.48	0.48
4:R:34:THR:HG23	4:R:181:MET:O	2.14	0.48
7:U:107:GLU:HG3	19:U:424:HOH:O	2.12	0.48
11:Y:173:VAL:HG12	11:Y:191:ASP:HA	1.95	0.48
12:Z:8:ASN:ND2	12:Z:58:HIS:H	2.09	0.48
1:O:51:GLN:HG2	1:O:56:TYR:CD2	2.49	0.48
4:R:149:ASP:HB2	4:R:150:PRO:CD	2.43	0.48
9:W:124:ASP:HB3	9:W:126:ILE:H	1.78	0.48
11:Y:72:GLU:O	11:Y:72:GLU:HG2	2.12	0.48
2:B:31:GLY:HA2	2:B:49:ARG:HH11	1.77	0.48
4:D:149:ASP:HB2	4:D:150:PRO:CD	2.42	0.48
11:K:173:VAL:HG12	11:K:191:ASP:HA	1.95	0.48
3:Q:91:GLN:HE21	10:X:62:LYS:HG3	1.79	0.48
4:D:34:THR:HG23	4:D:181:MET:O	2.13	0.48
8:H:210:PRO:HB2	9:I:200:LYS:HB3	1.95	0.48
10:X:44:LEU:HD11	10:X:102:LEU:HD13	1.96	0.48
7:G:72:THR:HG22	7:G:74:SER:H	1.79	0.48
11:K:3:THR:HG22	11:K:100:MET:HE1	1.94	0.48
9:I:46:ASP:O	9:I:47:ARG:HB2	2.13	0.48
5:S:2:GLN:HE22	6:T:5:THR:H	1.62	0.48
6:T:108:LEU:HD11	6:T:137:LEU:HB3	1.96	0.48
9:W:46:ASP:O	9:W:47:ARG:HB2	2.14	0.48
2:B:89:LEU:HG	2:B:113:LEU:HD13	1.96	0.48
4:D:65:HIS:CE1	4:D:98:THR:HB	2.49	0.47
9:I:113:PRO:O	9:I:114:LYS:HB2	2.14	0.47
10:J:181:ARG:HG2	10:J:190:ASN:HA	1.96	0.47
1:O:147:GLN:HE21	1:O:157:TRP:HE1	1.62	0.47
6:T:152:ASP:HB2	6:T:153:PRO:CD	2.44	0.47
12:Z:22:ILE:HG21	12:Z:175:VAL:HG21	1.95	0.47
6:F:152:ASP:HB2	6:F:153:PRO:CD	2.45	0.47
10:X:143:LEU:HD13	10:X:163:CYS:SG	2.55	0.47
11:K:72:GLU:O	11:K:73:ARG:HB3	2.14	0.47
12:L:110:ILE:HB	12:L:122:TYR:HB2	1.96	0.47
3:Q:175:TYR:CZ	3:Q:180:ILE:HD11	2.50	0.47
5:S:2:GLN:HE22	6:T:5:THR:CA	2.23	0.47
7:U:12:ILE:HG13	7:U:14:ILE:HG12	1.96	0.47
6:F:168:ALA:HB1	6:F:171:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:122:SER:HB3	9:I:136:VAL:HB	1.96	0.47
10:J:80:ALA:O	10:J:84:THR:HG23	2.13	0.47
14:N:38:HIS:CD2	14:N:39:GLN:H	2.33	0.47
6:F:108:LEU:HD11	6:F:137:LEU:HB3	1.96	0.47
10:J:143:LEU:HD13	10:J:163:CYS:SG	2.55	0.47
3:Q:131:LEU:HD23	3:Q:145:GLN:HB3	1.95	0.47
12:Z:8:ASN:HA	12:Z:30:SER:O	2.13	0.47
2:P:89:LEU:HG	2:P:113:LEU:HD13	1.97	0.47
4:R:65:HIS:CE1	4:R:98:THR:HB	2.49	0.47
9:W:113:PRO:O	9:W:114:LYS:HB2	2.15	0.47
7:G:12:ILE:HG13	7:G:14:ILE:HG12	1.96	0.47
12:L:46:LEU:HB3	12:L:72:LEU:HD11	1.97	0.47
12:L:137:ALA:H	12:L:146:GLN:HE21	1.63	0.47
5:S:206:ASN:C	5:S:206:ASN:HD22	2.18	0.47
9:W:122:SER:HB3	9:W:136:VAL:HB	1.97	0.47
1:A:40:ALA:HB2	1:A:180:ASP:HA	1.97	0.47
2:B:122:GLN:HG3	3:C:124:ARG:HG3	1.95	0.47
14:N:168:SER:O	17:N:201:04C:H33	2.14	0.47
3:Q:19:GLU:HA	3:Q:22:GLN:NE2	2.30	0.47
6:T:168:ALA:HB1	6:T:171:ALA:HB3	1.96	0.47
12:Z:46:LEU:HB3	12:Z:72:LEU:HD11	1.96	0.47
9:I:61:THR:O	9:I:65:ARG:HG3	2.14	0.47
5:S:168:TYR:OH	5:S:190:ARG:HD2	2.15	0.47
2:P:86:THR:HA	2:P:89:LEU:HD12	1.97	0.47
9:W:61:THR:O	9:W:65:ARG:HG3	2.14	0.47
11:Y:72:GLU:O	11:Y:73:ARG:HB3	2.14	0.47
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.63	0.47
1:A:147:GLN:HE21	1:A:157:TRP:HE1	1.62	0.46
5:E:106:VAL:HA	5:E:109:ILE:HD12	1.96	0.46
14:N:188:ILE:HG22	14:N:193:LEU:HD12	1.97	0.46
3:Q:11:PRO:HA	4:R:18:TYR:CD2	2.51	0.46
5:S:167:THR:O	5:S:171:ARG:HG3	2.15	0.46
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.95	0.46
3:C:175:TYR:CZ	3:C:180:ILE:HD11	2.50	0.46
5:E:206:ASN:C	5:E:206:ASN:HD22	2.18	0.46
10:J:161:ARG:HE	10:J:161:ARG:HB2	1.52	0.46
11:K:20:ALA:HB3	11:K:28:SER:HB3	1.97	0.46
5:S:106:VAL:HA	5:S:109:ILE:HD12	1.96	0.46
2:B:86:THR:HA	2:B:89:LEU:HD12	1.97	0.46
4:D:149:ASP:HB2	4:D:150:PRO:HD2	1.98	0.46
10:J:44:LEU:HD11	10:J:102:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:90:TYR:HB2	14:N:94:LEU:HD12	1.96	0.46
10:X:181:ARG:HG2	10:X:190:ASN:HA	1.97	0.46
5:E:167:THR:O	5:E:171:ARG:HG3	2.15	0.46
14:N:97:HIS:CG	14:N:115:MET:HB3	2.50	0.46
10:X:80:ALA:O	10:X:84:THR:HG23	2.14	0.46
3:C:19:GLU:HA	3:C:22:GLN:NE2	2.30	0.46
7:G:140:ILE:HG22	7:G:150:VAL:HG22	1.98	0.46
7:G:142:ILE:HD13	7:G:221:VAL:HA	1.98	0.46
9:I:153:TRP:CH2	9:I:155:PRO:HA	2.51	0.46
7:U:49:ILE:HG13	19:U:413:HOH:O	2.15	0.46
11:Y:19:ARG:O	17:Y:301:04C:H34	2.16	0.46
1:A:70:HIS:CE1	1:A:103:PRO:HB3	2.51	0.46
6:F:3:ILE:HD12	6:F:15:SER:HB2	1.97	0.46
12:L:64:LEU:CD2	12:L:108:ASN:HD21	2.28	0.46
14:N:134:ILE:HG21	14:N:158:ALA:O	2.15	0.46
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	1.97	0.46
12:Z:64:LEU:CD2	12:Z:108:ASN:HD21	2.28	0.46
1:O:70:HIS:CE1	1:O:103:PRO:HB3	2.51	0.46
9:W:97:LYS:HG3	9:W:102:TYR:CE1	2.50	0.46
11:Y:154:ASP:O	11:Y:158:ARG:HB2	2.16	0.46
8:H:153:GLU:HG3	8:H:154:LEU:N	2.31	0.46
9:I:97:LYS:HG3	9:I:102:TYR:CE1	2.51	0.46
11:K:11:GLY:HA2	11:K:104:TRP:HZ3	1.81	0.46
7:U:229:LEU:O	7:U:233:GLU:HB2	2.16	0.46
11:Y:4:LEU:CD2	11:Y:159:ALA:HB3	2.46	0.46
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.51	0.46
7:G:229:LEU:O	7:G:233:GLU:HB2	2.16	0.46
9:I:163:PHE:CE1	9:I:197:ARG:HD3	2.51	0.46
13:M:46:ASN:ND2	13:M:49:THR:H	2.14	0.46
1:O:40:ALA:HB2	1:O:180:ASP:HA	1.98	0.46
6:T:34:SER:OG	6:T:65:ARG:NH1	2.49	0.46
8:H:48:VAL:HB	8:H:51:ASP:HB2	1.99	0.45
9:I:35:THR:HG22	9:I:37:ASP:H	1.82	0.45
9:I:47:ARG:HG3	9:I:189:ILE:CG2	2.47	0.45
11:K:50:ALA:CB	12:L:127:VAL:HG12	2.46	0.45
13:M:46:ASN:ND2	13:M:48:SER:H	2.13	0.45
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.51	0.45
5:E:168:TYR:OH	5:E:190:ARG:HD2	2.15	0.45
1:O:149:ASP:HB2	1:O:150:PRO:CD	2.46	0.45
1:A:149:ASP:HB2	1:A:150:PRO:CD	2.46	0.45
7:U:72:THR:HG22	7:U:74:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG12	3:C:99:ASP:H	1.82	0.45
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.98	0.45
4:R:149:ASP:HB2	4:R:150:PRO:HD2	1.98	0.45
6:T:75:MET:HE2	6:T:137:LEU:HD21	1.99	0.45
7:U:140:ILE:HG22	7:U:150:VAL:HG22	1.98	0.45
8:V:48:VAL:HB	8:V:51:ASP:HB2	1.97	0.45
9:W:35:THR:HG22	9:W:37:ASP:H	1.81	0.45
6:F:34:SER:OG	6:F:65:ARG:NH1	2.50	0.45
7:G:71:ILE:HG21	7:G:113:LEU:HD11	1.99	0.45
6:T:2:SER:HA	6:T:21:PHE:CE2	2.52	0.45
9:W:153:TRP:CH2	9:W:155:PRO:HA	2.51	0.45
10:X:24:ASN:CG	10:X:25:ILE:H	2.20	0.45
1:A:83:ARG:NH2	7:G:157:GLY:O	2.50	0.45
2:B:214:THR:HG22	19:B:434:HOH:O	2.17	0.45
11:K:154:ASP:O	11:K:158:ARG:HB2	2.16	0.45
6:T:3:ILE:HD12	6:T:15:SER:HB2	1.99	0.45
7:U:142:ILE:HD13	7:U:221:VAL:HA	1.97	0.45
12:Z:45:LYS:HB2	12:Z:203:ILE:HD13	1.97	0.45
1:A:73:LEU:HD21	1:A:135:ILE:HG12	1.99	0.45
11:K:4:LEU:CD2	11:K:159:ALA:HB3	2.46	0.45
7:U:72:THR:HG22	7:U:73:GLU:N	2.32	0.45
7:U:154:ASP:HB3	7:U:156:ALA:H	1.82	0.45
4:D:83:LYS:HD2	4:D:111:LEU:HD11	1.99	0.45
14:N:78:ALA:O	14:N:82:VAL:HG13	2.17	0.45
7:U:195:GLU:HG2	7:U:241:LEU:HG	1.99	0.45
1:A:53:SER:HB3	1:A:56:TYR:CD1	2.52	0.45
2:B:43:LEU:HB2	19:B:434:HOH:O	2.16	0.45
5:E:2:GLN:HE22	6:F:5:THR:N	2.14	0.45
5:E:35:LEU:HD13	5:E:184:LEU:HD22	1.99	0.45
7:G:200:CYS:O	7:G:204:VAL:HG23	2.17	0.45
12:L:123:SER:CB	12:L:136:LYS:HG2	2.47	0.45
11:Y:113:TYR:HD2	11:Y:121:LEU:HD12	1.82	0.45
3:C:107:THR:HG21	3:C:144:TYR:HB3	1.99	0.44
2:P:32:THR:HG21	2:P:199:THR:HG21	1.99	0.44
9:W:163:PHE:CE1	9:W:197:ARG:HD3	2.51	0.44
12:Z:123:SER:CB	12:Z:136:LYS:HG2	2.47	0.44
13:M:12:LEU:HB2	13:M:23:ALA:HB3	1.99	0.44
7:U:200:CYS:O	7:U:204:VAL:HG23	2.17	0.44
9:W:47:ARG:HG3	9:W:189:ILE:CG2	2.46	0.44
9:W:171:LEU:CD2	9:W:199:LEU:HD13	2.47	0.44
11:Y:11:GLY:HA2	11:Y:104:TRP:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:SER:HA	6:F:21:PHE:CE2	2.52	0.44
11:K:113:TYR:HD2	11:K:121:LEU:HD12	1.82	0.44
13:M:149:LEU:HD11	13:M:175:VAL:HG21	1.99	0.44
13:M:193:THR:OG1	13:M:194:GLU:N	2.50	0.44
7:U:71:ILE:HG21	7:U:113:LEU:HD11	1.99	0.44
12:L:76:LYS:HB2	12:L:76:LYS:HE3	1.87	0.44
13:M:59:ASP:CB	13:M:108:ASN:HD21	2.27	0.44
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.51	0.44
8:V:153:GLU:HG3	8:V:154:LEU:N	2.31	0.44
3:C:119:GLN:HG3	4:D:127:ARG:HG3	1.99	0.44
5:E:154:ARG:NH1	5:E:154:ARG:CG	2.77	0.44
7:U:72:THR:HG21	19:U:424:HOH:O	2.18	0.44
3:C:107:THR:HG23	3:C:132:ILE:HD13	1.99	0.44
9:I:171:LEU:CD2	9:I:199:LEU:HD13	2.47	0.44
2:P:16:ARG:HD2	2:P:21:GLU:OE2	2.18	0.44
3:Q:97:VAL:HG12	3:Q:99:ASP:H	1.82	0.44
9:W:27:PHE:HB3	9:W:35:THR:HB	1.99	0.44
2:B:32:THR:HG21	2:B:199:THR:HG21	1.99	0.44
1:O:53:SER:HB3	1:O:56:TYR:CD1	2.52	0.44
3:Q:107:THR:HG21	3:Q:144:TYR:HB3	1.99	0.44
17:V:301:04C:H37	18:V:302:IOD:I	2.88	0.44
4:D:69:ALA:HB3	4:D:134:LEU:HB2	2.00	0.44
7:G:195:GLU:HG2	7:G:241:LEU:HG	2.00	0.44
10:J:24:ASN:CG	10:J:25:ILE:H	2.20	0.44
2:P:202:VAL:O	2:P:203:SER:HB3	2.18	0.44
9:W:106:PRO:HG2	9:W:123:LEU:HB2	1.99	0.44
2:B:16:ARG:HD2	2:B:21:GLU:OE2	2.18	0.44
2:B:107:GLU:O	2:B:111:THR:OG1	2.34	0.44
3:Q:119:GLN:HG3	4:R:127:ARG:HG3	2.00	0.44
3:Q:224:ILE:HG13	3:Q:225:GLU:N	2.33	0.44
14:N:80:ALA:HA	14:N:100:VAL:HG11	1.98	0.43
5:S:2:GLN:HE22	6:T:5:THR:N	2.16	0.43
4:R:83:LYS:HD2	4:R:111:LEU:HD11	2.00	0.43
1:A:6:SER:O	2:B:126:LYS:NZ	2.51	0.43
1:A:71:ILE:HG21	1:A:109:LEU:HD22	2.01	0.43
7:G:155:PRO:HD3	19:G:425:HOH:O	2.17	0.43
11:K:14:VAL:O	11:K:176:MET:HA	2.18	0.43
3:Q:34:VAL:CG1	3:Q:190:VAL:HG22	2.48	0.43
