Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2016 – 11:40 PM EDT

PDB ID	:	5LEY
Title	:	Human 20S proteasome complex with Oprozomib at 1.9 Angstrom
Authors	:	Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on	:	2016-06-30
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

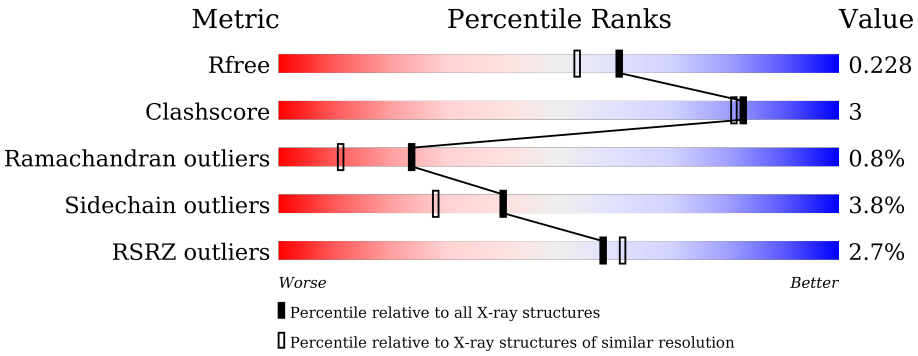
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	234	2% 84% 11%
1	O	234	7% 87% 8%
2	B	261	3% 85% 8% 5%
2	P	261	7% 81% 11% 5%
3	C	248	6% 81% 11%
3	Q	248	11% 81% 13%

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Mol	Chain	Length	Quality of chain
4	D	241	4% 86% 9%
4	R	241	2% 86% 10%
5	E	263	4% 78% 9% 11%
5	S	263	3% 79% 10% 10%
6	F	255	78% 12% 6%
6	T	255	4% 77% 14% 6%
7	G	246	2% 91% 6%
7	U	246	5% 85% 9%
8	H	234	2% 86% 6% 6%
8	V	234	3% 85% 7% 6%
9	I	205	90% 9%
9	W	205	94% 5%
10	J	201	81% 14%
10	X	201	87% 7%
11	K	204	85% 11%
11	Y	204	85% 11%
12	L	213	92% 8%
12	Z	213	93% 7%
13	M	219	89% 9%
13	a	219	91% 7%
14	N	205	% 91% 6%
14	b	205	94% 5%
15	c	4	100%
15	d	4	100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CL	B	302	-	-	X	-
16	CL	M	301	-	-	-	X
16	CL	S	301	-	-	-	X
16	CL	b	302	-	-	-	X
19	1PE	H	306	-	-	-	X
19	1PE	I	303	-	-	-	X
19	1PE	I	304	-	-	-	X
19	1PE	L	301	-	-	-	X
19	1PE	M	305	-	-	-	X
19	1PE	W	303	-	-	-	X
7	YCM	U	137	-	-	X	-
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51947 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
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	240	Total	C	N	O	S	0	0	0
			1825	1139	321	360	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	236	Total	C	N	O	S	0	3	0
			1853	1160	335	347	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1545	974	269	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1570	991	278	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			
15	d	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total Cl 1 1	0	0
16	K	4	Total Cl 4 4	0	0
16	B	2	Total Cl 2 2	0	0
16	W	1	Total Cl 1 1	0	0
16	N	3	Total Cl 3 3	0	0
16	S	3	Total Cl 3 3	0	0
16	E	3	Total Cl 3 3	0	0
16	b	4	Total Cl 4 4	0	0
16	V	2	Total Cl 2 2	0	0
16	A	4	Total Cl 4 4	0	0
16	R	2	Total Cl 2 2	0	0
16	M	4	Total Cl 4 4	0	0
16	D	2	Total Cl 2 2	0	0
16	I	1	Total Cl 1 1	0	0
16	a	3	Total Cl 3 3	0	0
16	U	1	Total Cl 1 1	0	0
16	G	2	Total Cl 2 2	0	0
16	Q	2	Total Cl 2 2	0	0
16	H	2	Total Cl 2 2	0	0
16	C	2	Total Cl 2 2	0	0
16	O	4	Total Cl 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	Y	5	Total Cl 5 5	0	0
16	F	1	Total Cl 1 1	0	0

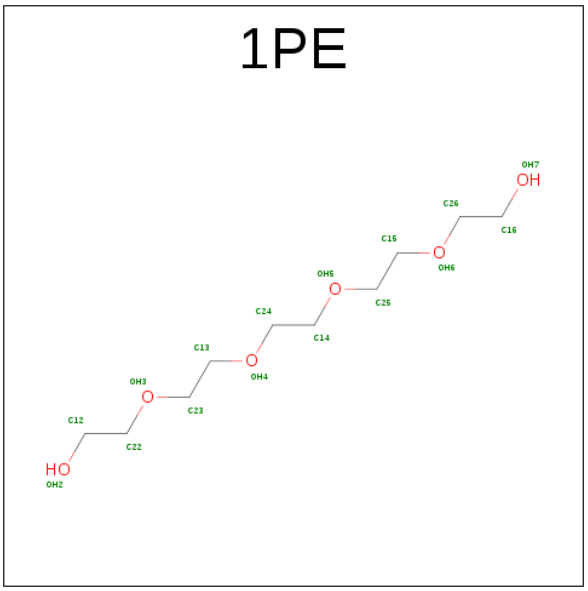
- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total K 1 1	0	0
17	b	1	Total K 1 1	0	0
17	Z	1	Total K 1 1	0	0
17	N	1	Total K 1 1	0	0
17	U	1	Total K 1 1	0	0
17	L	1	Total K 1 1	0	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	J	1	Total Mg 1 1	0	0
18	K	1	Total Mg 1 1	0	0
18	H	2	Total Mg 2 2	0	0
18	I	2	Total Mg 2 2	0	0
18	V	1	Total Mg 1 1	0	0
18	W	1	Total Mg 1 1	0	0
18	X	1	Total Mg 1 1	0	0
18	L	1	Total Mg 1 1	0	0

- Molecule 19 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	H	1	Total C O 16 10 6	0	0
19	H	1	Total C O 16 10 6	0	0
19	I	1	Total C O 16 10 6	0	0
19	I	1	Total C O 16 10 6	0	0
19	L	1	Total C O 16 10 6	0	0
19	M	1	Total C O 16 10 6	0	0
19	V	1	Total C O 16 10 6	0	0
19	W	1	Total C O 16 10 6	0	0
19	Z	1	Total C O 16 10 6	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	109	Total O 109 109	0	0
20	B	120	Total O 120 120	0	0
20	C	76	Total O 76 76	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	93	Total O 93 93	0	0
20	E	137	Total O 137 137	0	0
20	F	180	Total O 180 180	0	0
20	G	187	Total O 187 187	0	0
20	H	157	Total O 157 157	0	0
20	I	155	Total O 155 155	0	0
20	J	133	Total O 133 133	0	0
20	K	98	Total O 98 98	0	0
20	L	124	Total O 124 124	0	0
20	M	148	Total O 148 148	0	0
20	N	168	Total O 168 168	0	0
20	O	89	Total O 89 89	0	0
20	P	117	Total O 117 117	0	0
20	Q	74	Total O 74 74	0	0
20	R	122	Total O 122 122	0	0
20	S	118	Total O 118 118	0	0
20	T	92	Total O 92 92	0	0
20	U	102	Total O 102 102	0	0
20	V	112	Total O 112 112	0	0
20	W	111	Total O 111 111	0	0
20	X	124	Total O 124 124	0	0

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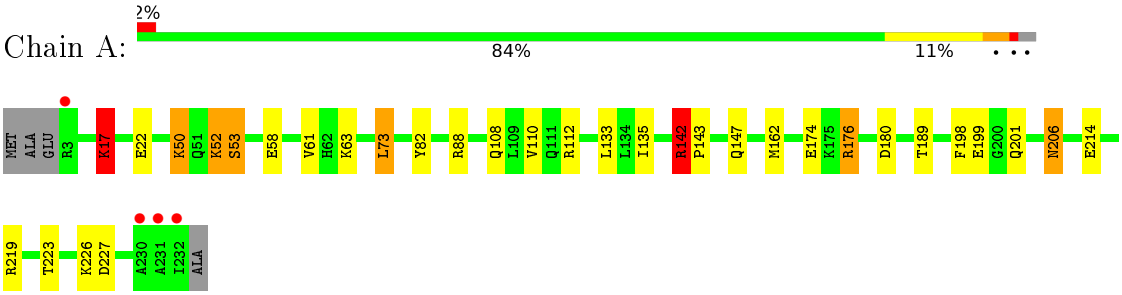
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	Y	137	Total O 137 137	0	0
20	Z	164	Total O 164 164	0	0
20	a	167	Total O 167 167	0	0
20	b	126	Total O 126 126	0	0
20	c	1	Total O 1 1	0	0
20	d	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

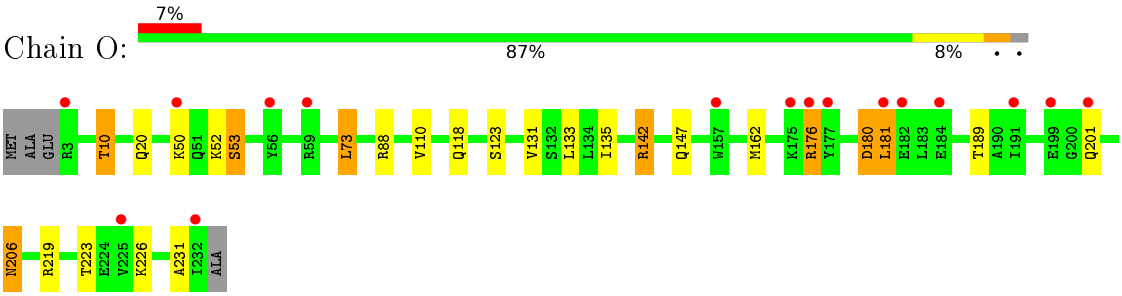
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



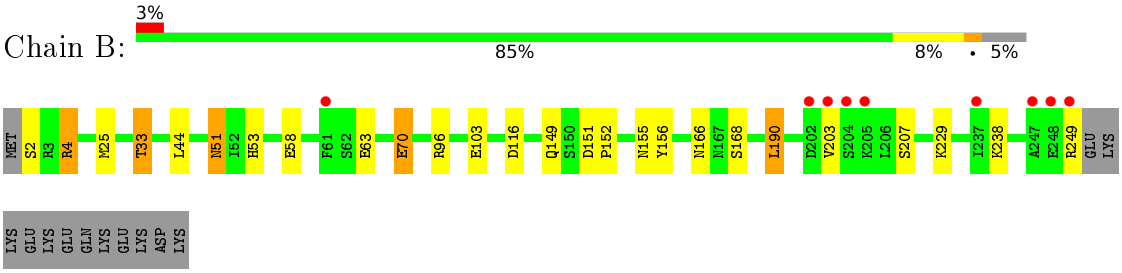
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



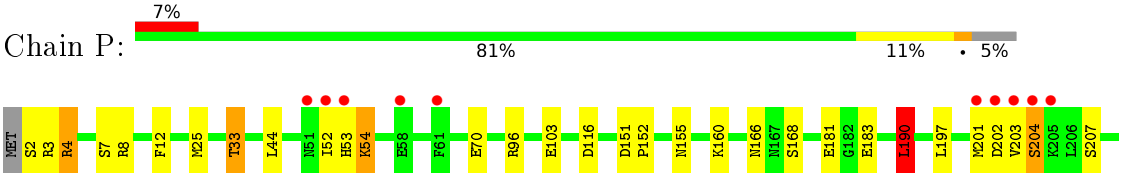
- Molecule 2: Proteasome subunit alpha type-4

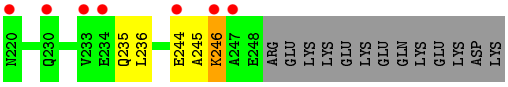
Chain B:



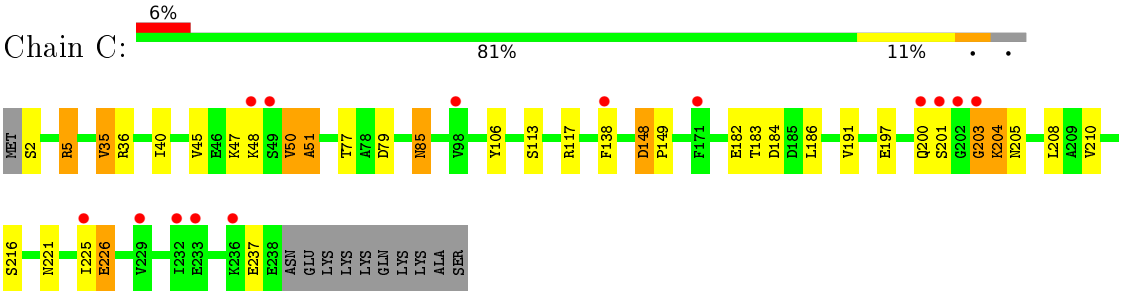
- Molecule 2: Proteasome subunit alpha type-4

Chain P:

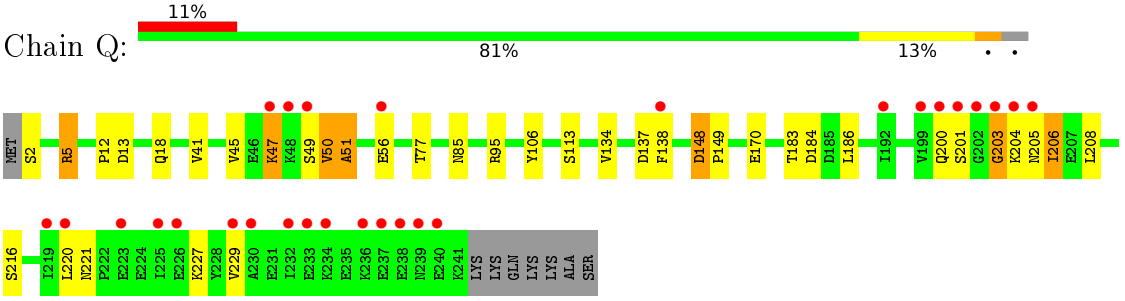




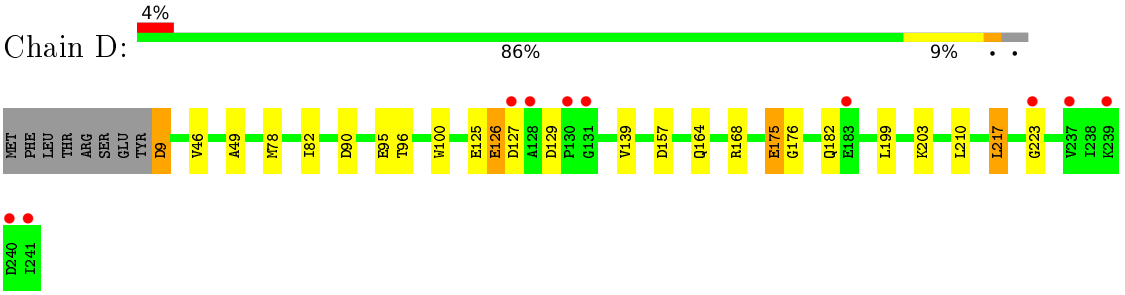
• Molecule 3: Proteasome subunit alpha type-7



