Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 PM GMT

PDB ID	:	4JT0
Title	:	Yeast 20S proteasome in complex with the dimerized linear mimetic of TMC-95A - yCP:4a
Authors	:	Desvergne, A.; Genin, E.; Marechal, X.; Gallastegui, N.; Dufau, L.; Richy, N.; Groll, M.; Vidal, J.; Reboud-Ravaux, M.
Deposited on	:	2013-03-22
Resolution	:	3.10 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 ⓘ symbol.

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

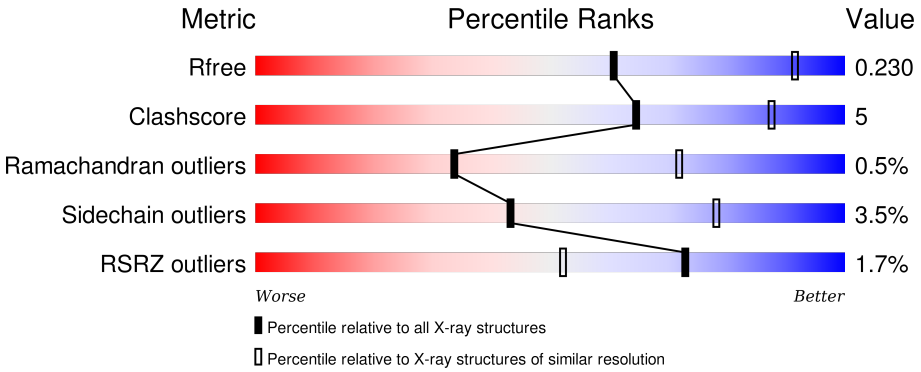
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	250	2% 88% 12%
1	O	250	2% 87% 13%
2	B	258	3% 76% 18% • 5%
2	P	258	4% 76% 17% • 5%
3	C	254	3% 74% 20% • 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	4% 75% 19% 5%
4	D	260	3% 82% 11% 7%
4	R	260	3% 81% 12% 7%
5	E	234	2% 79% 19%
5	S	234	% 79% 19%
6	F	288	% 72% 11% 15%
6	T	288	2% 71% 13% 15%
7	G	252	2% 81% 15%
7	U	252	2% 81% 15%
8	H	232	% 86% 10%
8	V	232	% 85% 10%
9	I	205	84% 16%
9	W	205	% 84% 16%
10	J	198	% 82% 18%
10	X	198	2% 82% 18%
11	K	212	% 88% 10%
11	Y	212	% 89% 9%
12	L	222	85% 14%
12	Z	222	85% 14%
13	M	233	87% 12%
13	a	233	97%
14	N	196	92% 8%
14	b	196	98%
15	c	4	100%
16	d	7	71% 29%

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
17	MES	K	301	-	-	-	X
17	MES	Y	301	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 51001 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- 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	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

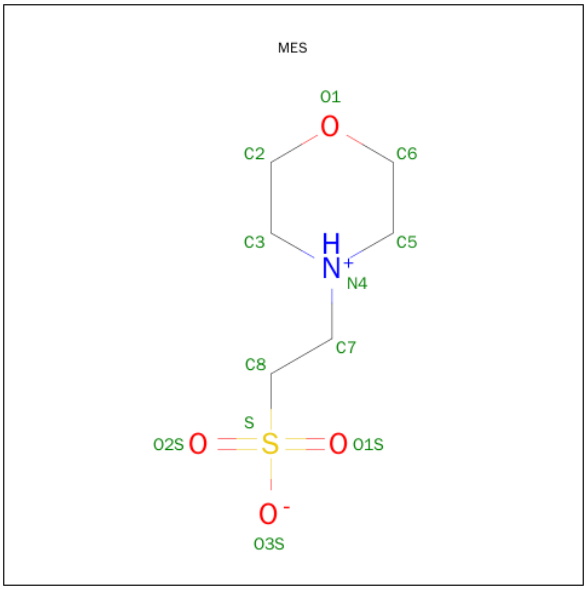
- Molecule 15 is a protein called TMC-95A mimic ligand yCP:4a fragment P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			48	37	5	6			

- Molecule 16 is a protein called TMC-95A mimic ligand yCP:4a fragment Q.

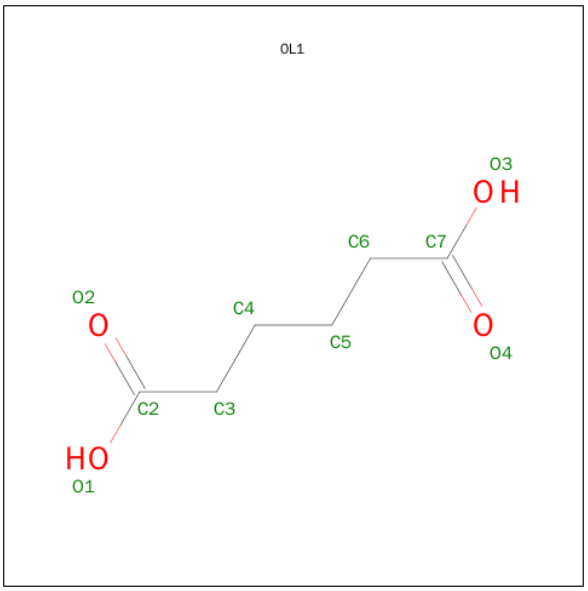
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	d	5	Total	C	N	O	0	0	0
			52	40	5	7			

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is HEXANEDIOIC ACID (three-letter code: 0L1) (formula: $C_6H_{10}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	c	1	Total C O 4 3 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	57	Total O 57 57	0	0
19	B	39	Total O 39 39	0	0
19	C	41	Total O 41 41	0	0
19	D	39	Total O 39 39	0	0
19	E	21	Total O 21 21	0	0
19	F	46	Total O 46 46	0	0
19	G	63	Total O 63 63	0	0
19	H	51	Total O 51 51	0	0
19	I	65	Total O 65 65	0	0
19	J	55	Total O 55 55	0	0
19	K	47	Total O 47 47	0	0

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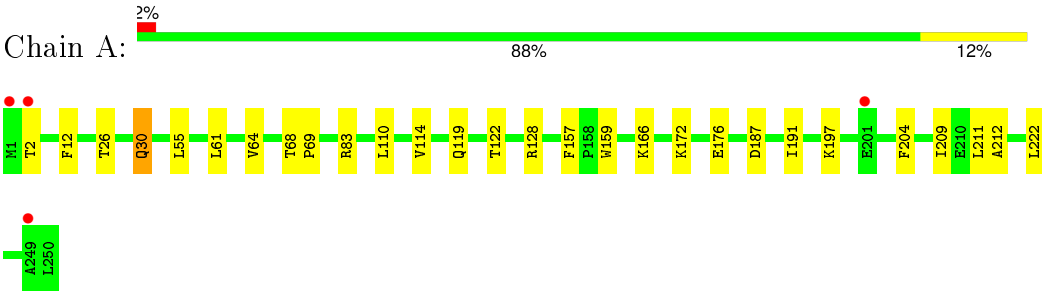
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	L	60	Total O 60 60	0	0
19	M	72	Total O 72 72	0	0
19	N	59	Total O 59 59	0	0
19	O	34	Total O 34 34	0	0
19	P	29	Total O 29 29	0	0
19	Q	27	Total O 27 27	0	0
19	R	30	Total O 30 30	0	0
19	S	21	Total O 21 21	0	0
19	T	40	Total O 40 40	0	0
19	U	58	Total O 58 58	0	0
19	V	48	Total O 48 48	0	0
19	W	57	Total O 57 57	0	0
19	X	44	Total O 44 44	0	0
19	Y	46	Total O 46 46	0	0
19	Z	49	Total O 49 49	0	0
19	a	75	Total O 75 75	0	0
19	b	61	Total O 61 61	0	0
19	d	1	Total O 1 1	0	0

3 Residue-property plots

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.

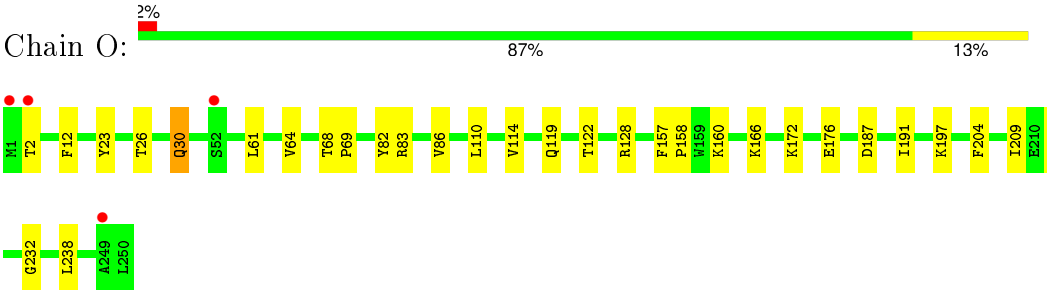
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



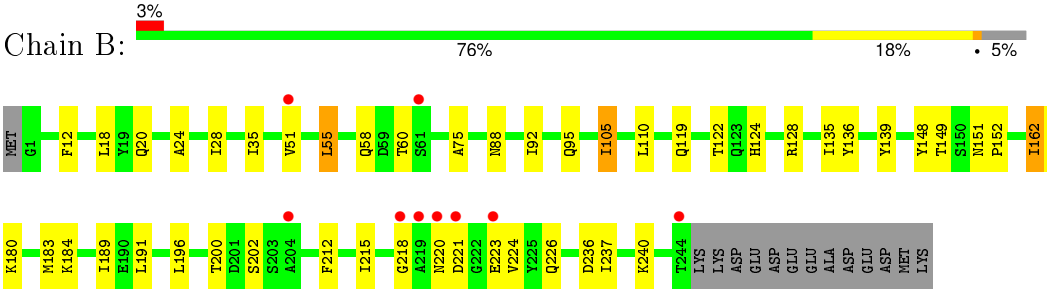
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