8:H:63:MET:CE	8:H:74:PRO:HB3	2.48	0.43
9:I:19:VAL:HG23	9:I:189:ILE:HB	2.01	0.43
11:K:164:THR:HG22	11:K:170:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:104:ASN:ND2	19:M:437:HOH:O	2.50	0.43
1:O:68:THR:HG23	1:O:70:HIS:H	1.83	0.43
2:P:123:PHE:HB3	3:Q:123:ARG:HB3	2.00	0.43
1:A:78:MET:CE	1:A:130:GLY:HA3	2.48	0.43
2:B:202:VAL:O	2:B:203:SER:HB3	2.18	0.43
1:O:78:MET:CE	1:O:130:GLY:HA3	2.48	0.43
12:Z:140:SER:HB2	19:Z:423:HOH:O	2.17	0.43
1:A:68:THR:HG23	1:A:70:HIS:H	1.83	0.43
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.30	0.43
3:C:11:PRO:HA	4:D:18:TYR:CD2	2.53	0.43
3:C:25:VAL:HG23	3:C:73:ALA:O	2.19	0.43
6:F:83:ASP:OD2	6:F:129:ARG:NH2	2.52	0.43
9:I:27:PHE:HB3	9:I:35:THR:HB	1.99	0.43
2:P:107:GLU:O	2:P:111:THR:OG1	2.34	0.43
6:T:123:THR:O	7:U:131:ARG:NH1	2.52	0.43
6:T:241:GLU:HA	6:T:244:LYS:NZ	2.33	0.43
1:A:58:GLU:HG2	1:A:205:ASP:HB3	2.01	0.43
5:S:35:LEU:HD13	5:S:184:LEU:HD22	1.99	0.43
8:V:18:THR:HB	8:V:30:SER:HA	2.01	0.43
1:A:110:VAL:HG22	1:A:135:ILE:HD13	2.00	0.43
3:C:34:VAL:CG1	3:C:190:VAL:HG22	2.48	0.43
11:K:15:ALA:HB2	11:K:176:MET:HG3	2.00	0.43
1:O:162:MET:HA	1:O:166:TYR:HB2	2.00	0.43
3:Q:25:VAL:O	3:Q:161:GLY:HA2	2.19	0.43
5:S:23:MET:HA	5:S:146:PRO:HG2	2.01	0.43
9:I:29:ILE:O	9:I:31:ALA:N	2.52	0.43
2:P:122:GLN:HG3	3:Q:124:ARG:HG3	2.01	0.43
3:C:25:VAL:O	3:C:161:GLY:HA2	2.19	0.43
7:G:85:ASP:OD1	7:G:131:ARG:NH2	2.52	0.43
1:O:73:LEU:HD21	1:O:135:ILE:HG12	1.99	0.43
11:Y:38:ASN:HB3	11:Y:39:PRO:HD2	2.01	0.43
1:A:55:LEU:HD21	7:G:178:LEU:HB3	2.01	0.42
2:B:123:PHE:HB3	3:C:123:ARG:HB3	2.00	0.42
2:B:228:LYS:O	2:B:232:VAL:HG23	2.19	0.42
5:E:23:MET:HA	5:E:146:PRO:HG2	2.01	0.42
10:J:16:ALA:HA	10:J:179:SER:O	2.18	0.42
17:K:301:04C:H41	17:K:301:04C:H29	1.85	0.42
13:M:94:ARG:HA	13:M:94:ARG:NE	2.34	0.42
3:Q:107:THR:HG23	3:Q:132:ILE:HD13	1.99	0.42
4:R:69:ALA:HB3	4:R:134:LEU:HB2	2.00	0.42
7:U:85:ASP:OD1	7:U:131:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:14:VAL:O	11:Y:176:MET:HA	2.18	0.42
11:Y:15:ALA:HB2	11:Y:176:MET:HG3	2.00	0.42
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	2.01	0.42
1:A:127:ARG:HG3	7:G:126:GLN:HG3	2.01	0.42
5:E:102:VAL:O	5:E:106:VAL:HG23	2.19	0.42
2:P:228:LYS:O	2:P:232:VAL:HG23	2.19	0.42
9:W:70:LEU:HD11	9:W:81:ILE:HG21	2.01	0.42
3:C:224:ILE:HG13	3:C:225:GLU:N	2.33	0.42
4:D:190:SER:O	4:D:194:LEU:HB2	2.19	0.42
9:I:70:LEU:HD11	9:I:81:ILE:HG21	2.01	0.42
4:R:190:SER:O	4:R:194:LEU:HB2	2.19	0.42
5:S:102:VAL:O	5:S:106:VAL:HG23	2.18	0.42
8:V:122:LEU:HD13	8:V:125:THR:HB	2.01	0.42
9:W:19:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
10:X:16:ALA:HA	10:X:179:SER:O	2.19	0.42
2:B:33:CYS:HB3	2:B:163:ILE:HD12	2.02	0.42
7:G:72:THR:HG22	7:G:73:GLU:N	2.34	0.42
1:O:55:LEU:HG	7:U:179:GLU:HG3	2.01	0.42
1:O:110:VAL:HG22	1:O:135:ILE:HD13	2.00	0.42
6:F:99:ARG:NH1	13:M:69:GLN:OE1	2.52	0.42
7:G:154:ASP:HB3	7:G:156:ALA:H	1.83	0.42
2:P:13:PRO:HA	3:Q:20:TYR:CD2	2.53	0.42
7:U:113:LEU:O	7:U:117:ILE:HG12	2.19	0.42
11:Y:164:THR:HG22	11:Y:170:SER:HB3	2.01	0.42
3:C:147:ASP:HB2	3:C:148:PRO:HD2	2.01	0.42
1:O:58:GLU:HG2	1:O:205:ASP:HB3	2.01	0.42
2:P:33:CYS:HB3	2:P:163:ILE:HD12	2.02	0.42
3:Q:11:PRO:HA	4:R:18:TYR:CE2	2.54	0.42
7:U:71:ILE:HD11	7:U:77:CYS:SG	2.60	0.42
11:Y:102:CYS:SG	11:Y:111:LEU:HD13	2.60	0.42
1:A:147:GLN:HG3	1:A:162:MET:CE	2.50	0.42
1:A:162:MET:HA	1:A:166:TYR:HB2	2.00	0.42
1:A:198:PHE:O	1:A:199:GLU:HB2	2.20	0.42
8:H:18:THR:HB	8:H:30:SER:HA	2.01	0.42
3:Q:25:VAL:HG23	3:Q:73:ALA:O	2.19	0.42
7:U:49:ILE:HG21	7:U:78:VAL:HB	2.01	0.42
9:W:29:ILE:O	9:W:31:ALA:N	2.52	0.42
11:Y:64:ARG:HD3	11:Y:64:ARG:HA	1.88	0.42
9:I:6:ASN:ND2	9:I:56:ALA:H	2.18	0.42
17:K:301:04C:O13	18:K:302:IOD:I	3.08	0.42
5:S:69:ILE:HG22	5:S:131:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:GLN:HG3	6:F:129:ARG:HG3	2.01	0.42
7:G:71:ILE:HD11	7:G:77:CYS:SG	2.60	0.42
8:H:77:ALA:O	8:H:80:THR:HG22	2.19	0.42
5:S:118:GLN:HG3	6:T:129:ARG:HG3	2.02	0.42
7:U:49:ILE:CG2	7:U:78:VAL:HB	2.50	0.42
5:E:46:LEU:HB2	5:E:192:LEU:HD11	2.02	0.42
6:F:75:MET:HE2	6:F:137:LEU:HD21	2.02	0.42
9:I:183:GLY:HA2	9:I:201:ALA:HB3	2.02	0.42
10:J:4:LEU:HB2	10:J:132:HIS:HB2	2.02	0.42
3:Q:147:ASP:HB2	3:Q:148:PRO:HD2	2.01	0.42
9:W:6:ASN:ND2	9:W:56:ALA:H	2.18	0.42
12:L:136:LYS:HA	12:L:146:GLN:HE22	1.85	0.41
8:V:77:ALA:O	8:V:80:THR:HG22	2.20	0.41
8:H:122:LEU:CD1	8:H:125:THR:HB	2.50	0.41
8:H:126:ALA:HB3	8:H:135:VAL:HG22	2.02	0.41
9:I:1:SER:HB3	9:I:4:SER:HB2	2.02	0.41
4:R:20:ILE:HA	4:R:23:ILE:HD12	2.01	0.41
8:V:173:VAL:HG13	8:V:190:SER:HB3	2.01	0.41
1:A:74:VAL:HG12	1:A:75:TYR:H	1.85	0.41
3:C:94:ARG:HB3	10:J:62:LYS:CE	2.51	0.41
6:F:39:ILE:HG22	6:F:162:GLY:CA	2.46	0.41
7:G:113:LEU:O	7:G:117:ILE:HG12	2.19	0.41
7:G:209:PHE:HB2	7:G:213:GLU:HB2	2.01	0.41
13:M:122:LEU:HG	13:M:137:LEU:HD12	2.02	0.41
14:N:77:LEU:HD22	14:N:81:ASN:ND2	2.35	0.41
1:O:71:ILE:HG21	1:O:109:LEU:HD22	2.01	0.41
1:O:83:ARG:NH2	7:U:157:GLY:O	2.53	0.41
5:S:46:LEU:HB2	5:S:192:LEU:HD11	2.02	0.41
8:V:122:LEU:CD1	8:V:125:THR:HB	2.49	0.41
10:X:4:LEU:HB2	10:X:132:HIS:HB2	2.02	0.41
6:F:113:ASP:O	6:F:117:MET:HG2	2.20	0.41
11:K:3:THR:HG22	11:K:100:MET:HE2	2.02	0.41
11:K:102:CYS:SG	11:K:111:LEU:HD13	2.60	0.41
13:M:46:ASN:HD21	13:M:49:THR:CG2	2.33	0.41
5:E:2:GLN:HE22	6:F:5:THR:H	1.68	0.41
9:I:90:VAL:HG21	9:I:108:ILE:HD11	2.03	0.41
9:I:106:PRO:HG2	9:I:123:LEU:HB2	2.02	0.41
11:K:38:ASN:HB3	11:K:39:PRO:HD2	2.01	0.41
4:R:20:ILE:HD13	4:R:150:PRO:HD2	2.02	0.41
7:U:53:LYS:HB2	7:U:215:GLU:HG3	2.03	0.41
7:U:106:TYR:OH	8:V:66:HIS:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:50:ALA:CB	12:Z:127:VAL:HG12	2.51	0.41
3:C:42:LEU:O	3:C:207:LEU:HB2	2.21	0.41
1:O:83:ARG:HH11	1:O:83:ARG:CG	2.29	0.41
3:Q:42:LEU:O	3:Q:207:LEU:HB2	2.21	0.41
3:Q:94:ARG:HB3	10:X:62:LYS:CE	2.51	0.41
6:T:39:ILE:HG22	6:T:162:GLY:CA	2.45	0.41
8:V:7:VAL:HG22	8:V:12:VAL:HG12	2.02	0.41
1:A:142:ARG:HA	1:A:143:PRO:HD3	1.95	0.41
3:C:25:VAL:HG21	3:C:129:SER:CB	2.50	0.41
7:G:49:ILE:HG21	7:G:78:VAL:HB	2.02	0.41
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.01	0.41
7:U:209:PHE:HB2	7:U:213:GLU:HB2	2.01	0.41
9:W:117:LYS:HA	9:W:118:PRO:HD3	1.92	0.41
2:B:157:GLY:HA3	3:C:57:THR:HG21	2.02	0.41
3:C:47:LYS:HE3	3:C:206:GLU:HB2	2.03	0.41
4:D:174:GLN:HE21	5:E:52:GLU:HG2	1.85	0.41
7:G:51:THR:OG1	7:G:78:VAL:HG21	2.20	0.41
8:H:173:VAL:HG13	8:H:190:SER:HB3	2.02	0.41
12:L:28:ARG:NH2	19:L:425:HOH:O	2.52	0.41
9:W:183:GLY:HA2	9:W:201:ALA:HB3	2.03	0.41
9:I:144:GLN:HE21	9:I:144:GLN:N	2.16	0.41
10:J:43:LEU:HD12	10:J:183:ILE:HD11	2.02	0.41
10:J:119:ASP:HB3	10:J:121:LEU:H	1.85	0.41
13:M:43:MET:SD	13:M:64:LYS:HG3	2.60	0.41
14:N:41:ILE:HD13	14:N:79:ALA:HB2	2.02	0.41
1:O:68:THR:HG22	1:O:71:ILE:HB	2.03	0.41
1:O:74:VAL:HG12	1:O:75:TYR:H	1.85	0.41
2:P:179:LYS:O	2:P:183:MET:HG2	2.21	0.41
7:U:51:THR:OG1	7:U:78:VAL:HG21	2.21	0.41
8:V:19:ARG:HG3	8:V:26:VAL:HG13	2.03	0.41
9:W:90:VAL:HG21	9:W:108:ILE:HD11	2.03	0.41
3:C:118:THR:O	4:D:127:ARG:NH1	2.54	0.41
3:C:169:GLU:HA	3:C:172:GLU:HG3	2.03	0.41
8:V:126:ALA:HB3	8:V:135:VAL:HG22	2.02	0.41
8:H:7:VAL:HG22	8:H:12:VAL:HG12	2.03	0.40
11:K:82:LEU:O	11:K:86:MET:HG3	2.22	0.40
14:N:143:LYS:O	14:N:146:MET:HG3	2.21	0.40
3:Q:47:LYS:HE3	3:Q:206:GLU:HB2	2.03	0.40
4:R:74:ILE:H	4:R:74:ILE:HD12	1.86	0.40
10:X:169:LYS:HG2	10:X:170:ARG:HG2	2.03	0.40
12:Z:76:LYS:HB2	12:Z:76:LYS:HE3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG23	1:A:226:ARG:HH21	1.86	0.40
3:C:91:GLN:HE21	10:J:62:LYS:HG3	1.85	0.40
4:D:20:ILE:HA	4:D:23:ILE:HD12	2.01	0.40
12:L:180:ILE:HA	19:L:429:HOH:O	2.20	0.40
1:O:147:GLN:HG3	1:O:162:MET:CE	2.50	0.40
1:O:223:THR:HG23	1:O:226:ARG:HH21	1.86	0.40
10:X:43:LEU:HD12	10:X:183:ILE:HD11	2.03	0.40
1:A:14:PRO:HA	2:B:22:TYR:CD2	2.57	0.40
2:B:179:LYS:O	2:B:183:MET:HG2	2.21	0.40
3:C:211:ARG:H	3:C:211:ARG:HG2	1.73	0.40
6:F:111:LEU:O	6:F:115:VAL:HG23	2.21	0.40
7:G:49:ILE:CG2	7:G:78:VAL:HB	2.51	0.40
11:K:120:ARG:HG3	19:K:406:HOH:O	2.21	0.40
14:N:45:LEU:HG	19:N:310:HOH:O	2.21	0.40
2:P:23:ALA:O	2:P:27:ILE:HD12	2.21	0.40
6:T:215:TRP:HB3	6:T:220:THR:HG21	2.04	0.40
8:V:137:LEU:HD13	8:V:141:ARG:HE	1.86	0.40
9:W:1:SER:HB3	9:W:4:SER:HB2	2.02	0.40
12:Z:136:LYS:HA	12:Z:146:GLN:HE22	1.85	0.40
1:A:68:THR:HG22	1:A:71:ILE:HB	2.03	0.40
4:D:20:ILE:HD13	4:D:150:PRO:HD2	2.02	0.40
5:E:69:ILE:HG22	5:E:131:ILE:HG12	2.02	0.40
3:Q:145:GLN:HG2	3:Q:158:ASN:HD22	1.86	0.40
6:T:113:ASP:O	6:T:117:MET:HG2	2.20	0.40
10:X:161:ARG:HE	10:X:161:ARG:HB2	1.49	0.40
12:Z:13:LEU:HD11	12:Z:149:LEU:CD1	2.47	0.40
12:Z:176:LYS:O	12:Z:180:ILE:HG13	2.22	0.40
3:C:94:ARG:HB3	10:J:62:LYS:HE3	2.03	0.40
12:L:31:GLU:HB2	12:L:36:HIS:CD2	2.56	0.40
1:O:198:PHE:O	1:O:199:GLU:HB2	2.20	0.40
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:146:ASP:O	13:M:206:GLN:NE2[2_655]	2.08	0.12

