



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4INR
Title : Yeast 20S proteasome in complex with the vinyl sulfone LU102
Authors : Geurink, P.P.; van der Linden, W.A.; Mirabella, A.C.; Gallastegui, N.; de Bruin, G.; Blom, A.E.M.; Voges, M.J.; Mock, E.D.; Florea, B.I.; van der Marel, G.A.; Driessen, C.; van der Stelt, M.; Groll, M.; Overkleeft, H.S.; Kisselev, A.F.
Deposited on : 2013-01-06
Resolution : 2.70 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

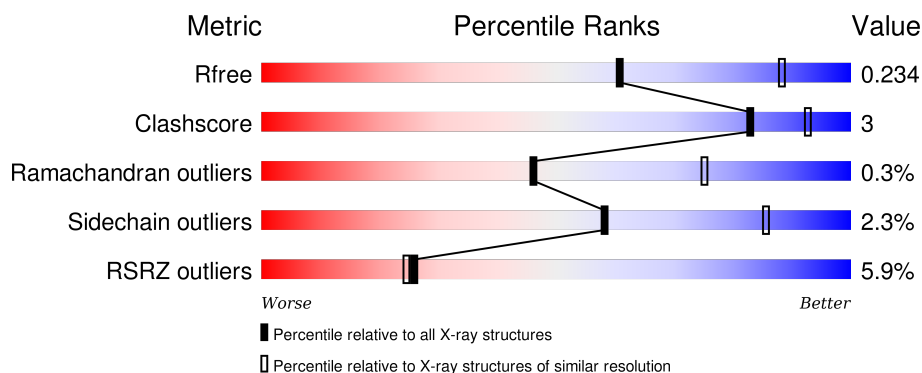
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	<div> <div>3%</div> <div>93%</div> <div>7%</div> </div>
1	O	250	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
2	B	258	<div> <div>9%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
2	P	258	<div> <div>11%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
3	C	254	<div> <div>12%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

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
15	1G1	H	301	-	-	-	X
15	1G1	V	301	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51061 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 component Y7.

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 component Y13.

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 component PRE6.

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 component PUP2.

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 component PRE5.

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 Proteasome component C1.

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 component C7-alpha.

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 component PUP1.

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 component PUP3.

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 component C11.

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 component PRE2.

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 component C5.

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			

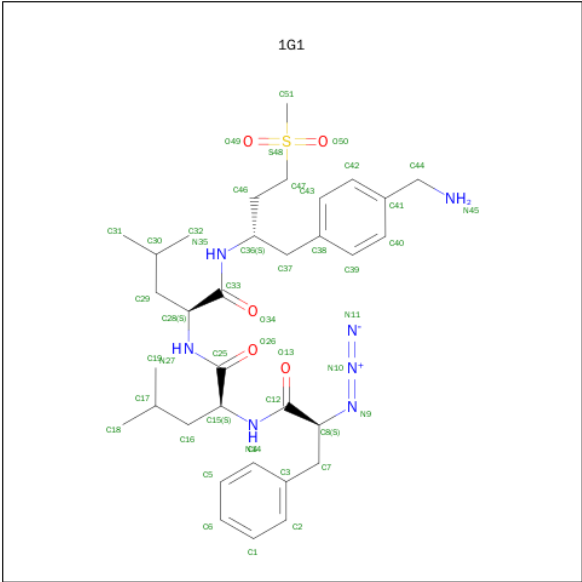
- Molecule 13 is a protein called Proteasome component PRE4.

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 component PRE3.

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 N3PHE-LEU-LEU-PHE(4-NH₂CH₂)-METHYL VINYL SULFONE, BOUND FORM (three-letter code: 1G1) (formula: C₃₃H₄₉N₇O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	K	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	V	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	Y	1	Total	C	N	O	S	0	0
			46	33	7	5	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O	0	0
			58	58		
16	B	37	Total	O	0	0
			37	37		
16	C	43	Total	O	0	0
			43	43		
16	D	37	Total	O	0	0
			37	37		
16	E	21	Total	O	0	0
			21	21		
16	F	47	Total	O	0	0
			47	47		
16	G	60	Total	O	0	0
			60	60		
16	H	54	Total	O	0	0
			54	54		

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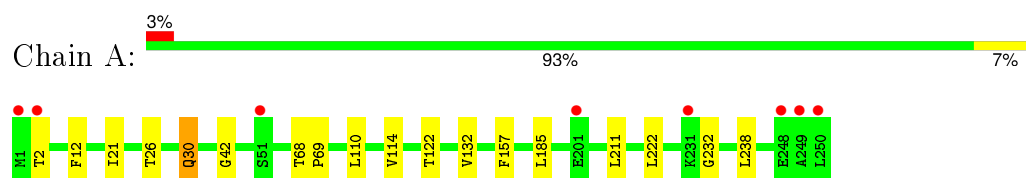
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	68	Total 68	O 68	0	0
16	J	53	Total 53	O 53	0	0
16	K	48	Total 48	O 48	0	0
16	L	57	Total 57	O 57	0	0
16	M	75	Total 75	O 75	0	0
16	N	55	Total 55	O 55	0	0
16	O	35	Total 35	O 35	0	0
16	P	28	Total 28	O 28	0	0
16	Q	29	Total 29	O 29	0	0
16	R	27	Total 27	O 27	0	0
16	S	17	Total 17	O 17	0	0
16	T	42	Total 42	O 42	0	0
16	U	60	Total 60	O 60	0	0
16	V	50	Total 50	O 50	0	0
16	W	57	Total 57	O 57	0	0
16	X	46	Total 46	O 46	0	0
16	Y	52	Total 52	O 52	0	0
16	Z	49	Total 49	O 49	0	0
16	a	77	Total 77	O 77	0	0
16	b	57	Total 57	O 57	0	0

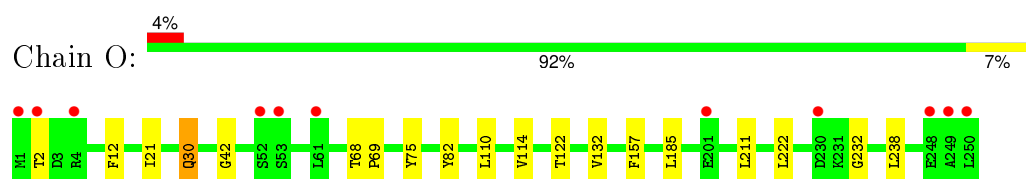
3 Residue-property plots [i](#)

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.