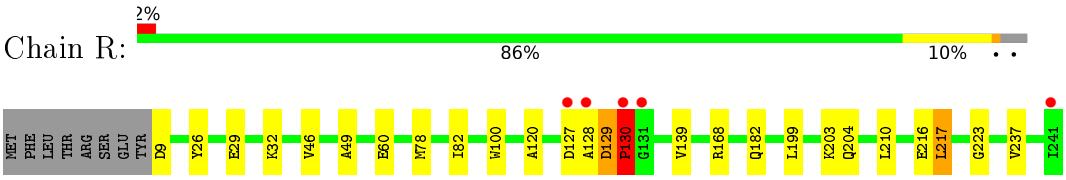
• Molecule 3: Proteasome subunit alpha type-7



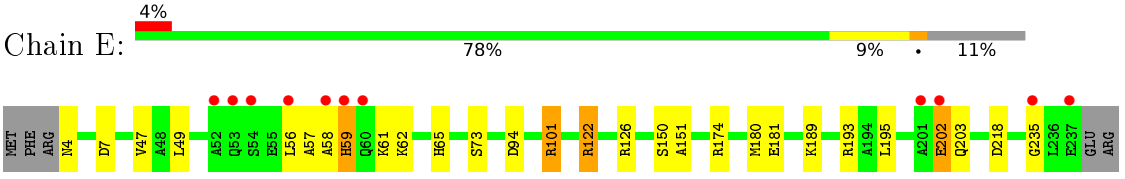
• Molecule 4: Proteasome subunit alpha type-5



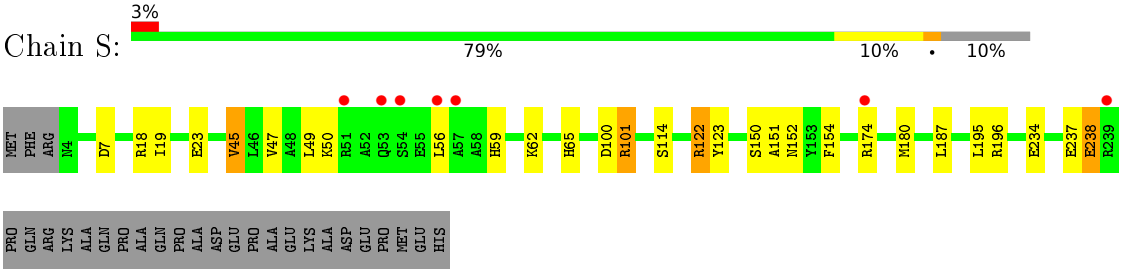
• Molecule 4: Proteasome subunit alpha type-5



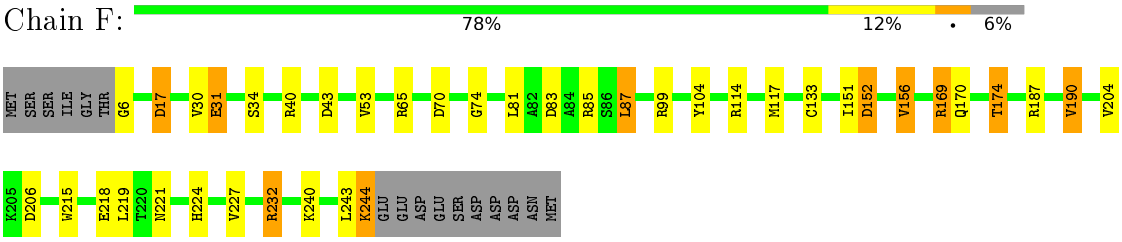
• Molecule 5: Proteasome subunit alpha type-1



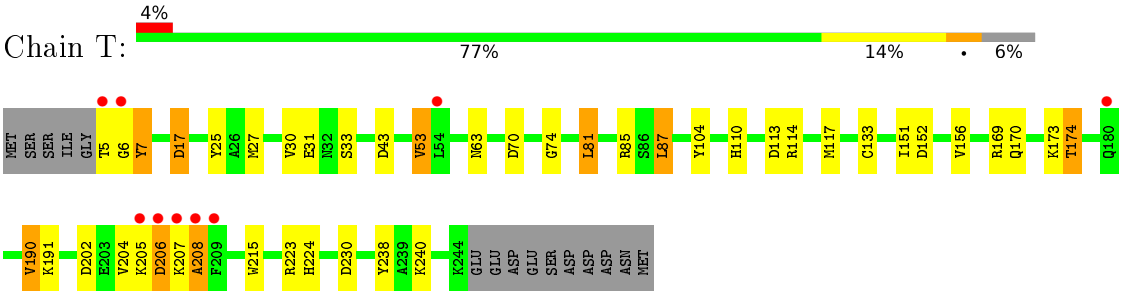
• Molecule 5: Proteasome subunit alpha type-1



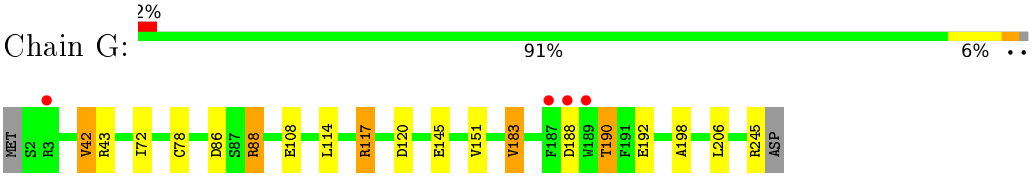
• Molecule 6: Proteasome subunit alpha type-3



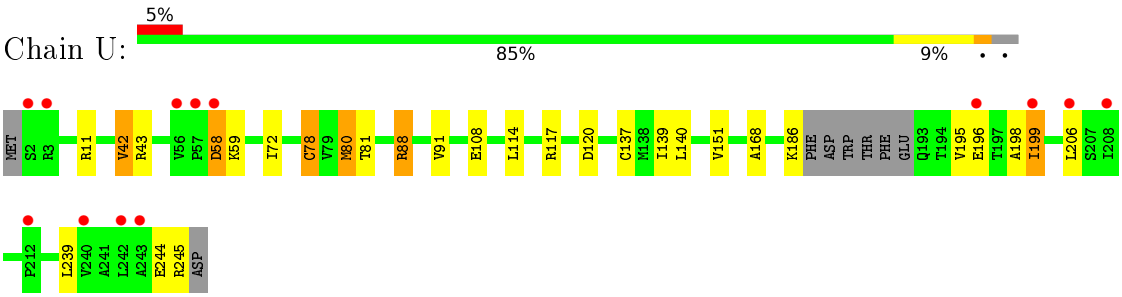
• Molecule 6: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-6

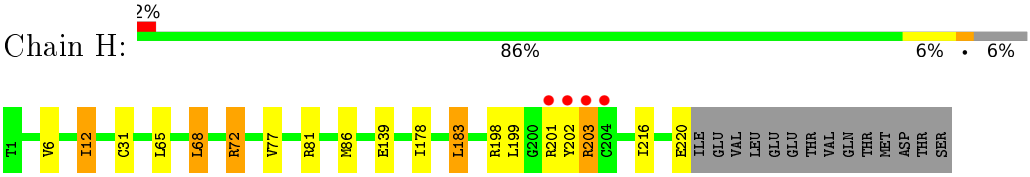


• Molecule 7: Proteasome subunit alpha type-6



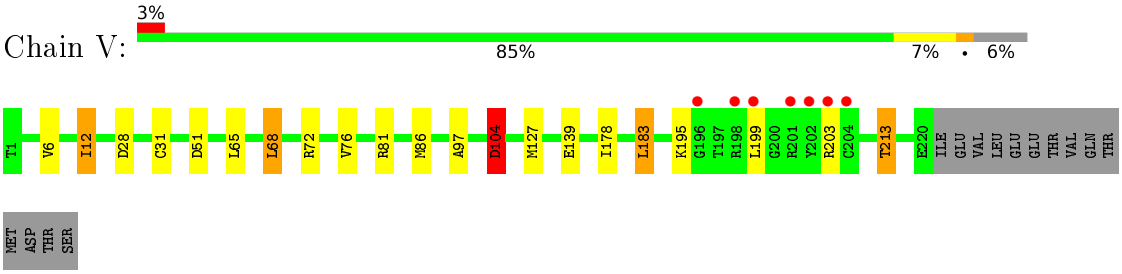
• Molecule 8: Proteasome subunit beta type-7

Chain H:



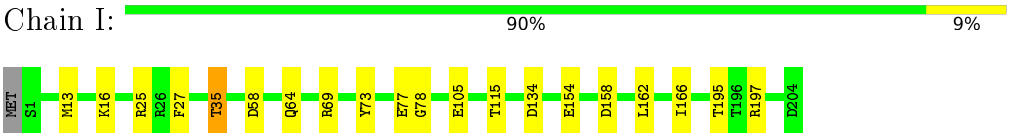
• Molecule 8: Proteasome subunit beta type-7

Chain V:



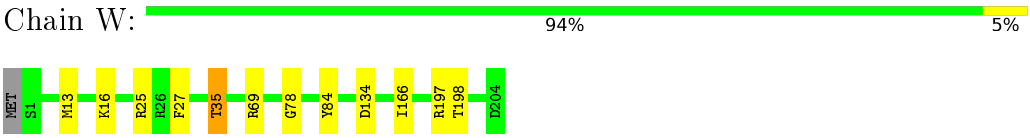
• Molecule 9: Proteasome subunit beta type-3

Chain I:



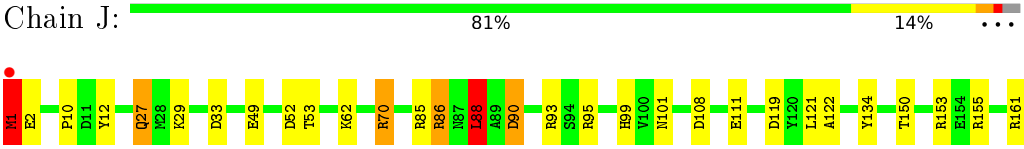
• Molecule 9: Proteasome subunit beta type-3

Chain W:



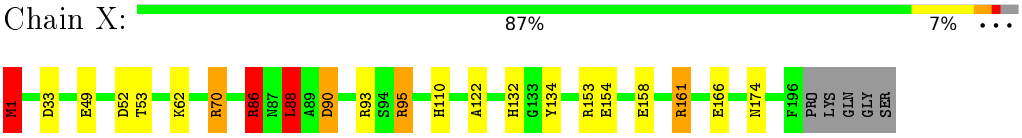
• Molecule 10: Proteasome subunit beta type-2

Chain J:



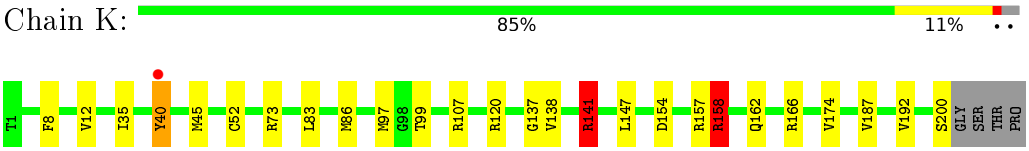
• Molecule 10: Proteasome subunit beta type-2

Chain X:



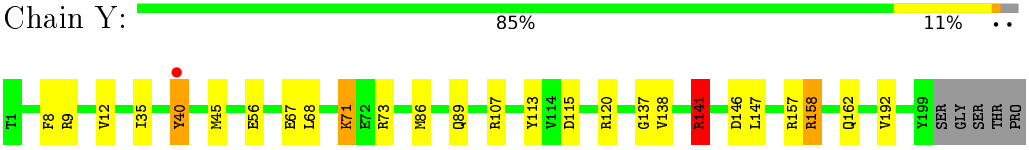
• Molecule 11: Proteasome subunit beta type-5

Chain K:



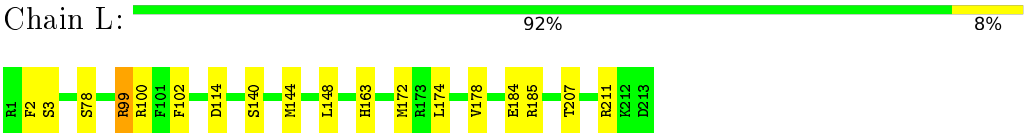
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



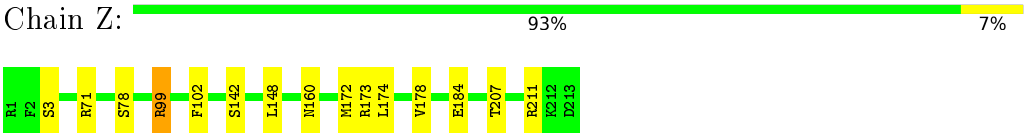
• Molecule 12: Proteasome subunit beta type-1

Chain L:



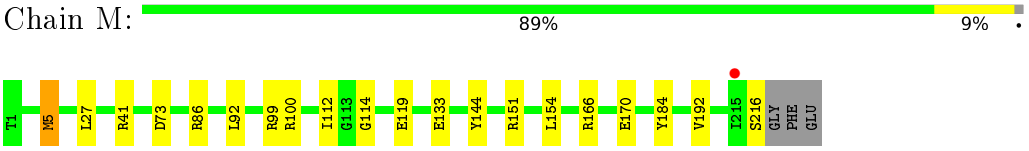
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



