



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:44 PM UTC

PDB ID : 4QV0 / pdb_00004qv0
Title : yCP beta5-A49T-A50V-double mutant
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-14
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

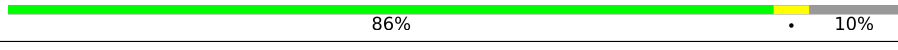
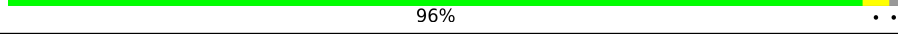
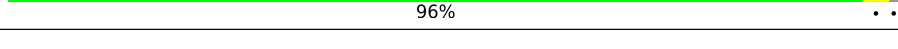
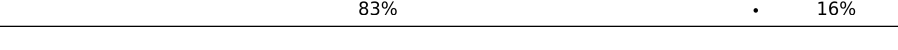
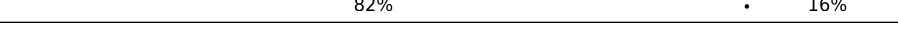
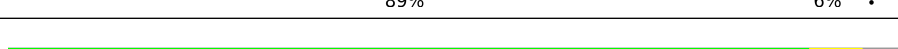
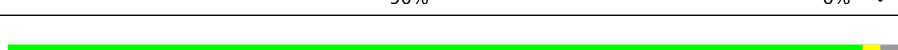
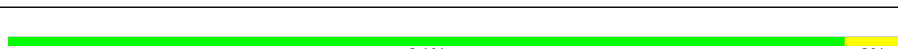
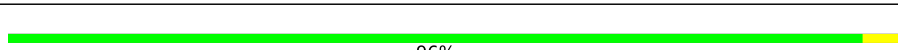
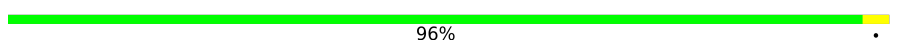
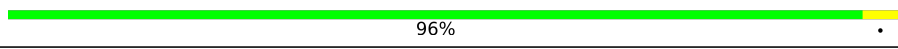
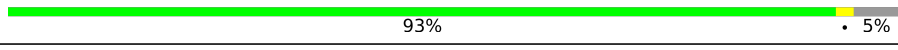
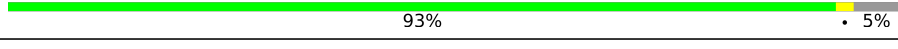
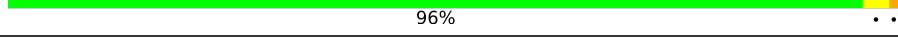
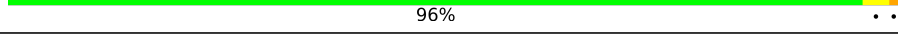
The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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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	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49529 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	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	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
			1648	1048	280	313	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1648	1048	280	313	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	49	THR	ALA	engineered mutation	UNP P30656
K	50	VAL	ALA	engineered mutation	UNP P30656
Y	49	THR	ALA	engineered mutation	UNP P30656
Y	50	VAL	ALA	engineered mutation	UNP P30656

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total 1	Mg 1	0	0
15	H	1	Total 1	Mg 1	0	0
15	K	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	V	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Cl 1	0	0
16	U	1	Total 1	Cl 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	3	Total 3	O 3	0	0
17	B	5	Total 5	O 5	0	0
17	C	3	Total 3	O 3	0	0
17	D	7	Total 7	O 7	0	0
17	E	5	Total 5	O 5	0	0
17	F	12	Total 12	O 12	0	0
17	G	2	Total 2	O 2	0	0
17	H	5	Total 5	O 5	0	0
17	I	2	Total 2	O 2	0	0