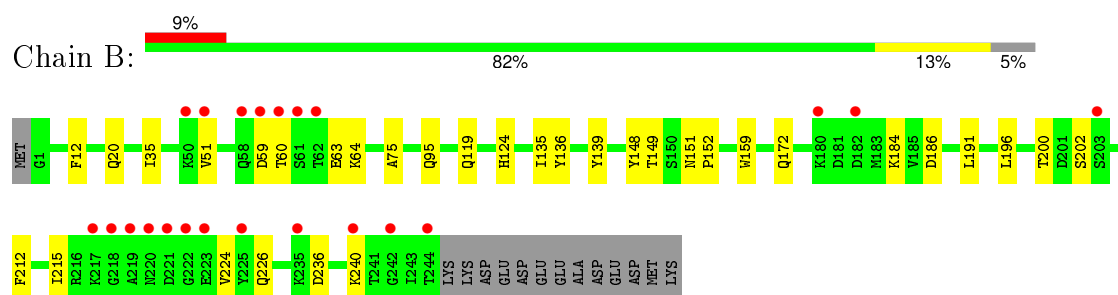
- Molecule 1: Proteasome component Y7



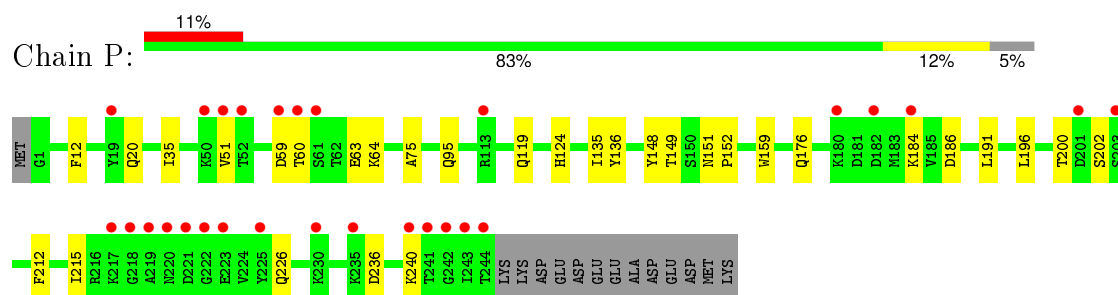
- Molecule 1: Proteasome component Y7



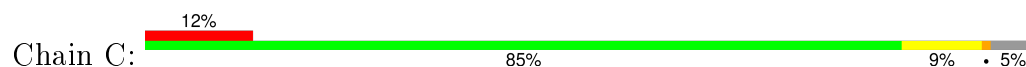
- Molecule 2: Proteasome component Y13

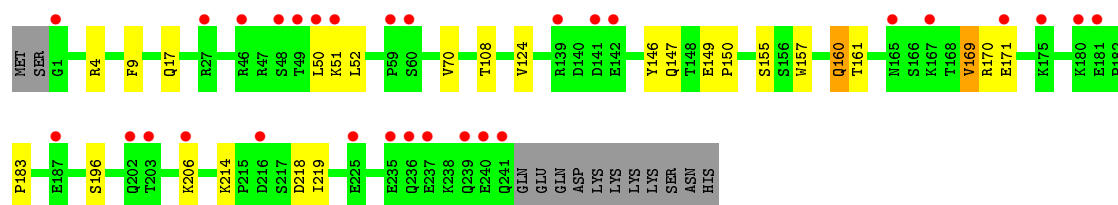


- Molecule 2: Proteasome component Y13

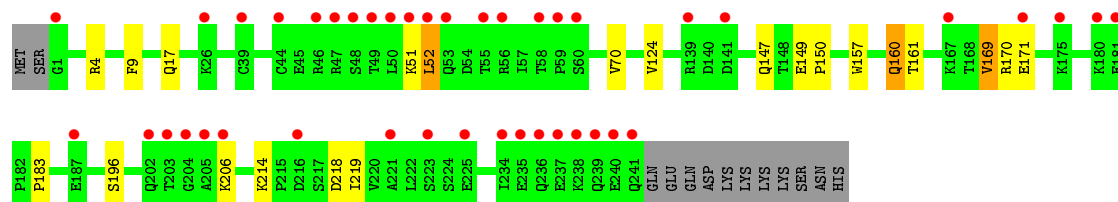
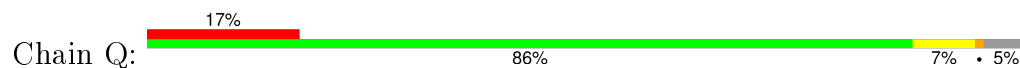


- Molecule 3: Proteasome component PRE6

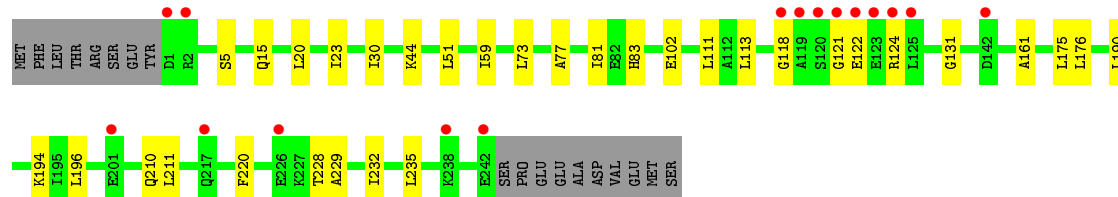
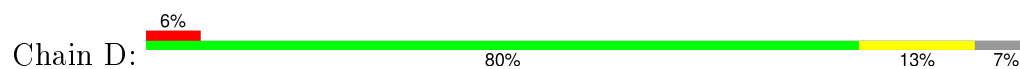




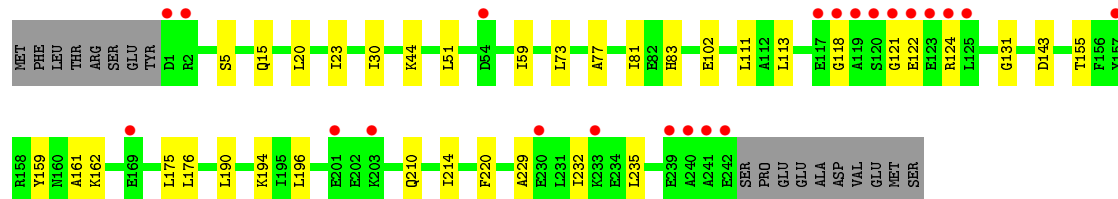
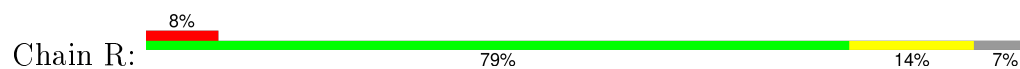
• Molecule 3: Proteasome component PRE6