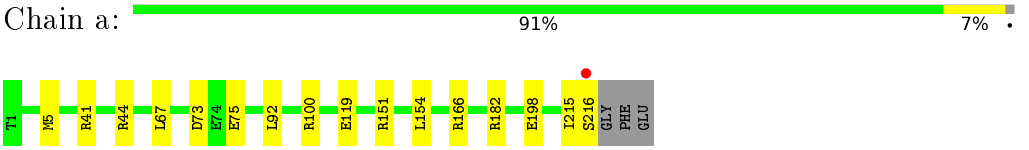
• Molecule 13: Proteasome subunit beta type-4

Chain M:



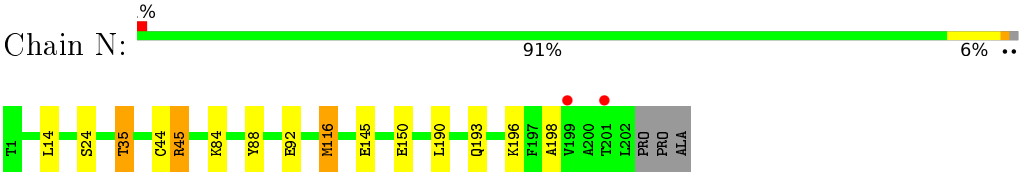
• Molecule 13: Proteasome subunit beta type-4

Chain a:



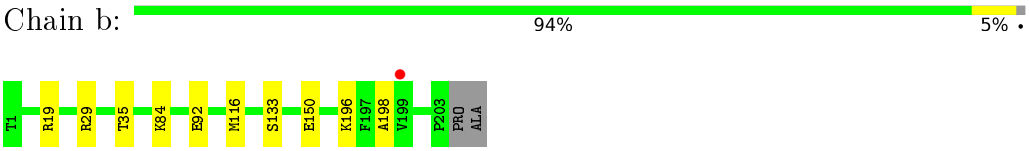
• Molecule 14: Proteasome subunit beta type-6

Chain N:



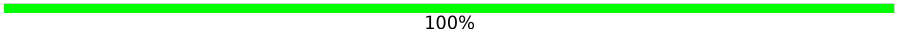
• Molecule 14: Proteasome subunit beta type-6

Chain b:



- Molecule 15: bound Oprozomib

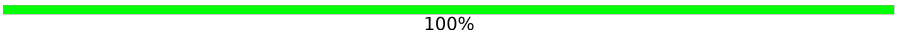
Chain c:



There are no outlier residues recorded for this chain.

- Molecule 15: bound Oprozomib

Chain d:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.39Å 202.65Å 315.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 1.90 106.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (170.45-1.90) 97.8 (106.69-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.188 , 0.225 0.195 , 0.228	Depositor DCC
R_{free} test set	27607 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	51947	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6V9, CL, K, 6V1, 1PE, OAS, YCM, 6VA

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	0.92	2/1833 (0.1%)	0.94	5/2489 (0.2%)
1	O	0.81	1/1778 (0.1%)	0.92	7/2419 (0.3%)
2	B	0.99	4/1958 (0.2%)	1.01	6/2645 (0.2%)
2	P	0.89	2/1934 (0.1%)	0.96	7/2617 (0.3%)
3	C	0.95	2/1818 (0.1%)	1.05	8/2469 (0.3%)
3	Q	0.91	1/1839 (0.1%)	1.01	6/2497 (0.2%)
4	D	0.95	3/1789 (0.2%)	0.97	5/2424 (0.2%)
4	R	1.06	2/1780 (0.1%)	1.05	6/2408 (0.2%)
5	E	0.94	2/1842 (0.1%)	1.00	7/2493 (0.3%)
5	S	0.92	1/1878 (0.1%)	0.97	5/2541 (0.2%)
6	F	1.09	5/1935 (0.3%)	1.16	26/2605 (1.0%)
6	T	1.00	3/1894 (0.2%)	1.11	16/2556 (0.6%)
7	G	1.09	2/1909 (0.1%)	0.98	7/2579 (0.3%)
7	U	0.92	2/1804 (0.1%)	0.95	7/2441 (0.3%)
8	H	1.05	1/1697 (0.1%)	1.17	11/2299 (0.5%)
8	V	0.88	2/1655 (0.1%)	1.01	8/2251 (0.4%)
9	I	1.03	2/1648 (0.1%)	1.24	14/2219 (0.6%)
9	W	0.84	1/1630 (0.1%)	1.11	12/2197 (0.5%)
10	J	1.06	1/1613 (0.1%)	1.28	14/2180 (0.6%)
10	X	0.97	2/1599 (0.1%)	1.24	13/2163 (0.6%)
11	K	1.01	2/1576 (0.1%)	1.11	12/2131 (0.6%)
11	Y	1.10	4/1610 (0.2%)	1.20	14/2172 (0.6%)
12	L	0.93	3/1672 (0.2%)	1.05	6/2257 (0.3%)
12	Z	1.09	4/1675 (0.2%)	1.11	6/2257 (0.3%)
13	M	1.04	2/1728 (0.1%)	1.06	7/2339 (0.3%)
13	a	1.09	3/1724 (0.2%)	1.07	8/2336 (0.3%)
14	N	1.13	4/1548 (0.3%)	1.00	4/2095 (0.2%)
14	b	1.08	3/1554 (0.2%)	1.00	5/2104 (0.2%)
All	All	0.99	66/48920 (0.1%)	1.06	252/66183 (0.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	5
3	C	0	1
3	Q	0	2
4	D	0	5
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
12	L	0	1
12	Z	0	1
13	a	0	1
All	All	1	26

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	13.81	1.40	1.25
14	N	150	GLU	CG-CD	11.07	1.68	1.51
12	Z	3	SER	CB-OG	10.22	1.55	1.42
13	a	75	GLU	CD-OE1	10.04	1.36	1.25
14	b	150	GLU	CG-CD	9.59	1.66	1.51
7	U	108	GLU	CD-OE1	9.00	1.35	1.25
3	Q	13	ASP	CB-CG	7.92	1.68	1.51
14	N	92	GLU	CG-CD	7.27	1.62	1.51
4	R	216	GLU	CD-OE2	7.24	1.33	1.25
14	b	133	SER	CB-OG	7.20	1.51	1.42
4	D	126	GLU	CD-OE2	7.13	1.33	1.25
2	P	103	GLU	CD-OE2	7.04	1.33	1.25
12	Z	78	SER	CB-OG	-6.99	1.33	1.42
2	B	103	GLU	CD-OE2	6.91	1.33	1.25
11	K	40	TYR	CE1-CZ	6.80	1.47	1.38
7	G	108	GLU	CD-OE2	6.65	1.32	1.25
10	J	153	ARG	NE-CZ	-6.64	1.24	1.33
14	b	92	GLU	CD-OE2	6.54	1.32	1.25
2	B	103	GLU	CD-OE1	6.49	1.32	1.25
2	B	70	GLU	CD-OE1	6.34	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	100	TRP	CE3-CZ3	6.32	1.49	1.38
13	a	119	GLU	CG-CD	6.22	1.61	1.51
6	F	218	GLU	CD-OE2	6.21	1.32	1.25
3	C	182	GLU	CG-CD	6.16	1.61	1.51
9	I	69	ARG	CD-NE	-6.15	1.35	1.46
6	F	104	TYR	CG-CD1	6.04	1.47	1.39
6	T	7	TYR	N-CA	6.03	1.58	1.46
13	a	119	GLU	CD-OE2	5.99	1.32	1.25
5	E	7	ASP	CB-CG	-5.97	1.39	1.51
4	D	100	TRP	CE3-CZ3	5.90	1.48	1.38
14	N	24	SER	CB-OG	-5.90	1.34	1.42
13	M	119	GLU	CG-CD	5.85	1.60	1.51
6	F	104	TYR	CE2-CZ	5.84	1.46	1.38
12	L	78	SER	CB-OG	-5.79	1.34	1.42
2	B	168	SER	CB-OG	-5.78	1.34	1.42
12	Z	142	SER	CB-OG	-5.78	1.34	1.42
7	U	108	GLU	CD-OE2	5.76	1.31	1.25
8	H	6	VAL	CB-CG1	-5.73	1.40	1.52
12	L	140	SER	CB-OG	-5.70	1.34	1.42
11	K	40	TYR	CG-CD1	5.66	1.46	1.39
13	M	119	GLU	CD-OE2	5.56	1.31	1.25
10	X	153	ARG	CZ-NH1	-5.52	1.25	1.33
4	D	100	TRP	CE2-CZ2	5.46	1.49	1.39
11	Y	40	TYR	CE1-CZ	5.41	1.45	1.38
6	T	25	TYR	CG-CD1	5.40	1.46	1.39
6	F	6	GLY	C-O	5.36	1.32	1.23
11	Y	113	TYR	CE1-CZ	-5.36	1.31	1.38
5	S	114	SER	CB-OG	-5.36	1.35	1.42
8	V	104[A]	ASP	CB-CG	-5.36	1.40	1.51
8	V	104[B]	ASP	CB-CG	-5.36	1.40	1.51
6	T	104	TYR	CE2-CZ	5.32	1.45	1.38
1	A	17	LYS	CD-CE	5.31	1.64	1.51
3	C	182	GLU	CD-OE2	-5.29	1.19	1.25
2	P	168	SER	CB-OG	-5.28	1.35	1.42
1	A	82	TYR	CE1-CZ	5.28	1.45	1.38
1	O	123	SER	CB-OG	-5.19	1.35	1.42
14	N	88	TYR	CE1-CZ	5.19	1.45	1.38
10	X	154	GLU	CG-CD	5.19	1.59	1.51
11	Y	40	TYR	CG-CD1	5.19	1.45	1.39
6	F	31	GLU	CD-OE2	5.15	1.31	1.25
9	I	105	GLU	CD-OE2	5.12	1.31	1.25
11	Y	67	GLU	CD-OE2	5.08	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	99	ARG	CD-NE	-5.07	1.37	1.46
12	L	2	PHE	CB-CG	-5.06	1.42	1.51
5	E	4	ASN	N-CA	5.06	1.56	1.46
9	W	84	TYR	CE1-CZ	5.03	1.45	1.38