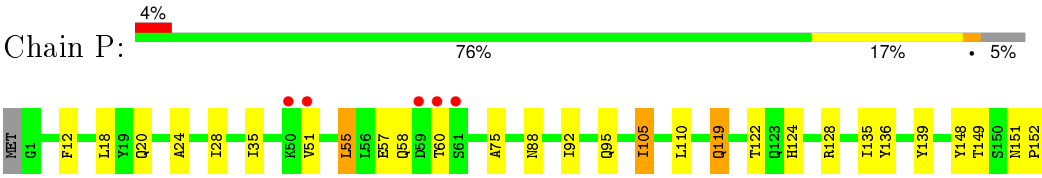
- Molecule 2: Proteasome subunit alpha type-3

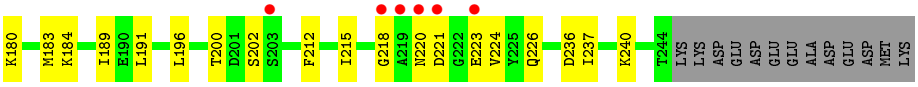
Chain B:



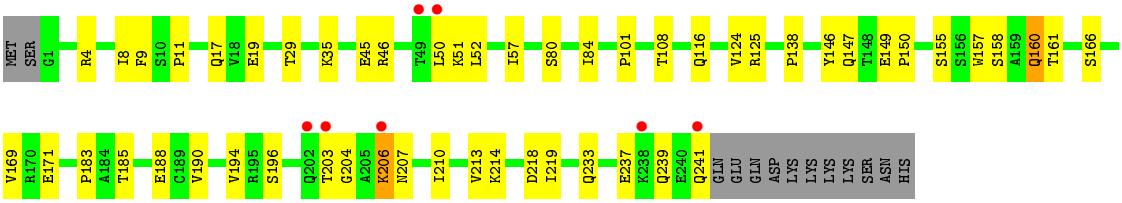
- Molecule 2: Proteasome subunit alpha type-3

Chain P:

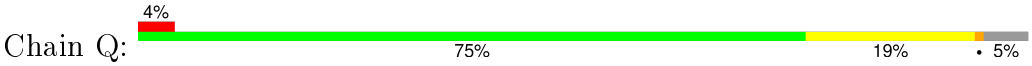


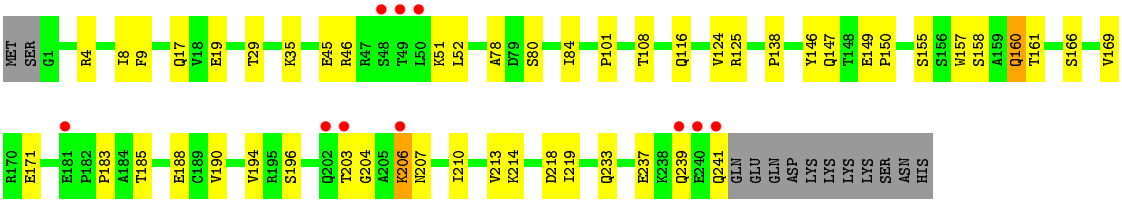


• Molecule 3: Proteasome subunit alpha type-4

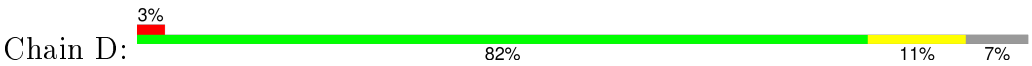


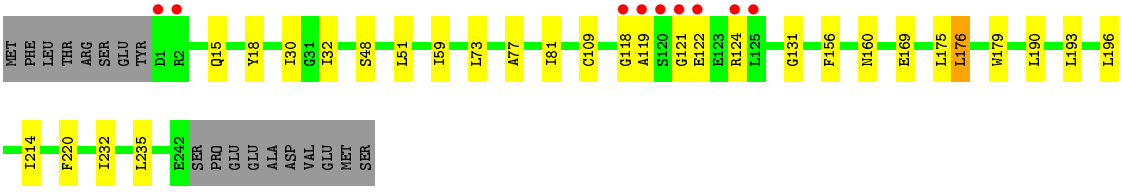
• Molecule 3: Proteasome subunit alpha type-4



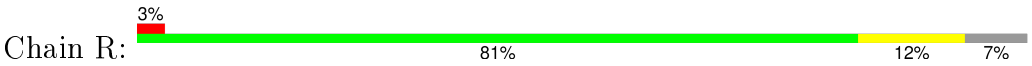


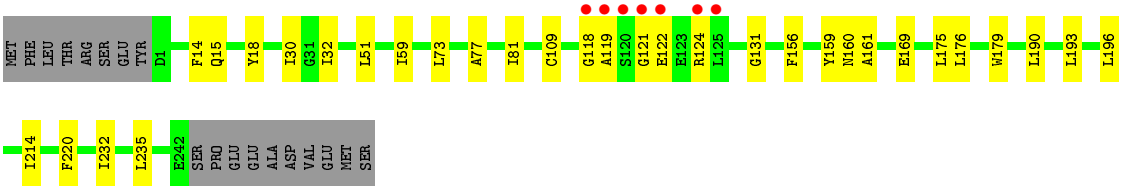
• Molecule 4: Proteasome subunit alpha type-5



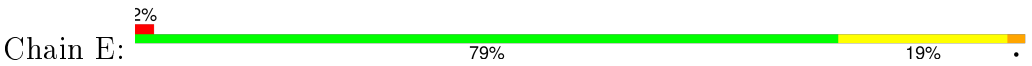


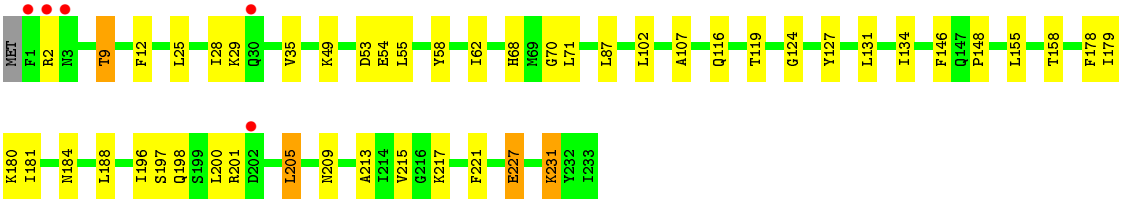
• Molecule 4: Proteasome subunit alpha type-5



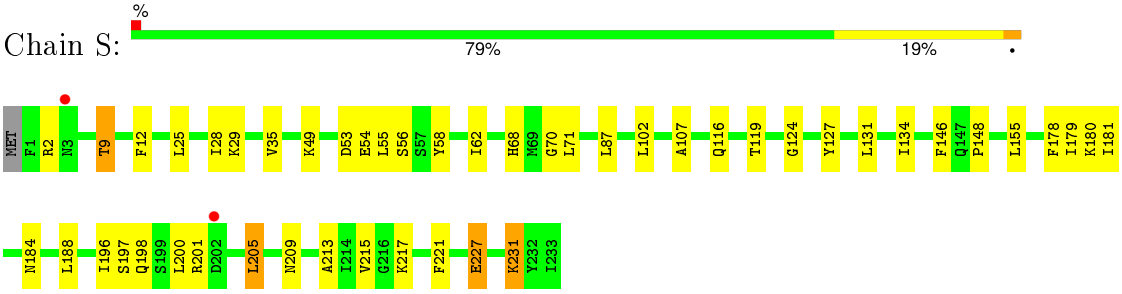


• Molecule 5: Proteasome subunit alpha type-6

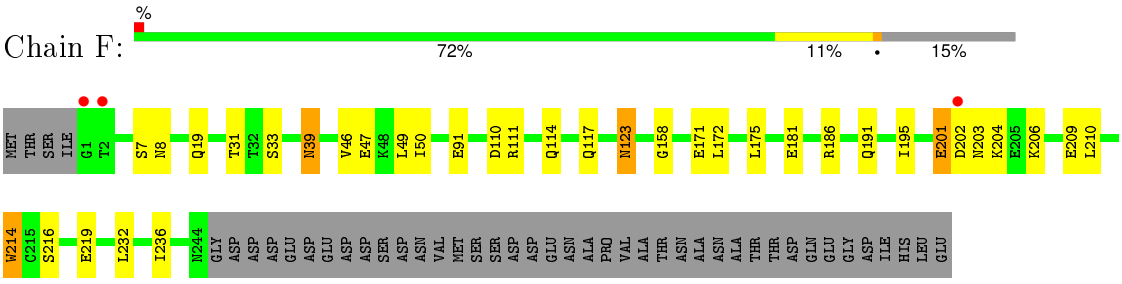




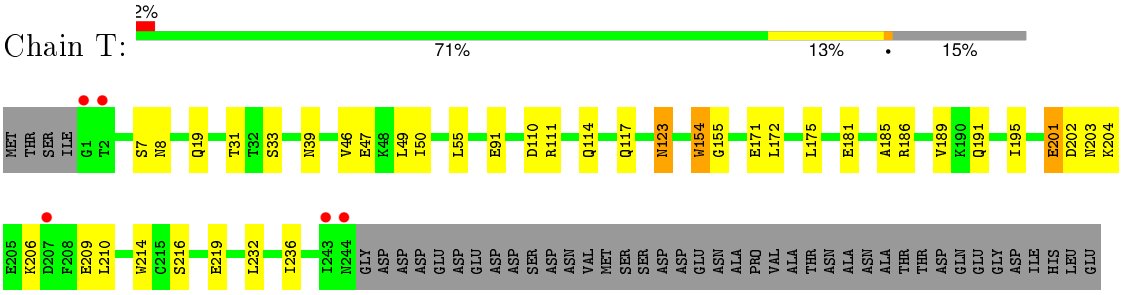
• Molecule 5: Proteasome subunit alpha type-6