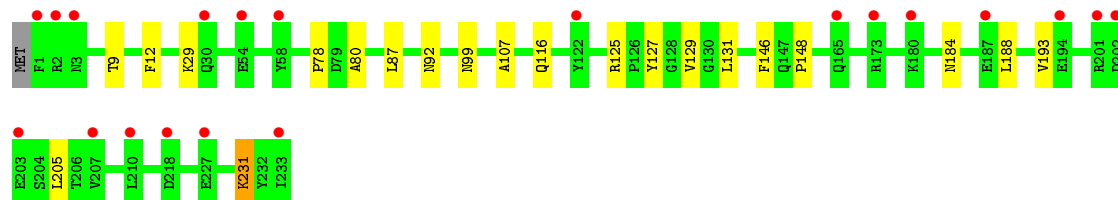
• Molecule 4: Proteasome component PUP2



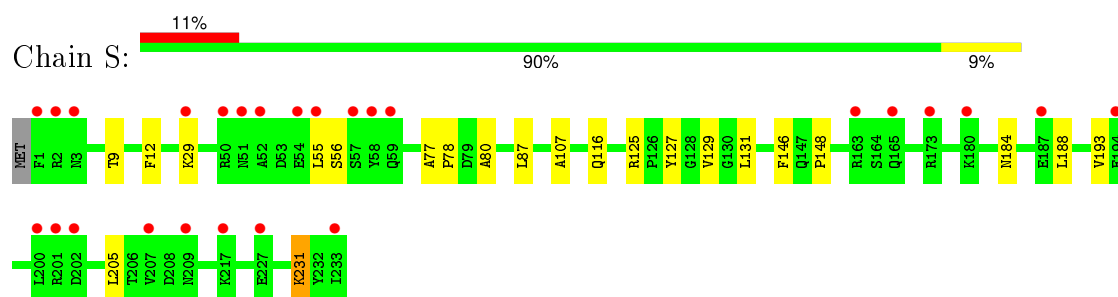
• Molecule 4: Proteasome component PUP2



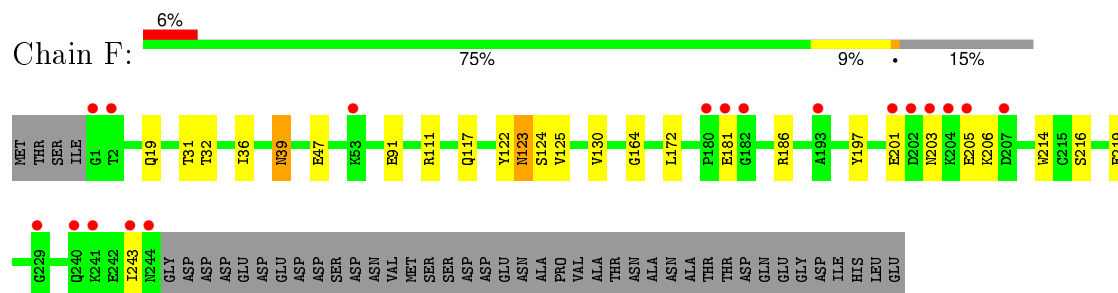
• Molecule 5: Proteasome component PRE5



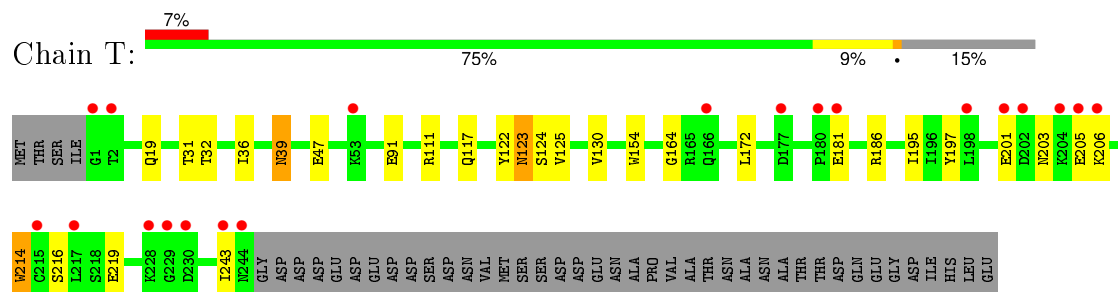
• Molecule 5: Proteasome component PRE5



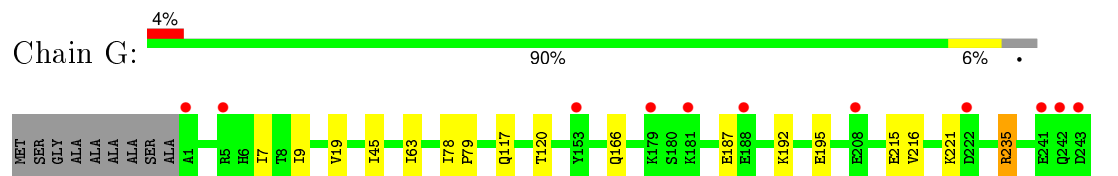
- Molecule 6: Proteasome component C1



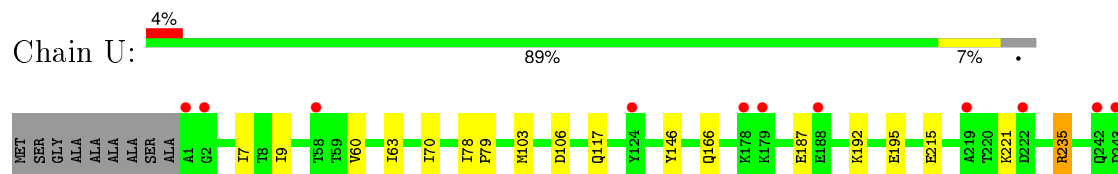
- Molecule 6: Proteasome component C1



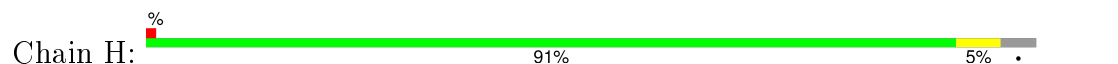
- Molecule 7: Proteasome component C7-alpha



- Molecule 7: Proteasome component C7-alpha

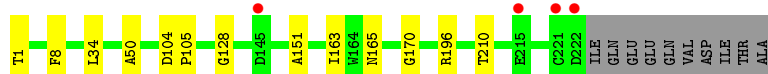
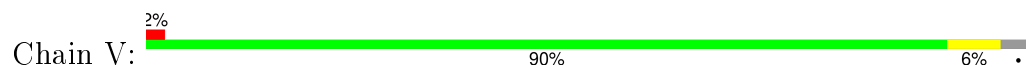


- Molecule 8: Proteasome component PUP1

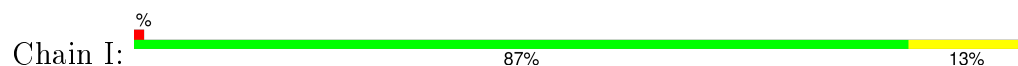




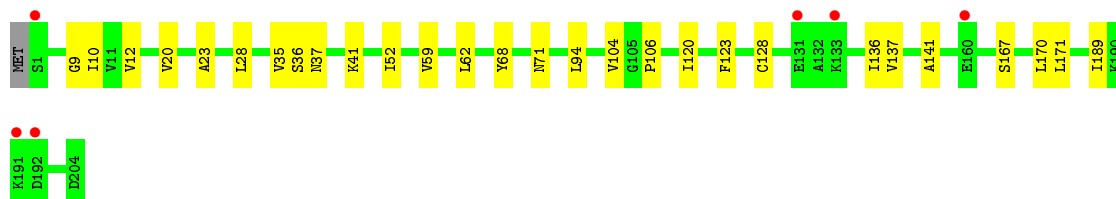
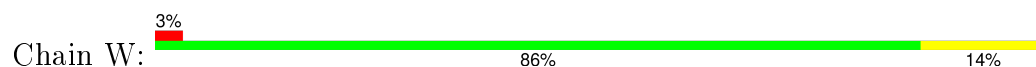
- Molecule 8: Proteasome component PUP1



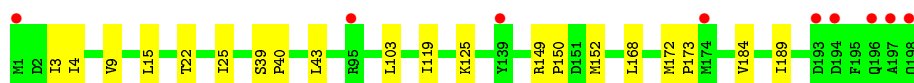
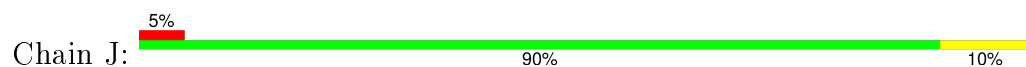
- Molecule 9: Proteasome component PUP3



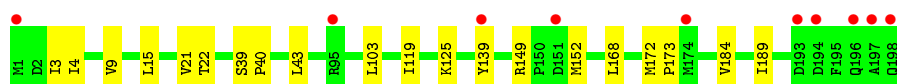
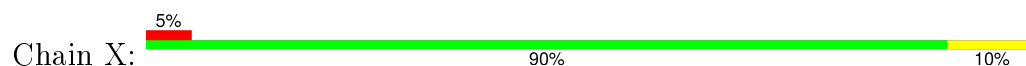
- Molecule 9: Proteasome component PUP3



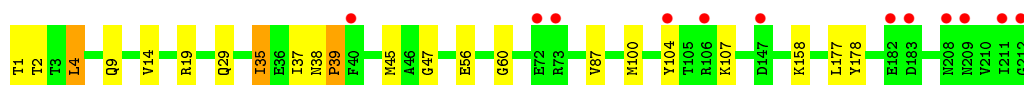
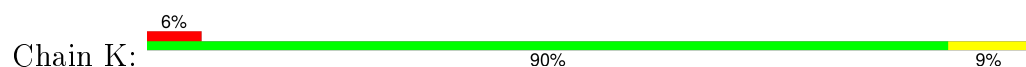
- Molecule 10: Proteasome component C11



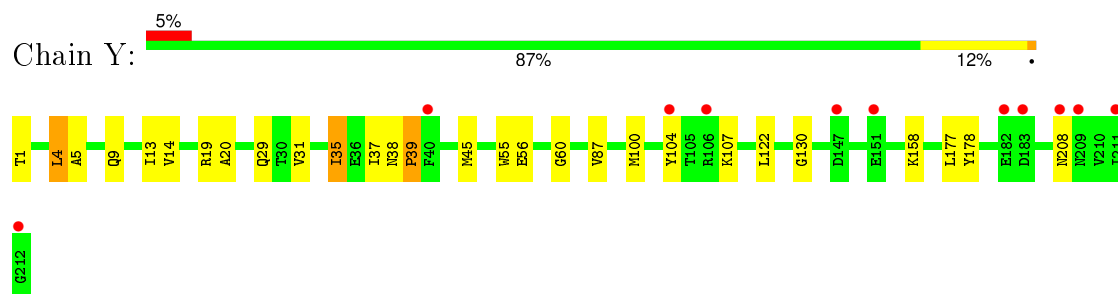
- Molecule 10: Proteasome component C11



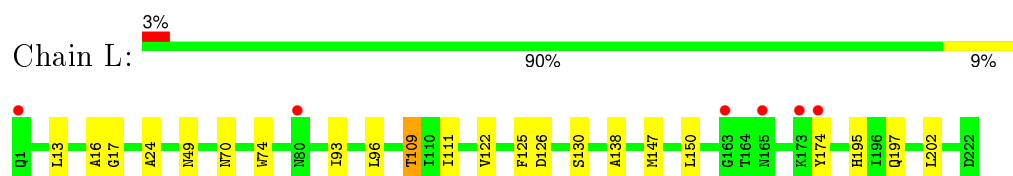
- Molecule 11: Proteasome component PRE2



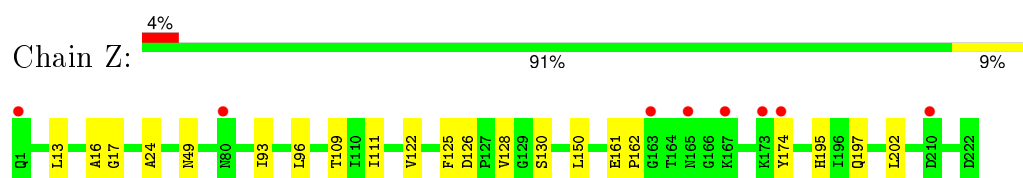
- Molecule 11: Proteasome component PRE2