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	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	12	37
1	O	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	12	37
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	66
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	66
3	C	236/248 (95%)	222 (94%)	14 (6%)	0	100	100
3	Q	236/248 (95%)	221 (94%)	15 (6%)	0	100	100
4	D	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	34	66
4	R	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	34	66
5	E	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
5	S	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
6	F	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	34	66
6	T	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	34	66
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
7	U	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
8	H	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	17	48
8	V	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	17	48
9	I	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	45
9	W	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	45
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	29	61
10	X	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	29	61
11	K	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
11	Y	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
12	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
12	Z	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
14	b	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
All	All	6188/6446 (96%)	5953 (96%)	213 (3%)	22 (0%)	34	66

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
9	I	30	GLN
6	T	216	VAL
9	W	30	GLN
1	A	40	ALA
1	A	198	PHE
1	A	199	GLU
2	B	203	SER
10	J	24	ASN
1	O	40	ALA
1	O	198	PHE
1	O	199	GLU
2	P	203	SER
10	X	24	ASN
4	D	112	ALA
9	I	47	ARG
4	R	112	ALA
9	W	47	ARG
8	H	195	PRO
8	V	195	PRO
8	H	194	GLU
8	V	194	GLU

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	189/191 (99%)	175 (93%)	14 (7%)	13	38
1	O	189/191 (99%)	174 (92%)	15 (8%)	12	34
2	B	208/221 (94%)	190 (91%)	18 (9%)	10	30
2	P	208/221 (94%)	190 (91%)	18 (9%)	10	30
3	C	202/211 (96%)	178 (88%)	24 (12%)	5	15
3	Q	202/211 (96%)	178 (88%)	24 (12%)	5	15
4	D	195/203 (96%)	186 (95%)	9 (5%)	27	60
4	R	195/203 (96%)	186 (95%)	9 (5%)	27	60
5	E	204/224 (91%)	191 (94%)	13 (6%)	17	45
5	S	204/224 (91%)	191 (94%)	13 (6%)	17	45
6	F	200/211 (95%)	189 (94%)	11 (6%)	21	53
6	T	200/211 (95%)	189 (94%)	11 (6%)	21	53
7	G	207/210 (99%)	197 (95%)	10 (5%)	25	58
7	U	207/210 (99%)	197 (95%)	10 (5%)	25	58
8	H	169/183 (92%)	151 (89%)	18 (11%)	6	20
8	V	169/183 (92%)	151 (89%)	18 (11%)	6	20
9	I	174/175 (99%)	163 (94%)	11 (6%)	18	46
9	W	174/175 (99%)	163 (94%)	11 (6%)	18	46
10	J	166/171 (97%)	158 (95%)	8 (5%)	25	58
10	X	166/171 (97%)	158 (95%)	8 (5%)	25	58
11	K	165/166 (99%)	151 (92%)	14 (8%)	10	31
11	Y	165/166 (99%)	151 (92%)	14 (8%)	10	31
12	L	178/178 (100%)	170 (96%)	8 (4%)	27	61
12	Z	178/178 (100%)	168 (94%)	10 (6%)	21	52
13	M	178/180 (99%)	167 (94%)	11 (6%)	18	47
13	a	178/180 (99%)	167 (94%)	11 (6%)	18	47
14	N	155/155 (100%)	143 (92%)	12 (8%)	13	35
14	b	155/155 (100%)	144 (93%)	11 (7%)	14	40
All	All	5180/5358 (97%)	4816 (93%)	364 (7%)	15	41

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	ARG
1	A	19	VAL
1	A	28	VAL
1	A	54	ILE
1	A	83	ARG
1	A	115	SER
1	A	140	GLU
1	A	189	THR
1	A	201	GLN
1	A	207	ILE
1	A	209	VAL
1	A	226	ARG
1	A	229	LEU
2	B	43	LEU
2	B	49	ARG
2	B	75	VAL
2	B	97	LEU
2	B	111	THR
2	B	163	ILE
2	B	177	ASP
2	B	179	LYS
2	B	182	GLU
2	B	184	THR
2	B	191	LEU
2	B	208	GLU
2	B	216	THR
2	B	217	ARG
2	B	234	GLN
2	B	240	GLU
2	B	242	GLU
2	B	243	GLU
3	C	4	ARG
3	C	34	VAL
3	C	41	VAL
3	C	46	LYS
3	C	56	ARG
3	C	76	THR
3	C	101	VAL
3	C	106	ILE
3	C	124	ARG
3	C	138	ASP
3	C	140	THR

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Mol	Chain	Res	Type
3	C	145	GLN
3	C	162	ARG
3	C	171	LEU
3	C	177	ASP
3	C	185	LEU
3	C	186	THR
3	C	195	LEU
3	C	212	ARG
3	C	217	LYS
3	C	220	ASN
3	C	223	GLU
3	C	231	ILE
3	C	236	GLU
4	D	12	ARG
4	D	28	THR
4	D	118	GLU
4	D	127	ARG
4	D	140	GLU
4	D	183	LEU
4	D	201	LYS
4	D	228	GLU
4	D	229	VAL
5	E	1	ASN
5	E	7	VAL
5	E	35	LEU
5	E	98	ARG
5	E	153	CYS
5	E	154	ARG
5	E	163	GLN
5	E	179	CYS
5	E	180	ASN
5	E	184	LEU
5	E	204	THR
5	E	206	ASN
5	E	226	VAL
6	F	30	VAL
6	F	37	ILE
6	F	66	LEU
6	F	129	ARG
6	F	133	CYS
6	F	181	MET
6	F	203	GLU

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Mol	Chain	Res	Type
6	F	205	LYS
6	F	214	SER
6	F	225	GLU
6	F	230	ASP
7	G	59	LEU
7	G	74	SER
7	G	80	THR
7	G	103	LYS
7	G	111	ASP
7	G	113	LEU
7	G	131	ARG
7	G	178	LEU
7	G	209	PHE
7	G	222	GLU
8	H	6	LEU
8	H	21	THR
8	H	23	ASP
8	H	32	GLU
8	H	40	LYS
8	H	56	THR
8	H	68	LEU
8	H	76	VAL
8	H	100	VAL
8	H	119	TYR
8	H	122	LEU
8	H	127	LEU
8	H	155	LEU
8	H	173	VAL
8	H	185	LEU
8	H	193	THR
8	H	197	GLN
8	H	216	VAL
9	I	33	MET
9	I	67	LYS
9	I	84	TYR
9	I	115	THR
9	I	116	PHE
9	I	117	LYS
9	I	131	VAL
9	I	142	SER
9	I	144	GLN
9	I	171	LEU

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Mol	Chain	Res	Type
9	I	192	ASP
10	J	1	MET
10	J	8	GLN
10	J	47	VAL
10	J	84	THR
10	J	85	ARG
10	J	86	ARG
10	J	143	LEU
10	J	161	ARG
11	K	9	GLN
11	K	13	ILE
11	K	27	SER
11	K	29	LEU
11	K	30	ARG
11	K	35	ILE
11	K	64	ARG
11	K	82	LEU
11	K	87	MET
11	K	88	LEU
11	K	115	ASP
11	K	121	LEU
11	K	139	MET
11	K	158	ARG
12	L	31	GLU
12	L	45	LYS
12	L	63	THR
12	L	133	ASP
12	L	160	ASN
12	L	162	GLU
12	L	166	LEU
12	L	173	ARG
13	M	3	ASN
13	M	35	ARG
13	M	44	ARG
13	M	46	ASN
13	M	49	THR
13	M	94	ARG
13	M	100	ARG
13	M	109	THR
13	M	152	GLU
13	M	168	LEU
13	M	192	VAL