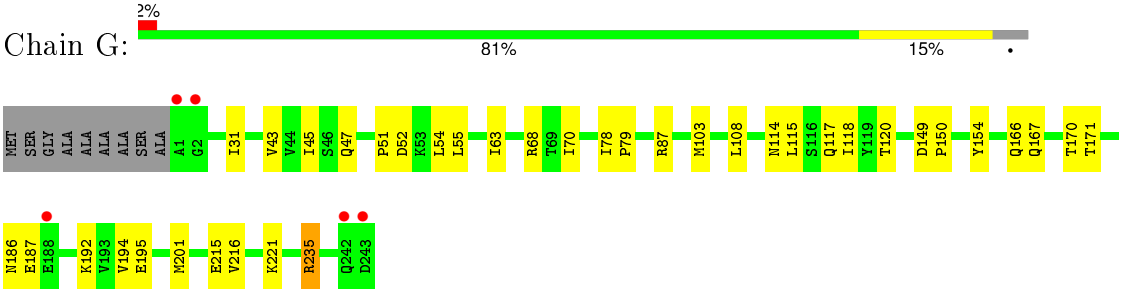
• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 6: Probable proteasome subunit alpha type-7

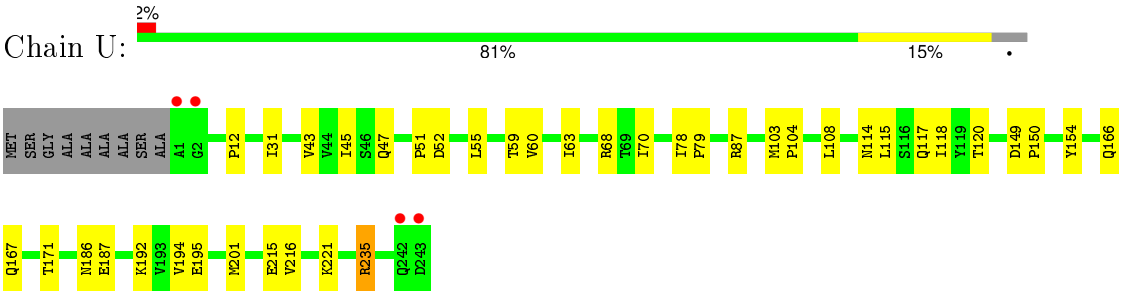


• Molecule 7: Proteasome subunit alpha type-1



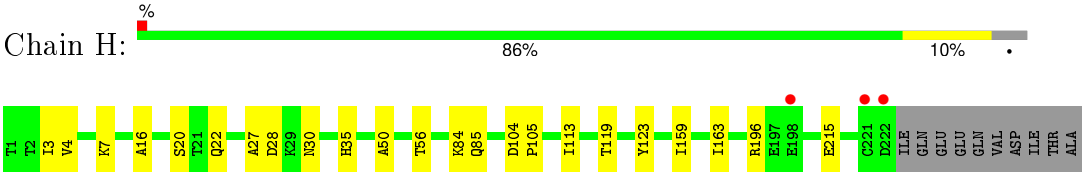
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



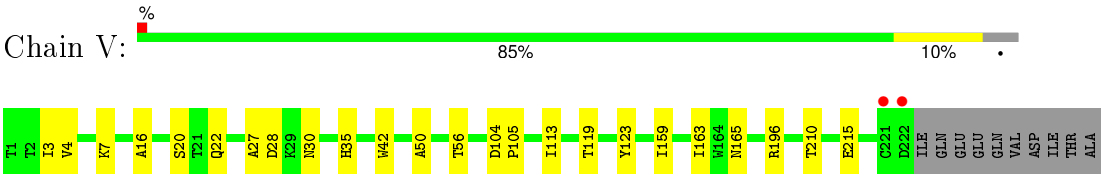
• Molecule 8: Proteasome subunit beta type-2

Chain H:



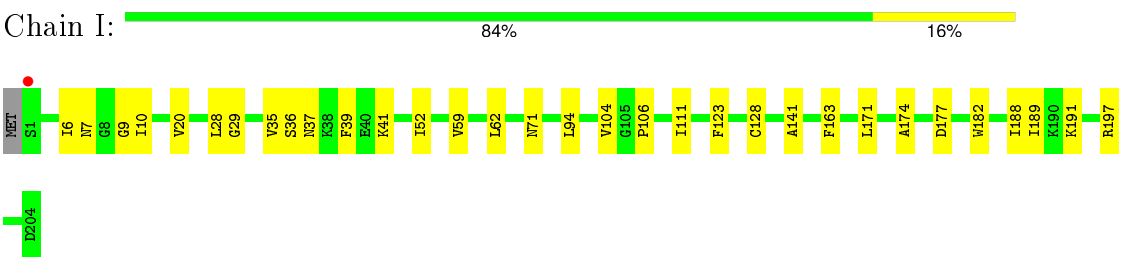
• Molecule 8: Proteasome subunit beta type-2

Chain V:



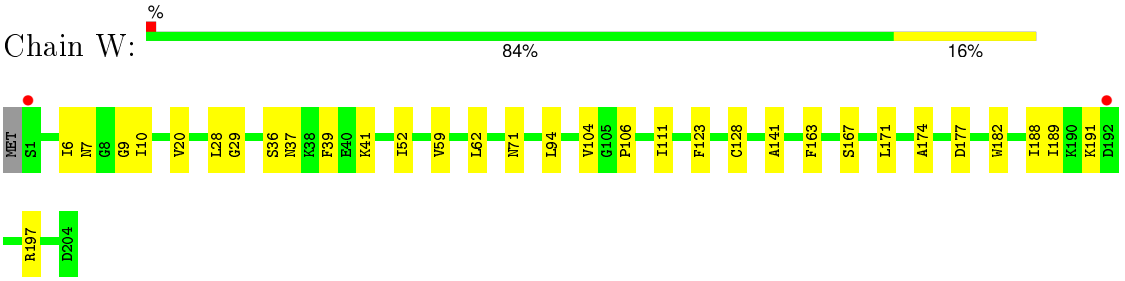
• Molecule 9: Proteasome subunit beta type-3

Chain I:



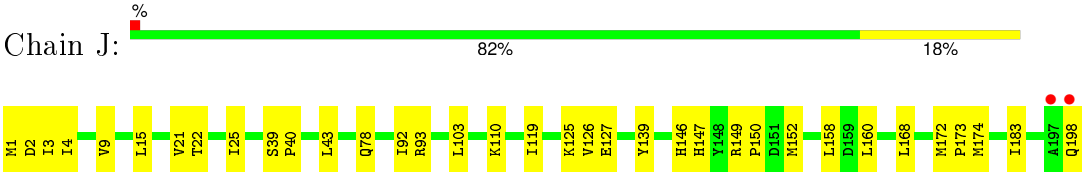
• Molecule 9: Proteasome subunit beta type-3

Chain W:



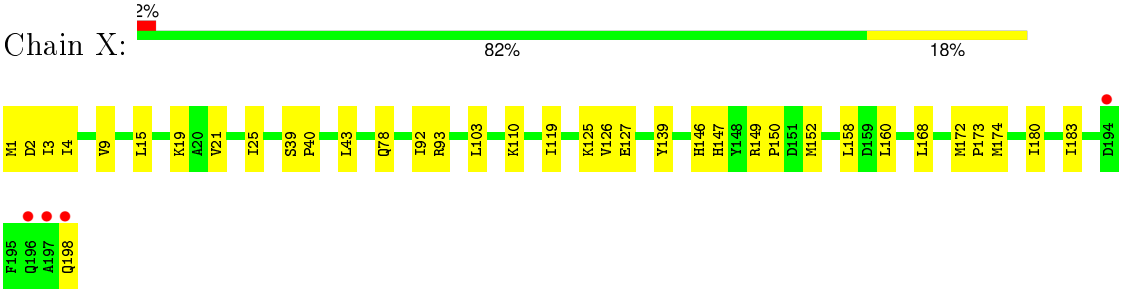
• Molecule 10: Proteasome subunit beta type-4

Chain J:



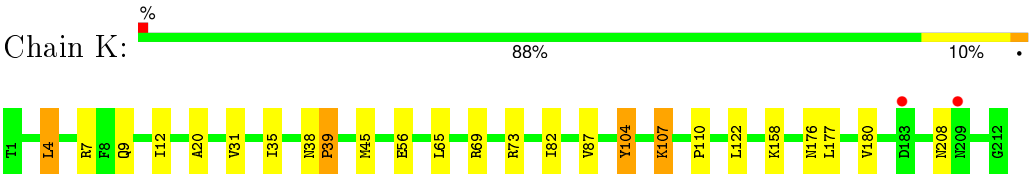
• Molecule 10: Proteasome subunit beta type-4

Chain X:



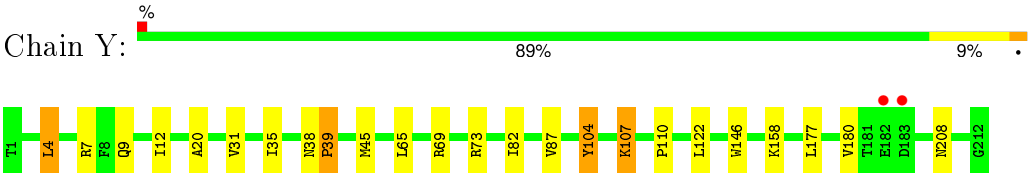
• Molecule 11: Proteasome subunit beta type-5

Chain K:



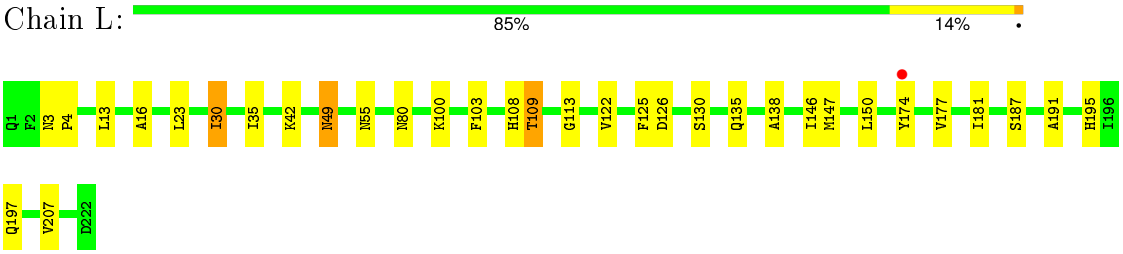
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