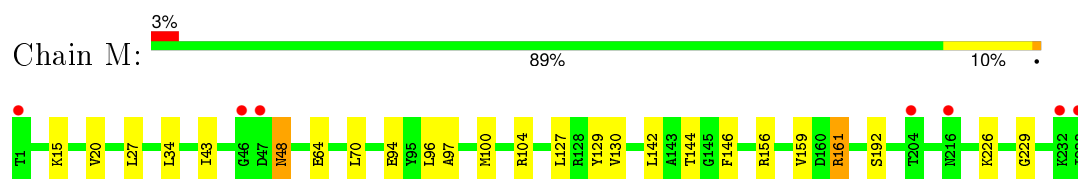
- Molecule 12: Proteasome component C5



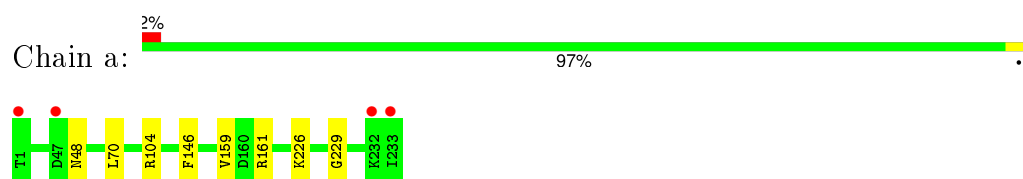
- Molecule 12: Proteasome component C5



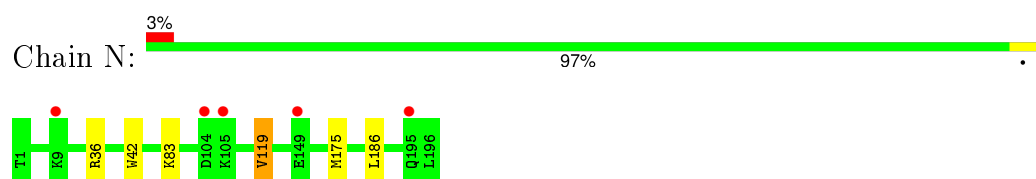
- Molecule 13: Proteasome component PRE4



- Molecule 13: Proteasome component PRE4

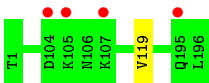


- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.32Å 301.05Å 144.32Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.70) 98.9 (15.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.231 0.228 , 0.234	Depositor DCC
R_{free} test set	14301 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 286015 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51061	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1G1