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Mol	Chain	Res	Type
14	N	20	VAL
14	N	27	VAL
14	N	28	ASN
14	N	37	LEU
14	N	58	MET
14	N	77	LEU
14	N	82	VAL
14	N	100	VAL
14	N	143	LYS
14	N	153	ARG
14	N	191	ASP
14	N	199	GLU
1	O	2	LYS
1	O	3	ARG
1	O	19	VAL
1	O	28	VAL
1	O	54	ILE
1	O	59	ARG
1	O	83	ARG
1	O	115	SER
1	O	140	GLU
1	O	189	THR
1	O	201	GLN
1	O	207	ILE
1	O	209	VAL
1	O	226	ARG
1	O	229	LEU
2	P	43	LEU
2	P	49	ARG
2	P	75	VAL
2	P	97	LEU
2	P	111	THR
2	P	163	ILE
2	P	177	ASP
2	P	179	LYS
2	P	182	GLU
2	P	184	THR
2	P	191	LEU
2	P	208	GLU
2	P	216	THR
2	P	217	ARG
2	P	234	GLN

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Mol	Chain	Res	Type
2	P	240	GLU
2	P	242	GLU
2	P	243	GLU
3	Q	4	ARG
3	Q	34	VAL
3	Q	41	VAL
3	Q	46	LYS
3	Q	56	ARG
3	Q	76	THR
3	Q	101	VAL
3	Q	106	ILE
3	Q	124	ARG
3	Q	138	ASP
3	Q	140	THR
3	Q	145	GLN
3	Q	162	ARG
3	Q	171	LEU
3	Q	177	ASP
3	Q	185	LEU
3	Q	186	THR
3	Q	195	LEU
3	Q	212	ARG
3	Q	217	LYS
3	Q	220	ASN
3	Q	223	GLU
3	Q	231	ILE
3	Q	236	GLU
4	R	12	ARG
4	R	28	THR
4	R	118	GLU
4	R	127	ARG
4	R	140	GLU
4	R	183	LEU
4	R	201	LYS
4	R	228	GLU
4	R	229	VAL
5	S	1	ASN
5	S	7	VAL
5	S	35	LEU
5	S	98	ARG
5	S	153	CYS
5	S	154	ARG

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Mol	Chain	Res	Type
5	S	163	GLN
5	S	179	CYS
5	S	180	ASN
5	S	184	LEU
5	S	204	THR
5	S	206	ASN
5	S	226	VAL
6	T	30	VAL
6	T	37	ILE
6	T	66	LEU
6	T	129	ARG
6	T	133	CYS
6	T	181	MET
6	T	203	GLU
6	T	205	LYS
6	T	214	SER
6	T	225	GLU
6	T	230	ASP
7	U	59	LEU
7	U	74	SER
7	U	80	THR
7	U	83	THR
7	U	111	ASP
7	U	113	LEU
7	U	131	ARG
7	U	178	LEU
7	U	209	PHE
7	U	222	GLU
8	V	6	LEU
8	V	21	THR
8	V	23	ASP
8	V	32	GLU
8	V	40	LYS
8	V	56	THR
8	V	68	LEU
8	V	76	VAL
8	V	100	VAL
8	V	119	TYR
8	V	122	LEU
8	V	127	LEU
8	V	155	LEU
8	V	173	VAL

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Mol	Chain	Res	Type
8	V	185	LEU
8	V	193	THR
8	V	197	GLN
8	V	216	VAL
9	W	33	MET
9	W	67	LYS
9	W	84	TYR
9	W	115	THR
9	W	116	PHE
9	W	123	LEU
9	W	131	VAL
9	W	142	SER
9	W	144	GLN
9	W	171	LEU
9	W	192	ASP
10	X	1	MET
10	X	8	GLN
10	X	47	VAL
10	X	84	THR
10	X	85	ARG
10	X	86	ARG
10	X	143	LEU
10	X	161	ARG
11	Y	9	GLN
11	Y	13	ILE
11	Y	27	SER
11	Y	29	LEU
11	Y	30	ARG
11	Y	35	ILE
11	Y	64	ARG
11	Y	82	LEU
11	Y	87	MET
11	Y	88	LEU
11	Y	115	ASP
11	Y	121	LEU
11	Y	139	MET
11	Y	158	ARG
12	Z	31	GLU
12	Z	45	LYS
12	Z	63	THR
12	Z	133	ASP
12	Z	160	ASN

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Mol	Chain	Res	Type
12	Z	162	GLU
12	Z	166	LEU
12	Z	173	ARG
12	Z	180	ILE
12	Z	212	LYS
13	a	3	ASN
13	a	35	ARG
13	a	44	ARG
13	a	46	ASN
13	a	49	THR
13	a	94	ARG
13	a	100	ARG
13	a	109	THR
13	a	152	GLU
13	a	168	LEU
13	a	192	VAL
14	b	27	VAL
14	b	28	ASN
14	b	37	LEU
14	b	58	MET
14	b	77	LEU
14	b	82	VAL
14	b	100	VAL
14	b	143	LYS
14	b	153	ARG
14	b	191	ASP
14	b	199	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	139	ASN
1	A	147	GLN
1	A	165	ASN
1	A	206	ASN
2	B	39	ASN
2	B	68	ASN
2	B	87	ASN
2	B	94	GLN
2	B	122	GLN
2	B	154	ASN

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Mol	Chain	Res	Type
2	B	176	GLN
3	C	22	GLN
3	C	91	GLN
3	C	174	ASN
3	C	220	ASN
4	D	106	GLN
4	D	174	GLN
4	D	196	GLN
4	D	213	GLN
5	E	2	GLN
5	E	40	HIS
5	E	143	GLN
5	E	163	GLN
5	E	172	HIS
7	G	89	GLN
7	G	126	GLN
8	H	66	HIS
8	H	106	ASN
8	H	143	GLN
8	H	186	GLN
9	I	6	ASN
9	I	39	GLN
9	I	64	GLN
9	I	144	GLN
10	J	8	GLN
10	J	27	GLN
10	J	32	HIS
10	J	61	GLN
10	J	174	ASN
11	K	10	HIS
11	K	117	ASN
11	K	124	GLN
12	L	8	ASN
12	L	58	HIS
12	L	108	ASN
12	L	146	GLN
12	L	152	GLN
12	L	159	GLN
13	M	46	ASN
13	M	104	ASN
13	M	108	ASN
13	M	157	GLN

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Mol	Chain	Res	Type
13	M	208	ASN
14	N	28	ASN
14	N	81	ASN
14	N	157	ASN
1	O	111	GLN
1	O	139	ASN
1	O	147	GLN
1	O	165	ASN
1	O	206	ASN
2	P	39	ASN
2	P	68	ASN
2	P	94	GLN
2	P	122	GLN
2	P	154	ASN
3	Q	22	GLN
3	Q	91	GLN
3	Q	174	ASN
3	Q	220	ASN
4	R	106	GLN
4	R	174	GLN
4	R	196	GLN
4	R	213	GLN
5	S	2	GLN
5	S	40	HIS
5	S	143	GLN
5	S	163	GLN
5	S	172	HIS
7	U	67	HIS
7	U	89	GLN
7	U	126	GLN
8	V	66	HIS
8	V	91	GLN
8	V	106	ASN
8	V	143	GLN
8	V	186	GLN
9	W	6	ASN
9	W	39	GLN
9	W	64	GLN
9	W	80	GLN
9	W	144	GLN
10	X	27	GLN
10	X	61	GLN

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Mol	Chain	Res	Type
10	X	132	HIS
10	X	174	ASN
11	Y	10	HIS
11	Y	38	ASN
11	Y	117	ASN
11	Y	124	GLN
12	Z	8	ASN
12	Z	58	HIS
12	Z	108	ASN
12	Z	146	GLN
12	Z	151	ASN
13	a	46	ASN
13	a	104	ASN
13	a	108	ASN
13	a	157	GLN
13	a	208	ASN
14	b	28	ASN
14	b	38	HIS
14	b	66	HIS
14	b	81	ASN
14	b	97	HIS
14	b	157	ASN

5.3.3 RNA (i)

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 60 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	04C	K	301	11	44,44,44	1.20	2 (4%)	56,58,58	1.00	2 (3%)
17	04C	V	301	8	44,44,44	1.18	3 (6%)	56,58,58	0.99	5 (8%)
17	04C	b	201	14	44,44,44	1.28	4 (9%)	56,58,58	1.17	6 (10%)
17	04C	Y	301	11	44,44,44	1.23	2 (4%)	56,58,58	1.36	7 (12%)
17	04C	H	301	8	44,44,44	1.14	2 (4%)	56,58,58	0.96	3 (5%)
17	04C	N	201	14	44,44,44	1.24	3 (6%)	56,58,58	1.19	7 (12%)

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
17	04C	K	301	11	-	12/44/52/52	0/3/3/3
17	04C	V	301	8	-	15/44/52/52	0/3/3/3
17	04C	b	201	14	-	11/44/52/52	0/3/3/3
17	04C	Y	301	11	-	15/44/52/52	0/3/3/3
17	04C	H	301	8	-	21/44/52/52	0/3/3/3
17	04C	N	201	14	-	12/44/52/52	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	04C	C10-C9	3.39	1.59	1.53
17	K	301	04C	C10-C9	3.19	1.59	1.53
17	K	301	04C	C12-C10	3.09	1.56	1.52
17	b	201	04C	C10-C9	3.07	1.59	1.53
17	b	201	04C	C12-C10	3.06	1.56	1.52
17	Y	301	04C	C10-C9	3.01	1.58	1.53
17	V	301	04C	C10-C9	2.81	1.58	1.53
17	Y	301	04C	C12-C10	2.80	1.56	1.52
17	H	301	04C	C12-C10	2.77	1.56	1.52
17	b	201	04C	C7-C6	2.76	1.57	1.51
17	V	301	04C	C12-C10	2.65	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	04C	C10-C9	2.60	1.58	1.53
17	N	201	04C	C12-C10	2.57	1.55	1.52
17	N	201	04C	C7-C6	2.44	1.57	1.51
17	V	301	04C	C9-C8	2.22	1.57	1.53
17	b	201	04C	C9-C8	2.12	1.57	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	04C	C32-N31-C36	4.61	119.20	108.83
17	b	201	04C	C11-C10-C12	-4.28	104.25	109.88
17	Y	301	04C	C33-C32-N31	4.27	116.58	110.10
17	K	301	04C	C11-C10-C12	-4.22	104.33	109.88
17	N	201	04C	C11-C10-C12	-3.94	104.70	109.88
17	Y	301	04C	C35-C36-N31	3.93	116.06	110.10
17	N	201	04C	C6-C7-C8	3.48	119.37	113.33
17	H	301	04C	C11-C10-C12	-3.29	105.55	109.88
17	V	301	04C	C11-C10-C12	-3.17	105.71	109.88
17	Y	301	04C	C11-C10-C12	-2.76	106.25	109.88
17	H	301	04C	C7-C8-N22	-2.66	106.19	110.07
17	Y	301	04C	C6-C7-C8	2.62	117.88	113.33
17	N	201	04C	C40-C24-N25	-2.59	105.33	110.79
17	V	301	04C	C7-C8-N22	-2.56	106.33	110.07
17	b	201	04C	C6-C7-C8	2.38	117.47	113.33
17	N	201	04C	C12-C10-C9	2.36	115.47	110.99
17	Y	301	04C	C7-C8-N22	-2.36	106.63	110.07
17	b	201	04C	C40-C24-N25	-2.30	105.94	110.79
17	b	201	04C	C12-C10-C9	2.25	115.26	110.99
17	b	201	04C	C30-N31-C32	2.24	114.57	111.09
17	V	301	04C	C6-C7-C8	2.18	117.13	113.33
17	N	201	04C	C7-C8-C9	-2.17	106.65	111.11
17	V	301	04C	C30-N31-C36	2.16	114.45	111.09
17	H	301	04C	C32-N31-C36	2.15	113.66	108.83
17	b	201	04C	C30-N31-C36	2.08	114.32	111.09
17	K	301	04C	C32-N31-C36	2.08	113.51	108.83
17	Y	301	04C	C7-C8-C9	-2.08	106.84	111.11
17	V	301	04C	O37-C29-C30	-2.07	117.46	121.08
17	N	201	04C	C7-C8-N22	-2.06	107.07	110.07
17	N	201	04C	C32-N31-C36	2.02	113.37	108.83