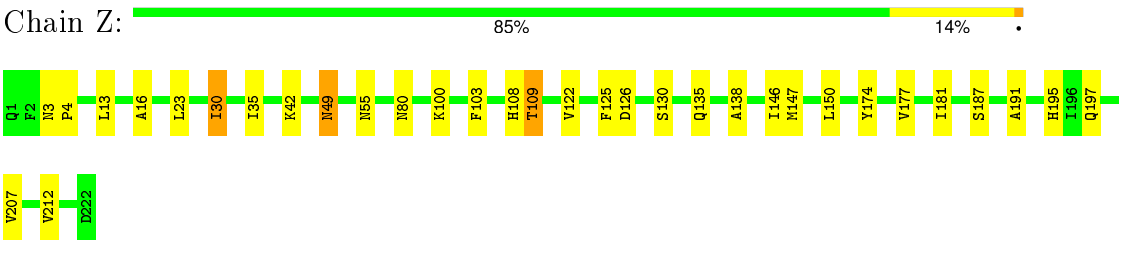
• Molecule 12: Proteasome subunit beta type-6

Chain L:



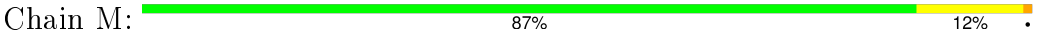
• Molecule 12: Proteasome subunit beta type-6

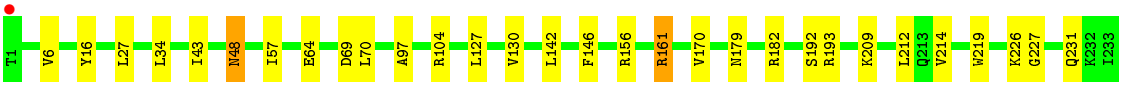
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

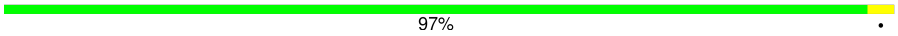
Chain M:





• Molecule 13: Proteasome subunit beta type-7

Chain a:

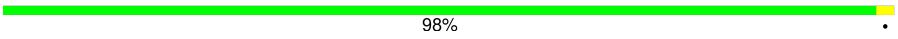


• Molecule 14: Proteasome subunit beta type-1

Chain N:

• Molecule 14: Proteasome subunit beta type-1

Chain b:



• Molecule 15: TMC-95A mimic ligand yCP:4a fragment P

Chain c:

There are no outlier residues recorded for this chain.

• Molecule 16: TMC-95A mimic ligand yCP:4a fragment Q

Chain d:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.70Å 301.40Å 144.60Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10 15.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-3.10) 99.7 (15.00-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.216 , 0.223 0.223 , 0.230	Depositor DCC
R_{free} test set	9543 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 190851 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	51001	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, 0L1, RE0, ABN, MES, TY5

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	0.37	1/1952 (0.1%)	0.48	0/2642
1	O	0.37	0/1952	0.48	0/2642
2	B	0.34	0/1934	0.49	0/2618
2	P	0.34	0/1934	0.49	0/2618
3	C	0.34	0/1919	0.49	0/2598
3	Q	0.34	0/1919	0.49	0/2598
4	D	0.36	0/1886	0.51	0/2541
4	R	0.36	0/1886	0.51	0/2541
5	E	0.31	0/1823	0.48	0/2463
5	S	0.31	0/1823	0.48	0/2463
6	F	0.41	1/1936 (0.1%)	0.48	0/2614
6	T	0.41	1/1936 (0.1%)	0.48	0/2614
7	G	0.34	0/1959	0.48	0/2652
7	U	0.34	0/1959	0.48	0/2652
8	H	0.44	0/1715	0.48	0/2326
8	V	0.44	1/1715 (0.1%)	0.48	0/2326
9	I	0.34	0/1611	0.49	0/2174
9	W	0.34	0/1611	0.49	0/2174
10	J	0.31	0/1613	0.48	0/2173
10	X	0.31	0/1613	0.48	0/2173
11	K	0.50	0/1681	0.51	1/2274 (0.0%)
11	Y	0.50	1/1681 (0.1%)	0.51	1/2274 (0.0%)
12	L	0.36	0/1795	0.48	0/2420
12	Z	0.36	0/1795	0.48	0/2420
13	M	0.36	1/1855 (0.1%)	0.50	0/2514
13	a	0.36	0/1855	0.50	0/2514
14	N	0.39	0/1541	0.45	0/2087
14	b	0.39	0/1541	0.45	0/2087
15	c	0.84	0/4	0.69	0/4
16	d	0.85	0/4	0.73	0/4
All	All	0.37	6/50448 (0.0%)	0.49	2/68200 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	146	TRP	CD2-CE2	5.03	1.47	1.41
6	F	214	TRP	CD2-CE2	5.03	1.47	1.41
8	V	42	TRP	CD2-CE2	5.02	1.47	1.41
13	M	219	TRP	CD2-CE2	5.02	1.47	1.41
1	A	159	TRP	CD2-CE2	5.01	1.47	1.41
6	T	154	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CA-CB-CG	5.18	127.21	115.30
11	K	4	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	21	0
1	O	1915	0	1929	22	0
2	B	1904	0	1904	33	0
2	P	1904	0	1904	31	0
3	C	1890	0	1903	31	0
3	Q	1890	0	1903	28	0
4	D	1861	0	1839	16	0
4	R	1861	0	1839	16	0
5	E	1795	0	1800	28	0
5	S	1795	0	1800	28	0
6	F	1896	0	1889	21	0
6	T	1896	0	1889	22	0
7	G	1921	0	1913	18	0
7	U	1921	0	1913	23	0
8	H	1684	0	1688	13	0
8	V	1684	0	1688	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1581	0	1574	21	0
9	W	1581	0	1574	21	0
10	J	1585	0	1590	25	0
10	X	1585	0	1590	27	0
11	K	1644	0	1595	14	0
11	Y	1644	0	1595	12	0
12	L	1757	0	1711	17	0
12	Z	1757	0	1711	17	0
13	M	1824	0	1832	17	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	c	48	0	35	0	0
16	d	52	0	37	0	0
17	K	12	0	13	0	0
17	Y	12	0	13	0	0
18	c	4	0	2	0	0
19	A	57	0	0	0	0
19	B	39	0	0	1	0
19	C	41	0	0	0	0
19	D	39	0	0	0	0
19	E	21	0	0	0	0
19	F	46	0	0	0	0
19	G	63	0	0	0	0
19	H	51	0	0	0	0
19	I	65	0	0	0	0
19	J	55	0	0	1	0
19	K	47	0	0	0	0
19	L	60	0	0	0	0
19	M	72	0	0	0	0
19	N	59	0	0	0	0
19	O	34	0	0	0	0
19	P	29	0	0	0	0
19	Q	27	0	0	0	0
19	R	30	0	0	0	0
19	S	21	0	0	0	0
19	T	40	0	0	0	0
19	U	58	0	0	0	0
19	V	48	0	0	0	0
19	W	57	0	0	0	0
19	X	44	0	0	0	0
19	Y	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	49	0	0	0	0
19	a	75	0	0	0	0
19	b	61	0	0	0	0
19	d	1	0	0	0	0
All	All	51001	0	49396	472	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 5.