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	0.36	0/1952	0.46	0/2642
1	O	0.36	0/1952	0.46	0/2642
2	B	0.33	0/1934	0.46	0/2618
2	P	0.33	0/1934	0.46	0/2618
3	C	0.33	0/1919	0.47	0/2598
3	Q	0.33	0/1919	0.47	0/2598
4	D	0.36	0/1886	0.47	0/2541
4	R	0.36	0/1886	0.47	0/2541
5	E	0.31	0/1823	0.45	0/2463
5	S	0.31	0/1823	0.45	0/2463
6	F	0.41	0/1936	0.45	0/2614
6	T	0.41	1/1936 (0.1%)	0.45	0/2614
7	G	0.34	0/1959	0.46	0/2652
7	U	0.34	0/1959	0.46	0/2652
8	H	0.44	1/1715 (0.1%)	0.46	0/2326
8	V	0.44	0/1715	0.47	0/2326
9	I	0.34	0/1611	0.46	0/2174
9	W	0.34	0/1611	0.47	0/2174
10	J	0.31	0/1613	0.45	0/2173
10	X	0.31	0/1613	0.45	0/2173
11	K	0.50	0/1681	0.49	1/2274 (0.0%)
11	Y	0.50	1/1681 (0.1%)	0.49	1/2274 (0.0%)
12	L	0.36	1/1795 (0.1%)	0.45	0/2420
12	Z	0.36	0/1795	0.45	0/2420
13	M	0.36	0/1855	0.48	0/2514
13	a	0.36	0/1855	0.48	0/2514
14	N	0.39	0/1541	0.44	0/2087
14	b	0.39	0/1541	0.44	0/2087
All	All	0.37	4/50440 (0.0%)	0.46	2/68192 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	214	TRP	CD2-CE2	5.06	1.47	1.41
12	L	74	TRP	CD2-CE2	5.01	1.47	1.41
8	H	164	TRP	CD2-CE2	5.01	1.47	1.41
11	Y	55	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.33	127.56	115.30
11	K	4	LEU	CA-CB-CG	5.24	127.36	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	9	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	15	0
3	Q	1890	0	1903	12	0
4	D	1861	0	1839	16	0
4	R	1861	0	1839	18	0
5	E	1795	0	1800	11	0
5	S	1795	0	1800	12	0
6	F	1896	0	1889	14	0
6	T	1896	0	1889	16	0
7	G	1921	0	1913	7	0
7	U	1921	0	1913	8	0
8	H	1684	0	1687	6	0
8	V	1684	0	1687	12	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	16	0
10	J	1585	0	1590	13	0
10	X	1585	0	1590	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1594	10	0
11	Y	1644	0	1594	15	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	16	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	H	46	0	48	1	0
15	K	46	0	48	1	0
15	V	46	0	48	4	0
15	Y	46	0	48	6	0
16	A	58	0	0	0	0
16	B	37	0	0	0	0
16	C	43	0	0	0	0
16	D	37	0	0	0	0
16	E	21	0	0	0	0
16	F	47	0	0	0	0
16	G	60	0	0	0	0
16	H	54	0	0	0	0
16	I	68	0	0	0	0
16	J	53	0	0	0	0
16	K	48	0	0	0	0
16	L	57	0	0	0	0
16	M	75	0	0	0	0
16	N	55	0	0	0	0
16	O	35	0	0	0	0
16	P	28	0	0	0	0
16	Q	29	0	0	0	0
16	R	27	0	0	0	0
16	S	17	0	0	0	0
16	T	42	0	0	0	0
16	U	60	0	0	0	0
16	V	50	0	0	0	0
16	W	57	0	0	0	0
16	X	46	0	0	1	0
16	Y	52	0	0	3	0
16	Z	49	0	0	0	0
16	a	77	0	0	0	0
16	b	57	0	0	0	0
All	All	51061	0	49484	285	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 (285) 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)
15:Y:301:1G1:H19	16:Y:442:HOH:O	1.74	0.87
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.66	0.77
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.66	0.76
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.71
5:S:12:PHE:H	6:T:19:GLN:HE22	1.39	0.71
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.70	0.71
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.37	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.38	0.70
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.56	0.70
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.56	0.69
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.56	0.69
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.75	0.68
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.75	0.68
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.76	0.66
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.77	0.66
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.79	0.65
13:M:48:ASN:H	13:M:48:ASN:HD22	1.47	0.63
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.79	0.63
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.80	0.62
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.82	0.61
1:A:12:PHE:H	2:B:20:GLN:HE22	1.48	0.61
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.82	0.61
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.61
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.84	0.60
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.84	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.59
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.85	0.59
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.83	0.58
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.85	0.58
15:Y:301:1G1:H8	16:Y:442:HOH:O	2.04	0.58
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.69	0.58
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.84	0.58
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.85	0.58
1:O:12:PHE:H	2:P:20:GLN:HE22	1.50	0.58
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.85	0.58
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.51	0.58
11:K:35:ILE:HB	11:K:45:MET:HE3	1.86	0.58
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.86	0.57
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.86	0.57
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.70	0.57
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.85	0.57
11:K:107:LYS:H	11:K:107:LYS:HD2	1.70	0.57
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.68	0.56
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.87	0.56
11:Y:20:ALA:HA	16:Y:442:HOH:O	2.06	0.56
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.88	0.56
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.87	0.56
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.86	0.56
6:F:39:ASN:HD22	6:F:39:ASN:N	2.04	0.56
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.54	0.55
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.89	0.55
6:T:39:ASN:HD22	6:T:39:ASN:N	2.05	0.55
11:K:47:GLY:H	15:K:301:1G1:H5	1.71	0.55
2:P:200:THR:HG22	2:P:202:SER:H	1.72	0.55
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.87	0.55
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.88	0.54
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.55	0.54
12:L:195:HIS:HD2	12:L:197:GLN:H	1.56	0.54
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.89	0.54
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.89	0.54
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.89	0.53
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.90	0.53
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.89	0.53
6:T:31:THR:HG21	6:T:47:GLU:O	2.09	0.53
8:V:1:THR:N	15:V:301:1G1:H5	2.23	0.52
9:I:106:PRO:HD2	9:I:123:PHE:HB2	1.91	0.52
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.90	0.52
6:F:39:ASN:HD22	6:F:39:ASN:H	1.57	0.52
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.90	0.52
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.90	0.52
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.08	0.52
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.92	0.52
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.91	0.52
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.92	0.52
10:J:168:LEU:O	10:J:172:MET:HB2	2.09	0.52
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.92	0.51
6:T:36:ILE:HG12	6:T:172:LEU:HD11	1.92	0.51
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.92	0.51
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.93	0.51
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.93	0.51
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.76	0.51
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.93	0.51
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.92	0.51
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.93	0.51
1:A:68:THR:HB	1:A:69:PRO:HD2	1.93	0.51
11:Y:31:VAL:HG11	15:Y:301:1G1:H18	1.93	0.50
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.93	0.50
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.92	0.50
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.93	0.50
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.93	0.50
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.93	0.50
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.91	0.50
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.94	0.50
6:F:31:THR:HG21	6:F:47:GLU:O	2.11	0.50
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.94	0.50
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.94	0.49
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.94	0.49
7:G:78:ILE:N	7:G:79:PRO:HD2	2.26	0.49
8:V:210:THR:HG21	9:W:167:SER:HB3	1.95	0.49
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.78	0.49
7:U:78:ILE:N	7:U:79:PRO:HD2	2.26	0.49
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.94	0.49
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.94	0.49
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.61	0.49
6:T:39:ASN:H	6:T:39:ASN:HD22	1.61	0.49
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.95	0.49
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.95	0.49
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.95	0.48
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.94	0.48
2:B:200:THR:HG22	2:B:202:SER:H	1.78	0.48
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.96	0.48
2:B:149:THR:HG22	2:B:159:TRP:HE1	1.78	0.48
9:W:12:VAL:HG23	9:W:137:VAL:HG12	1.95	0.48
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.96	0.48
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.95	0.48
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.95	0.48
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.96	0.48
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.62	0.48
13:M:161:ARG:NH1	13:M:161:ARG:HG3	2.27	0.48
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.95	0.47
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.94	0.47
6:F:36:ILE:HG12	6:F:172:LEU:HD11	1.95	0.47
11:K:14:VAL:HB	11:K:178:TYR:HB2	1.95	0.47
1:O:110:LEU:O	1:O:114:VAL:HG23	2.15	0.47
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.63	0.47
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.96	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.96	0.47
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.97	0.47
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.96	0.47
9:I:23:ALA:HB1	9:I:170:LEU:HD22	1.95	0.47
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.95	0.47
8:V:1:THR:N	15:V:301:1G1:C47	2.78	0.47
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.96	0.47
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.61	0.47
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.97	0.47
2:P:149:THR:HG22	2:P:159:TRP:HE1	1.78	0.47
1:A:110:LEU:O	1:A:114:VAL:HG23	2.15	0.47
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.80	0.47
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.97	0.47
5:E:231:LYS:H	5:E:231:LYS:HD2	1.78	0.47
8:V:1:THR:O	8:V:128:GLY:HA3	2.15	0.47
11:Y:14:VAL:HB	11:Y:178:TYR:HB2	1.97	0.47
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.96	0.47
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.96	0.47
5:S:231:LYS:HD2	5:S:231:LYS:H	1.80	0.46
5:S:127:TYR:O	5:S:148:PRO:HB3	2.15	0.46
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.96	0.46
9:I:12:VAL:HG23	9:I:137:VAL:HG12	1.97	0.46
10:X:168:LEU:O	10:X:172:MET:HB2	2.14	0.46
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.62	0.46
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.97	0.46
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.97	0.46
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.50	0.46
15:H:301:1G1:H20	15:H:301:1G1:H5	1.66	0.46
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.96	0.46
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:229:ALA:HA	4:R:232:ILE:HD12	1.96	0.46
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.97	0.46
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.98	0.46
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.46
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.97	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.97	0.46
8:V:1:THR:H3	15:V:301:1G1:C47	2.29	0.46
4:D:229:ALA:HA	4:D:232:ILE:HD12	1.97	0.46
5:E:127:TYR:O	5:E:148:PRO:HB3	2.16	0.46
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.98	0.46
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.50	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.45
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.98	0.45
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.80	0.45
4:R:5:SER:HB2	5:S:125:ARG:HD3	1.98	0.45
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.99	0.45
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.99	0.45
4:D:161:ALA:HB1	4:D:175:LEU:HD22	1.98	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.99	0.45
6:F:122:TYR:HB2	6:F:125:VAL:HG22	1.97	0.45
4:R:77:ALA:O	4:R:81:ILE:HG12	2.16	0.45
6:T:122:TYR:HB2	6:T:125:VAL:HG22	1.98	0.45
8:H:210:THR:HG21	9:I:167:SER:HB3	1.98	0.45
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.98	0.45
15:Y:301:1G1:C33	15:Y:301:1G1:H4	2.47	0.45
9:W:62:LEU:HD11	9:W:104:VAL:HG21	1.98	0.45
4:R:155:THR:HG22	5:S:77:ALA:HB3	1.99	0.44
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.99	0.44
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.44
9:W:120:ILE:HD12	9:W:136:ILE:HG12	1.99	0.44
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.99	0.44
1:O:42:GLY:HA3	1:O:185:LEU:HD13	1.99	0.44
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.98	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.98	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.99	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.44
5:E:193:VAL:HG13	5:E:205:LEU:HD11	1.99	0.44
9:W:23:ALA:HB1	9:W:170:LEU:HD22	1.98	0.44
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.82	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.44
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.99	0.44
5:S:193:VAL:HG13	5:S:205:LEU:HD11	1.99	0.44
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.00	0.44
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.53	0.44
11:Y:1:THR:N	15:Y:301:1G1:H5	2.33	0.44
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	2.00	0.44
6:F:197:TYR:HB3	6:F:243:ILE:HD12	2.00	0.43
1:A:42:GLY:HA3	1:A:185:LEU:HD13	2.00	0.43
9:I:28:LEU:HB3	9:I:36:SER:HB3	2.00	0.43
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.99	0.43
4:R:113:LEU:HD12	5:S:78:PRO:HB2	1.99	0.43
4:D:194:LYS:HB2	4:D:235:LEU:HD21	2.00	0.43
6:T:197:TYR:HB3	6:T:243:ILE:HD12	2.00	0.43
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.83	0.43
2:B:236:ASP:O	2:B:240:LYS:HG2	2.17	0.43
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.99	0.43
6:F:123:ASN:HD22	6:F:124:SER:N	2.17	0.43
7:U:70:ILE:HD11	7:U:103:MET:O	2.18	0.43
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.43
2:P:236:ASP:O	2:P:240:LYS:HG2	2.19	0.43
9:I:52:ILE:HB	9:I:59:VAL:HG13	2.01	0.43
4:R:194:LYS:HB2	4:R:235:LEU:HD21	2.00	0.43
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.00	0.43
4:D:77:ALA:O	4:D:81:ILE:HG12	2.18	0.43
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.01	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.49	0.43
7:U:7:ILE:HG13	7:U:9:ILE:HG12	2.01	0.43
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.84	0.43
2:P:176:GLN:HG3	3:Q:52:LEU:HD13	2.01	0.43
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.01	0.42
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.54	0.42
4:D:20:LEU:HA	4:D:23:ILE:HD12	2.02	0.42
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.00	0.42
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.29	0.42
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.68	0.42
11:K:19:ARG:HH21	11:K:29:GLN:HE22	1.66	0.42
6:T:32:THR:HB	6:T:164:GLY:H	1.84	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.42
9:I:62:LEU:HD11	9:I:104:VAL:HG21	2.02	0.42
12:L:138:ALA:HB3	12:L:147:MET:HG2	2.02	0.41
9:W:35:VAL:HG13	16:X:222:HOH:O	2.19	0.41
12:Z:161:GLU:HA	12:Z:162:PRO:HD3	1.93	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.41
4:D:83:HIS:CG	4:D:111:LEU:HD11	2.55	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
12:L:17:GLY:HA2	12:L:174:TYR:HE1	1.86	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.55	0.41
12:Z:93:ILE:HA	12:Z:96:LEU:HD12	2.02	0.41
11:Y:35:ILE:HB	11:Y:45:MET:HE3	2.03	0.41
11:K:1:THR:CG2	11:K:2:THR:N	2.83	0.41
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.21	0.41
1:O:30:GLN:HE21	1:O:30:GLN:HA	1.85	0.41
6:F:32:THR:HB	6:F:164:GLY:H	1.85	0.41
13:M:48:ASN:HD22	13:M:48:ASN:N	2.11	0.41
10:J:172:MET:HA	10:J:173:PRO:HD3	1.85	0.41
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.56	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.02	0.41
2:B:172:GLN:HG2	3:C:50:LEU:HD12	2.03	0.41
4:R:83:HIS:CG	4:R:111:LEU:HD11	2.55	0.41
15:Y:301:1G1:H3	15:Y:301:1G1:H20	1.86	0.41
7:G:45:ILE:HG13	7:G:216:VAL:HG22	2.03	0.41
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.57	0.41
13:M:15:LYS:HB3	13:M:20:VAL:HG12	2.02	0.41
8:V:1:THR:H1	15:V:301:1G1:H5	1.84	0.40
1:A:26:THR:O	1:A:30:GLN:HG2	2.21	0.40
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.56	0.40
4:R:161:ALA:HB1	4:R:175:LEU:HD22	2.04	0.40
6:T:172:LEU:HD22	6:T:195:ILE:HD13	2.03	0.40
13:M:43:ILE:HG12	13:M:64:GLU:HG3	2.03	0.40
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.87	0.40
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.03	0.40
7:G:19:VAL:HG21	7:G:120:THR:HG23	2.03	0.40
5:E:99:ASN:HB2	13:M:94:GLU:HG2	2.02	0.40
4:D:211:LEU:HD12	4:D:228:THR:HG23	2.03	0.40
12:L:93:ILE:HA	12:L:96:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:20:LEU:HA	4:R:23:ILE:HD12	2.03	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%)	241 (97%)	6 (2%)	1 (0%)	39	69
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	39	69
2	P	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	39	69
3	C	239/254 (94%)	231 (97%)	6 (2%)	2 (1%)	24	51
3	Q	239/254 (94%)	232 (97%)	5 (2%)	2 (1%)	24	51
4	D	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	15	37
4	R	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	15	37
5	E	231/234 (99%)	224 (97%)	7 (3%)	0	100	100
5	S	231/234 (99%)	224 (97%)	7 (3%)	0	100	100
6	F	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
6	T	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
7	U	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	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	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	34	63
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	34	63
11	Y	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	34	63
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	39	69
13	a	231/233 (99%)	222 (96%)	8 (4%)	1 (0%)	39	69
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6588 (96%)	6111 (97%)	181 (3%)	20 (0%)	46	75