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	X	86	ARG	NE-CZ-NH2	-21.50	109.55	120.30
10	J	86	ARG	NE-CZ-NH2	-21.33	109.63	120.30
10	J	86	ARG	NE-CZ-NH1	20.61	130.60	120.30
10	X	86	ARG	NE-CZ-NH1	18.78	129.69	120.30
9	I	69	ARG	NE-CZ-NH1	17.32	128.96	120.30
9	W	69	ARG	NE-CZ-NH1	16.30	128.45	120.30
12	Z	99	ARG	NE-CZ-NH2	-15.80	112.40	120.30
8	H	72	ARG	NE-CZ-NH2	-15.71	112.44	120.30
12	L	99	ARG	NE-CZ-NH2	-15.71	112.44	120.30
9	I	25[A]	ARG	NE-CZ-NH1	13.88	127.24	120.30
9	I	25[B]	ARG	NE-CZ-NH1	13.88	127.24	120.30
12	Z	99	ARG	NE-CZ-NH1	13.29	126.95	120.30
8	H	72	ARG	NE-CZ-NH1	13.23	126.91	120.30
9	W	69	ARG	NE-CZ-NH2	-11.86	114.37	120.30
9	I	69	ARG	NE-CZ-NH2	-11.70	114.45	120.30
12	L	99	ARG	NE-CZ-NH1	11.57	126.08	120.30
10	X	153	ARG	NE-CZ-NH1	-11.28	114.66	120.30
7	U	88	ARG	NE-CZ-NH1	10.37	125.48	120.30
7	G	117	ARG	NE-CZ-NH1	10.30	125.45	120.30
14	b	29	ARG	NE-CZ-NH1	10.08	125.34	120.30
4	R	120[A]	ALA	C-N-CA	9.99	146.69	121.70
4	R	120[B]	ALA	C-N-CA	9.99	146.69	121.70
2	P	96	ARG	NE-CZ-NH1	9.95	125.28	120.30
11	Y	157	ARG	NE-CZ-NH1	9.87	125.24	120.30
9	W	25[A]	ARG	NE-CZ-NH1	9.83	125.21	120.30
9	W	25[B]	ARG	NE-CZ-NH1	9.83	125.21	120.30
11	Y	157	ARG	NE-CZ-NH2	-9.61	115.50	120.30
2	B	4	ARG	NE-CZ-NH1	9.28	124.94	120.30
2	B	96	ARG	NE-CZ-NH1	9.17	124.89	120.30
7	U	117	ARG	NE-CZ-NH1	9.14	124.87	120.30
4	D	9	ASP	CB-CG-OD1	9.06	126.45	118.30
14	N	92	GLU	OE1-CD-OE2	-9.05	112.43	123.30
12	Z	172	MET	CG-SD-CE	-8.98	85.83	100.20
11	Y	141[A]	ARG	NE-CZ-NH1	8.82	124.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	141[B]	ARG	NE-CZ-NH1	8.82	124.71	120.30
9	W	16[A]	LYS	C-N-CA	8.78	143.65	121.70
9	W	16[B]	LYS	C-N-CA	8.78	143.65	121.70
6	F	117	MET	CG-SD-CE	8.77	114.22	100.20
11	Y	158	ARG	NE-CZ-NH1	8.52	124.56	120.30
10	J	86	ARG	CD-NE-CZ	8.48	135.47	123.60
9	I	16[A]	LYS	C-N-CA	8.41	142.73	121.70
9	I	16[B]	LYS	C-N-CA	8.41	142.73	121.70
13	M	5	MET	CG-SD-CE	8.30	113.48	100.20
4	R	9	ASP	CB-CG-OD1	8.29	125.76	118.30
6	T	27	MET	CG-SD-CE	8.25	113.41	100.20
13	M	151	ARG	NE-CZ-NH1	8.21	124.41	120.30
6	F	114	ARG	NE-CZ-NH2	-8.09	116.26	120.30
6	T	117	MET	CG-SD-CE	8.06	113.10	100.20
12	L	172	MET	CG-SD-CE	-8.00	87.41	100.20
6	T	114	ARG	NE-CZ-NH2	-7.96	116.32	120.30
3	C	117	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	B	4	ARG	NE-CZ-NH2	-7.88	116.36	120.30
11	K	141	ARG	NE-CZ-NH1	7.87	124.24	120.30
11	K	86	MET	CG-SD-CE	7.86	112.78	100.20
13	a	5	MET	CG-SD-CE	7.85	112.76	100.20
6	T	43	ASP	CB-CG-OD2	7.78	125.31	118.30
8	V	72	ARG	NE-CZ-NH2	-7.78	116.41	120.30
11	Y	115	ASP	CB-CG-OD2	7.78	125.30	118.30
9	I	25[A]	ARG	NE-CZ-NH2	-7.77	116.42	120.30
9	I	25[B]	ARG	NE-CZ-NH2	-7.77	116.42	120.30
7	U	88	ARG	NE-CZ-NH2	-7.76	116.42	120.30
6	F	190	VAL	CB-CA-C	-7.68	96.80	111.40
8	H	81	ARG	NE-CZ-NH2	-7.63	116.49	120.30
13	M	151	ARG	NE-CZ-NH2	-7.58	116.51	120.30
11	Y	120	ARG	NE-CZ-NH1	7.56	124.08	120.30
5	E	122	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	O	181	LEU	CA-CB-CG	7.49	132.52	115.30
7	G	120	ASP	CB-CG-OD1	7.47	125.02	118.30
6	F	206	ASP	CB-CG-OD1	-7.44	111.60	118.30
2	P	4	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	219	ARG	NE-CZ-NH1	7.29	123.94	120.30
11	K	157	ARG	NE-CZ-NH2	-7.25	116.67	120.30
11	K	154	ASP	CB-CG-OD2	7.24	124.82	118.30
11	Y	158	ARG	NE-CZ-NH2	-7.24	116.68	120.30
8	H	198	ARG	NE-CZ-NH1	7.22	123.91	120.30
11	K	157	ARG	NE-CZ-NH1	7.21	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	86	MET	CG-SD-CE	7.14	111.62	100.20
8	H	198	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	219	ARG	NE-CZ-NH2	-6.99	116.81	120.30
6	F	206	ASP	CB-CG-OD2	6.99	124.59	118.30
11	K	120	ARG	NE-CZ-NH1	6.94	123.77	120.30
10	X	90	ASP	CB-CG-OD1	6.93	124.53	118.30
5	S	122	ARG	NE-CZ-NH2	-6.90	116.85	120.30
10	X	86	ARG	CD-NE-CZ	6.88	133.22	123.60
6	T	6	GLY	C-N-CA	6.87	138.87	121.70
7	U	80[A]	MET	CG-SD-CE	6.82	111.12	100.20
7	U	80[B]	MET	CG-SD-CE	6.82	111.12	100.20
8	H	72	ARG	CD-NE-CZ	6.82	133.15	123.60
10	J	33	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	73	LEU	CA-CB-CG	6.81	130.97	115.30
6	T	17	ASP	CB-CG-OD1	-6.81	112.17	118.30
10	J	88	LEU	CB-CG-CD2	6.70	122.39	111.00
6	T	169	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	B	96	ARG	NE-CZ-NH2	-6.66	116.97	120.30
10	X	93	ARG	NE-CZ-NH1	6.61	123.60	120.30
6	T	190	VAL	CB-CA-C	-6.59	98.88	111.40
8	H	86	MET	CG-SD-CE	-6.56	89.70	100.20
6	F	17	ASP	CB-CG-OD1	-6.54	112.41	118.30
9	I	58	ASP	CB-CG-OD2	6.50	124.15	118.30
6	T	113	ASP	CB-CG-OD2	-6.48	112.47	118.30
11	K	107	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	P	96	ARG	NE-CZ-NH2	-6.42	117.09	120.30
3	Q	5	ARG	NE-CZ-NH1	6.40	123.50	120.30
7	G	117	ARG	NE-CZ-NH2	-6.39	117.10	120.30
10	J	93	ARG	NE-CZ-NH1	6.39	123.50	120.30
9	I	197	ARG	NE-CZ-NH1	6.39	123.49	120.30
3	Q	5	ARG	NE-CZ-NH2	-6.38	117.11	120.30
7	G	245	ARG	NE-CZ-NH1	6.38	123.49	120.30
13	a	166	ARG	NE-CZ-NH2	-6.36	117.12	120.30
6	F	43	ASP	CB-CG-OD1	6.34	124.00	118.30
5	E	94	ASP	CB-CG-OD2	6.32	123.99	118.30
13	M	166	ARG	NE-CZ-NH2	-6.30	117.15	120.30
6	F	87	LEU	CB-CG-CD1	6.27	121.67	111.00
12	Z	71	ARG	NE-CZ-NH2	6.26	123.43	120.30
12	Z	99	ARG	CD-NE-CZ	6.26	132.36	123.60
7	G	88	ARG	NE-CZ-NH2	-6.24	117.18	120.30
11	K	158	ARG	NE-CZ-NH2	-6.22	117.19	120.30
14	b	116	MET	CG-SD-CE	-6.21	90.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	232[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
6	F	232[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
8	V	72	ARG	NE-CZ-NH1	6.19	123.40	120.30
11	Y	107	ARG	NE-CZ-NH1	6.19	123.39	120.30
6	F	232[A]	ARG	NE-CZ-NH1	6.16	123.38	120.30
6	F	232[B]	ARG	NE-CZ-NH1	6.16	123.38	120.30
14	N	116	MET	CG-SD-CE	-6.12	90.41	100.20
7	U	11	ARG	NE-CZ-NH1	6.11	123.35	120.30
4	D	157	ASP	CB-CG-OD1	6.11	123.80	118.30
3	Q	13	ASP	CB-CA-C	6.10	122.60	110.40
11	K	158	ARG	NE-CZ-NH1	6.09	123.34	120.30
9	W	25[A]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
9	W	25[B]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	O	73	LEU	CA-CB-CG	6.07	129.26	115.30
1	O	88	ARG	NE-CZ-NH2	-6.07	117.27	120.30
9	I	134	ASP	CB-CG-OD1	6.04	123.74	118.30
9	W	134	ASP	CB-CG-OD1	6.04	123.74	118.30
5	E	122	ARG	NE-CZ-NH1	6.03	123.32	120.30
6	F	83	ASP	CB-CG-OD2	-6.03	112.88	118.30
14	N	45	ARG	NE-CZ-NH2	-6.02	117.29	120.30
9	W	197	ARG	NE-CZ-NH1	6.01	123.31	120.30
10	J	161	ARG	NE-CZ-NH2	-6.00	117.30	120.30
12	L	99	ARG	CD-NE-CZ	5.99	131.99	123.60
4	D	90	ASP	CB-CG-OD1	-5.99	112.91	118.30
5	E	126	ARG	NE-CZ-NH1	5.98	123.29	120.30
4	D	168	ARG	NE-CZ-NH2	-5.95	117.32	120.30
6	F	156	VAL	CG1-CB-CG2	-5.95	101.38	110.90
3	C	79	ASP	CB-CG-OD2	-5.94	112.95	118.30
13	a	151	ARG	NE-CZ-NH1	5.93	123.27	120.30
8	V	12	ILE	CG1-CB-CG2	-5.93	98.36	111.40
13	a	41	ARG	NE-CZ-NH1	5.93	123.26	120.30
11	Y	115	ASP	CB-CG-OD1	-5.92	112.97	118.30
6	F	70	ASP	CB-CG-OD1	5.88	123.59	118.30
8	H	12	ILE	CG1-CB-CG2	-5.86	98.51	111.40
14	N	45	ARG	NE-CZ-NH1	5.86	123.23	120.30
6	T	114	ARG	NE-CZ-NH1	5.85	123.22	120.30
4	D	168	ARG	NE-CZ-NH1	5.84	123.22	120.30
7	G	86	ASP	CB-CG-OD1	5.84	123.55	118.30
6	F	40	ARG	NE-CZ-NH1	5.80	123.20	120.30
8	V	81	ARG	NE-CZ-NH2	-5.79	117.40	120.30
13	M	99	ARG	NE-CZ-NH1	5.79	123.19	120.30
14	b	29	ARG	CB-CA-C	-5.78	98.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	7	TYR	N-CA-CB	5.77	120.98	110.60
7	G	183	VAL	CB-CA-C	-5.76	100.45	111.40
10	X	70	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	O	73	LEU	CB-CA-C	-5.76	99.26	110.20
9	I	25[A]	ARG	CD-NE-CZ	5.75	131.65	123.60
9	I	25[B]	ARG	CD-NE-CZ	5.75	131.65	123.60
3	C	5	ARG	NE-CZ-NH1	5.73	123.17	120.30
3	Q	220	LEU	CA-C-N	5.73	129.80	117.20
5	S	174	ARG	NE-CZ-NH1	5.72	123.16	120.30
14	b	29	ARG	NE-CZ-NH2	-5.72	117.44	120.30
3	Q	137	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	O	219	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	B	116	ASP	CB-CG-OD1	5.71	123.44	118.30
5	E	174	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	73	LEU	CB-CA-C	-5.69	99.39	110.20
6	F	114	ARG	NE-CZ-NH1	5.66	123.13	120.30
13	M	73	ASP	CB-CG-OD1	5.65	123.38	118.30
3	C	36	ARG	NE-CZ-NH1	5.64	123.12	120.30
10	J	70	ARG	NE-CZ-NH2	-5.63	117.48	120.30
10	J	85	ARG	NE-CZ-NH2	-5.61	117.50	120.30
6	F	169[A]	ARG	NE-CZ-NH2	-5.60	117.50	120.30
6	F	169[B]	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	P	116	ASP	CB-CG-OD1	5.58	123.32	118.30
10	X	33	ASP	CB-CG-OD1	5.56	123.30	118.30
5	S	122	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	O	142	ARG	NE-CZ-NH1	5.53	123.06	120.30
8	H	77	VAL	CB-CA-C	-5.53	100.90	111.40
11	Y	71	LYS	CD-CE-NZ	5.50	124.36	111.70
1	A	142	ARG	NE-CZ-NH1	5.47	123.03	120.30
4	R	120[A]	ALA	N-CA-C	-5.47	96.24	111.00
4	R	120[B]	ALA	N-CA-C	-5.47	96.24	111.00
14	b	19	ARG	NE-CZ-NH2	-5.46	117.57	120.30
10	X	70	ARG	NE-CZ-NH1	5.45	123.03	120.30
10	X	161	ARG	NE-CZ-NH2	-5.45	117.58	120.30
8	V	86	MET	CG-SD-CE	-5.44	91.50	100.20
13	M	41	ARG	NE-CZ-NH1	5.43	123.01	120.30
6	T	70	ASP	CB-CG-OD1	5.39	123.16	118.30
10	J	161	ARG	NE-CZ-NH1	5.39	123.00	120.30
12	L	114	ASP	CB-CG-OD1	5.38	123.14	118.30
6	T	87	LEU	CB-CG-CD1	5.38	120.14	111.00
3	C	5	ARG	NE-CZ-NH2	-5.37	117.61	120.30
10	X	88	LEU	CB-CG-CD2	5.37	120.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	120	ARG	NE-CZ-NH2	-5.37	117.62	120.30
5	S	7	ASP	CB-CG-OD1	-5.35	113.49	118.30
10	J	52	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	C	85[A]	ASN	CB-CA-C	5.28	120.96	110.40
3	C	85[B]	ASN	CB-CA-C	5.28	120.96	110.40
12	L	100	ARG	NE-CZ-NH1	5.28	122.94	120.30
10	J	184	ASP	CB-CG-OD1	5.26	123.04	118.30
6	F	85	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	P	4	ARG	NE-CZ-NH2	-5.25	117.67	120.30
5	E	122	ARG	CG-CD-NE	-5.24	100.80	111.80
2	B	2	SER	N-CA-CB	5.22	118.34	110.50
3	Q	220	LEU	C-N-CA	5.22	134.75	121.70
11	K	166	ARG	NE-CZ-NH1	5.20	122.90	120.30
8	V	51	ASP	CB-CG-OD2	-5.20	113.62	118.30
9	I	158	ASP	CB-CG-OD1	5.19	122.97	118.30
6	T	230	ASP	CB-CG-OD2	5.18	122.96	118.30
8	H	203	ARG	NE-CZ-NH1	5.18	122.89	120.30
11	Y	56	GLU	CA-CB-CG	-5.17	102.03	113.40
4	R	168	ARG	NE-CZ-NH2	-5.16	117.72	120.30
6	F	169[A]	ARG	NE-CZ-NH1	5.16	122.88	120.30
6	F	169[B]	ARG	NE-CZ-NH1	5.16	122.88	120.30
7	U	120	ASP	CB-CG-OD1	5.15	122.94	118.30
8	V	68	LEU	CB-CG-CD1	5.14	119.74	111.00
8	V	28	ASP	CB-CG-OD1	5.13	122.92	118.30
6	F	85	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	P	3	ARG	NE-CZ-NH2	-5.13	117.73	120.30
6	F	152	ASP	CB-CG-OD1	5.12	122.91	118.30
13	a	182	ARG	NE-CZ-NH1	5.12	122.86	120.30
10	J	153	ARG	NE-CZ-NH2	-5.11	117.74	120.30
11	K	45	MET	CG-SD-CE	5.11	108.38	100.20
13	a	67	LEU	CA-CB-CG	5.11	127.05	115.30
6	T	169	ARG	NE-CZ-NH2	-5.10	117.75	120.30
10	X	161	ARG	NE-CZ-NH1	5.08	122.84	120.30
10	J	90	ASP	CB-CG-OD1	5.08	122.87	118.30
1	O	219	ARG	NE-CZ-NH1	5.08	122.84	120.30
8	H	68	LEU	CB-CG-CD1	5.07	119.62	111.00
5	S	100	ASP	CB-CG-OD2	5.07	122.86	118.30
13	a	44	ARG	NE-CZ-NH1	5.05	122.83	120.30
5	E	193	ARG	NE-CZ-NH1	5.04	122.82	120.30
6	T	17	ASP	CB-CG-OD2	5.04	122.84	118.30
9	W	25[A]	ARG	CD-NE-CZ	5.03	130.65	123.60
9	W	25[B]	ARG	CD-NE-CZ	5.03	130.65	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	73	ASP	CB-CG-OD1	5.03	122.83	118.30
3	C	197	GLU	OE1-CD-OE2	5.02	129.33	123.30
6	F	40	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	P	190	LEU	CB-CG-CD1	5.02	119.54	111.00
12	Z	99	ARG	CG-CD-NE	-5.02	101.26	111.80
10	X	52	ASP	CB-CG-OD2	-5.02	113.78	118.30
11	K	120	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	F	99	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
4	D	223	GLY	Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
12	L	99	ARG	Sidechain
2	P	202	ASP	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
10	X	86	ARG	Sidechain
12	Z	99	ARG	Sidechain
13	a	215	ILE	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	1788	0	1761	16	0
1	O	1741	0	1683	8	0
2	B	1922	0	1913	9	0
2	P	1898	0	1861	15	0
3	C	1798	0	1718	20	0
3	Q	1825	0	1751	17	0
4	D	1762	0	1709	9	0
4	R	1753	0	1726	12	0
5	E	1822	0	1779	12	0
5	S	1853	0	1796	24	0
6	F	1888	0	1882	12	0
6	T	1856	0	1816	14	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	20	0
8	H	1664	0	1681	8	0
8	V	1622	0	1595	6	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	19	0
10	X	1576	0	1561	12	0
11	K	1545	0	1495	7	0
11	Y	1570	0	1547	12	0
12	L	1636	0	1625	5	0
12	Z	1642	0	1635	5	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	0	0
14	N	1519	0	1496	5	0
14	b	1524	0	1496	0	0
15	c	37	0	6	0	0
15	d	37	0	6	0	0
16	A	4	0	0	1	0
16	B	2	0	0	2	0
16	C	2	0	0	1	0
16	D	2	0	0	0	0
16	E	3	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	H	2	0	0	1	0
16	I	1	0	0	0	0
16	K	4	0	0	0	0
16	M	4	0	0	1	0
16	N	3	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	1	0
16	R	2	0	0	1	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	2	0	0	0	0
16	W	1	0	0	0	0
16	Y	5	0	0	0	0
16	a	3	0	0	0	0
16	b	4	0	0	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	H	32	0	44	0	0
19	I	32	0	44	1	0
19	L	16	0	22	0	0
19	M	16	0	22	1	0
19	V	16	0	22	1	0
19	W	16	0	22	0	0
19	Z	16	0	22	0	0
20	A	109	0	0	4	0
20	B	120	0	0	0	0
20	C	76	0	0	1	0
20	D	93	0	0	3	0
20	E	137	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	180	0	0	4	0
20	G	187	0	0	4	0
20	H	157	0	0	4	0
20	I	155	0	0	1	0
20	J	133	0	0	2	0
20	K	98	0	0	0	0
20	L	124	0	0	0	0
20	M	148	0	0	1	0
20	N	168	0	0	0	0
20	O	89	0	0	1	0
20	P	117	0	0	2	0
20	Q	74	0	0	1	0
20	R	122	0	0	2	0
20	S	118	0	0	4	0
20	T	92	0	0	2	0
20	U	102	0	0	1	0
20	V	112	0	0	2	0
20	W	111	0	0	1	0
20	X	124	0	0	3	0
20	Y	137	0	0	0	0
20	Z	164	0	0	0	0
20	a	167	0	0	0	0
20	b	126	0	0	0	0
20	c	1	0	0	0	0
20	d	1	0	0	0	0
All	All	51947	0	47542	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (279) 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)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.25	0.99
10:X:1:MET:HE1	10:X:134:TYR:H	1.30	0.96
5:S:65[A]:HIS:CE1	20:S:404:HOH:O	2.27	0.87
16:R:301:CL:CL	20:R:506:HOH:O	2.29	0.86
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.60	0.84
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.78	0.84
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.07	0.81
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.61	0.80
7:U:137:YCM:HD3	7:U:168:ALA:HB1	1.64	0.79
7:U:137:YCM:OZ1	7:U:139:ILE:HG13	1.83	0.78
10:J:99[A]:HIS:CD2	20:J:406:HOH:O	2.36	0.78
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.66	0.77
8:V:195:LYS:CB	20:V:495:HOH:O	2.31	0.77
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.29	0.77