All (472) 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)
2:B:189:ILE:HG21	2:B:237:ILE:HD11	1.38	1.05
2:P:189:ILE:HG21	2:P:237:ILE:HD11	1.37	1.04
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.53	0.89
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.53	0.88
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.60	0.82
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.60	0.82
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.49	0.78
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.49	0.76
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.53	0.73
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.54	0.73
1:O:12:PHE:H	2:P:20:GLN:HE22	1.36	0.72
2:B:189:ILE:CG2	2:B:237:ILE:HD11	2.20	0.71
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.57	0.70
2:P:189:ILE:CG2	2:P:237:ILE:HD11	2.19	0.70
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.56	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.40	0.69
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.72	0.69
1:A:176:GLU:HG2	2:B:55:LEU:HD21	1.75	0.69
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.58	0.69
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.58	0.69
2:P:200:THR:HG22	2:P:202:SER:H	1.58	0.68
2:B:12:PHE:H	3:C:17:GLN:HE22	1.39	0.68
10:J:173:PRO:HB2	10:X:174:MET:HE1	1.73	0.68
2:B:200:THR:HG22	2:B:202:SER:H	1.58	0.68
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.58	0.68
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.23	0.67
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.76	0.67
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.77	0.67
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.43	0.67
1:A:12:PHE:H	2:B:20:GLN:HE22	1.41	0.67
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.77	0.67
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.77	0.67
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.23	0.67
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.77	0.66
6:T:210:LEU:HD23	6:T:236:ILE:HD13	1.77	0.66
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.77	0.66
6:F:210:LEU:HD23	6:F:236:ILE:HD13	1.77	0.66
6:F:50:ILE:HD11	6:F:209:GLU:HB2	1.78	0.65
5:S:12:PHE:H	6:T:19:GLN:HE22	1.43	0.65
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.78	0.65
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.77	0.65
1:A:176:GLU:HG2	2:B:55:LEU:CD2	2.27	0.65
6:F:191:GLN:O	6:F:195:ILE:HG12	1.96	0.65
6:T:191:GLN:O	6:T:195:ILE:HG12	1.97	0.64
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.80	0.63
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.80	0.63
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.82	0.62
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.82	0.62
11:K:208:ASN:ND2	10:X:150:PRO:HG3	2.13	0.62
5:E:12:PHE:H	6:F:19:GLN:HE22	1.47	0.62
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.82	0.61
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.82	0.61
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.64	0.61
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.83	0.61
14:N:51:ASP:O	14:N:55:ILE:HG12	1.99	0.61
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.82	0.61
13:M:48:ASN:H	13:M:48:ASN:HD22	1.47	0.60
1:O:204:PHE:CE1	1:O:209:ILE:HD11	2.36	0.60
6:T:31:THR:HG21	6:T:47:GLU:O	2.02	0.60
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.83	0.60
1:A:204:PHE:CE1	1:A:209:ILE:HD11	2.35	0.60
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.82	0.60
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.83	0.60
6:F:31:THR:HG21	6:F:47:GLU:O	2.02	0.60
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.81	0.60
11:K:107:LYS:H	11:K:107:LYS:HD2	1.67	0.60
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.47	0.60
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.67	0.59
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.84	0.59
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.83	0.59
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.83	0.59
7:G:70:ILE:HG21	7:G:108:LEU:HD23	1.84	0.59
7:U:70:ILE:HG21	7:U:108:LEU:HD23	1.84	0.59
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.85	0.59
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.49	0.58
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.68	0.58
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.83	0.58
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.85	0.58
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.67	0.58
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.86	0.58
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.68	0.58
9:W:163:PHE:HD1	9:W:188:ILE:HD11	1.68	0.58
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.85	0.58
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.86	0.57
1:A:110:LEU:O	1:A:114:VAL:HG23	2.04	0.57
10:J:150:PRO:HG3	11:Y:208:ASN:ND2	2.20	0.57
8:H:35:HIS:CB	8:H:56:THR:HG21	2.34	0.57
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.87	0.57
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.86	0.57
1:O:110:LEU:O	1:O:114:VAL:HG23	2.05	0.57
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.87	0.57
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.87	0.57
9:I:163:PHE:HD1	9:I:188:ILE:HD11	1.68	0.57
5:S:205:LEU:HD23	5:S:205:LEU:H	1.70	0.56
6:T:232:LEU:O	6:T:236:ILE:HG12	2.06	0.56
8:V:35:HIS:CB	8:V:56:THR:HG21	2.34	0.56
5:E:205:LEU:HD23	5:E:205:LEU:H	1.71	0.56
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.86	0.56
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.88	0.56
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.87	0.56
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.88	0.56
2:B:180:LYS:HG3	2:B:183:MET:HG3	1.87	0.56
6:F:232:LEU:O	6:F:236:ILE:HG12	2.06	0.55
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.88	0.55
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.88	0.55
11:K:73:ARG:NH2	11:K:104:TYR:O	2.40	0.55
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.86	0.55
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.54	0.55
1:A:187:ASP:O	1:A:191:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.88	0.55
1:O:187:ASP:O	1:O:191:ILE:HG12	2.06	0.55
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.88	0.55
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.86	0.55
2:P:88:ASN:O	2:P:92:ILE:HG12	2.07	0.55
13:M:43:ILE:HG12	13:M:64:GLU:HG3	1.88	0.55
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.40	0.55
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.88	0.55
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.87	0.55
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.88	0.55
7:G:114:ASN:O	7:G:118:ILE:HD12	2.07	0.55
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.88	0.55
2:P:180:LYS:HG3	2:P:183:MET:HG3	1.87	0.54
7:U:114:ASN:O	7:U:118:ILE:HD12	2.07	0.54
10:J:168:LEU:O	10:J:172:MET:HB2	2.07	0.54
4:R:77:ALA:O	4:R:81:ILE:HG12	2.08	0.54
6:F:175:LEU:HD21	6:F:191:GLN:HG2	1.89	0.54
5:S:35:VAL:HG23	5:S:196:ILE:HD12	1.90	0.54
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.88	0.54
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.87	0.54
4:D:77:ALA:O	4:D:81:ILE:HG12	2.08	0.54
1:A:176:GLU:CG	2:B:55:LEU:HD21	2.37	0.54
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.90	0.54
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.90	0.54
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.57	0.53
3:Q:29:THR:HB	3:Q:45:GLU:HG3	1.89	0.53
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.43	0.53
2:B:88:ASN:O	2:B:92:ILE:HG12	2.07	0.53
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.90	0.53
13:M:48:ASN:HD22	13:M:48:ASN:N	2.05	0.53
10:X:168:LEU:O	10:X:172:MET:HB2	2.08	0.53
10:X:1:MET:HG2	10:X:2:ASP:H	1.73	0.53
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.91	0.53
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.91	0.53
12:Z:30:ILE:HG22	12:Z:35:ILE:HA	1.91	0.53
7:G:52:ASP:HB3	7:G:55:LEU:HG	1.91	0.53
9:I:28:LEU:HB3	9:I:36:SER:HB3	1.91	0.53
3:C:29:THR:HB	3:C:45:GLU:HG3	1.89	0.53
5:E:35:VAL:HG23	5:E:196:ILE:HD12	1.90	0.53
2:P:162:ILE:HD13	2:P:163:SER:H	1.74	0.53
10:J:1:MET:HG2	10:J:2:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.90	0.53
6:T:175:LEU:HD21	6:T:191:GLN:HG2	1.89	0.52
12:L:30:ILE:HG22	12:L:35:ILE:HA	1.91	0.52
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.44	0.52
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.90	0.52
4:R:190:LEU:HD12	4:R:235:LEU:HB2	1.91	0.52
3:C:185:THR:HB	3:C:188:GLU:HG2	1.91	0.52
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.91	0.52
4:D:190:LEU:HD12	4:D:235:LEU:HB2	1.92	0.52
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.91	0.52
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.56	0.52
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.74	0.52
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.90	0.52
2:B:162:ILE:HD13	2:B:163:SER:H	1.74	0.52
7:U:52:ASP:HB3	7:U:55:LEU:HG	1.92	0.52
10:J:1:MET:HG2	10:J:2:ASP:N	2.25	0.51
9:W:111:ILE:HG21	9:W:191:LYS:HG2	1.92	0.51
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.93	0.51
2:P:189:ILE:HG21	2:P:237:ILE:CD1	2.26	0.51
10:J:158:LEU:HD21	10:J:183:ILE:HD11	1.92	0.51
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.09	0.51
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.51
2:P:24:ALA:O	2:P:28:ILE:HG12	2.11	0.51
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.91	0.51
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.11	0.51
10:X:158:LEU:HD21	10:X:183:ILE:HD11	1.92	0.51
3:C:190:VAL:O	3:C:194:VAL:HG23	2.11	0.51
2:B:24:ALA:O	2:B:28:ILE:HG12	2.11	0.50
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.57	0.50
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.92	0.50
9:I:111:ILE:HG21	9:I:191:LYS:HG2	1.92	0.50
13:M:6:VAL:HG12	13:M:57:ILE:HD12	1.93	0.50
5:S:25:LEU:HA	5:S:28:ILE:HD12	1.93	0.50
10:X:1:MET:HG2	10:X:2:ASP:N	2.26	0.50
10:X:158:LEU:HD13	10:X:198:GLN:HE22	1.76	0.50
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.94	0.50
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.93	0.50
7:U:87:ARG:CZ	7:U:115:LEU:HD21	2.41	0.50
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.92	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.58	0.50
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:52:ILE:HG22	9:W:59:VAL:HG22	1.94	0.50
10:J:158:LEU:HD13	10:J:198:GLN:HE22	1.77	0.50
5:E:25:LEU:HA	5:E:28:ILE:HD12	1.92	0.50
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.92	0.50
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.92	0.49
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.94	0.49
7:G:87:ARG:CZ	7:G:115:LEU:HD21	2.41	0.49
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.31	0.49
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.94	0.49
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.93	0.49
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.11	0.49
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.78	0.49
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.95	0.49
2:B:162:ILE:CD1	2:B:163:SER:H	2.26	0.49
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.95	0.49
9:I:52:ILE:HG22	9:I:59:VAL:HG22	1.95	0.48
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.78	0.48
10:X:92:ILE:HG23	10:X:93:ARG:HG3	1.95	0.48
2:P:162:ILE:CD1	2:P:163:SER:H	2.26	0.48
3:Q:239:GLN:C	3:Q:241:GLN:H	2.17	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.13	0.48
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.79	0.48
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.95	0.48
9:W:163:PHE:CD1	9:W:188:ILE:HD11	2.48	0.48
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.44	0.48
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.78	0.48
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.44	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.94	0.48
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.94	0.48
5:E:49:LYS:HB3	5:E:58:TYR:HB3	1.95	0.48
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.31	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
1:O:30:GLN:HE21	1:O:30:GLN:HA	1.79	0.48
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	1.95	0.48
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.96	0.48
1:O:197:LYS:HA	1:O:204:PHE:CE1	2.49	0.48
11:K:35:ILE:HB	11:K:45:MET:CE	2.44	0.48
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.27	0.48
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.49	0.48
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.94	0.47
2:B:223:GLU:HG2	2:B:224:VAL:H	1.79	0.47
2:P:223:GLU:HG2	2:P:224:VAL:H	1.79	0.47
6:T:201:GLU:O	6:T:204:LYS:HD2	2.14	0.47
3:C:239:GLN:C	3:C:241:GLN:H	2.17	0.47
10:J:92:ILE:HG23	10:J:93:ARG:HG3	1.95	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.96	0.47
9:I:163:PHE:CD1	9:I:188:ILE:HD11	2.48	0.47
5:E:9:THR:HG21	5:E:119:THR:HA	1.96	0.47
5:S:49:LYS:HB3	5:S:58:TYR:HB3	1.95	0.47
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.95	0.47
9:I:35:VAL:HG13	19:J:241:HOH:O	2.15	0.47