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	04C	C6-C7-C8-N22
17	H	301	04C	C6-C7-C8-C9
17	H	301	04C	C11-C10-C9-O21
17	H	301	04C	C9-C10-C12-O13
17	H	301	04C	C11-C10-C12-O13
17	K	301	04C	C30-C29-N28-C27
17	K	301	04C	C6-C7-C8-N22
17	K	301	04C	C6-C7-C8-C9
17	N	201	04C	C9-C10-C12-O13
17	N	201	04C	C11-C10-C12-O13
17	V	301	04C	C6-C7-C8-C9
17	V	301	04C	C11-C10-C9-O21
17	Y	301	04C	C6-C7-C8-N22
17	Y	301	04C	C6-C7-C8-C9
17	Y	301	04C	C11-C10-C9-C8
17	Y	301	04C	C12-C10-C9-C8
17	b	201	04C	C9-C10-C12-O13
17	b	201	04C	C11-C10-C12-O13
17	H	301	04C	C47-C44-O45-C46
17	H	301	04C	C43-C44-O45-C46
17	K	301	04C	C47-C44-O45-C46
17	N	201	04C	C47-C44-O45-C46
17	Y	301	04C	C47-C44-O45-C46
17	Y	301	04C	C43-C44-O45-C46
17	K	301	04C	O37-C29-N28-C27
17	K	301	04C	C43-C44-O45-C46
17	N	201	04C	C43-C44-O45-C46
17	V	301	04C	C47-C44-O45-C46
17	V	301	04C	C43-C44-O45-C46
17	b	201	04C	C43-C44-O45-C46
17	b	201	04C	C47-C44-O45-C46
17	b	201	04C	C23-C24-C40-C41
17	b	201	04C	N25-C24-C40-C41
17	H	301	04C	N25-C24-C40-C41
17	H	301	04C	C23-C24-C40-C41
17	K	301	04C	C23-C24-C40-C41
17	V	301	04C	C5-C6-C7-C8
17	Y	301	04C	C5-C6-C7-C8
17	V	301	04C	N25-C24-C40-C41
17	V	301	04C	C1-C6-C7-C8
17	K	301	04C	C1-C6-C7-C8
17	K	301	04C	N25-C24-C40-C41
17	K	301	04C	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	Y	301	04C	C1-C6-C7-C8
17	Y	301	04C	C11-C10-C9-O21
17	H	301	04C	C11-C10-C9-C8
17	V	301	04C	C11-C10-C9-C8
17	V	301	04C	C6-C7-C8-N22
17	H	301	04C	O37-C29-C30-N31
17	V	301	04C	C29-C30-N31-C32
17	H	301	04C	N28-C29-C30-N31
17	V	301	04C	N28-C29-C30-N31
17	V	301	04C	C23-C24-C40-C41
17	H	301	04C	C1-C6-C7-C8
17	V	301	04C	O37-C29-C30-N31
17	H	301	04C	C5-C6-C7-C8
17	Y	301	04C	C12-C10-C9-O21
17	b	201	04C	C11-C10-C9-O21
17	H	301	04C	C29-C30-N31-C36
17	H	301	04C	C29-C30-N31-C32
17	N	201	04C	C29-C30-N31-C36
17	N	201	04C	C29-C30-N31-C32
17	V	301	04C	C29-C30-N31-C36
17	N	201	04C	C1-C6-C7-C8
17	b	201	04C	C1-C6-C7-C8
17	N	201	04C	C5-C6-C7-C8
17	b	201	04C	C5-C6-C7-C8
17	b	201	04C	C11-C10-C9-C8
17	H	301	04C	O49-C23-N22-C8
17	Y	301	04C	C29-C30-N31-C32
17	H	301	04C	O39-C26-N25-C24
17	N	201	04C	N25-C24-C40-C41
17	H	301	04C	C23-C24-N25-C26
17	Y	301	04C	O49-C23-N22-C8
17	K	301	04C	C26-C27-N28-C29
17	N	201	04C	N22-C23-C24-N25
17	H	301	04C	C27-C26-N25-C24
17	N	201	04C	O49-C23-C24-N25
17	Y	301	04C	N25-C24-C40-C41
17	H	301	04C	C12-C10-C9-C8
17	V	301	04C	C12-C10-C9-C8
17	Y	301	04C	C26-C27-N28-C29
17	N	201	04C	N22-C8-C9-C10
17	b	201	04C	N22-C8-C9-C10
17	K	301	04C	O49-C23-N22-C8

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Mol	Chain	Res	Type	Atoms
17	Y	301	04C	C23-C24-C40-C41

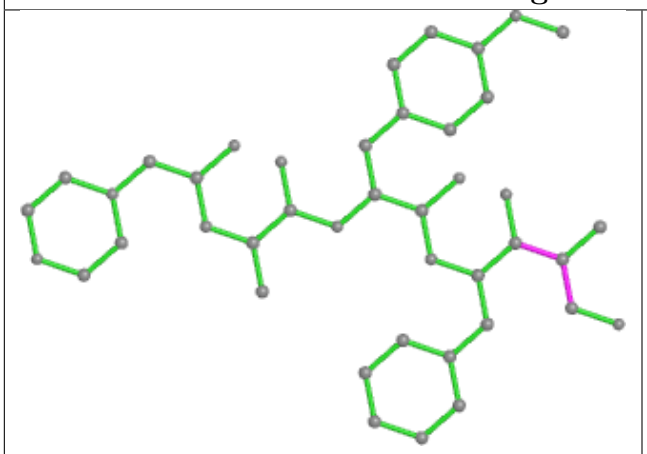
There are no ring outliers.

4 monomers are involved in 10 short contacts:

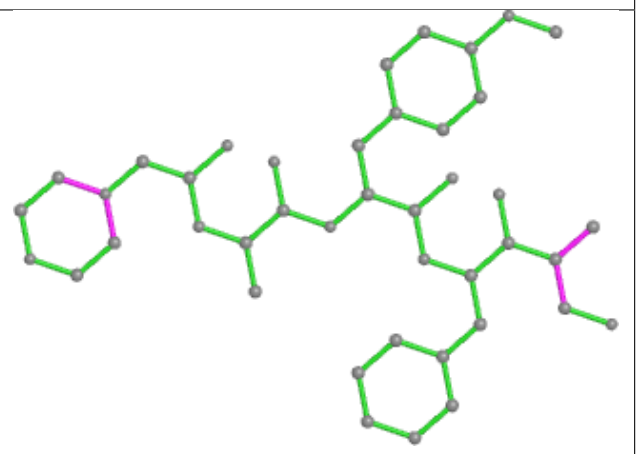
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	04C	3	0
17	V	301	04C	1	0
17	Y	301	04C	3	0
17	N	201	04C	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