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
3	C	52	LEU
4	D	121	GLY
1	O	2	THR
3	Q	52	LEU
2	B	51	VAL
3	C	183	PRO
4	D	122	GLU
11	K	39	PRO
2	P	51	VAL
3	Q	183	PRO
11	Y	39	PRO
4	D	118	GLY
4	R	122	GLU
13	a	229	GLY
13	M	229	GLY
4	R	121	GLY
10	X	9	VAL
10	J	9	VAL
4	R	118	GLY

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	92
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	92
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	75
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	75
3	C	213/226 (94%)	206 (97%)	7 (3%)	45	76
3	Q	213/226 (94%)	206 (97%)	7 (3%)	45	76
4	D	198/215 (92%)	194 (98%)	4 (2%)	63	87
4	R	198/215 (92%)	192 (97%)	6 (3%)	48	79
5	E	192/193 (100%)	186 (97%)	6 (3%)	47	78
5	S	192/193 (100%)	186 (97%)	6 (3%)	47	78
6	F	201/239 (84%)	192 (96%)	9 (4%)	34	65
6	T	201/239 (84%)	192 (96%)	9 (4%)	34	65
7	G	207/210 (99%)	203 (98%)	4 (2%)	65	88
7	U	207/210 (99%)	203 (98%)	4 (2%)	65	88
8	H	181/190 (95%)	179 (99%)	2 (1%)	80	94
8	V	181/190 (95%)	179 (99%)	2 (1%)	80	94
9	I	172/173 (99%)	170 (99%)	2 (1%)	78	93
9	W	172/173 (99%)	170 (99%)	2 (1%)	78	93
10	J	175/175 (100%)	175 (100%)	0	100	100
10	X	175/175 (100%)	175 (100%)	0	100	100
11	K	169/169 (100%)	163 (96%)	6 (4%)	42	73
11	Y	169/169 (100%)	163 (96%)	6 (4%)	42	73
12	L	185/185 (100%)	183 (99%)	2 (1%)	80	94
12	Z	185/185 (100%)	183 (99%)	2 (1%)	80	94
13	M	199/199 (100%)	192 (96%)	7 (4%)	43	74
13	a	199/199 (100%)	192 (96%)	7 (4%)	43	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	161 (99%)	1 (1%)	90	97
14	b	162/162 (100%)	161 (99%)	1 (1%)	90	97
All	All	5332/5522 (97%)	5210 (98%)	122 (2%)	58	85

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	132	VAL
1	A	157	PHE
2	B	59	ASP
2	B	60	THR
2	B	119	GLN
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
2	B	212	PHE
3	C	4	ARG
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
5	E	9	THR
5	E	29	LYS
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	130	VAL
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU

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Mol	Chain	Res	Type
6	F	203	ASN
6	F	214	TRP
7	G	117	GLN
7	G	166	GLN
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	87	VAL
11	K	100	MET
11	K	104	TYR
12	L	49	ASN
12	L	109	THR
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	226	LYS
14	N	119	VAL
1	O	30	GLN
1	O	132	VAL
1	O	157	PHE
2	P	59	ASP
2	P	60	THR
2	P	119	GLN
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
2	P	212	PHE
3	Q	4	ARG
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU

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Mol	Chain	Res	Type
3	Q	206	LYS
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN
6	T	214	TRP
7	U	117	GLN
7	U	166	GLN
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	87	VAL
11	Y	100	MET
11	Y	104	TYR
12	Z	49	ASN
12	Z	128	VAL
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE

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Mol	Chain	Res	Type
13	a	159	VAL
13	a	161	ARG
13	a	226	LYS
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
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	241	GLN
4	D	15	GLN
4	D	210	GLN
4	D	225	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
7	G	30	ASN
7	G	83	ASN

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Mol	Chain	Res	Type
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	30	ASN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
10	J	118	GLN
10	J	147	HIS
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	70	ASN
12	L	80	ASN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
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
3	Q	17	GLN

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Mol	Chain	Res	Type
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
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
7	U	6	HIS
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	186	ASN
8	V	30	ASN
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	118	GLN
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN

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Mol	Chain	Res	Type
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	1G1	H	301	8	46,47,47	1.19	3 (6%)	54,63,63	1.15	6 (11%)
15	1G1	K	301	11	46,47,47	1.15	3 (6%)	54,63,63	0.96	3 (5%)
15	1G1	V	301	8	46,47,47	1.27	3 (6%)	54,63,63	1.13	2 (3%)
15	1G1	Y	301	11	46,47,47	1.18	3 (6%)	54,63,63	0.98	1 (1%)

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	1G1	H	301	8	-	0/51/51/51	0/2/2/2
15	1G1	K	301	11	-	1/51/51/51	0/2/2/2
15	1G1	V	301	8	-	1/51/51/51	0/2/2/2
15	1G1	Y	301	11	-	0/51/51/51	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	1G1	C47-S48	2.36	1.81	1.78
15	H	301	1G1	C46-C36	2.47	1.57	1.52
15	K	301	1G1	C46-C36	2.51	1.57	1.52
15	H	301	1G1	C47-S48	2.62	1.81	1.78
15	V	301	1G1	C46-C36	2.63	1.58	1.52
15	Y	301	1G1	C47-S48	2.67	1.81	1.78
15	Y	301	1G1	C46-C36	2.99	1.58	1.52
15	V	301	1G1	C47-S48	3.17	1.82	1.78
15	K	301	1G1	C46-C47	3.44	1.56	1.52
15	Y	301	1G1	C46-C47	3.50	1.56	1.52
15	H	301	1G1	C46-C47	3.91	1.56	1.52
15	V	301	1G1	C46-C47	4.32	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	301	1G1	C46-C36-C37	-3.21	106.25	112.05
15	K	301	1G1	C46-C36-C37	-2.77	107.04	112.05
15	H	301	1G1	C37-C38-C43	-2.39	115.90	120.90
15	K	301	1G1	C37-C38-C43	-2.27	116.15	120.90
15	H	301	1G1	C46-C36-N35	-2.16	107.53	110.27
15	V	301	1G1	O50-S48-C51	-2.01	106.70	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	301	1G1	O49-S48-C47	2.10	109.62	108.28
15	H	301	1G1	O50-S48-C47	2.27	109.74	108.28
15	K	301	1G1	C38-C37-C36	3.28	121.39	114.32
15	H	301	1G1	C38-C37-C36	3.95	122.84	114.32
15	Y	301	1G1	O49-S48-C47	4.45	111.13	108.28
15	V	301	1G1	O49-S48-C47	5.26	111.65	108.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	V	301	1G1	C8-N9-N10-N11
15	K	301	1G1	C8-N9-N10-N11