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.30	0.47
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.96	0.47
6:T:49:LEU:HD22	6:T:206:LYS:HB2	1.96	0.47
7:G:78:ILE:N	7:G:79:PRO:HD2	2.30	0.47
2:B:105:ILE:HD12	2:B:110:LEU:HB2	1.96	0.47
3:C:46:ARG:HB2	3:C:207:ASN:HA	1.95	0.47
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.97	0.47
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.49	0.47
2:P:105:ILE:HD12	2:P:110:LEU:HB2	1.96	0.47
2:B:189:ILE:HG21	2:B:237:ILE:CD1	2.26	0.47
12:L:100:LYS:HE3	12:L:103:PHE:O	2.15	0.47
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.96	0.47
8:V:7:LYS:HG3	8:V:123:TYR:HA	1.95	0.47
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.96	0.47
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.96	0.46
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.96	0.46
5:S:134:ILE:HD12	5:S:215:VAL:HG12	1.97	0.46
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.15	0.46
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.44	0.46
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.49	0.46
5:E:28:ILE:HD11	5:E:148:PRO:HG2	1.97	0.46
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.97	0.46
6:F:49:LEU:HD22	6:F:206:LYS:HB2	1.96	0.46
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.96	0.46
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.97	0.46
7:U:78:ILE:N	7:U:79:PRO:HD2	2.30	0.46
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.98	0.46
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.30	0.46
5:S:28:ILE:HD11	5:S:148:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.97	0.46
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.96	0.46
3:C:46:ARG:HD2	3:C:206:LYS:O	2.16	0.46
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.16	0.46
5:S:127:TYR:O	5:S:148:PRO:HB3	2.16	0.46
1:O:119:GLN:O	1:O:122:THR:HB	2.16	0.46
5:E:68:HIS:HE1	5:E:102:LEU:O	1.99	0.46
6:F:201:GLU:O	6:F:204:LYS:HD2	2.16	0.46
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.15	0.46
9:I:106:PRO:HB2	9:I:123:PHE:CD2	2.51	0.46
1:A:197:LYS:HA	1:A:204:PHE:CE1	2.50	0.46
9:W:106:PRO:HB2	9:W:123:PHE:CD2	2.51	0.46
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.98	0.46
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.97	0.46
3:Q:194:VAL:HG22	3:Q:210:ILE:HD11	1.98	0.46
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.51	0.46
5:S:68:HIS:HE1	5:S:102:LEU:O	1.99	0.45
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.96	0.45
3:C:194:VAL:HG22	3:C:210:ILE:HD11	1.98	0.45
1:A:26:THR:O	1:A:30:GLN:HG2	2.17	0.45
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.51	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.82	0.45
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.47	0.45
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.81	0.45
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.99	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.45
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.82	0.45
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.15	0.45
5:E:127:TYR:O	5:E:148:PRO:HB3	2.16	0.45
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.82	0.45
5:E:134:ILE:HD12	5:E:215:VAL:HG12	1.98	0.45
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.99	0.45
1:A:119:GLN:O	1:A:122:THR:HB	2.17	0.45
5:E:231:LYS:H	5:E:231:LYS:HD2	1.82	0.45
5:E:179:ILE:HG23	5:E:180:LYS:HG3	1.99	0.45
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.99	0.45
12:Z:135:GLN:HG3	12:Z:174:TYR:OH	2.17	0.45
7:G:31:ILE:HG23	7:G:47:GLN:HB2	1.99	0.45
5:S:197:SER:HA	5:S:200:LEU:HG	1.99	0.45
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:179:ILE:HG23	5:S:180:LYS:HG3	1.99	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.45
8:H:159:ILE:O	8:H:163:ILE:HD12	2.17	0.44
5:S:155:LEU:HD23	6:T:55:LEU:HA	1.99	0.44
12:L:135:GLN:HG3	12:L:174:TYR:OH	2.17	0.44
12:L:146:ILE:HD11	12:L:191:ALA:HB2	2.00	0.44
1:O:172:LYS:O	1:O:176:GLU:HG3	2.17	0.44
12:L:49:ASN:HA	12:L:49:ASN:HD22	1.67	0.44
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.00	0.44
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.00	0.44
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.44
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.00	0.44
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.99	0.44
1:A:172:LYS:O	1:A:176:GLU:HG3	2.17	0.44
6:F:8:ASN:HB3	6:F:123:ASN:HA	2.00	0.44
11:K:7:ARG:HD2	11:K:110:PRO:O	2.18	0.44
1:A:176:GLU:HA	2:B:55:LEU:HD11	2.00	0.44
2:P:18:LEU:HD13	2:P:122:THR:HG23	2.00	0.44
11:K:35:ILE:HB	11:K:45:MET:HE2	2.00	0.44
8:V:159:ILE:O	8:V:163:ILE:HD12	2.18	0.44
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.99	0.44
1:A:68:THR:HB	1:A:69:PRO:HD2	2.00	0.44
6:T:8:ASN:HB3	6:T:123:ASN:HA	1.99	0.44
6:T:171:GLU:HB3	6:T:195:ILE:HD12	1.99	0.44
1:O:26:THR:O	1:O:30:GLN:HG2	2.17	0.44
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.98	0.44
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.82	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.99	0.44
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.00	0.44
5:S:231:LYS:HD2	5:S:231:LYS:H	1.82	0.44
11:K:12:ILE:HB	11:K:180:VAL:HB	1.99	0.44
2:B:223:GLU:HG2	2:B:224:VAL:N	2.33	0.44
2:P:223:GLU:HG2	2:P:224:VAL:N	2.33	0.44
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.53	0.44
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.99	0.44
1:O:160:LYS:HD2	2:P:55:LEU:HA	2.00	0.44
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.53	0.44
5:S:178:PHE:HA	5:S:181:ILE:HG12	1.99	0.44
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.00	0.44
3:Q:160:GLN:CA	3:Q:160:GLN:HE21	2.23	0.43
9:I:10:ILE:HD11	9:I:174:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:15:LEU:HD12	10:X:43:LEU:HD23	2.00	0.43
12:Z:146:ILE:HD11	12:Z:191:ALA:HB2	1.99	0.43
5:E:178:PHE:HA	5:E:181:ILE:HG12	2.00	0.43
5:E:197:SER:HA	5:E:200:LEU:HG	1.99	0.43
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.82	0.43
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.82	0.43
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.47	0.43
2:B:18:LEU:HD13	2:B:122:THR:HG23	2.00	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.18	0.43
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.98	0.43
3:Q:233:GLN:O	3:Q:237:GLU:HG2	2.18	0.43
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.67	0.43
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.99	0.43
10:X:4:ILE:HG22	10:X:103:LEU:HD12	2.01	0.43
5:S:178:PHE:HA	5:S:181:ILE:CG1	2.49	0.43
1:O:68:THR:HB	1:O:69:PRO:HD2	2.00	0.43
6:F:171:GLU:HB3	6:F:195:ILE:HD12	1.99	0.43
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	2.01	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
5:E:70:GLY:HA3	5:E:221:PHE:CZ	2.54	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.83	0.43
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.53	0.43
10:J:25:ILE:O	10:X:139:TYR:OH	2.37	0.42
5:E:178:PHE:HA	5:E:181:ILE:CG1	2.49	0.42
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.01	0.42
7:G:45:ILE:HD13	7:G:216:VAL:HG22	2.00	0.42
12:Z:177:VAL:O	12:Z:181:ILE:HG12	2.19	0.42
7:U:45:ILE:HD13	7:U:216:VAL:HG22	2.00	0.42
9:W:10:ILE:HD11	9:W:174:ALA:HB2	2.00	0.42
3:C:213:VAL:HG23	3:C:219:ILE:HG12	2.01	0.42
8:H:215:GLU:HG3	9:I:197:ARG:HG2	2.00	0.42
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.01	0.42
3:C:80:SER:O	3:C:84:ILE:HD12	2.20	0.42
3:C:101:PRO:HG2	3:C:138:PRO:HG3	2.01	0.42
12:L:177:VAL:O	12:L:181:ILE:HG12	2.19	0.42
5:S:227:GLU:CD	5:S:227:GLU:H	2.23	0.42
12:Z:49:ASN:HD22	12:Z:49:ASN:HA	1.67	0.42
3:Q:166:SER:HA	3:Q:169:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:GLN:O	3:C:237:GLU:HG2	2.19	0.42
10:J:15:LEU:HD12	10:J:43:LEU:HD23	2.00	0.42
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.49	0.42
12:Z:146:ILE:HD12	12:Z:187:SER:HB3	2.02	0.42
3:Q:213:VAL:HG23	3:Q:219:ILE:HG12	2.01	0.42
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.34	0.42
10:X:152:MET:HE1	10:X:160:LEU:HD22	2.02	0.42
12:L:146:ILE:HD12	12:L:187:SER:HB3	2.01	0.42
10:J:4:ILE:HG22	10:J:103:LEU:HD12	2.02	0.42
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.55	0.42
14:N:126:ILE:HD13	14:N:126:ILE:H	1.84	0.42
9:I:7:ASN:HA	9:I:29:GLY:O	2.20	0.42
6:F:158:GLY:O	7:G:54:LEU:HB3	2.20	0.42
4:R:32:ILE:HD11	4:R:175:LEU:HD22	2.02	0.42
10:J:152:MET:HE1	10:J:160:LEU:HD22	2.01	0.42
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.01	0.42
2:P:236:ASP:O	2:P:240:LYS:HG2	2.20	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.42
3:C:166:SER:HA	3:C:169:VAL:CG1	2.49	0.41
1:O:222:LEU:HD13	1:O:232:GLY:HA2	2.02	0.41
1:A:211:LEU:HD22	1:A:238:LEU:HD12	2.02	0.41
11:K:176:ASN:HA	11:K:176:ASN:HD22	1.71	0.41
1:A:222:LEU:HD13	1:A:232:GLY:HA2	2.01	0.41
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.02	0.41
14:N:82:PHE:HB3	14:N:113:ILE:HD13	2.01	0.41
3:C:35:LYS:HD3	3:C:158:SER:HA	2.02	0.41
4:R:119:ALA:HA	5:S:124:GLY:HA2	2.01	0.41
4:D:32:ILE:HD11	4:D:175:LEU:HD22	2.02	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.00	0.41
6:T:185:ALA:O	6:T:189:VAL:HG23	2.20	0.41
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.02	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.02	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
1:O:23:TYR:CE1	7:U:12:PRO:HA	2.55	0.41
5:E:227:GLU:CD	5:E:227:GLU:H	2.23	0.41
2:B:236:ASP:O	2:B:240:LYS:HG2	2.20	0.41
14:N:59:VAL:HG22	14:N:81:VAL:HG12	2.02	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.41
3:Q:101:PRO:HG2	3:Q:138:PRO:HG3	2.01	0.41
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.01	0.41
3:Q:35:LYS:HD3	3:Q:158:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:180:LYS:CG	2:P:183:MET:HG3	2.50	0.41
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.03	0.41
4:R:14:PHE:HD2	4:R:18:TYR:HH	1.68	0.41
1:O:158:PRO:HB2	2:P:57:GLU:HB3	2.01	0.41
7:U:103:MET:HA	7:U:104:PRO:HD3	1.93	0.41
12:L:138:ALA:HB3	12:L:147:MET:HG2	2.03	0.41
5:E:155:LEU:HD13	5:E:158:THR:HB	2.03	0.41
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	2.03	0.41
9:W:28:LEU:HB2	9:W:39:PHE:CB	2.51	0.41
12:L:113:GLY:HA2	12:L:207:VAL:HG11	2.03	0.41
10:X:19:LYS:HD3	10:X:180:ILE:HG13	2.03	0.41
3:Q:80:SER:O	3:Q:84:ILE:HD12	2.20	0.41
4:R:193:LEU:HD21	4:R:232:ILE:HG13	2.03	0.41
1:O:211:LEU:HD22	1:O:238:LEU:HD12	2.02	0.41
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.02	0.40
4:D:193:LEU:HD21	4:D:232:ILE:HG13	2.03	0.40
10:X:147:HIS:HB2	10:X:160:LEU:HD11	2.03	0.40
9:I:28:LEU:HB2	9:I:39:PHE:CB	2.51	0.40
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.02	0.40
4:D:109:CYS:SG	4:D:156:PHE:HB3	2.62	0.40
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.03	0.40
3:C:157:TRP:CZ3	4:D:48:SER:HB3	2.57	0.40
3:Q:155:SER:HB2	4:R:51:LEU:HD21	2.04	0.40
1:O:82:TYR:O	1:O:86:VAL:HG23	2.22	0.40
6:F:110:ASP:O	6:F:114:GLN:HG2	2.22	0.40
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	2.03	0.40
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.03	0.40
8:V:210:THR:HG21	9:W:167:SER:HB3	2.02	0.40
6:T:110:ASP:O	6:T:114:GLN:HG2	2.21	0.40
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.62	0.40
6:F:39:ASN:N	6:F:39:ASN:HD22	2.19	0.40
8:H:84:LYS:HG3	8:H:85:GLN:N	2.36	0.40
19:B:301:HOH:O	3:C:57:ILE:HD11	2.22	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	248/250 (99%)	237 (96%)	9 (4%)	2 (1%)	24	63
1	O	248/250 (99%)	237 (96%)	9 (4%)	2 (1%)	24	63
2	B	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	16	52
2	P	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	16	52
3	C	239/254 (94%)	229 (96%)	7 (3%)	3 (1%)	15	50
3	Q	239/254 (94%)	229 (96%)	7 (3%)	3 (1%)	15	50
4	D	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	15	50
4	R	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	15	50
5	E	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	15	50
5	S	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	15	50
6	F	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
6	T	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	241/252 (96%)	230 (95%)	10 (4%)	1 (0%)	39	75
7	U	241/252 (96%)	230 (95%)	10 (4%)	1 (0%)	39	75
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	34	72
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	34	72
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	34	72
11	Y	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	34	72
12	L	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
12	Z	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
13	M	231/233 (99%)	222 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	c	1/4 (25%)	1 (100%)	0	0	100	100
16	d	1/7 (14%)	1 (100%)	0	0	100	100
All	All	6314/6599 (96%)	6048 (96%)	232 (4%)	34 (0%)	34	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
2	B	218	GLY
2	B	221	ASP
5	E	2	ARG
5	E	201	ARG
2	P	218	GLY
2	P	221	ASP
5	S	2	ARG
5	S	201	ARG
1	A	166	LYS
3	C	203	THR
4	D	121	GLY
4	D	122	GLU
5	E	217	LYS
11	K	39	PRO
1	O	166	LYS
3	Q	203	THR
4	R	121	GLY
4	R	122	GLU
5	S	217	LYS
11	Y	39	PRO
1	A	2	THR
2	B	51	VAL
10	J	9	VAL
1	O	2	THR
2	P	51	VAL
3	Q	183	PRO
10	X	9	VAL
3	C	183	PRO