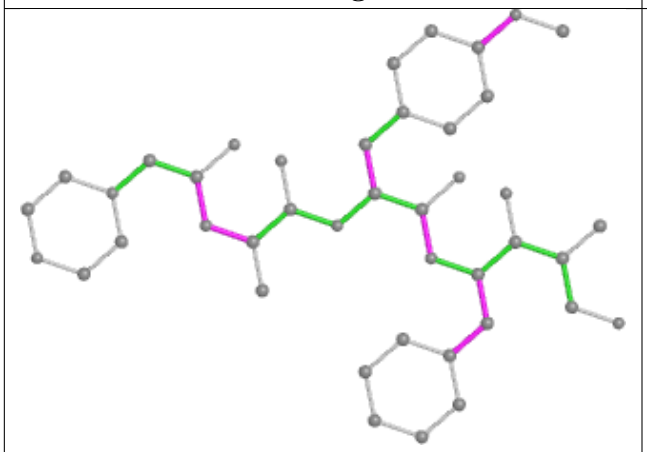
Ligand 04C K 301



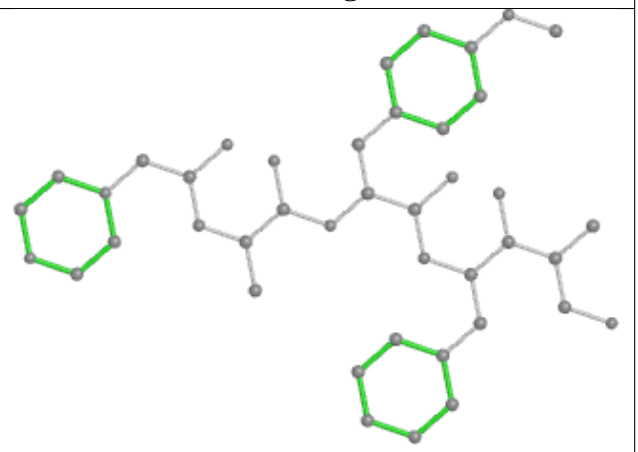
Bond lengths



Bond angles

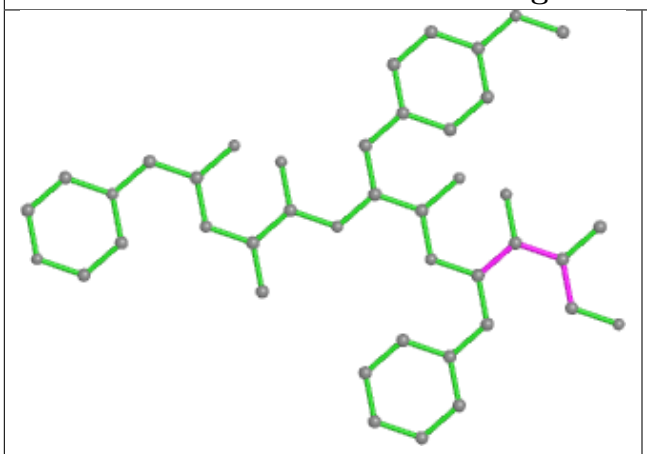


Torsions

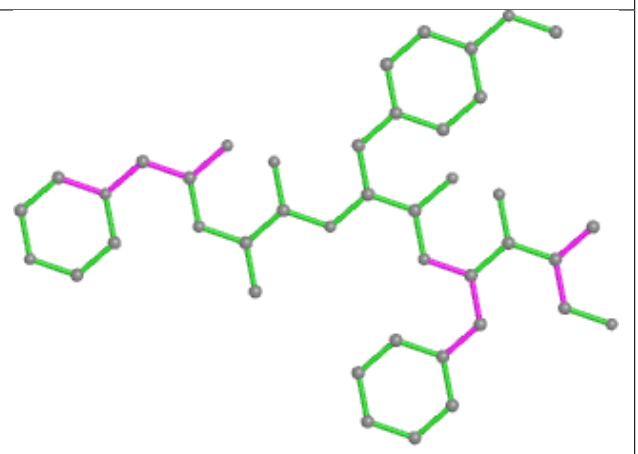


Rings

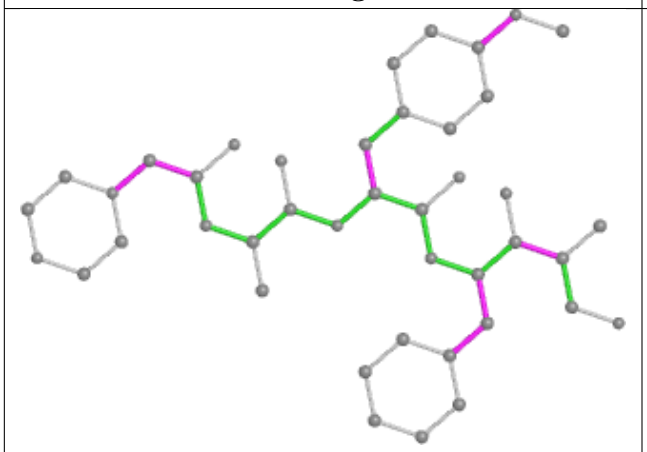
Ligand 04C V 301



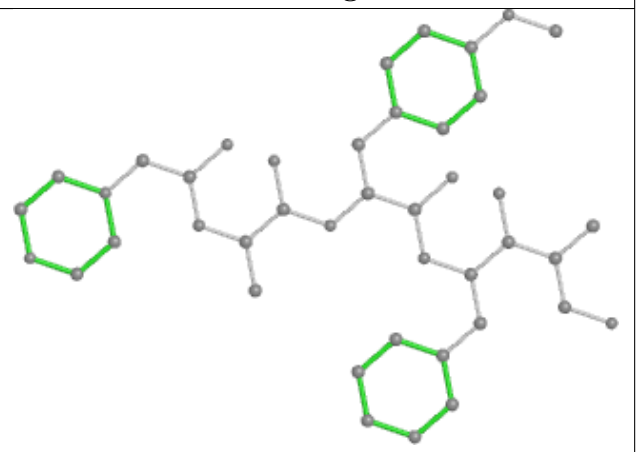
Bond lengths



Bond angles

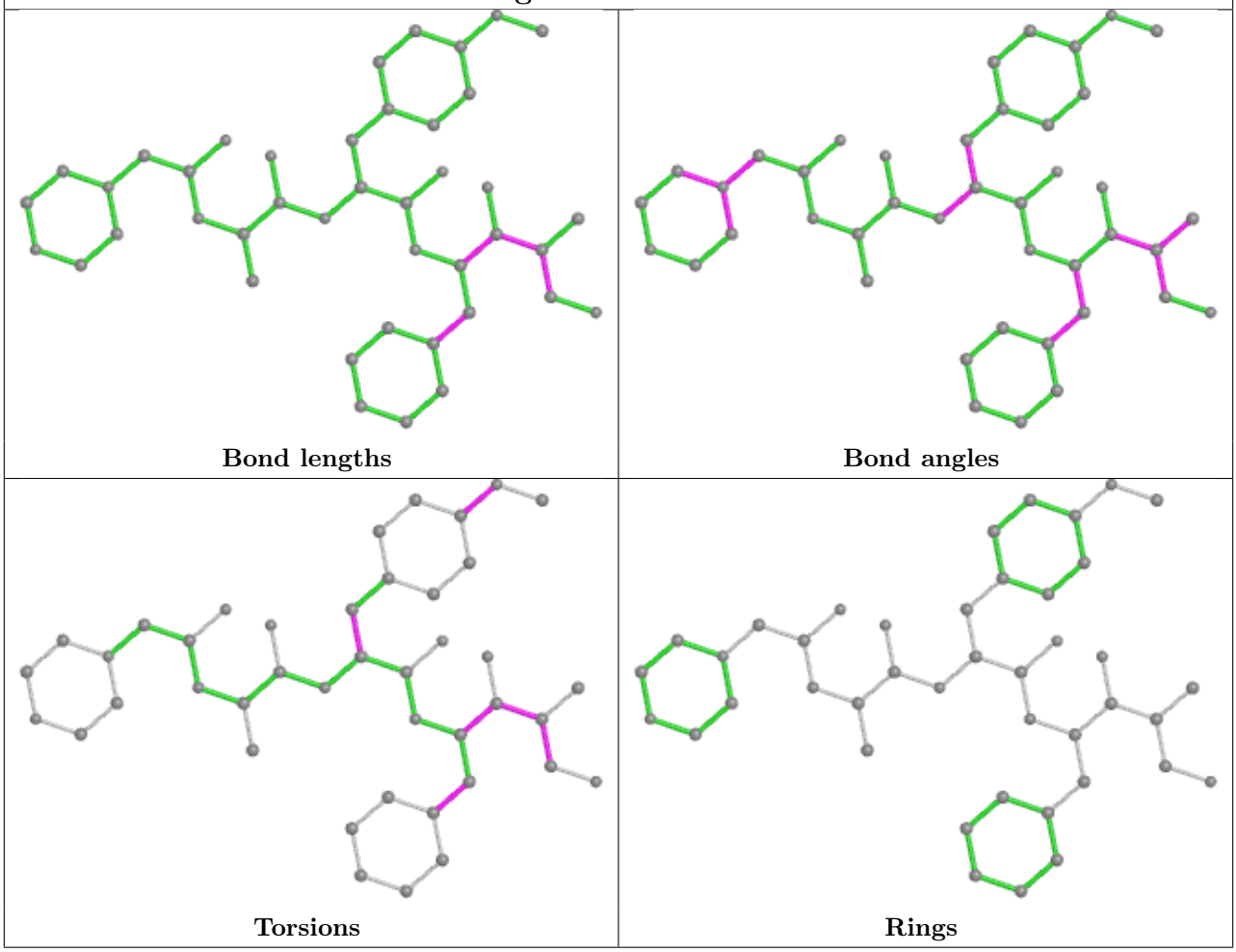


Torsions

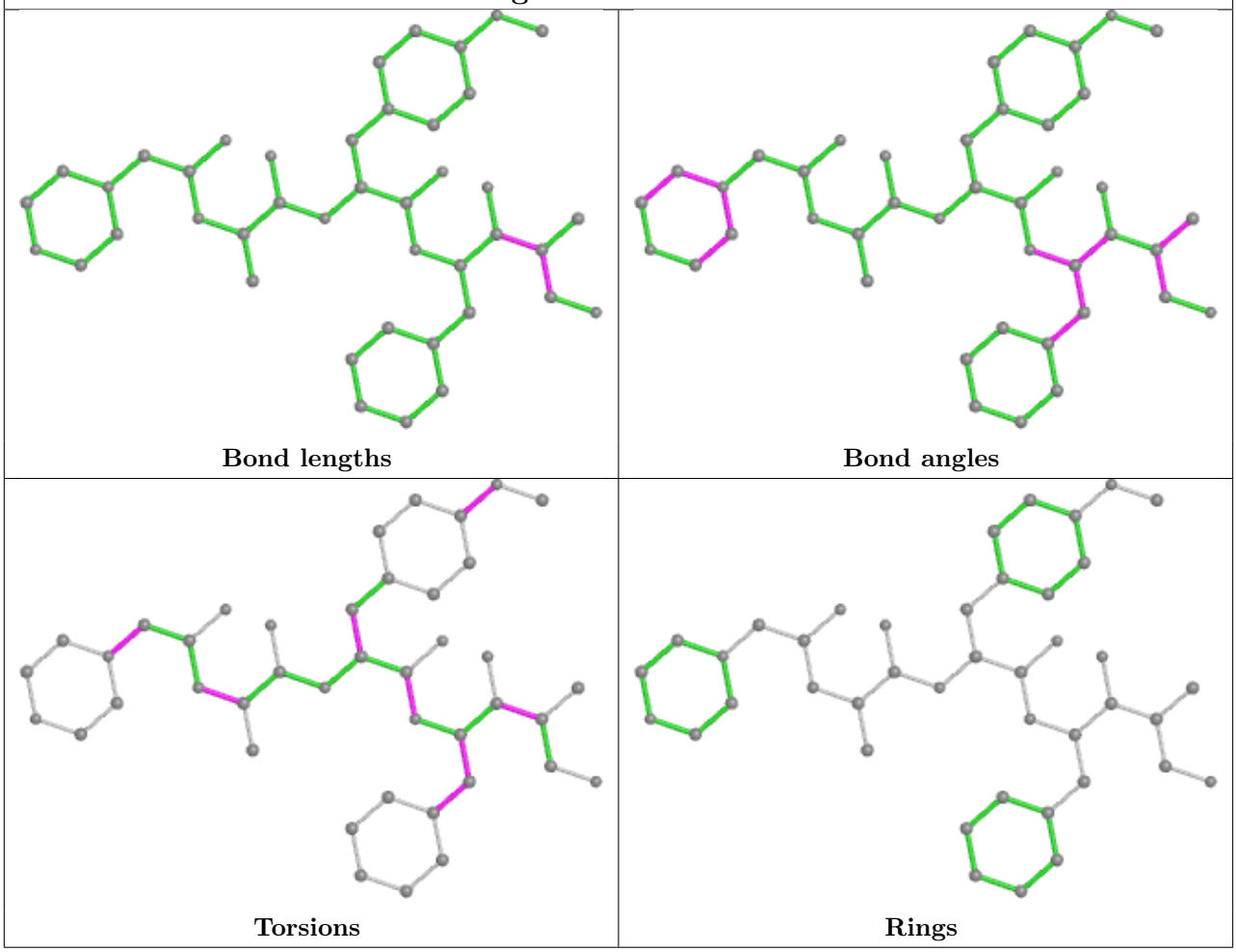


Rings

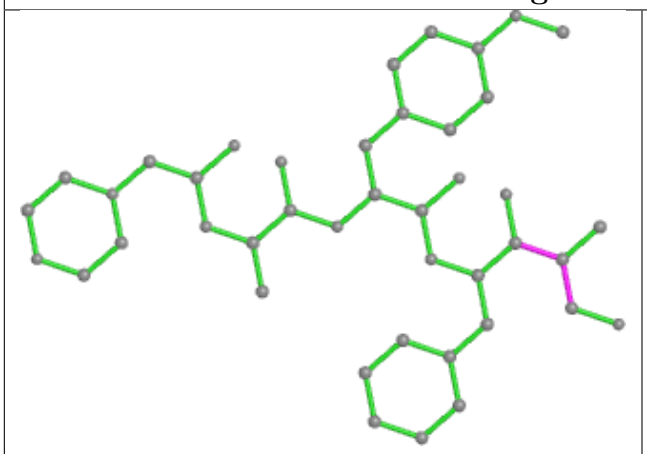
Ligand 04C b 201



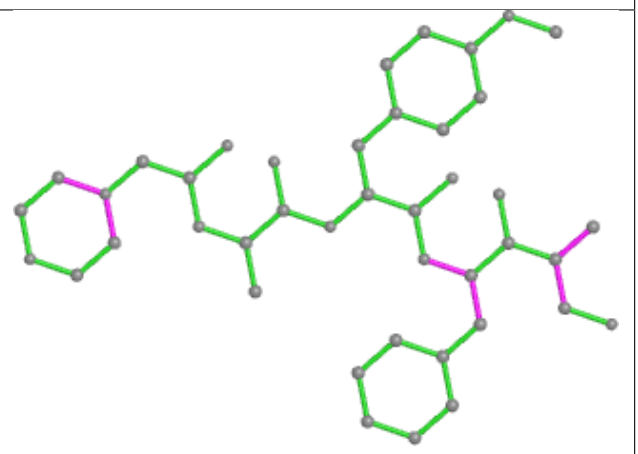
Ligand 04C Y 301



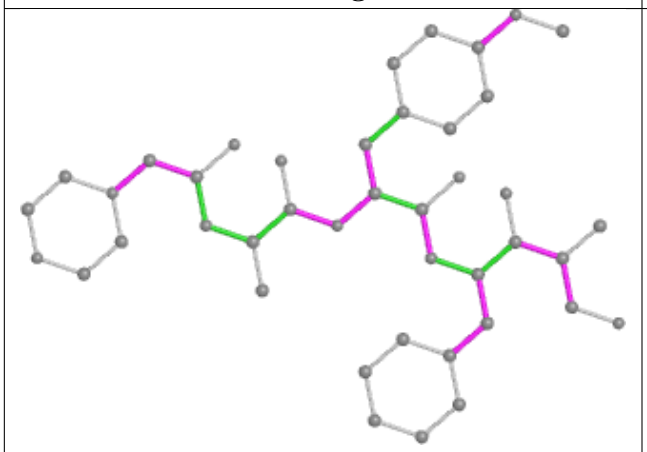
Ligand 04C H 301



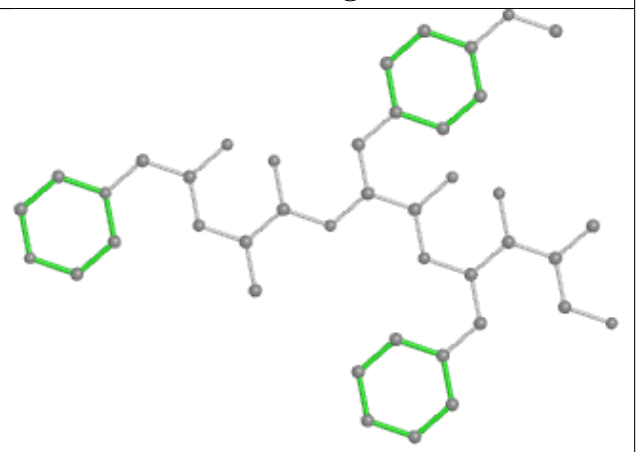
Bond lengths



Bond angles

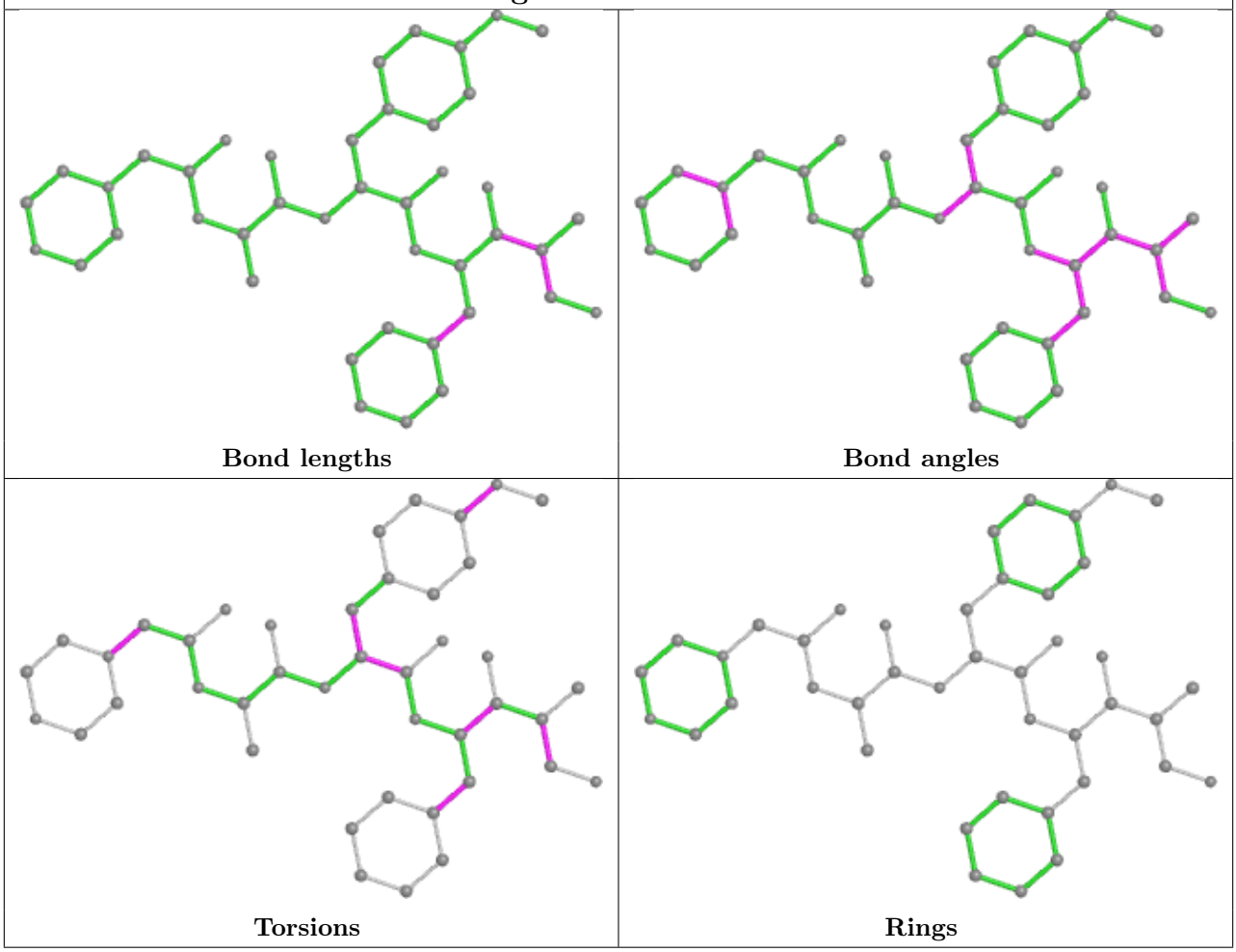


Torsions



Rings

Ligand 04C N 201



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	230/234 (98%)	0.10	11 (4%)	30	27	44, 68, 95, 106	0
1	O	230/234 (98%)	0.03	4 (1%)	70	69	35, 52, 86, 96	0
2	B	248/261 (95%)	0.24	15 (6%)	21	18	45, 72, 121, 149	0
2	P	248/261 (95%)	0.00	12 (4%)	30	27	32, 57, 99, 142	0
3	C	238/248 (95%)	0.64	31 (13%)	3	2	51, 87, 150, 194	0
3	Q	238/248 (95%)	0.47	27 (11%)	5	4	41, 74, 132, 174	0
4	D	233/241 (96%)	0.55	18 (7%)	13	10	41, 91, 150, 200	0
4	R	233/241 (96%)	0.39	12 (5%)	27	23	43, 83, 125, 154	0
5	E	238/263 (90%)	0.19	11 (4%)	32	29	34, 66, 107, 128	0
5	S	238/263 (90%)	0.08	8 (3%)	45	40	35, 61, 102, 122	0
6	F	244/255 (95%)	0.17	6 (2%)	57	55	37, 67, 103, 117	0
6	T	244/255 (95%)	0.09	10 (4%)	37	32	34, 57, 93, 111	0
7	G	243/246 (98%)	0.21	12 (4%)	29	26	47, 70, 108, 129	0
7	U	243/246 (98%)	0.08	16 (6%)	18	14	32, 57, 99, 117	0
8	H	219/234 (93%)	-0.12	6 (2%)	54	50	11, 50, 94, 125	0
8	V	219/234 (93%)	-0.24	6 (2%)	54	50	4, 41, 78, 103	0
9	I	204/205 (99%)	-0.08	4 (1%)	65	63	33, 55, 82, 101	0
9	W	204/205 (99%)	-0.25	2 (0%)	82	82	27, 42, 64, 82	0
10	J	196/201 (97%)	-0.16	3 (1%)	73	73	38, 50, 72, 83	0
10	X	196/201 (97%)	-0.26	1 (0%)	91	91	32, 48, 67, 83	0
11	K	201/204 (98%)	-0.08	3 (1%)	73	73	9, 47, 72, 87	0
11	Y	201/204 (98%)	0.15	4 (1%)	65	63	5, 57, 82, 94	0
12	L	213/213 (100%)	-0.20	2 (0%)	84	84	29, 42, 64, 86	0
12	Z	213/213 (100%)	-0.14	1 (0%)	91	91	41, 49, 67, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	-0.30	1 (0%)	91	91	29, 38, 61, 82	0
13	a	216/219 (98%)	-0.24	1 (0%)	91	91	36, 44, 61, 82	0
14	N	199/199 (100%)	-0.19	1 (0%)	91	91	4, 43, 61, 72	0
14	b	199/199 (100%)	-0.20	0	100	100	3, 41, 61, 70	0
All	All	6244/6446 (96%)	0.05	228 (3%)	41	37	3, 56, 111, 200	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	5	THR	7.7
3	C	49	VAL	7.7
4	D	123	GLY	7.4
4	R	123	GLY	7.3
6	F	1	SER	6.5
4	R	122	PRO	6.5
7	U	1	SER	6.5
4	R	233	ILE	6.2
8	H	199	ALA	5.7
13	M	216	SER	5.7
3	Q	236	GLU	5.5
3	C	233	LYS	5.5
7	G	242	ALA	5.4
3	Q	238	ASN	5.2
5	E	238	GLN	5.1
3	C	200	SER	4.8
7	G	1	SER	4.8
3	C	203	LYS	4.7
4	D	233	ILE	4.7
1	A	1	ALA	4.7
8	V	199	ALA	4.7
5	S	52	GLU	4.7
3	Q	200	SER	4.7
2	B	237	LYS	4.6
2	B	247	GLU	4.6
3	C	238	ASN	4.6
3	C	237	GLU	4.5
7	G	187	ASP	4.4
7	G	2	ARG	4.3
3	Q	178	ASP	4.3
4	D	232	ASP	4.3
2	B	244	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
6	T	5	THR	4.2
2	P	248	ARG	4.1
3	Q	45	GLU	4.1
4	D	122	PRO	4.0
4	D	201	LYS	3.9
7	U	186	PHE	3.9
6	T	1	SER	3.9
3	C	199	GLN	3.9
4	D	199	GLU	3.8
5	E	52	GLU	3.8
3	Q	55	GLU	3.8
5	S	199	GLU	3.8
7	U	2	ARG	3.8
7	G	243	GLU	3.7
7	U	3	GLY	3.7
6	F	3	ILE	3.7
5	S	238	GLN	3.7
5	E	53	LEU	3.7
4	D	171	SER	3.7
3	C	45	GLU	3.6
2	B	53	LYS	3.6
3	Q	199	GLN	3.6
5	E	235	GLU	3.6
1	A	2	LYS	3.5
13	a	216	SER	3.5
8	H	201	ARG	3.5
5	E	237	PRO	3.5
7	G	185	LYS	3.4
3	Q	232	GLU	3.4
8	V	201	ARG	3.4
5	E	199	GLU	3.4
3	Q	233	LYS	3.3
4	D	177	TYR	3.3
6	T	204	VAL	3.3
9	I	116	PHE	3.3
3	C	48	SER	3.3
8	V	200	GLY	3.3
1	O	2	LYS	3.3
3	C	236	GLU	3.2
2	B	203	SER	3.2
2	P	203	SER	3.2
2	B	204	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
6	T	3	ILE	3.1
2	P	202	VAL	3.1
6	T	207	LYS	3.1
7	G	186	PHE	3.1
4	R	215	GLY	3.1
5	S	237	PRO	3.1
6	F	207	LYS	3.1
3	C	232	GLU	3.1
7	U	6	ALA	3.0
4	R	224	GLU	3.0
9	I	114	LYS	3.0
10	J	95	ARG	3.0
2	P	244	ALA	3.0
4	R	199	GLU	3.0
8	H	197	GLN	3.0
3	Q	181	GLU	3.0
3	Q	182	THR	3.0