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	301	1G1	1	0
15	K	301	1G1	1	0
15	V	301	1G1	4	0
15	Y	301	1G1	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	0.17	8 (3%) 51 51	61, 76, 101, 119	0
1	O	250/250 (100%)	0.20	11 (4%) 38 37	63, 81, 106, 123	0
2	B	244/258 (94%)	0.48	22 (9%) 12 9	58, 80, 121, 136	0
2	P	244/258 (94%)	0.55	28 (11%) 6 5	62, 82, 117, 134	0
3	C	241/254 (94%)	0.47	30 (12%) 5 4	59, 82, 123, 156	0
3	Q	241/254 (94%)	0.79	42 (17%) 2 1	68, 97, 148, 191	0
4	D	242/260 (93%)	0.33	16 (6%) 22 20	61, 82, 108, 127	0
4	R	242/260 (93%)	0.49	22 (9%) 11 9	65, 89, 120, 138	0
5	E	233/234 (99%)	0.39	20 (8%) 13 10	66, 90, 117, 125	0
5	S	233/234 (99%)	0.49	26 (11%) 7 5	68, 94, 125, 135	0
6	F	244/288 (84%)	0.22	18 (7%) 17 15	63, 81, 113, 137	0
6	T	244/288 (84%)	0.23	20 (8%) 14 11	63, 82, 118, 140	0
7	G	243/252 (96%)	0.12	11 (4%) 37 36	60, 76, 99, 129	0
7	U	243/252 (96%)	0.17	11 (4%) 37 36	61, 75, 97, 129	0
8	H	222/232 (95%)	0.10	3 (1%) 78 77	59, 70, 86, 104	0
8	V	222/232 (95%)	0.09	4 (1%) 71 72	58, 69, 86, 109	0
9	I	204/205 (99%)	-0.16	3 (1%) 76 76	55, 67, 81, 88	0
9	W	204/205 (99%)	-0.06	6 (2%) 55 55	58, 67, 84, 94	0
10	J	198/198 (100%)	0.15	9 (4%) 37 36	54, 67, 87, 123	0
10	X	198/198 (100%)	0.16	10 (5%) 32 30	58, 68, 84, 124	0
11	K	212/212 (100%)	0.17	12 (5%) 27 26	54, 68, 89, 95	0
11	Y	212/212 (100%)	0.15	11 (5%) 31 30	57, 70, 92, 100	0
12	L	222/222 (100%)	-0.04	6 (2%) 58 58	55, 68, 96, 104	0
12	Z	222/222 (100%)	0.02	8 (3%) 46 46	56, 70, 96, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.07	7 (3%) 54 54	53, 69, 86, 101	0
13	a	233/233 (100%)	-0.05	4 (1%) 73 74	55, 68, 82, 96	0
14	N	196/196 (100%)	-0.10	5 (2%) 59 59	57, 65, 82, 89	0
14	b	196/196 (100%)	-0.11	4 (2%) 68 69	55, 64, 82, 89	0
All	All	6368/6588 (96%)	0.20	377 (5%) 26 24	53, 74, 113, 191	0

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	197	ALA	10.2
4	R	119	ALA	10.0
10	X	198	GLN	9.7
2	P	220	ASN	9.7
2	P	219	ALA	9.6
4	D	120	SER	9.6
7	U	243	ASP	9.4
4	D	119	ALA	9.4
10	X	197	ALA	9.2
4	R	120	SER	9.2
10	J	198	GLN	9.1
7	G	1	ALA	8.9
2	P	51	VAL	8.7
2	B	220	ASN	8.5
3	C	49	THR	8.5
8	V	222	ASP	8.4
7	U	1	ALA	8.0
2	B	219	ALA	7.9
3	Q	240	GLU	7.9
6	F	1	GLY	7.8
4	D	118	GLY	7.7
3	Q	241	GLN	7.7
3	Q	49	THR	7.6
11	Y	104	TYR	7.6
3	C	50	LEU	7.5
4	R	121	GLY	7.4
9	W	1	SER	7.4
3	Q	50	LEU	7.4
8	H	222	ASP	7.2
2	B	51	VAL	7.2
4	D	121	GLY	7.1
3	Q	48	SER	7.0