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.66	0.77
10:J:185:LYS:NZ	20:J:401:HOH:O	2.15	0.76
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.01	0.74
4:D:96:THR:OG1	20:D:401:HOH:O	2.06	0.74
6:F:221:ASN:HB2	20:F:557:HOH:O	1.87	0.73
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.71	0.73
5:S:152[B]:ASN:ND2	20:S:401:HOH:O	2.22	0.72
7:G:188:ASP:O	7:G:190:THR:HG22	1.89	0.72
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.24	0.71
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.73	0.70
9:I:35:THR:HG21	20:I:450:HOH:O	1.91	0.69
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.39	0.69
10:X:1:MET:HE1	10:X:134:TYR:N	2.06	0.69
14:N:35:THR:CG2	14:N:45:ARG:HE	2.05	0.69
1:A:88[B]:ARG:NH2	20:A:401:HOH:O	2.22	0.68
5:S:101:ARG:NH1	20:S:403:HOH:O	2.27	0.68
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.76	0.67
5:E:58:ALA:O	5:E:59:HIS:CB	2.43	0.67
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.43	0.66
2:P:25[B]:MET:CE	2:P:25[B]:MET:HA	2.25	0.66
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.43	0.66
1:O:10:THR:HG23	20:O:404:HOH:O	1.95	0.66
20:H:541:HOH:O	12:Z:160:ASN:CB	2.43	0.66
5:E:47:VAL:CG1	5:E:195:LEU:HD22	2.26	0.65
5:S:65[A]:HIS:ND1	20:S:404:HOH:O	2.28	0.65
7:U:58:ASP:O	7:U:59:LYS:CB	2.44	0.65
4:R:129:ASP:CB	4:R:130:PRO:CD	2.75	0.65
16:C:302:CL:CL	20:C:446:HOH:O	2.51	0.64
7:U:137:YCM:HD3	7:U:168:ALA:CB	2.26	0.64
13:M:170:GLU:OE1	20:M:401:HOH:O	2.15	0.64
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.27	0.64
3:C:47:LYS:CB	3:C:48:LYS:HA	2.28	0.63
5:S:47:VAL:CG1	5:S:195:LEU:HD22	2.27	0.62
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.17	0.62
7:U:195:VAL:O	7:U:199:ILE:HG23	1.99	0.62
12:L:144:MET:CE	12:L:185:ARG:HB2	2.31	0.61
10:X:95:ARG:HB2	10:X:95:ARG:HH11	1.65	0.61
3:C:47:LYS:CB	3:C:48:LYS:CA	2.79	0.60
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.41	0.59
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.69	0.58
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.87	0.58
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.01	0.58
5:E:49:LEU:O	5:E:62:LYS:HD2	2.04	0.58
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.85	0.57
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.86	0.57
5:S:49:LEU:O	5:S:62:LYS:HD2	2.04	0.57
20:D:458:HOH:O	5:E:57:ALA:HB2	2.05	0.57
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.87	0.57
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.05	0.57
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.51	0.56
7:U:80[A]:MET:HE3	7:U:91:VAL:HG23	1.87	0.56
1:A:52:LYS:CB	20:A:492:HOH:O	2.53	0.56
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.86	0.56
2:P:246:LYS:N	2:P:246:LYS:HE3	2.22	0.55
2:P:25[B]:MET:HE1	20:P:435:HOH:O	2.06	0.55
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.38	0.55
2:P:160:LYS:HE2	2:P:181:GLU:OE1	2.07	0.54
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.88	0.54
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.37	0.54
6:T:205:LYS:O	6:T:206:ASP:CG	2.45	0.54
2:P:25[B]:MET:HA	2:P:25[B]:MET:HE2	1.90	0.54
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.55	0.54
10:X:110:HIS:HB2	20:X:513:HOH:O	2.09	0.53
13:M:5:MET:HE2	14:N:116:MET:HB3	1.89	0.53
4:R:78:MET:HG3	4:R:82:ILE:CD1	2.37	0.53
3:C:50:VAL:O	3:C:51:ALA:HB3	2.07	0.53
9:W:35:THR:HG21	20:W:444:HOH:O	2.09	0.53
7:G:145:GLU:CB	20:G:547:HOH:O	2.56	0.52
20:Q:453:HOH:O	4:R:60:GLU:HG3	2.09	0.52
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.43	0.52
16:B:301:CL:CL	16:B:302:CL:CL	3.01	0.52
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.09	0.52
9:W:13:MET:HE1	9:W:166:ILE:N	2.25	0.52
1:A:214:GLU:HB3	20:A:499:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:203:ARG:NH2	9:I:154:GLU:OE1	2.38	0.51
9:I:73:TYR:CE1	9:I:77:GLU:OE2	2.64	0.51
5:S:234:GLU:HA	5:S:234:GLU:OE2	2.10	0.51
3:Q:203:GLY:HA2	3:Q:229:VAL:HG11	1.93	0.51
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.43	0.51
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.59	0.50
7:U:81:THR:HB	7:U:137:YCM:CD	2.42	0.50
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.41	0.50
4:R:182:GLN:HA	5:S:56:LEU:HD11	1.92	0.50
16:A:302:CL:CL	16:B:302:CL:CL	43.33	0.50
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.94	0.50
10:J:49:GLU:O	10:J:53:THR:HG23	2.10	0.50
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.93	0.50
4:D:129:ASP:HA	20:D:477:HOH:O	2.11	0.50
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.93	0.50
7:G:42:VAL:HG13	7:G:198:ALA:HB2	1.94	0.50
10:X:49:GLU:O	10:X:53:THR:HG23	2.12	0.50
11:K:40:TYR:CD2	11:K:73:ARG:CZ	2.95	0.49
8:V:213:THR:HB	9:W:198:THR:OG1	2.12	0.49
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.12	0.49
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.95	0.49
3:C:183:THR:OG1	3:C:184:ASP:N	2.45	0.49
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.27	0.49
8:H:203:ARG:N	20:H:404:HOH:O	2.46	0.49
8:V:178:ILE:HG12	8:V:183:LEU:HD12	1.93	0.49
2:B:33:THR:HB	2:B:166:ASN:O	2.11	0.49
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.93	0.49
20:G:508:HOH:O	8:H:72:ARG:HD3	2.12	0.49
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.40	0.49
1:A:63:LYS:NZ	20:A:405:HOH:O	2.45	0.48
16:M:302:CL:CL	16:M:303:CL:CL	3.05	0.48
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.28	0.48
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.42	0.48
8:H:216:ILE:HD13	9:I:195:THR:HG23	1.94	0.48
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.43	0.48
3:C:50:VAL:O	3:C:51:ALA:CB	2.61	0.48
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.43	0.48
2:P:155:ASN:ND2	20:P:402:HOH:O	2.38	0.48
11:Y:40:TYR:CD2	11:Y:73:ARG:NH1	2.82	0.48
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.14	0.48
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:43:ARG:HB3	7:U:151:VAL:CG1	2.43	0.48
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.14	0.48
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.95	0.48
8:H:178:ILE:HG12	8:H:183:LEU:HD12	1.96	0.47
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.96	0.47
10:X:161:ARG:HD3	20:X:492:HOH:O	2.14	0.47
10:X:132:HIS:HD2	20:X:470:HOH:O	1.97	0.47
1:A:174:GLU:OE1	2:B:53:HIS:NE2	2.46	0.47
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.41	0.47
6:F:30:VAL:HG22	6:F:133[A]:CYS:HA	1.97	0.47
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.43	0.47
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.14	0.47
3:C:226:GLU:HG3	3:C:226:GLU:O	2.13	0.47
14:N:190:LEU:H	14:N:193:GLN:HE21	1.61	0.47
4:R:29:GLU:OE2	4:R:32:LYS:HE2	2.14	0.47
6:T:110:HIS:HD2	20:T:346:HOH:O	1.97	0.47
5:E:65:HIS:HB2	20:E:439:HOH:O	2.15	0.47
13:M:27:LEU:HD22	13:M:184:TYR:HB2	1.97	0.47
11:Y:68:LEU:O	11:Y:71:LYS:HE3	2.14	0.47
6:F:204:VAL:HG22	20:F:409:HOH:O	2.13	0.46
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.64	0.46
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.97	0.46
1:A:17:LYS:HE2	1:A:22:GLU:OE2	2.15	0.46
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.55	0.46
2:P:197:LEU:HB3	2:P:201:MET:HE3	1.97	0.46
6:F:219:LEU:HD22	20:F:433:HOH:O	2.14	0.46
2:P:33:THR:HB	2:P:166:ASN:O	2.14	0.46
11:K:158:ARG:HD2	11:K:162:GLN:HE21	1.80	0.46
2:P:2:SER:HB3	5:S:123:TYR:CE2	2.51	0.46
2:P:8:ARG:HH21	3:Q:5:ARG:HD2	1.80	0.46
7:U:42:VAL:HG13	7:U:198:ALA:HB2	1.98	0.46
11:Y:40:TYR:CZ	11:Y:73:ARG:HB3	2.51	0.46
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.16	0.46
2:B:44:LEU:HD12	2:B:44:LEU:C	2.37	0.46
4:D:78:MET:HG3	4:D:82:ILE:CD1	2.44	0.46
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.16	0.46
11:K:40:TYR:CD2	11:K:73:ARG:NH1	2.84	0.45
4:D:203:LYS:HE2	4:D:210:LEU:HB3	1.98	0.45
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.16	0.45
7:U:81:THR:OG1	7:U:137:YCM:NZ2	2.46	0.45
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.16	0.45
5:E:218:ASP:OD1	5:E:218:ASP:N	2.49	0.45
9:I:73:TYR:CE1	9:I:77:GLU:CD	2.90	0.45
3:Q:183:THR:OG1	3:Q:184:ASP:N	2.50	0.45
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.45	0.45
5:S:196:ARG:NH2	5:S:238:GLU:CB	2.80	0.45
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.49	0.45
11:K:137:GLY:O	11:K:141:ARG:HG2	2.17	0.45
7:G:43:ARG:HB3	7:G:151:VAL:HG23	1.99	0.45
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.37	0.45
6:T:30:VAL:HG22	6:T:133[A]:CYS:HA	1.98	0.45
1:A:133:LEU:O	1:A:147:GLN:HA	2.17	0.44
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.97	0.44
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.48	0.44
3:Q:106:TYR:C	3:Q:106:TYR:CD1	2.90	0.44
3:Q:12:PRO:HA	4:R:26:TYR:CD2	2.53	0.44
13:M:114:GLY:HA2	13:M:192:VAL:HG11	2.00	0.44
3:C:106:TYR:C	3:C:106:TYR:CD1	2.90	0.44
3:C:183:THR:HG23	3:C:186:LEU:H	1.83	0.44
8:H:201:ARG:NH1	20:H:406:HOH:O	2.49	0.44
1:O:10:THR:HB	1:O:20:GLN:HB2	1.99	0.44
1:A:206:ASN:HD22	1:A:206:ASN:C	2.22	0.44
13:M:144:TYR:CZ	19:M:305:1PE:H242	2.53	0.44
7:U:80[A]:MET:CE	7:U:91:VAL:HG23	2.47	0.44
6:T:53:VAL:HG12	6:T:208:ALA:HB1	2.00	0.43
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.98	0.43
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.18	0.43
6:F:170:GLN:O	6:F:174:THR:HG23	2.18	0.43
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.43
10:J:12:TYR:CD1	10:J:182:ILE:HD11	2.52	0.43
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.99	0.43
6:T:191:LYS:HB3	6:T:238:TYR:CD1	2.54	0.43
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.18	0.43
7:U:137:YCM:CD	7:U:137:YCM:C	2.97	0.43
5:S:237:GLU:O	5:S:238:GLU:CB	2.66	0.43
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.49	0.43
10:X:86:ARG:HD3	10:X:90:ASP:OD1	2.19	0.43
14:N:190:LEU:H	14:N:193:GLN:NE2	2.17	0.42
1:O:133:LEU:O	1:O:147:GLN:HA	2.19	0.42
1:O:110:VAL:HG22	1:O:135:ILE:HD12	2.01	0.42
3:Q:95:ARG:HG2	16:Q:301:CL:CL	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18[B]:ARG:CG	5:S:19:ILE:N	2.80	0.42
1:A:198:PHE:O	1:A:199:GLU:CB	2.67	0.42
5:E:150:SER:O	5:E:151:ALA:HB3	2.20	0.42
4:R:203:LYS:HE2	4:R:210:LEU:HB3	2.01	0.42
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.54	0.42
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.49	0.42
4:D:182:GLN:HA	5:E:56:LEU:HD11	2.00	0.42
3:Q:183:THR:HG23	3:Q:186:LEU:H	1.84	0.42
3:Q:85:ASN:OD1	10:X:70:ARG:NH2	2.52	0.42
11:Y:40:TYR:HB3	11:Y:73:ARG:NH1	2.34	0.42
3:C:47:LYS:CB	3:C:48:LYS:O	2.68	0.42
6:F:151:ILE:HA	6:F:156:VAL:O	2.20	0.42
6:F:34:SER:OG	6:F:65:ARG:NH1	2.52	0.42
3:Q:50:VAL:O	3:Q:51:ALA:CB	2.68	0.42
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.50	0.42
11:K:83:LEU:CD2	11:K:99:THR:HG21	2.50	0.42
11:Y:158:ARG:HE	11:Y:162:GLN:NE2	2.14	0.42
16:H:304:CL:CL	20:H:521:HOH:O	2.59	0.42
5:S:196:ARG:HH22	5:S:238:GLU:CB	2.33	0.42
11:Y:137:GLY:O	11:Y:141[A]:ARG:HG2	2.20	0.42
7:G:117:ARG:NH2	20:G:404:HOH:O	2.44	0.41
13:M:112:ILE:HD12	13:M:112:ILE:N	2.35	0.41
4:R:199:LEU:HD12	4:R:237:VAL:CG1	2.50	0.41
6:T:170:GLN:O	6:T:174:THR:HG23	2.20	0.41
7:U:244:GLU:O	7:U:245:ARG:C	2.59	0.41
2:B:25[B]:MET:SD	2:B:152:PRO:HD2	2.61	0.41
6:F:243:LEU:O	6:F:244:LYS:C	2.59	0.41
7:U:88:ARG:HD2	7:U:88:ARG:HA	1.89	0.41
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.21	0.41
13:M:92:LEU:CD2	13:M:112:ILE:HD11	2.49	0.41
1:O:206:ASN:HD22	1:O:206:ASN:C	2.24	0.41
5:S:150:SER:O	5:S:151:ALA:HB3	2.20	0.41
7:U:186:LYS:N	20:U:404:HOH:O	2.53	0.41
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.50	0.41
3:C:35:VAL:HG13	3:C:191:VAL:HG22	2.03	0.41
7:G:192:GLU:HG3	20:G:407:HOH:O	2.21	0.41
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.19	0.41
2:P:44:LEU:HD12	2:P:44:LEU:C	2.41	0.41
10:J:108:ASP:HB3	10:J:111:GLU:HB2	2.03	0.41
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.51	0.41
10:J:1[A]:MET:HG2	10:J:2:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:148:LEU:HD23	12:L:178:VAL:HG12	2.03	0.41
1:O:180:ASP:N	1:O:180:ASP:OD1	2.54	0.41
2:B:149:GLN:O	2:B:156:TYR:HA	2.20	0.41
19:I:303:1PE:H122	10:J:90:ASP:HB3	2.03	0.41
10:J:121:LEU:O	10:J:122:ALA:HB3	2.21	0.41
6:T:151:ILE:HA	6:T:156:VAL:O	2.21	0.41
1:A:110:VAL:HG22	1:A:135:ILE:HD12	2.02	0.41
4:R:204:GLN:NE2	20:R:405:HOH:O	2.54	0.41
12:Z:148:LEU:HG	12:Z:148:LEU:O	2.19	0.41
10:J:10:PRO:HG3	10:J:150:THR:HA	2.02	0.40
1:A:58[B]:GLU:H	1:A:58[B]:GLU:CD	2.25	0.40
5:E:202:GLU:HG2	5:E:203:GLN:N	2.35	0.40
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.57	0.40
11:K:52:CYS:SG	11:K:97:MET:HG3	2.62	0.40
19:V:304:1PE:H241	20:V:499:HOH:O	2.21	0.40
1:A:142:ARG:HG2	1:A:143:PRO:HD2	2.02	0.40
9:I:13[A]:MET:CE	9:I:162:LEU:HD12	2.51	0.40
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	2.04	0.40
5:S:45:VAL:CG1	5:S:187:LEU:HD23	2.51	0.40
6:T:207:LYS:HE2	20:T:376:HOH:O	2.22	0.40
6:T:81:LEU:HD13	6:T:85:ARG:CZ	2.51	0.40
8:H:199:LEU:HB3	12:Z:173:ARG:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	231/234 (99%)	219 (95%)	7 (3%)	5 (2%)	8 1
1	O	228/234 (97%)	217 (95%)	5 (2%)	6 (3%)	7 1
2	B	248/261 (95%)	238 (96%)	8 (3%)	2 (1%)	24 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	247/261 (95%)	232 (94%)	12 (5%)	3 (1%)	16 5
3	C	236/248 (95%)	220 (93%)	9 (4%)	7 (3%)	5 1
3	Q	237/248 (96%)	221 (93%)	6 (2%)	10 (4%)	3 0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15 4
4	R	232/241 (96%)	221 (95%)	7 (3%)	4 (2%)	11 2
5	E	232/263 (88%)	225 (97%)	6 (3%)	1 (0%)	39 27
5	S	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	39 27
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100 100
6	T	239/255 (94%)	232 (97%)	4 (2%)	3 (1%)	15 4
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100 100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	39 27
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	34 21
9	I	205/205 (100%)	201 (98%)	4 (2%)	0	100 100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100 100
10	J	195/201 (97%)	193 (99%)	2 (1%)	0	100 100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100 100
11	K	198/204 (97%)	195 (98%)	3 (2%)	0	100 100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100 100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100 100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100 100
13	M	215/219 (98%)	209 (97%)	6 (3%)	0	100 100
13	a	216/219 (99%)	208 (96%)	8 (4%)	0	100 100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	34 21
14	b	202/205 (98%)	200 (99%)	1 (0%)	1 (0%)	34 21
All	All	6208/6458 (96%)	6025 (97%)	134 (2%)	49 (1%)	24 11