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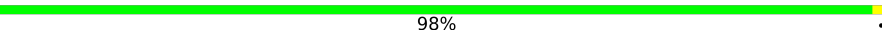
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	6	Total O 6 6	0	0
17	K	8	Total O 8 8	0	0
17	L	8	Total O 8 8	0	0
17	M	7	Total O 7 7	0	0
17	N	5	Total O 5 5	0	0
17	O	1	Total O 1 1	0	0
17	P	4	Total O 4 4	0	0
17	Q	8	Total O 8 8	0	0
17	R	1	Total O 1 1	0	0
17	S	5	Total O 5 5	0	0
17	T	5	Total O 5 5	0	0
17	U	6	Total O 6 6	0	0
17	V	4	Total O 4 4	0	0
17	W	3	Total O 3 3	0	0
17	X	10	Total O 10 10	0	0
17	Y	8	Total O 8 8	0	0
17	Z	3	Total O 3 3	0	0
17	a	8	Total O 8 8	0	0
17	b	3	Total O 3 3	0	0

3 Residue-property plots [i](#)

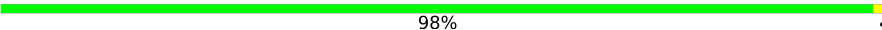
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98% .



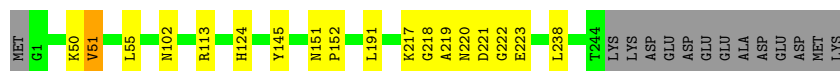
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 7% 5%



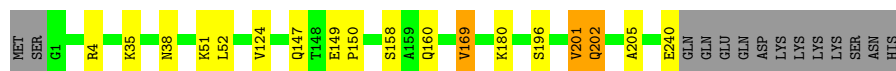
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 7% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% 6%

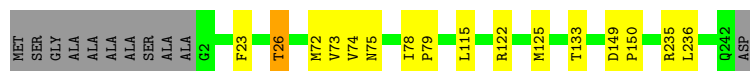


- Molecule 3: Proteasome subunit alpha type-4

Chain Q:  87% 6% 6%

WORLDWIDE
PDB
PROTEIN DATA BANK

Chain G:  89% 6% .

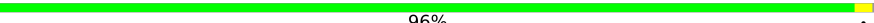


- Molecule 7: Proteasome subunit alpha type-1

Chain U:  90% 6% .

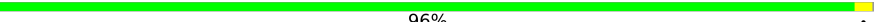


- Molecule 8: Proteasome subunit beta type-2

Chain H:  96% ..



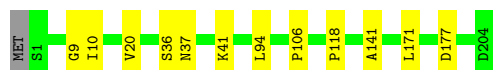
- Molecule 8: Proteasome subunit beta type-2

Chain V:  96% ..

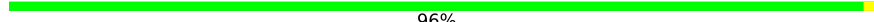


- Molecule 9: Proteasome subunit beta type-3

Chain I:  94% 6%



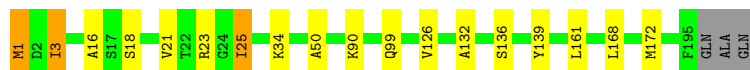
- Molecule 9: Proteasome subunit beta type-3

Chain W:  96% .

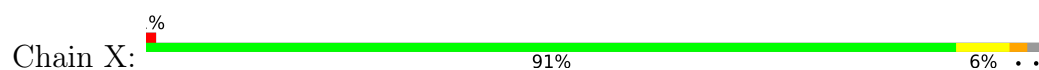


- Molecule 10: Proteasome subunit beta type-4

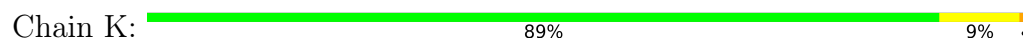
Chain J:  89% 8% ..