3	C	47	LYS	3.0
3	C	178	ASP	3.0
7	U	187	ASP	3.0
4	R	192	ILE	2.9
5	E	50	GLN	2.9
2	B	1	SER	2.9
3	C	234	GLU	2.9
1	O	3	ARG	2.9
1	A	178	ASN	2.9
3	Q	203	LYS	2.9
3	Q	46	LYS	2.9
5	E	234	GLU	2.9
8	H	196	VAL	2.9
4	D	215	GLY	2.8
2	P	219	SER	2.8
1	A	3	ARG	2.8
2	B	206	SER	2.8
3	C	137	PHE	2.8
2	P	246	ALA	2.8
11	K	73	ARG	2.8
3	Q	165	LYS	2.8
7	U	185	LYS	2.7
3	C	185	LEU	2.7
11	Y	9	GLN	2.7
3	C	211	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
11	Y	200	GLY	2.7
1	A	59	ARG	2.7
2	B	246	ALA	2.7
4	D	47	THR	2.7
6	T	219	LEU	2.7
3	C	204	ASN	2.6
3	C	179	ALA	2.6
3	Q	237	GLU	2.6
6	T	208	ALA	2.6
4	R	175	GLU	2.6
4	R	180	SER	2.6
5	E	198	ALA	2.6
11	Y	73	ARG	2.6
3	Q	47	LYS	2.6
4	D	200	GLU	2.6
7	U	4	SER	2.6
7	G	58	LYS	2.6
6	T	4	GLY	2.6
3	Q	48	SER	2.6
4	D	121	ASP	2.6
3	C	202	GLY	2.6
11	K	72	GLU	2.6
8	H	195	PRO	2.6
3	Q	137	PHE	2.5
11	K	9	GLN	2.5
5	E	200	GLN	2.5
6	T	60	GLU	2.5
7	U	184	LYS	2.5
3	C	162	ARG	2.5
4	D	49	PRO	2.5
3	C	55	GLU	2.5
2	P	247	GLU	2.5
1	A	180	ASP	2.5
3	Q	177	ASP	2.5
3	C	235	LYS	2.5
3	Q	212	ARG	2.4
12	Z	162	GLU	2.4
2	P	243	GLU	2.4
5	S	234	GLU	2.4
2	P	245	LYS	2.4
9	W	114	LYS	2.4
2	B	248	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
10	X	95	ARG	2.4
2	P	53	LYS	2.4
3	C	169	GLU	2.4
3	C	37	LYS	2.4
6	F	2	SER	2.4
1	A	203	THR	2.4
2	B	233	GLU	2.4
4	D	222	THR	2.4
4	R	121	ASP	2.4
1	O	201	GLN	2.4
5	S	53	LEU	2.4
7	G	238	LEU	2.3
7	U	207	ILE	2.3
3	Q	206	GLU	2.3
12	L	163	HIS	2.3
1	O	1	ALA	2.3
9	W	116	PHE	2.3
3	Q	49	VAL	2.3
7	G	184	LYS	2.3
2	B	178	TYR	2.3
3	C	206	GLU	2.3
5	S	235	GLU	2.3
3	C	175	TYR	2.3
6	F	142	ALA	2.3
5	S	233	LEU	2.2
1	A	179	GLU	2.2
2	B	18	TYR	2.2
4	R	188	LYS	2.2
2	B	219	SER	2.2
10	J	109	GLU	2.2
7	U	145	GLU	2.2
12	L	1	ARG	2.2
7	U	176	SER	2.2
1	A	201	GLN	2.2
7	G	10	ARG	2.2
14	N	191	ASP	2.2
3	C	16	PHE	2.2
2	B	29	HIS	2.2
4	D	220	MET	2.2
1	A	50	LYS	2.2
4	D	188	LYS	2.2
6	T	202	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	218	ILE	2.2
7	U	56	PRO	2.2
8	V	198	ARG	2.2
3	Q	213	ASP	2.1
4	D	25	LEU	2.1
3	C	46	LYS	2.1
3	Q	229	ALA	2.1
10	J	196	PHE	2.1
7	U	5	SER	2.1
5	E	171	ARG	2.1
11	Y	72	GLU	2.1
8	H	198	ARG	2.1
8	V	197	GLN	2.1
4	D	168	GLY	2.1
7	U	144	GLU	2.1
3	Q	235	LYS	2.1
1	A	13	SER	2.1
2	P	205	LEU	2.1
9	I	30	GLN	2.1
7	U	210	LYS	2.1
4	R	142	GLY	2.0
7	G	192	GLN	2.0
8	V	195	PRO	2.0
9	I	155	PRO	2.0
3	Q	195	LEU	2.0
2	P	201	ASP	2.0
3	C	172	GLU	2.0
3	Q	37	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th 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	B-factors(Å^2)	Q<0.9
16	K	L	303	1/1	0.70	0.69	31,31,31,31	0
16	K	B	301	1/1	0.72	0.32	55,55,55,55	0
16	K	K	303	1/1	0.74	0.18	51,51,51,51	0
15	CL	V	305	1/1	0.81	0.23	44,44,44,44	0
15	CL	a	303	1/1	0.82	0.14	44,44,44,44	0
15	CL	U	301	1/1	0.82	0.14	45,45,45,45	0
15	CL	S	302	1/1	0.82	0.13	45,45,45,45	0
15	CL	X	302	1/1	0.82	0.19	51,51,51,51	0
16	K	b	203	1/1	0.84	0.38	45,45,45,45	0
16	K	G	301	1/1	0.85	0.22	56,56,56,56	0
15	CL	R	302	1/1	0.85	0.22	59,59,59,59	0
16	K	Z	302	1/1	0.86	0.14	47,47,47,47	0
15	CL	P	301	1/1	0.86	0.19	39,39,39,39	0
16	K	S	303	1/1	0.88	0.27	50,50,50,50	0
15	CL	A	303	1/1	0.89	0.13	45,45,45,45	0
17	04C	Y	301	42/42	0.89	0.30	2,16,29,34	0
16	K	X	304	1/1	0.90	0.24	70,70,70,70	0
15	CL	a	304	1/1	0.90	0.12	44,44,44,44	0
15	CL	R	303	1/1	0.90	0.11	45,45,45,45	0
15	CL	L	302	1/1	0.90	0.15	24,24,24,24	0
15	CL	X	303	1/1	0.91	0.17	72,72,72,72	0
15	CL	M	304	1/1	0.91	0.09	48,48,48,48	0
17	04C	N	201	42/42	0.91	0.23	2,3,8,11	0
15	CL	E	301	1/1	0.91	0.20	42,42,42,42	0
17	04C	K	301	42/42	0.92	0.26	7,14,28,32	0
16	K	Z	304	1/1	0.92	0.21	40,40,40,40	0
15	CL	J	301	1/1	0.92	0.07	35,35,35,35	0
17	04C	b	201	42/42	0.93	0.22	2,3,12,17	0
17	04C	V	301	42/42	0.94	0.16	3,5,24,25	0
15	CL	X	301	1/1	0.94	0.24	46,46,46,46	0
17	04C	H	301	42/42	0.94	0.20	6,13,19,20	0
15	CL	V	306	1/1	0.95	0.12	40,40,40,40	0
15	CL	A	302	1/1	0.95	0.12	32,32,32,32	0
16	K	M	305	1/1	0.95	0.20	37,37,37,37	0
16	K	Z	303	1/1	0.95	0.07	24,24,24,24	0
15	CL	R	301	1/1	0.96	0.12	32,32,32,32	0
15	CL	D	301	1/1	0.96	0.10	35,35,35,35	0
16	K	a	305	1/1	0.96	0.43	37,37,37,37	0
15	CL	Q	301	1/1	0.96	0.16	39,39,39,39	0
15	CL	Q	302	1/1	0.96	0.09	37,37,37,37	0
15	CL	S	301	1/1	0.97	0.18	35,35,35,35	0