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Mol	Chain	Res	Type
4	D	118	GLY
7	G	51	PRO
4	R	118	GLY
7	U	51	PRO

5.3.2 Protein sidechains

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	209/209 (100%)	206 (99%)	3 (1%)	74	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	90
2	B	203/216 (94%)	192 (95%)	11 (5%)	27	64
2	P	203/216 (94%)	192 (95%)	11 (5%)	27	64
3	C	213/226 (94%)	204 (96%)	9 (4%)	36	73
3	Q	213/226 (94%)	204 (96%)	9 (4%)	36	73
4	D	198/215 (92%)	194 (98%)	4 (2%)	63	86
4	R	198/215 (92%)	194 (98%)	4 (2%)	63	86
5	E	192/193 (100%)	180 (94%)	12 (6%)	22	58
5	S	192/193 (100%)	180 (94%)	12 (6%)	22	58
6	F	201/239 (84%)	190 (94%)	11 (6%)	27	63
6	T	201/239 (84%)	190 (94%)	11 (6%)	27	63
7	G	207/210 (99%)	199 (96%)	8 (4%)	39	75
7	U	207/210 (99%)	199 (96%)	8 (4%)	39	75
8	H	181/190 (95%)	179 (99%)	2 (1%)	80	93
8	V	181/190 (95%)	179 (99%)	2 (1%)	80	93
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	84
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	84
10	J	175/175 (100%)	172 (98%)	3 (2%)	68	89
10	X	175/175 (100%)	172 (98%)	3 (2%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	169/169 (100%)	161 (95%)	8 (5%)	32 70
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32 70
12	L	185/185 (100%)	179 (97%)	6 (3%)	46 79
12	Z	185/185 (100%)	179 (97%)	6 (3%)	46 79
13	M	199/199 (100%)	192 (96%)	7 (4%)	43 78
13	a	199/199 (100%)	192 (96%)	7 (4%)	43 78
14	N	162/162 (100%)	158 (98%)	4 (2%)	55 84
14	b	162/162 (100%)	158 (98%)	4 (2%)	55 84
All	All	5332/5522 (97%)	5148 (96%)	184 (4%)	43 78

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	LEU
1	A	157	PHE
2	B	55	LEU
2	B	58	GLN
2	B	60	THR
2	B	105	ILE
2	B	119	GLN
2	B	149	THR
2	B	162	ILE
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
3	C	4	ARG
3	C	8	ILE
3	C	19	GLU
3	C	51	LYS
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	171	GLU
3	C	206	LYS
4	D	124	ARG
4	D	169	GLU
4	D	176	LEU

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Mol	Chain	Res	Type
4	D	214	ILE
5	E	9	THR
5	E	29	LYS
5	E	53	ASP
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	198	GLN
5	E	205	LEU
5	E	227	GLU
5	E	231	LYS
6	F	7	SER
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	202	ASP
6	F	203	ASN
6	F	214	TRP
7	G	68	ARG
7	G	117	GLN
7	G	154	TYR
7	G	166	GLN
7	G	186	ASN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
8	H	30	ASN
8	H	196	ARG
9	I	6	ILE
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	78	GLN
10	J	110	LYS
10	J	127	GLU
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	82	ILE
11	K	87	VAL
11	K	104	TYR
11	K	107	LYS
12	L	23	LEU
12	L	30	ILE
12	L	49	ASN
12	L	80	ASN
12	L	108	HIS
12	L	109	THR
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	226	LYS
14	N	119	VAL
14	N	126	ILE
14	N	149	GLU
14	N	187	ILE
1	O	30	GLN
1	O	61	LEU
1	O	157	PHE
2	P	55	LEU
2	P	58	GLN
2	P	60	THR
2	P	105	ILE
2	P	119	GLN
2	P	149	THR
2	P	162	ILE
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	8	ILE
3	Q	19	GLU
3	Q	51	LYS

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Mol	Chain	Res	Type
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	171	GLU
3	Q	206	LYS
4	R	124	ARG
4	R	169	GLU
4	R	176	LEU
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	53	ASP
5	S	54	GLU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	198	GLN
5	S	205	LEU
5	S	227	GLU
5	S	231	LYS
6	T	7	SER
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	214	TRP
7	U	68	ARG
7	U	117	GLN
7	U	154	TYR
7	U	166	GLN
7	U	186	ASN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	30	ASN
8	V	196	ARG

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Mol	Chain	Res	Type
9	W	6	ILE
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	78	GLN
10	X	110	LYS
10	X	127	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	82	ILE
11	Y	87	VAL
11	Y	104	TYR
11	Y	107	LYS
12	Z	23	LEU
12	Z	30	ILE
12	Z	49	ASN
12	Z	80	ASN
12	Z	108	HIS
12	Z	109	THR
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	226	LYS
14	b	119	VAL
14	b	126	ILE
14	b	149	GLU
14	b	187	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN

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Mol	Chain	Res	Type
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	236	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN
5	E	4	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	66	HIS

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Mol	Chain	Res	Type
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
9	I	156	ASN
10	J	37	GLN
10	J	55	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS
10	J	191	GLN
10	J	198	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN

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Mol	Chain	Res	Type
3	Q	17	GLN
3	Q	77	ASN
3	Q	92	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	236	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	4	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
9	W	156	ASN

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Mol	Chain	Res	Type
10	X	37	GLN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	191	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
15	TY5	c	1	18,15	19,20,21	1.27	2 (10%)	22,25,27	0.87	1 (4%)
15	RE0	c	3	15	15,17,18	1.27	1 (6%)	21,25,27	2.07	5 (23%)
16	ACA	d	3	16	3,3,8	0.73	0	1,2,8	0.67	0
16	TY5	d	4	16	19,20,21	1.23	0	22,25,27	0.81	1 (4%)
16	RE0	d	6	16	15,17,18	1.26	1 (6%)	21,25,27	2.10	5 (23%)