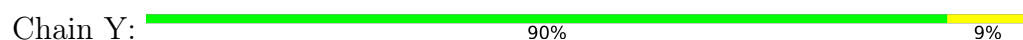
- Molecule 10: Proteasome subunit beta type-4



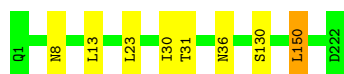
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



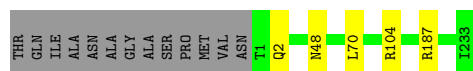
- Molecule 12: Proteasome subunit beta type-6



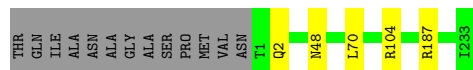
- Molecule 12: Proteasome subunit beta type-6



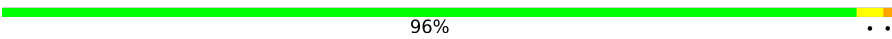
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7

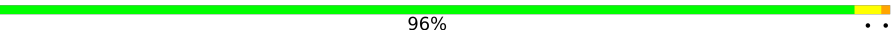


- Molecule 14: Proteasome subunit beta type-1

Chain N:  96% ..



● Molecule 14: Proteasome subunit beta type-1

Chain b:  96% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.80Å 300.21Å 144.40Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10 15.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-3.10) 97.2 (15.00-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.159 , 0.197 (Not available) , 0.199	Depositor DCC
R_{free} test set	9273 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49529	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.69	0/2642
2	B	0.41	0/1934	0.68	0/2618
2	P	0.40	0/1934	0.68	0/2618
3	C	0.39	0/1910	0.70	1/2586 (0.0%)
3	Q	0.39	0/1910	0.70	1/2586 (0.0%)
4	D	0.38	0/1837	0.65	0/2475
4	R	0.39	0/1837	0.65	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.39	0/1800	0.66	0/2433
6	F	0.39	0/1932	0.70	0/2609
6	T	0.39	0/1932	0.70	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.38	0/1945	0.67	0/2634
8	H	0.37	0/1750	0.63	0/2373
8	V	0.37	0/1750	0.63	0/2373
9	I	0.38	0/1611	0.66	0/2174
9	W	0.38	0/1611	0.66	0/2174
10	J	0.40	0/1589	0.67	0/2142
10	X	0.40	0/1589	0.66	0/2142
11	K	0.37	0/1685	0.69	1/2280 (0.0%)
11	Y	0.37	0/1685	0.71	1/2280 (0.0%)
12	L	0.37	0/1795	0.66	0/2420
12	Z	0.38	0/1795	0.66	0/2420
13	M	0.39	0/1855	0.68	0/2514
13	a	0.39	0/1855	0.67	0/2514
14	N	0.37	0/1541	0.66	0/2087
14	b	0.36	0/1541	0.66	0/2087
All	All	0.38	0/50272	0.67	4/67974 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	49	THR	N-CA-C	9.89	120.92	108.45
11	K	49	THR	N-CA-C	6.35	117.87	108.60
3	C	201	VAL	N-CA-C	5.69	116.42	110.62
3	Q	201	VAL	N-CA-C	5.60	116.33	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	48	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	1	0
8	V	1719	0	1719	1	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	13	0
10	X	1561	0	1569	10	0
11	K	1648	0	1601	17	0
11	Y	1648	0	1601	17	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	0	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	3	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	3	0	0	0	0
17	B	5	0	0	0	0
17	C	3	0	0	0	0
17	D	7	0	0	0	0
17	E	5	0	0	0	0
17	F	12	0	0	0	0
17	G	2	0	0	0	0
17	H	5	0	0	0	0
17	I	2	0	0	0	0
17	J	6	0	0	0	0
17	K	8	0	0	0	0
17	L	8	0	0	0	0
17	M	7	0	0	0	0
17	N	5	0	0	0	0
17	O	1	0	0	0	0
17	P	4	0	0	0	0
17	Q	8	0	0	0	0
17	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	5	0	0	0	0
17	T	5	0	0	0	0
17	U	6	0	0	0	0
17	V	4	0	0	0	0
17	W	3	0	0	0	0
17	X	10	0	0	0	0
17	Y	8	0	0	0	0
17	Z	3	0	0	0	0
17	a	8	0	0	0	0
17	b	3	0	0	0	0
All	All	49529	0	49142	112	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 1.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:25:ILE:O	10:X:139:TYR:OH	2.21	0.59
11:K:53:GLN:O	11:K:57:THR:HG23	2.05	0.57
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.04	0.56
14:b:152:VAL:HA	14:b:175:MET:HE1	1.88	0.56
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.54
14:N:152:VAL:HA	14:N:175:MET:HE1	1.89	0.54
11:Y:35:ILE:HD11	11:Y:57:THR:HG22	1.90	0.54
11:K:35:ILE:HD11	11:K:57:THR:HG22	1.89	0.54
11:Y:48:GLY:C	11:Y:49:THR:HG23	2.33	0.54
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
11:K:35:ILE:HB	11:K:45:MET:HE3	1.92	0.52
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.92	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.50
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.11	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.50
3:C:201:VAL:O	3:C:202:GLN:HB3	2.12	0.50
11:K:50:VAL:HB	12:L:130:SER:HB3	1.93	0.50
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.77	0.50
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.46	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:ILE:HB	11:K:45:MET:CE	2.42	0.49
11:K:52:CYS:SG	11:K:97:MET:HG2	2.53	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
11:Y:48:GLY:C	11:Y:49:THR:CG2	2.85	0.49
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.94	0.49
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.42	0.49
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.78	0.49