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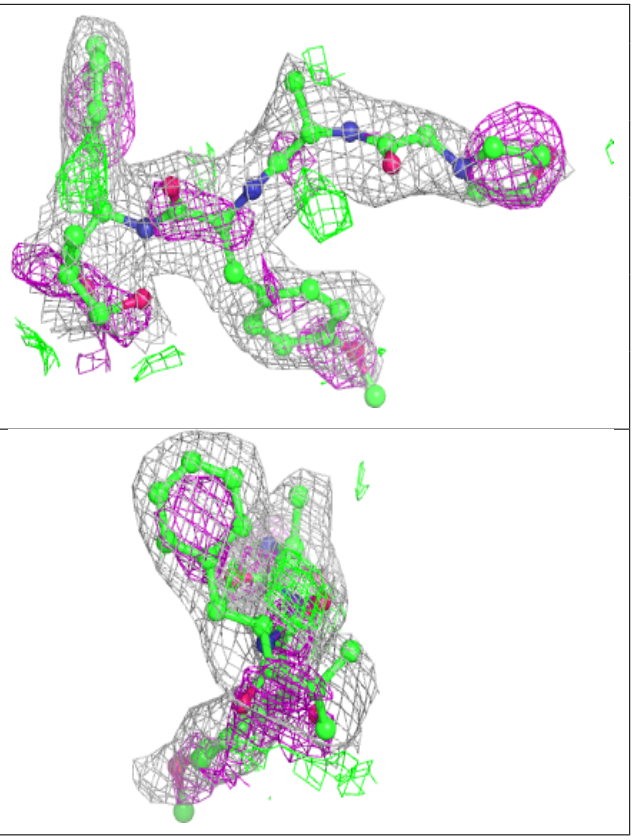
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CL	M	301	1/1	0.97	0.08	39,39,39,39	0
15	CL	O	301	1/1	0.97	0.09	33,33,33,33	0
15	CL	O	302	1/1	0.97	0.08	44,44,44,44	0
16	K	I	302	1/1	0.97	0.45	41,41,41,41	0
15	CL	a	301	1/1	0.97	0.10	33,33,33,33	0
15	CL	a	302	1/1	0.97	0.07	29,29,29,29	0
15	CL	Z	301	1/1	0.98	0.19	26,26,26,26	0
15	CL	Q	304	1/1	0.98	0.04	29,29,29,29	0
15	CL	V	304	1/1	0.98	0.09	33,33,33,33	0
15	CL	M	302	1/1	0.98	0.14	30,30,30,30	0
15	CL	I	301	1/1	0.98	0.06	28,28,28,28	0
15	CL	N	203	1/1	0.98	0.09	36,36,36,36	0
15	CL	A	301	1/1	0.98	0.08	34,34,34,34	0
15	CL	Q	303	1/1	0.98	0.03	32,32,32,32	0
15	CL	H	303	1/1	0.99	0.07	31,31,31,31	0
15	CL	M	303	1/1	0.99	0.06	25,25,25,25	0
15	CL	W	301	1/1	0.99	0.12	28,28,28,28	0
15	CL	V	303	1/1	0.99	0.12	30,30,30,30	0
15	CL	L	301	1/1	0.99	0.05	32,32,32,32	0
18	IOD	H	302	1/1	0.99	0.07	49,49,49,49	0
18	IOD	N	202	1/1	0.99	0.02	48,48,48,48	0
18	IOD	Y	302	1/1	0.99	0.02	55,55,55,55	0
18	IOD	b	202	1/1	0.99	0.03	46,46,46,46	0
18	IOD	K	302	1/1	1.00	0.03	53,53,53,53	0
18	IOD	V	302	1/1	1.00	0.13	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

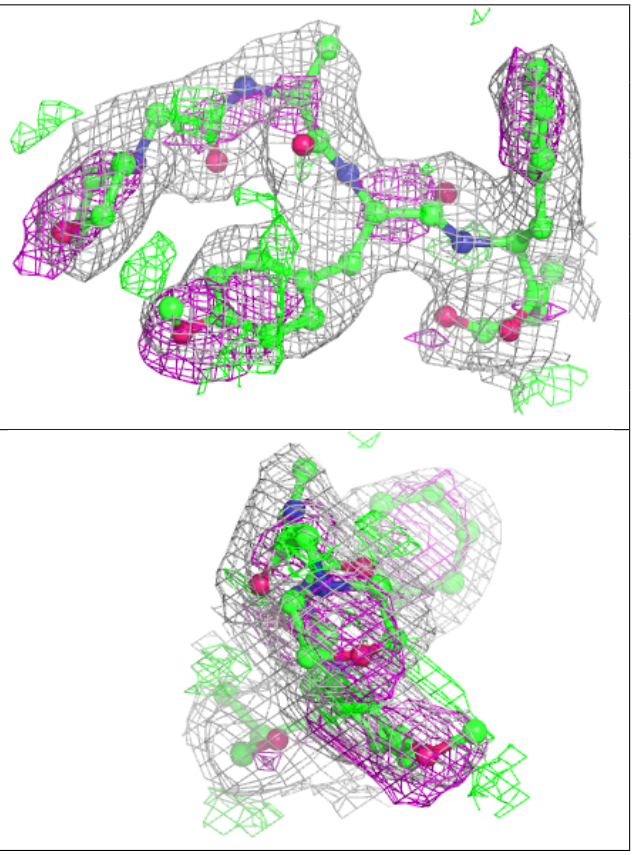
Electron density around 04C Y 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



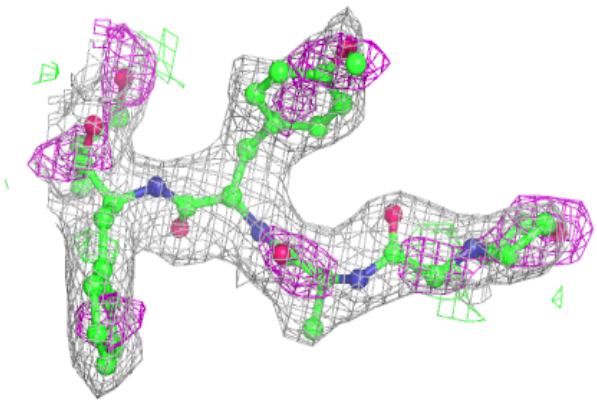
Electron density around 04C N 201:

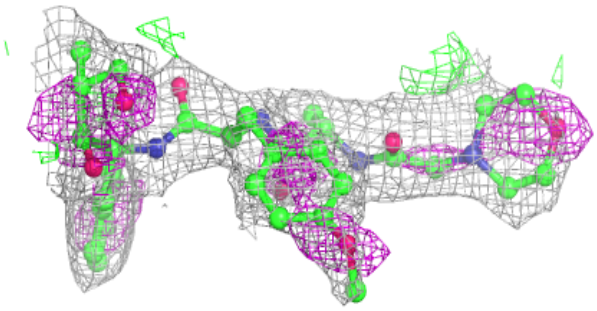
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

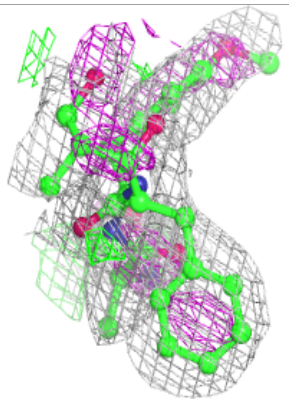


Electron density around 04C K 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

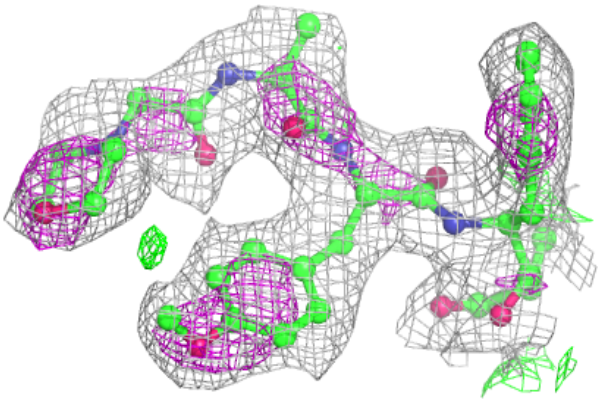


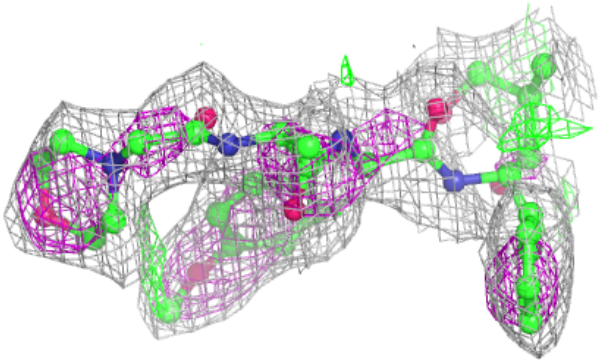


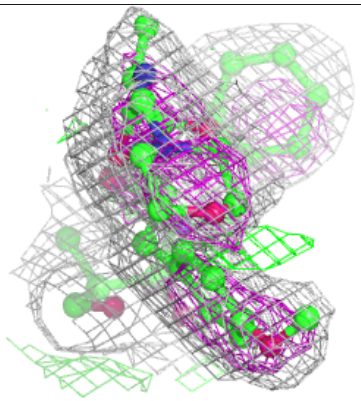


Electron density around 04C b 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

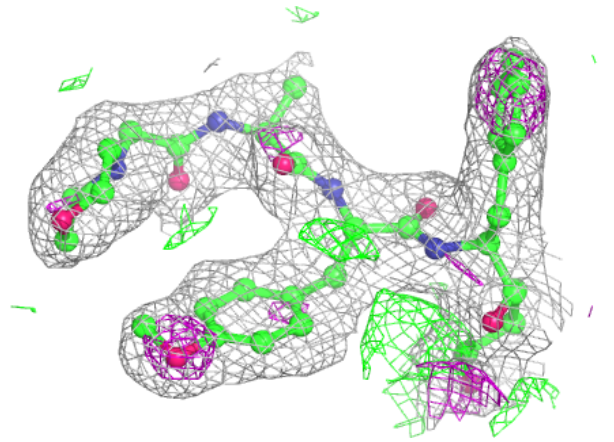


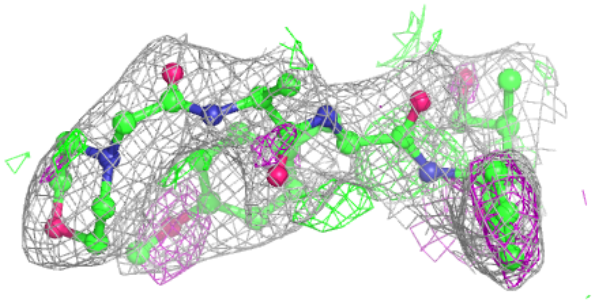


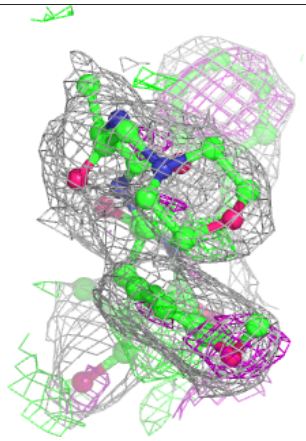


Electron density around 04C V 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

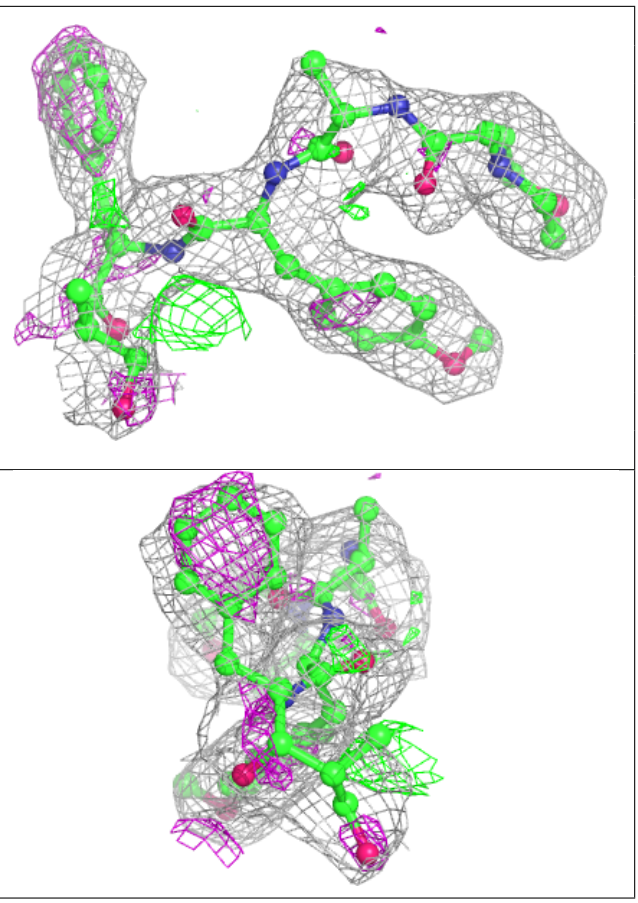






Electron density around 04C H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.