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER

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Mol	Chain	Res	Type
3	C	50	VAL
3	C	216	SER
1	O	50	LYS
1	O	52	LYS
1	O	53	SER
1	O	231	ALA
2	P	204	SER
3	Q	47	LYS
3	Q	200	GLN
3	Q	206	ILE
3	Q	221	ASN
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	206	ASP
3	C	51	ALA
4	D	176	GLY
5	E	59	HIS
2	P	54	LYS
3	Q	50	VAL
3	Q	51	ALA
3	Q	201	SER
3	Q	216	SER
4	R	128	ALA
6	T	7	TYR
1	A	176	ARG
3	C	200	GLN
14	N	198	ALA
1	O	176	ARG
3	Q	138	PHE
7	U	58	ASP
8	V	203	ARG
2	B	203	VAL
3	C	204	LYS
2	P	52	ILE
6	T	208	ALA
14	b	198	ALA
1	A	201	GLN
2	B	51	ASN
3	C	138	PHE
4	D	175[A]	GLU
4	D	175[B]	GLU

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Mol	Chain	Res	Type
4	R	127	ASP
1	O	201	GLN
3	C	203	GLY
3	Q	203	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	173 (94%)	12 (6%)	21	10
1	O	176/191 (92%)	164 (93%)	12 (7%)	20	9
2	B	199/221 (90%)	190 (96%)	9 (4%)	34	21
2	P	196/221 (89%)	183 (93%)	13 (7%)	21	10
3	C	179/210 (85%)	169 (94%)	10 (6%)	26	14
3	Q	184/210 (88%)	175 (95%)	9 (5%)	31	18
4	D	189/203 (93%)	182 (96%)	7 (4%)	41	29
4	R	187/203 (92%)	184 (98%)	3 (2%)	70	66
5	E	192/223 (86%)	183 (95%)	9 (5%)	32	20
5	S	195/223 (87%)	191 (98%)	4 (2%)	61	55
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	14
6	T	192/212 (91%)	181 (94%)	11 (6%)	25	13
7	G	202/207 (98%)	196 (97%)	6 (3%)	48	38
7	U	186/207 (90%)	182 (98%)	4 (2%)	60	53
8	H	181/195 (93%)	174 (96%)	7 (4%)	39	27
8	V	172/195 (88%)	162 (94%)	10 (6%)	25	13
9	I	176/174 (101%)	174 (99%)	2 (1%)	80	79
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	90
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	19
10	X	165/170 (97%)	159 (96%)	6 (4%)	42	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	154/159 (97%)	143 (93%)	11 (7%)	18 8
11	Y	158/159 (99%)	150 (95%)	8 (5%)	29 17
12	L	175/178 (98%)	169 (97%)	6 (3%)	44 33
12	Z	175/178 (98%)	172 (98%)	3 (2%)	68 64
13	M	180/181 (99%)	177 (98%)	3 (2%)	68 64
13	a	178/181 (98%)	173 (97%)	5 (3%)	51 41
14	N	158/159 (99%)	154 (98%)	4 (2%)	55 47
14	b	158/159 (99%)	155 (98%)	3 (2%)	65 59
All	All	5030/5366 (94%)	4833 (96%)	197 (4%)	40 27

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	50	LYS
1	A	53	SER
1	A	61	VAL
1	A	142	ARG
1	A	176	ARG
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	4	ARG
2	B	33	THR
2	B	58	GLU
2	B	70	GLU
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	238	LYS
2	B	249	ARG
3	C	2	SER
3	C	35	VAL
3	C	45	VAL
3	C	113	SER
3	C	148	ASP

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Mol	Chain	Res	Type
3	C	201	SER
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
3	C	226	GLU
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	126	GLU
4	D	139	VAL
4	D	199	LEU
4	D	217	LEU
5	E	61	LYS
5	E	73	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	122	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
8	H	12	ILE
8	H	31	CYS
8	H	65	LEU
8	H	68	LEU

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Mol	Chain	Res	Type
8	H	183	LEU
8	H	202	TYR
8	H	220	GLU
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	8	PHE
11	K	12	VAL
11	K	35	ILE
11	K	138	VAL
11	K	141	ARG
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
11	K	192	VAL
11	K	200	SER
12	L	3[A]	SER
12	L	3[B]	SER
12	L	102	PHE
12	L	163	HIS
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	216	SER
14	N	35	THR
14	N	84	LYS
14	N	145	GLU
14	N	196	LYS
1	O	10	THR
1	O	53	SER
1	O	118	GLN
1	O	131	VAL
1	O	142	ARG

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Mol	Chain	Res	Type
1	O	176	ARG
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	4	ARG
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	53	HIS
2	P	70	GLU
2	P	183	GLU
2	P	190	LEU
2	P	204	SER
2	P	207	SER
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
3	Q	2	SER
3	Q	45	VAL
3	Q	56	GLU
3	Q	113	SER
3	Q	148	ASP
3	Q	170	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	46	VAL
4	R	139	VAL
4	R	217	LEU
5	S	45	VAL
5	S	101	ARG
5	S	122	ARG
5	S	180	MET
6	T	17	ASP
6	T	31	GLU
6	T	33	SER
6	T	53	VAL
6	T	81	LEU
6	T	87	LEU

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Mol	Chain	Res	Type
6	T	174	THR
6	T	190	VAL
6	T	215	TRP
6	T	223	ARG
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL
8	V	12	ILE
8	V	31	CYS
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
9	W	35	THR
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
10	X	174	ASN
11	Y	8	PHE
11	Y	12	VAL
11	Y	89	GLN
11	Y	138	VAL
11	Y	141[A]	ARG
11	Y	141[B]	ARG
11	Y	147	LEU
11	Y	192	VAL
12	Z	102	PHE
12	Z	174	LEU
12	Z	207	THR
13	a	92	LEU
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER