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Mol	Chain	Res	Type	RSRZ
7	G	243	ASP	6.9
5	E	202	ASP	6.8
4	R	125	LEU	6.7
11	K	104	TYR	6.7
2	B	221	ASP	6.6
2	B	218	GLY	6.5
1	A	1	MET	6.5
8	V	221	CYS	6.3
2	P	221	ASP	6.2
3	Q	203	THR	6.2
11	Y	212	GLY	6.1
3	Q	205	ALA	6.1
3	Q	58	THR	6.1
8	H	221	CYS	6.0
5	E	1	PHE	6.0
5	S	1	PHE	6.0
1	A	250	LEU	5.9
4	R	124	ARG	5.9
3	C	241	GLN	5.8
13	M	233	ILE	5.8
2	P	225	TYR	5.7
4	R	118	GLY	5.7
4	R	1	ASP	5.7
5	S	2	ARG	5.5
9	I	1	SER	5.4
1	O	249	ALA	5.3
5	S	173	ARG	5.3
1	O	2	THR	5.3
5	S	54	GLU	5.3
1	O	250	LEU	5.3
4	D	122	GLU	5.2
5	S	52	ALA	5.1
3	Q	239	GLN	5.1
2	P	218	GLY	5.0
10	J	1	MET	5.0
12	L	173	LYS	5.0
5	E	2	ARG	4.9
5	S	202	ASP	4.9
12	L	174	TYR	4.9
6	F	202	ASP	4.9
7	G	242	GLN	4.9
2	B	50	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	2	THR	4.8
2	B	240	LYS	4.7
11	K	182	GLU	4.7
2	P	60	THR	4.7
10	X	1	MET	4.7
10	X	194	ASP	4.7
2	P	59	ASP	4.6
13	a	233	ILE	4.6
12	Z	174	TYR	4.6
4	D	124	ARG	4.6
4	R	122	GLU	4.6
11	K	212	GLY	4.5
3	Q	52	LEU	4.5
3	C	203	THR	4.4
3	Q	59	PRO	4.4
3	Q	202	GLN	4.4
5	E	233	ILE	4.4
1	O	1	MET	4.4
3	Q	175	LYS	4.4
7	U	242	GLN	4.3
2	P	61	SER	4.3
2	P	223	GLU	4.3
1	A	201	GLU	4.3
4	D	125	LEU	4.2
6	F	244	ASN	4.2
5	S	201	ARG	4.1
5	E	3	ASN	4.1
11	K	209	ASN	4.1
2	P	50	LYS	4.1
4	D	123	GLU	4.1
12	L	163	GLY	4.1
2	B	223	GLU	4.0
2	B	60	THR	4.0
11	K	183	ASP	4.0
6	T	1	GLY	3.9
13	M	1	THR	3.9
11	K	40	PHE	3.9
4	D	1	ASP	3.9
2	B	61	SER	3.9
6	T	244	ASN	3.9
3	Q	51	LYS	3.9
6	T	53	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	3.8
3	Q	237	GLU	3.8
4	R	2	ARG	3.8
8	H	198	GLU	3.8
5	E	30	GLN	3.8
5	S	58	TYR	3.8
3	C	240	GLU	3.7
12	Z	173	LYS	3.7
5	S	3	ASN	3.7
1	A	248	GLU	3.7
4	R	230	GLU	3.7
12	L	1	GLN	3.6
11	K	208	ASN	3.6
3	Q	236	GLN	3.6
6	F	241	LYS	3.6
2	B	217	LYS	3.5
3	Q	187	GLU	3.5
5	S	187	GLU	3.5
2	B	244	THR	3.5
4	R	239	GLU	3.5
11	Y	182	GLU	3.5
6	F	205	GLU	3.5
3	C	202	GLN	3.5
3	C	181	GLU	3.5
2	P	203	SER	3.4
5	E	203	GLU	3.4
6	T	2	THR	3.4
10	J	196	GLN	3.4
3	Q	235	GLU	3.4
10	X	196	GLN	3.4
11	Y	40	PHE	3.4
1	A	249	ALA	3.4
4	D	2	ARG	3.4
5	S	194	GLU	3.4
6	F	181	GLU	3.3
2	P	52	THR	3.3
13	a	1	THR	3.3
5	S	200	LEU	3.3
5	S	29	LYS	3.3
7	U	188	GLU	3.2
2	B	225	TYR	3.2
3	C	48	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	3.2
3	Q	204	GLY	3.2
3	C	206	LYS	3.2
5	S	180	LYS	3.2
13	M	232	LYS	3.2
13	a	232	LYS	3.2
6	F	243	ILE	3.1
9	W	192	ASP	3.1
3	Q	60	SER	3.1
3	C	175	LYS	3.1
3	Q	167	LYS	3.1
6	T	177	ASP	3.1
6	F	229	GLY	3.1
3	C	141	ASP	3.1
4	R	241	ALA	3.1
5	S	227	GLU	3.1
11	Y	209	ASN	3.1
7	G	222	ASP	3.1
3	Q	234	ILE	3.1
10	X	95	ARG	3.1
10	J	174	MET	3.1
13	M	47	ASP	3.1
3	C	225	GLU	3.1
3	Q	1	GLY	3.0
6	F	182	GLY	3.0
2	P	243	ILE	3.0
3	C	51	LYS	3.0
11	Y	147	ASP	3.0
6	F	2	THR	3.0
2	P	19	TYR	3.0
5	S	51	ASN	3.0
2	B	235	LYS	3.0
6	T	228	LYS	3.0
3	C	167	LYS	3.0
2	P	241	THR	3.0
2	P	222	GLY	3.0
10	J	139	TYR	3.0
3	Q	55	THR	2.9
2	B	58	GLN	2.9
11	Y	106	ARG	2.9
10	X	139	TYR	2.9
3	Q	216	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
11	Y	208	ASN	2.9
7	G	5	ARG	2.9
6	F	53	LYS	2.9
10	J	193	ASP	2.9
3	C	235	GLU	2.9
5	E	54	GLU	2.9
14	N	105	LYS	2.9
6	F	204	LYS	2.9
2	P	242	GLY	2.9
5	E	201	ARG	2.8
2	B	180	LYS	2.8
14	b	107	LYS	2.8
1	O	248	GLU	2.8
5	E	165	GLN	2.8
2	P	217	LYS	2.8
7	U	178	LYS	2.8
5	E	218	ASP	2.8
6	F	193	ALA	2.8
3	Q	141	ASP	2.8
6	T	230	ASP	2.8
2	P	184	LYS	2.8
4	D	242	GLU	2.8
9	I	131	GLU	2.8
2	P	180	LYS	2.7
6	T	205	GLU	2.7
6	T	206	LYS	2.7
3	Q	53	GLN	2.7
10	J	95	ARG	2.7
5	S	57	SER	2.7
3	C	239	GLN	2.7
10	J	194	ASP	2.7
11	K	106	ARG	2.7
5	E	207	VAL	2.7
3	C	59	PRO	2.7
7	G	181	LYS	2.7
2	P	182	ASP	2.7
5	E	173	ARG	2.7
6	T	229	GLY	2.7
3	Q	225	GLU	2.7
5	E	210	LEU	2.6
4	R	242	GLU	2.6
6	T	181	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	62	THR	2.6
4	R	117	GLU	2.6
7	U	219	ALA	2.6
3	Q	238	LYS	2.6
1	O	201	GLU	2.6
3	C	46	ARG	2.6
3	Q	47	ARG	2.5
14	b	195	GLN	2.5
4	R	240	ALA	2.5
2	P	113	ARG	2.5
5	S	233	ILE	2.5
2	B	203	SER	2.5
3	Q	223	SER	2.5
4	R	233	LYS	2.5
3	Q	181	GLU	2.5
5	E	194	GLU	2.5
3	C	139	ARG	2.5
5	E	227	GLU	2.5
3	C	187	GLU	2.5
4	R	157	TYR	2.5
1	A	231	LYS	2.5
1	O	4	ARG	2.5
11	K	147	ASP	2.5
3	Q	26	LYS	2.4
3	C	27	ARG	2.4
12	Z	163	GLY	2.4
11	Y	183	ASP	2.4
12	Z	165	ASN	2.4
9	W	160	GLU	2.4
12	Z	210	ASP	2.4
1	O	53	SER	2.4
5	S	50	ARG	2.4
6	T	217	LEU	2.4
6	T	166	GLN	2.4
7	U	2	GLY	2.4
3	C	142	GLU	2.4
2	P	235	LYS	2.4
3	Q	39	CYS	2.4
6	T	215	CYS	2.4
2	B	59	ASP	2.4
10	X	174	MET	2.4
4	D	201	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	R	169	GLU	2.4
2	B	182	ASP	2.4
5	S	209	ASN	2.4
11	Y	151	GLU	2.4
3	Q	56	ARG	2.4
3	Q	139	ARG	2.4
13	M	204	THR	2.4
7	U	222	ASP	2.3
13	M	216	ASN	2.3
1	O	61	LEU	2.3
5	E	122	TYR	2.3
4	D	217	GLN	2.3
11	K	211	ILE	2.3
6	T	201	GLU	2.3
6	T	204	LYS	2.3
7	G	153	TYR	2.3
5	S	55	LEU	2.3
9	W	191	LYS	2.3
14	b	105	LYS	2.3
14	N	195	GLN	2.3
6	F	207	ASP	2.3
4	D	238	LYS	2.3
6	T	243	ILE	2.3
4	R	201	GLU	2.3
7	G	179	LYS	2.3
3	C	180	LYS	2.3
14	N	104	ASP	2.2
6	T	202	ASP	2.2
2	P	240	LYS	2.2
5	E	180	LYS	2.2
6	F	201	GLU	2.2
14	N	149	GLU	2.2
6	F	203	ASN	2.2
1	O	230	ASP	2.2
10	X	151	ASP	2.2
12	Z	80	ASN	2.2
3	Q	171	GLU	2.2
5	S	163	ARG	2.2
7	U	124	TYR	2.2
1	O	52	SER	2.2
3	Q	44	CYS	2.2
13	a	47	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
7	U	179	LYS	2.2
14	N	9	LYS	2.2
14	b	104	ASP	2.2
13	M	46	GLY	2.2
3	Q	221	ALA	2.2
4	R	123	GLU	2.2
5	S	207	VAL	2.2
7	G	208	GLU	2.2
5	S	59	GLN	2.1
3	C	1	GLY	2.1
5	E	187	GLU	2.1
11	K	72	GLU	2.1
5	S	217	LYS	2.1
6	T	180	PRO	2.1
3	Q	46	ARG	2.1
8	V	215	GLU	2.1
2	P	230	LYS	2.1
3	C	236	GLN	2.1
9	W	133	LYS	2.1
12	Z	1	GLN	2.1
3	C	165	ASN	2.1
3	C	237	GLU	2.1
7	G	188	GLU	2.1
8	V	145	ASP	2.1
2	B	222	GLY	2.1
11	Y	211	ILE	2.1
12	L	80	ASN	2.1
3	C	171	GLU	2.1
12	Z	167	LYS	2.1
4	D	142	ASP	2.1
10	X	193	ASP	2.1
5	S	165	GLN	2.1
4	R	54	ASP	2.1
7	G	241	GLU	2.1
7	U	58	THR	2.1
12	L	165	ASN	2.1
6	F	240	GLN	2.1
3	C	216	ASP	2.1
3	C	60	SER	2.1
4	R	203	LYS	2.1
5	E	58	TYR	2.1
2	P	201	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
11	K	73	ARG	2.0
4	D	226	GLU	2.0
9	W	131	GLU	2.0
1	A	51	SER	2.0
6	T	198	LEU	2.0
6	F	180	PRO	2.0
2	P	244	THR	2.0
3	Q	180	LYS	2.0
9	I	2	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	1G1	V	301	46/46	0.86	0.30	2.46	65,72,84,84	0
15	1G1	H	301	46/46	0.83	0.30	2.22	65,70,83,83	0
15	1G1	Y	301	46/46	0.87	0.26	1.62	55,58,65,65	0
15	1G1	K	301	46/46	0.86	0.24	1.38	52,56,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.