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
15	TY5	c	1	18,15	-	0/9/11/13	0/2/2/2
15	RE0	c	3	15	-	0/5/23/25	0/2/2/2
16	ACA	d	3	16	-	0/0/1/6	0/0/0/0
16	TY5	d	4	16	-	0/9/11/13	0/2/2/2
16	RE0	d	6	16	-	0/5/23/25	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	1	TY5	C54-C53	2.04	1.43	1.38
15	c	1	TY5	C53-C52	2.08	1.43	1.38
16	d	6	RE0	CG-CD2	2.67	1.54	1.51
15	c	3	RE0	CG-CD2	2.72	1.54	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	6	RE0	CG-CD2-CE2	-5.39	106.41	108.80
15	c	3	RE0	CG-CD2-CE2	-5.21	106.49	108.80
16	d	6	RE0	CE2-NE1-CD1	-5.10	109.13	111.88
15	c	3	RE0	CE2-NE1-CD1	-5.07	109.14	111.88
16	d	4	TY5	O-C-CA	-3.14	117.30	125.49
15	c	1	TY5	O-C-CA	-3.14	117.32	125.49
15	c	3	RE0	O-C-CA	-2.89	117.96	125.49
16	d	6	RE0	O-C-CA	-2.87	118.02	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c	3	RE0	CZ2-CE2-NE1	-2.54	125.82	131.02
16	d	6	RE0	CZ2-CE2-NE1	-2.51	125.89	131.02
15	c	3	RE0	CD2-CE2-NE1	2.96	111.56	109.61
16	d	6	RE0	CD2-CE2-NE1	2.97	111.56	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MES	K	301	-	11,12,12	0.96	0	14,16,16	1.92	3 (21%)
17	MES	Y	301	-	11,12,12	1.04	0	14,16,16	2.28	6 (42%)
18	0L1	c	101	15	3,3,9	0.74	0	1,2,10	0.65	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
17	MES	K	301	-	-	0/6/14/14	0/1/1/1
17	MES	Y	301	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	0L1	c	101	15	-	0/0/1/7	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	MES	O2S-S-C8	-5.35	102.34	106.91
17	K	301	MES	O2S-S-C8	-5.04	102.61	106.91
17	K	301	MES	O1S-S-C8	2.31	108.88	106.91
17	Y	301	MES	O1S-S-C8	2.38	108.94	106.91
17	Y	301	MES	C6-C5-N4	2.61	114.08	110.12
17	Y	301	MES	C5-N4-C3	2.64	114.63	108.90
17	Y	301	MES	C2-C3-N4	2.84	114.43	110.12
17	Y	301	MES	O3S-S-O1S	2.96	118.51	111.61
17	K	301	MES	O3S-S-O1S	3.19	119.03	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.41	4 (1%)	74	55	48, 63, 84, 98	0
1	O	250/250 (100%)	-0.35	4 (1%)	74	55	55, 71, 92, 103	0
2	B	244/258 (94%)	-0.26	9 (3%)	45	22	52, 69, 98, 105	0
2	P	244/258 (94%)	-0.23	11 (4%)	37	17	57, 71, 97, 111	0
3	C	241/254 (94%)	-0.23	7 (2%)	55	31	50, 67, 101, 127	0
3	Q	241/254 (94%)	-0.09	10 (4%)	41	19	60, 82, 123, 152	0
4	D	242/260 (93%)	-0.29	9 (3%)	45	22	53, 68, 94, 107	0
4	R	242/260 (93%)	-0.21	7 (2%)	55	31	58, 75, 103, 118	0
5	E	233/234 (99%)	-0.31	5 (2%)	67	44	55, 73, 92, 101	0
5	S	233/234 (99%)	-0.23	2 (0%)	85	72	60, 80, 106, 115	0
6	F	244/288 (84%)	-0.40	3 (1%)	81	64	53, 67, 91, 104	0
6	T	244/288 (84%)	-0.35	5 (2%)	68	46	55, 74, 100, 116	0
7	G	243/252 (96%)	-0.43	5 (2%)	67	44	49, 64, 83, 114	0
7	U	243/252 (96%)	-0.39	4 (1%)	74	55	55, 66, 84, 110	0
8	H	222/232 (95%)	-0.53	3 (1%)	78	60	48, 57, 75, 86	0
8	V	222/232 (95%)	-0.52	2 (0%)	85	72	50, 59, 73, 92	0
9	I	204/205 (99%)	-0.66	1 (0%)	91	83	46, 56, 71, 76	0
9	W	204/205 (99%)	-0.59	2 (0%)	84	69	51, 58, 74, 84	0
10	J	198/198 (100%)	-0.50	2 (1%)	84	69	47, 57, 73, 108	0
10	X	198/198 (100%)	-0.46	4 (2%)	68	46	53, 59, 72, 102	0
11	K	212/212 (100%)	-0.45	2 (0%)	85	72	47, 62, 79, 86	0
11	Y	212/212 (100%)	-0.46	2 (0%)	85	72	52, 64, 83, 89	0
12	L	222/222 (100%)	-0.59	1 (0%)	91	83	48, 58, 82, 87	0
12	Z	222/222 (100%)	-0.55	0	100	100	51, 60, 81, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.57	1 (0%) 93 85	47, 58, 69, 71	0
13	a	233/233 (100%)	-0.55	1 (0%) 93 85	48, 57, 66, 69	0
14	N	196/196 (100%)	-0.62	0 100 100	48, 54, 68, 72	0
14	b	196/196 (100%)	-0.60	0 100 100	48, 55, 68, 77	0
15	c	1/4 (25%)	-0.11	0 100 100	57, 57, 57, 57	0
16	d	1/7 (14%)	0.89	0 100 100	62, 62, 62, 62	0
All	All	6370/6599 (96%)	-0.41	106 (1%) 73 52	46, 63, 94, 152	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	118	GLY	6.5
2	P	220	ASN	6.3
4	D	120	SER	6.1
6	F	1	GLY	6.1
2	B	219	ALA	6.1
4	R	119	ALA	5.9
2	B	220	ASN	5.9
3	C	49	THR	5.7
2	P	219	ALA	5.5
4	D	119	ALA	5.4
7	G	1	ALA	5.4
4	R	121	GLY	5.3
7	U	243	ASP	5.3
4	R	120	SER	5.1
4	D	118	GLY	5.0
10	X	198	GLN	4.9
7	G	243	ASP	4.8
10	J	197	ALA	4.8
10	J	198	GLN	4.4
3	C	241	GLN	4.3
9	W	1	SER	4.2
8	V	222	ASP	4.1
3	Q	239	GLN	4.1
7	U	1	ALA	4.1
1	A	2	THR	4.0
3	Q	50	LEU	4.0
3	C	50	LEU	3.6
3	Q	203	THR	3.6
4	D	121	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
6	T	1	GLY	3.4
8	V	221	CYS	3.4
2	B	218	GLY	3.4
3	Q	49	THR	3.3
3	Q	240	GLU	3.2
5	E	202	ASP	3.2
7	G	242	GLN	3.2
5	S	202	ASP	3.2
3	C	206	LYS	3.2
4	D	125	LEU	3.2
3	Q	206	LYS	3.2
10	X	197	ALA	3.1
9	I	1	SER	3.0
8	H	222	ASP	3.0
6	T	244	ASN	2.9
2	B	223	GLU	2.9
3	C	203	THR	2.9
2	P	223	GLU	2.9
2	B	61	SER	2.8
2	P	203	SER	2.8
2	P	51	VAL	2.8
4	R	124	ARG	2.8
1	A	1	MET	2.8
2	B	221	ASP	2.7
13	M	1	THR	2.7
8	H	198	GLU	2.7
3	Q	48	SER	2.7
7	U	242	GLN	2.7
2	P	60	THR	2.7
4	D	124	ARG	2.7
6	T	2	THR	2.7
3	Q	241	GLN	2.7
2	P	218	GLY	2.7
1	O	1	MET	2.7
8	H	221	CYS	2.6
2	P	50	LYS	2.6
4	R	125	LEU	2.6
5	S	3	ASN	2.5
5	E	3	ASN	2.5
4	D	2	ARG	2.5
1	O	249	ALA	2.5
4	D	1	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	183	ASP	2.5
10	X	196	GLN	2.5
7	G	2	GLY	2.5
6	F	2	THR	2.4
4	D	122	GLU	2.4
10	X	194	ASP	2.4
3	C	202	GLN	2.4
1	O	2	THR	2.4
12	L	174	TYR	2.4
3	Q	202	GLN	2.4
2	P	59	ASP	2.3
1	A	249	ALA	2.3
3	C	238	LYS	2.3
5	E	1	PHE	2.3
11	Y	183	ASP	2.3
11	K	209	ASN	2.3
13	a	1	THR	2.3
9	W	192	ASP	2.2
1	O	52	SER	2.2
2	B	51	VAL	2.2
5	E	30	GLN	2.2
2	P	221	ASP	2.2
5	E	2	ARG	2.2
6	T	243	ILE	2.2
11	Y	182	GLU	2.1
4	R	122	GLU	2.1
2	B	204	ALA	2.1
3	Q	181	GLU	2.1
6	F	202	ASP	2.1
7	U	2	GLY	2.1
2	P	61	SER	2.1
7	G	188	GLU	2.0
1	A	201	GLU	2.0
6	T	207	ASP	2.0
2	B	244	THR	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	RE0	c	3	16/17	0.94	0.21	-	55,56,57,57	0
16	ACA	d	3	4/9	0.88	0.45	-	65,65,65,65	0
16	RE0	d	6	16/17	0.88	0.24	-	60,61,62,62	0
15	TY5	c	1	19/20	0.81	0.44	-	59,61,64,64	0
16	TY5	d	4	19/20	0.81	0.42	-	64,66,69,69	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
17	MES	Y	301	12/12	0.89	0.31	4.18	63,65,66,66	0
17	MES	K	301	12/12	0.94	0.26	3.89	55,56,56,56	0
18	0L1	c	101	4/10	0.87	0.50	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.