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Mol	Chain	Res	Type
14	b	35	THR
14	b	84	LYS
14	b	196	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	102	GLN
2	B	109	GLN
3	C	54	GLN
4	D	227	HIS
5	E	65	HIS
6	F	143	ASN
8	H	116	HIS
8	H	153	ASN
8	H	193	ASN
9	I	161	HIS
10	J	87	ASN
10	J	101	ASN
11	K	162	GLN
12	L	157	ASN
13	M	47	ASN
13	M	162	GLN
14	N	193	GLN
1	O	62	HIS
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	109	GLN
3	Q	18	GLN
4	R	227	HIS
5	S	86	ASN
6	T	63	ASN
6	T	68	ASN
6	T	143	ASN
8	V	116	HIS
8	V	193	ASN
9	W	172	ASN

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Mol	Chain	Res	Type
10	X	24	ASN
10	X	132	HIS
10	X	174	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS
14	b	193	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	YCM	C	63	3	7,9,10	1.04	0	5,10,12	1.65	1 (20%)
5	6V1	E	148	5	11,15,16	1.22	2 (18%)	11,20,22	1.76	4 (36%)
7	YCM	G	137	7	7,9,10	3.06	4 (57%)	5,10,12	4.08	2 (40%)
7	6V1	G	161	7	11,15,16	1.44	3 (27%)	11,20,22	3.20	8 (72%)
7	6V1	G	47	7	11,15,16	1.97	4 (36%)	11,20,22	3.61	4 (36%)
10	6V1	J	91	10	11,15,16	1.85	2 (18%)	11,20,22	4.92	7 (63%)
3	YCM	Q	63	3	7,9,10	1.86	2 (28%)	5,10,12	2.88	3 (60%)
5	6V1	S	148	5	11,15,16	1.62	4 (36%)	11,20,22	1.83	3 (27%)
7	YCM	U	137	7	7,9,10	2.63	2 (28%)	5,10,12	5.29	3 (60%)
7	6V1	U	161	7	11,15,16	1.33	2 (18%)	11,20,22	2.86	7 (63%)
7	6V1	U	47	7	11,15,16	1.36	2 (18%)	11,20,22	3.52	4 (36%)
10	6V1	X	91	10	11,15,16	1.95	4 (36%)	11,20,22	5.34	6 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	6V9	c	1	15	6,8,9	0.76	0	2,10,12	3.34	1 (50%)
15	OAS	c	2	15	4,6,9	0.55	0	2,6,11	1.49	0
15	OAS	c	3	15	4,6,9	0.85	0	2,6,11	1.32	0
15	6V9	d	1	15	6,8,9	0.65	0	2,10,12	4.75	1 (50%)
15	OAS	d	2	15	4,6,9	1.03	0	2,6,11	3.37	1 (50%)
15	OAS	d	3	15	4,6,9	0.76	0	2,6,11	1.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YCM	C	63	3	-	0/6/8/10	0/0/0/0
5	6V1	E	148	5	-	0/6/25/27	0/1/1/1
7	YCM	G	137	7	-	0/6/8/10	0/0/0/0
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	0/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	0/6/8/10	0/0/0/0
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	YCM	U	137	7	-	0/6/8/10	0/0/0/0
7	6V1	U	161	7	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	0/6/25/27	0/1/1/1
15	6V9	c	1	15	-	0/0/2/4	0/1/1/1
15	OAS	c	2	15	-	0/3/5/9	0/0/0/0
15	OAS	c	3	15	-	0/3/5/9	0/0/0/0
15	6V9	d	1	15	-	0/0/2/4	0/1/1/1
15	OAS	d	2	15	-	0/3/5/9	0/0/0/0
15	OAS	d	3	15	-	0/3/5/9	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-5.76	1.70	1.81
7	U	137	YCM	CB-SG	-5.60	1.70	1.81
10	J	91	6V1	C1-SG	-4.63	1.77	1.83
3	Q	63	YCM	CD-SG	-4.16	1.72	1.81
7	G	47	6V1	C2-N3	-3.97	1.33	1.38
10	X	91	6V1	C1-SG	-3.91	1.78	1.83
5	S	148	6V1	C2-N3	-3.18	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	C4-N3	-2.93	1.33	1.38
5	E	148	6V1	C2-N3	-2.77	1.34	1.38
7	G	161	6V1	C4-N3	-2.74	1.33	1.38
7	U	47	6V1	C2-N3	-2.70	1.34	1.38
7	G	161	6V1	C1-C2	-2.41	1.50	1.52
7	U	47	6V1	C4-N3	-2.35	1.34	1.38
7	G	161	6V1	C2-N3	-2.34	1.35	1.38
7	U	161	6V1	C2-N3	-2.32	1.35	1.38
3	Q	63	YCM	CB-SG	-2.15	1.77	1.81
5	S	148	6V1	C4-N3	-2.11	1.34	1.38
10	X	91	6V1	C4-N3	-2.06	1.35	1.38
5	E	148	6V1	C1-C2	2.05	1.54	1.52
5	S	148	6V1	C1-C2	2.24	1.54	1.52
7	G	47	6V1	C5-C4	2.26	1.54	1.50
7	U	161	6V1	C1-C2	2.30	1.54	1.52
7	G	137	YCM	CD-CE	2.42	1.58	1.51
10	J	91	6V1	O7-C2	2.54	1.27	1.22
5	S	148	6V1	C5-C4	2.59	1.54	1.50
10	X	91	6V1	C1-C2	2.59	1.54	1.52
7	G	137	YCM	CE-NZ2	2.97	1.42	1.32
10	X	91	6V1	O7-C2	3.07	1.28	1.22
7	U	137	YCM	CD-CE	3.22	1.60	1.51
7	G	47	6V1	C1-SG	3.46	1.87	1.83
7	G	137	YCM	CD-SG	3.52	1.89	1.81

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	47	6V1	C5-C1-C2	-9.84	96.49	103.98
15	d	1	6V9	O1-C4-C3	-6.66	118.90	124.47
10	X	91	6V1	C6-N3-C4	-5.76	117.11	123.24
7	G	161	6V1	C5-C1-C2	-5.65	99.68	103.98
10	J	91	6V1	C6-N3-C4	-5.57	117.31	123.24
10	X	91	6V1	O7-C2-C1	-5.00	116.15	125.18
7	U	47	6V1	C5-C1-C2	-4.95	100.21	103.98
3	Q	63	YCM	CA-CB-SG	-4.91	101.24	112.84
15	c	1	6V9	O1-C4-C3	-4.47	120.73	124.47
7	U	161	6V1	O8-C4-C5	-4.10	121.89	127.38
10	X	91	6V1	O8-C4-C5	-4.01	122.00	127.38
7	U	161	6V1	C5-C1-C2	-3.83	101.07	103.98
10	J	91	6V1	O7-C2-C1	-3.55	118.77	125.18
7	G	161	6V1	O7-C2-C1	-3.39	119.06	125.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	91	6V1	O8-C4-C5	-3.33	122.92	127.38
7	G	161	6V1	O8-C4-C5	-3.08	123.25	127.38
5	S	148	6V1	O-C-CA	-2.79	118.24	125.72
3	Q	63	YCM	O-C-CA	-2.74	118.37	125.72
5	E	148	6V1	O-C-CA	-2.73	118.39	125.72
7	G	161	6V1	CA-CB-SG	-2.70	106.63	112.87
3	C	63	YCM	O-C-CA	-2.68	118.53	125.72
5	S	148	6V1	C5-C1-C2	-2.60	102.01	103.98
5	E	148	6V1	CA-CB-SG	-2.57	106.93	112.87
7	U	47	6V1	O8-C4-C5	-2.47	124.07	127.38
7	U	137	YCM	OZ1-CE-NZ2	-2.37	115.79	122.52
7	U	161	6V1	O7-C2-C1	-2.27	121.09	125.18
7	G	47	6V1	O7-C2-C1	-2.17	121.26	125.18
7	U	137	YCM	OZ1-CE-CD	-2.12	116.21	120.98
7	U	161	6V1	O-C-CA	-2.09	120.11	125.72
7	G	137	YCM	O-C-CA	-2.07	120.18	125.72
5	E	148	6V1	C6-N3-C4	2.20	125.58	123.24
5	E	148	6V1	C6-N3-C2	2.33	125.23	123.42
7	U	161	6V1	O8-C4-N3	2.35	126.83	123.91
7	G	161	6V1	C6-N3-C2	2.44	125.31	123.42
7	G	161	6V1	O7-C2-N3	2.44	127.56	124.19
10	J	91	6V1	C5-C1-C2	2.47	105.87	103.98
7	G	47	6V1	C6-N3-C2	2.72	125.53	123.42
7	U	47	6V1	C6-N3-C2	2.86	125.64	123.42
3	Q	63	YCM	CD-CE-NZ2	3.03	118.82	115.48
5	S	148	6V1	C6-N3-C2	3.50	126.14	123.42
7	G	161	6V1	O8-C4-N3	4.00	128.87	123.91
7	U	161	6V1	C6-N3-C2	4.14	126.63	123.42
7	G	161	6V1	CB-SG-C1	4.40	110.34	101.58
7	U	161	6V1	CB-SG-C1	4.53	110.58	101.58
15	d	2	OAS	C1A-OG-CB	4.72	131.50	112.39
7	G	47	6V1	CB-SG-C1	5.25	112.03	101.58
10	J	91	6V1	O7-C2-N3	6.36	132.99	124.19
10	X	91	6V1	O7-C2-N3	7.39	134.40	124.19
10	J	91	6V1	CB-SG-C1	7.93	117.35	101.58
10	X	91	6V1	CB-SG-C1	8.18	117.86	101.58
7	G	137	YCM	CD-CE-NZ2	8.56	124.92	115.48
7	U	47	6V1	CB-SG-C1	9.53	120.54	101.58
10	J	91	6V1	C6-N3-C2	9.70	130.97	123.42
10	X	91	6V1	C6-N3-C2	10.47	131.56	123.42
7	U	137	YCM	CD-CE-NZ2	11.22	127.85	115.48

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	137	YCM	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 83 ligands modelled in this entry, 74 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
19	1PE	H	305	-	15,15,15	0.60	0	14,14,14	0.67	0
19	1PE	H	306	-	15,15,15	0.61	0	14,14,14	0.50	0
19	1PE	I	303	-	15,15,15	0.57	0	14,14,14	1.02	1 (7%)
19	1PE	I	304	-	15,15,15	0.57	0	14,14,14	0.93	1 (7%)
19	1PE	L	301	-	15,15,15	0.64	0	14,14,14	0.77	0
19	1PE	M	305	-	15,15,15	0.58	0	14,14,14	0.38	0
19	1PE	V	304	-	15,15,15	0.78	0	14,14,14	0.84	1 (7%)
19	1PE	W	303	-	15,15,15	0.67	0	14,14,14	0.46	0
19	1PE	Z	301	-	15,15,15	0.66	0	14,14,14	0.59	0

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
19	1PE	H	305	-	-	0/13/13/13	0/0/0/0
19	1PE	H	306	-	-	0/13/13/13	0/0/0/0
19	1PE	I	303	-	-	0/13/13/13	0/0/0/0
19	1PE	I	304	-	-	0/13/13/13	0/0/0/0
19	1PE	L	301	-	-	0/13/13/13	0/0/0/0
19	1PE	M	305	-	-	0/13/13/13	0/0/0/0
19	1PE	V	304	-	-	0/13/13/13	0/0/0/0
19	1PE	W	303	-	-	0/13/13/13	0/0/0/0
19	1PE	Z	301	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	I	304	1PE	OH6-C15-C25	-2.30	100.20	110.40
19	V	304	1PE	OH5-C25-C15	2.03	119.42	110.40
19	I	303	1PE	C25-OH5-C14	2.46	123.82	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	303	1PE	1	0
19	M	305	1PE	1	0
19	V	304	1PE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/234 (98%)	-0.01	4 (1%) 73 76	30, 47, 80, 96	0
1	O	230/234 (98%)	0.39	16 (6%) 19 21	40, 62, 100, 123	0
2	B	248/261 (95%)	0.07	9 (3%) 46 50	34, 49, 89, 136	0
2	P	247/261 (94%)	0.30	17 (6%) 20 22	39, 58, 99, 134	0
3	C	236/248 (95%)	0.41	14 (5%) 26 29	34, 59, 102, 140	0
3	Q	239/248 (96%)	0.67	28 (11%) 6 7	35, 63, 118, 149	0
4	D	233/241 (96%)	0.29	10 (4%) 39 42	36, 56, 86, 121	0
4	R	233/241 (96%)	-0.00	5 (2%) 67 70	33, 44, 67, 92	0
5	E	233/263 (88%)	0.16	11 (4%) 35 38	29, 42, 87, 105	0
5	S	235/263 (89%)	0.10	7 (2%) 54 57	34, 48, 81, 106	0
6	F	239/255 (93%)	-0.02	0 100 100	26, 36, 57, 75	0
6	T	240/255 (94%)	0.27	9 (3%) 44 48	35, 51, 85, 110	0
7	G	241/246 (97%)	0.05	4 (1%) 73 76	27, 40, 74, 106	0
7	U	235/246 (95%)	0.37	13 (5%) 29 32	41, 59, 93, 129	0
8	H	220/234 (94%)	0.07	4 (1%) 71 74	28, 37, 68, 100	0
8	V	220/234 (94%)	0.05	7 (3%) 51 54	38, 49, 81, 103	0
9	I	204/205 (99%)	-0.08	0 100 100	29, 37, 58, 73	0
9	W	204/205 (99%)	-0.06	0 100 100	37, 49, 71, 78	0
10	J	195/201 (97%)	-0.11	1 (0%) 91 92	29, 40, 57, 70	0
10	X	195/201 (97%)	-0.13	0 100 100	33, 42, 56, 69	0
11	K	200/204 (98%)	-0.03	1 (0%) 91 92	33, 44, 68, 83	0
11	Y	199/204 (97%)	-0.08	1 (0%) 91 92	27, 36, 58, 69	0
12	L	213/213 (100%)	-0.00	0 100 100	33, 48, 70, 85	0
12	Z	213/213 (100%)	-0.06	0 100 100	28, 38, 60, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	0.02	1 (0%) 91 92	27, 39, 61, 89	0
13	a	216/219 (98%)	-0.06	1 (0%) 91 92	29, 40, 61, 81	0
14	N	202/205 (98%)	-0.02	2 (0%) 84 86	27, 35, 55, 87	0
14	b	203/205 (99%)	-0.07	1 (0%) 91 92	32, 40, 66, 96	0
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
All	All	6219/6466 (96%)	0.10	166 (2%) 58 61	26, 45, 84, 149	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	15.2
1	O	232	ILE	10.8
4	D	241	ILE	10.0
3	Q	232	ILE	8.3
5	E	54	SER	8.2
3	Q	234	LYS	8.0
2	P	203	VAL	7.5
3	C	49	SER	7.4
8	V	203	ARG	6.7
5	E	52	ALA	6.7
13	a	216	SER	6.6
7	U	2	SER	6.4
7	G	187	PHE	6.3
3	Q	202	GLY	6.2
3	Q	229	VAL	6.0
3	Q	200	GLN	6.0
2	B	61	PHE	5.9
3	Q	238	GLU	5.8
3	Q	233	GLU	5.6
2	P	61	PHE	5.6
3	Q	240	GLU	5.5
3	Q	48	LYS	5.5
11	K	40	TYR	5.5
3	Q	236	LYS	5.4
5	E	53	GLN	5.3
2	B	203	VAL	5.3
3	C	225	ILE	5.2
3	C	138	PHE	5.2
11	Y	40	TYR	5.1
4	R	241	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	O	177	TYR	5.0
5	E	56	LEU	4.9
3	Q	201	SER	4.8
3	Q	225	ILE	4.7
8	H	204	CYS	4.6
4	D	237	VAL	4.6
3	C	202	GLY	4.6
2	P	247	ALA	4.6
3	Q	47	LYS	4.6
2	P	205	LYS	4.5
3	Q	230	ALA	4.5
7	G	189	TRP	4.4
7	U	3	ARG	4.4
8	V	198	ARG	4.4
3	Q	203	GLY	4.4
1	O	201	GLN	4.3
3	Q	223	GLU	4.3
5	S	57	ALA	4.3
7	G	188	ASP	4.3
8	H	203	ARG	4.2
8	V	199	LEU	4.2
6	T	54	LEU	4.1
3	C	236	LYS	4.0
4	R	127	ASP	4.0
7	U	242	LEU	4.0
7	U	208	ILE	3.9
3	C	200	GLN	3.9
7	U	243	ALA	3.9
6	T	205	LYS	3.9
3	Q	239	ASN	3.8
6	T	206	ASP	3.8
7	U	206	LEU	3.7
5	S	54	SER	3.7
7	U	58	ASP	3.7
2	P	234	GLU	3.7
2	P	202	ASP	3.6
1	O	157	TRP	3.5
8	V	202	TYR	3.5
2	B	247	ALA	3.5
6	T	208	ALA	3.5
4	D	240	ASP	3.4
1	O	3	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
5	E	201	ALA	3.4
10	J	1[A]	MET	3.4
2	P	230	GLN	3.4
5	E	58	ALA	3.4
2	P	51	ASN	3.4
5	S	56	LEU	3.4
3	Q	192	ILE	3.4
3	C	48	LYS	3.3
3	Q	237	GLU	3.3
1	O	181	LEU	3.3
7	U	212	PRO	3.2
4	R	130	PRO	3.2
3	C	98	VAL	3.2
8	H	201	ARG	3.2
7	U	199	ILE	3.2
4	R	128	ALA	3.1
3	Q	226	GLU	3.0
1	O	184	GLU	3.0
7	U	57	PRO	3.0
5	E	59	HIS	3.0
3	Q	49	SER	3.0
1	O	59	ARG	2.9
6	T	209	PHE	2.9
3	C	233	GLU	2.9
3	Q	205	ASN	2.9
3	Q	219	ILE	2.9
2	P	220	ASN	2.9
2	P	58	GLU	2.8
1	A	231	ALA	2.8
5	S	53	GLN	2.8
5	E	237	GLU	2.8
1	O	176	ARG	2.8
2	P	233	VAL	2.8
3	C	201	SER	2.7
3	Q	204	LYS	2.7
7	G	3	ARG	2.7
8	H	202	TYR	2.7
5	E	235	GLY	2.7
13	M	215	ILE	2.7
6	T	5	THR	2.7
3	Q	138	PHE	2.7
1	O	175	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	223	GLY	2.6
3	C	229	VAL	2.6
2	B	248	GLU	2.6
5	E	60	GLN	2.6
2	B	202	ASP	2.6
5	S	239	ARG	2.6
6	T	207	LYS	2.5
5	S	174	ARG	2.5
2	B	249	ARG	2.5
7	U	56	VAL	2.5
3	C	232	ILE	2.4
4	D	130	PRO	2.4
3	Q	220	LEU	2.4
5	S	51	ARG	2.4
2	B	205	LYS	2.4
7	U	240	VAL	2.4
7	U	196	GLU	2.4
2	P	53	HIS	2.4
4	R	131	GLY	2.4
2	B	204	SER	2.3
1	O	50	LYS	2.3
3	C	171	PHE	2.3
1	A	230	ALA	2.3
1	A	232	ILE	2.3
4	D	239	LYS	2.3
6	T	6	GLY	2.2
4	D	183	GLU	2.2
1	O	225	VAL	2.2
6	T	180	GLN	2.2
14	N	201	THR	2.2
1	O	199	GLU	2.2
1	O	191	ILE	2.2
4	D	127	ASP	2.2
4	D	128	ALA	2.2
3	C	203	GLY	2.2
8	V	201	ARG	2.2
1	O	182	GLU	2.2
2	P	52	ILE	2.2
3	Q	56	GLU	2.1
4	D	131	GLY	2.1
14	N	199	VAL	2.1
14	b	199	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
8	V	196	GLY	2.1
8	V	204	CYS	2.1
1	O	56	TYR	2.1
1	A	3	ARG	2.1
2	P	246	LYS	2.1
2	P	244	GLU	2.1
5	E	202	GLU	2.1
2	P	201	MET	2.0
3	Q	199	VAL	2.0
2	B	237	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	6V9	d	1	8/9	0.99	0.09	-	33,33,35,36	0
10	6V1	J	91	15/16	0.93	0.19	-	33,51,56,57	0
5	6V1	S	148	15/16	0.94	0.16	-	37,61,67,67	0
3	YCM	C	63	10/11	0.90	0.10	-	52,53,61,61	0
7	6V1	U	47	15/16	0.83	0.28	-	73,107,113,116	0
7	6V1	G	47	15/16	0.95	0.16	-	38,57,61,61	0
15	OAS	d	3	7/10	0.98	0.10	-	27,28,29,30	0
5	6V1	E	148	15/16	0.93	0.14	-	33,49,59,60	0
7	YCM	U	137	10/11	0.85	0.24	-	51,60,74,76	0
7	YCM	G	137	10/11	0.92	0.10	-	31,40,53,56	0
7	6V1	U	161	15/16	0.93	0.13	-	53,71,79,80	0
7	6V1	G	161	15/16	0.96	0.12	-	33,51,58,61	0
15	OAS	c	2	7/10	0.96	0.12	-	34,37,41,44	0
3	YCM	Q	63	10/11	0.92	0.10	-	52,54,64,65	0
10	6V1	X	91	15/16	0.91	0.20	-	35,54,58,65	0
15	6V9	c	1	8/9	0.98	0.08	-	38,39,41,42	0
15	OAS	d	2	7/10	0.97	0.13	-	27,30,37,40	0
15	OAS	c	3	7/10	0.98	0.12	-	35,35,38,38	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	CL	S	301	1/1	0.96	0.29	9.71	65,65,65,65	0
19	1PE	I	304	16/16	0.82	0.22	9.46	53,62,77,81	0
19	1PE	M	305	16/16	0.79	0.24	9.17	70,73,87,90	0
16	CL	M	301	1/1	0.96	0.21	8.91	57,57,57,57	0
19	1PE	H	306	16/16	0.87	0.24	5.83	55,66,88,88	0
16	CL	b	302	1/1	0.96	0.14	3.26	62,62,62,62	0
19	1PE	L	301	16/16	0.84	0.13	3.06	53,64,70,71	0
19	1PE	I	303	16/16	0.89	0.14	2.67	50,55,61,67	0
19	1PE	W	303	16/16	0.87	0.12	2.01	52,61,70,71	0
19	1PE	Z	301	16/16	0.89	0.12	1.36	53,61,66,66	0
19	1PE	H	305	16/16	0.92	0.13	1.07	39,53,62,62	0
18	MG	H	302	1/1	0.99	0.11	1.03	34,34,34,34	0
19	1PE	V	304	16/16	0.90	0.12	0.91	44,54,78,83	0
16	CL	a	301	1/1	0.96	0.12	0.89	60,60,60,60	0
16	CL	D	301	1/1	0.92	0.15	0.67	66,66,66,66	0
18	MG	I	301	1/1	0.96	0.10	0.60	34,34,34,34	0
16	CL	Q	302	1/1	0.93	0.14	0.50	63,63,63,63	0
16	CL	U	301	1/1	0.98	0.11	-0.15	54,54,54,54	0
16	CL	M	302	1/1	0.94	0.11	-0.19	61,61,61,61	0
16	CL	E	301	1/1	0.99	0.11	-0.28	57,57,57,57	0
16	CL	N	301	1/1	0.97	0.10	-0.47	43,43,43,43	0
16	CL	G	301	1/1	0.98	0.10	-0.60	46,46,46,46	0
16	CL	B	302	1/1	0.97	0.10	-0.61	57,57,57,57	0
16	CL	S	302	1/1	0.96	0.08	-0.94	62,62,62,62	0
16	CL	b	304	1/1	0.97	0.08	-1.11	51,51,51,51	0
16	CL	b	303	1/1	0.97	0.09	-1.23	51,51,51,51	0
16	CL	A	304	1/1	0.98	0.09	-1.26	56,56,56,56	0
16	CL	E	303	1/1	0.98	0.07	-1.42	57,57,57,57	0
16	CL	A	301	1/1	0.97	0.06	-1.59	48,48,48,48	0
16	CL	F	301	1/1	0.98	0.06	-1.99	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	CL	O	301	1/1	0.95	0.07	-2.09	55,55,55,55	0
17	K	b	305	1/1	0.96	0.06	-2.32	46,46,46,46	0
18	MG	L	303	1/1	0.97	0.07	-2.35	39,39,39,39	0
16	CL	Y	303	1/1	0.95	0.04	-2.42	67,67,67,67	0
17	K	N	304	1/1	0.99	0.06	-2.80	41,41,41,41	0
16	CL	K	303	1/1	0.97	0.04	-2.81	69,69,69,69	0
18	MG	K	301	1/1	0.98	0.05	-3.31	35,35,35,35	0
16	CL	Y	304	1/1	0.95	0.06	-3.33	56,56,56,56	0
17	K	Z	302	1/1	0.99	0.06	-3.33	42,42,42,42	0
18	MG	W	301	1/1	0.93	0.07	-3.89	38,38,38,38	0
16	CL	S	303	1/1	0.97	0.05	-4.20	53,53,53,53	0
17	K	L	302	1/1	0.97	0.05	-4.59	50,50,50,50	0
16	CL	N	303	1/1	0.96	0.06	-4.69	47,47,47,47	0
18	MG	I	305	1/1	0.97	0.07	-4.76	30,30,30,30	0
17	K	U	302	1/1	0.97	0.04	-5.32	42,42,42,42	0
17	K	G	303	1/1	0.99	0.06	-9.45	35,35,35,35	0
16	CL	C	301	1/1	0.92	0.12	-	60,60,60,60	0
16	CL	P	301	1/1	0.96	0.06	-	52,52,52,52	0
16	CL	K	304	1/1	0.95	0.18	-	60,60,60,60	0
16	CL	I	302	1/1	0.97	0.08	-	44,44,44,44	0
16	CL	V	303	1/1	0.90	0.07	-	59,59,59,59	0
16	CL	C	302	1/1	0.96	0.12	-	62,62,62,62	0
16	CL	K	302	1/1	0.97	0.08	-	38,38,38,38	0
16	CL	D	302	1/1	0.95	0.14	-	61,61,61,61	0
18	MG	X	301	1/1	0.97	0.03	-	53,53,53,53	0
16	CL	B	301	1/1	0.96	0.08	-	41,41,41,41	0
18	MG	H	301	1/1	0.96	0.04	-	45,45,45,45	0
16	CL	N	302	1/1	0.98	0.07	-	47,47,47,47	0
18	MG	V	301	1/1	0.95	0.07	-	53,53,53,53	0
18	MG	J	301	1/1	0.96	0.04	-	51,51,51,51	0
16	CL	E	302	1/1	0.97	0.07	-	51,51,51,51	0
16	CL	a	302	1/1	0.97	0.08	-	47,47,47,47	0
16	CL	Y	305	1/1	0.95	0.17	-	59,59,59,59	0
16	CL	b	301	1/1	0.95	0.07	-	48,48,48,48	0
16	CL	V	302	1/1	0.88	0.08	-	56,56,56,56	0
16	CL	M	304	1/1	0.98	0.10	-	54,54,54,54	0
16	CL	Y	302	1/1	0.98	0.12	-	59,59,59,59	0
16	CL	O	304	1/1	0.94	0.11	-	62,62,62,62	0
16	CL	K	305	1/1	0.91	0.14	-	59,59,59,59	0
16	CL	A	303	1/1	0.98	0.06	-	49,49,49,49	0
16	CL	G	302	1/1	0.98	0.05	-	61,61,61,61	0
16	CL	O	302	1/1	0.94	0.06	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	CL	H	303	1/1	0.91	0.07	-	53,53,53,53	0
16	CL	Y	301	1/1	0.99	0.13	-	35,35,35,35	0
16	CL	R	301	1/1	0.93	0.10	-	57,57,57,57	0
16	CL	W	302	1/1	0.97	0.05	-	50,50,50,50	0
16	CL	a	303	1/1	0.94	0.09	-	56,56,56,56	0
16	CL	M	303	1/1	0.99	0.05	-	44,44,44,44	0
16	CL	O	303	1/1	0.84	0.18	-	85,85,85,85	0
16	CL	H	304	1/1	0.98	0.05	-	49,49,49,49	0
16	CL	Q	301	1/1	0.92	0.19	-	67,67,67,67	0
16	CL	A	302	1/1	0.88	0.09	-	65,65,65,65	0
16	CL	R	302	1/1	0.97	0.12	-	53,53,53,53	0

6.5 Other polymers

There are no such residues in this entry.