11:Y:52:CYS:SG	11:Y:97:MET:HG2	2.54	0.48
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.13	0.48
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.96	0.47
10:J:50:ALA:O	11:K:91:LYS:NZ	2.47	0.47
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.97	0.47
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.48	0.46
2:B:217:LYS:C	2:B:219:ALA:H	2.24	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.51	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.97	0.45
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.51	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.45
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.46	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
11:Y:50:VAL:HB	12:Z:130:SER:HB3	1.98	0.45
2:P:217:LYS:C	2:P:219:ALA:H	2.24	0.45
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.52	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.44
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.44
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.89	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.44
11:K:48:GLY:HA3	11:K:49:THR:HG23	1.99	0.44
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.00	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
11:Y:97:MET:HB2	11:Y:117:SER:HB3	1.99	0.43
11:K:97:MET:HB2	11:K:117:SER:HB3	1.99	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.49	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.43
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.00	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.43
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.52	0.43
11:K:35:ILE:HG23	11:K:37:ILE:HG13	2.00	0.42
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.00	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.42
11:Y:35:ILE:HG23	11:Y:37:ILE:HG13	2.01	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.01	0.42
10:J:25:ILE:O	10:J:25:ILE:HG12	2.20	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.45	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
11:K:49:THR:HB	11:K:51:ASP:H	1.84	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.41
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	2.03	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.02	0.41
2:B:221:ASP:O	2:B:223:GLU:N	2.54	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
2:B:145:TYR:OH	2:B:217:LYS:N	2.53	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.41
11:K:4:LEU:C	11:K:4:LEU:HD22	2.46	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.03	0.40
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.04	0.40
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.40
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.04	0.40
2:P:221:ASP:O	2:P:223:GLU:N	2.54	0.40
10:X:132:ALA:HB1	10:X:136:SER:HB2	2.04	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%)	239 (96%)	8 (3%)	1 (0%)	30	61
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	61
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	30
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	30
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	47
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	47
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
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	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6284/6614 (95%)	6098 (97%)	172 (3%)	14 (0%)	43	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
3	Q	202	GLN
2	B	218	GLY
2	B	222	GLY
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN

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%)	205 (98%)	4 (2%)	50	73
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	73
2	B	203/216 (94%)	198 (98%)	5 (2%)	42	69
2	P	203/216 (94%)	198 (98%)	5 (2%)	42	69
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	58
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	58
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	51
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	51
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	68
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	68
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	69
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	69
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	63
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	63
8	H	185/190 (97%)	183 (99%)	2 (1%)	65	78
8	V	185/190 (97%)	183 (99%)	2 (1%)	65	78
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	78
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	78
10	J	173/175 (99%)	167 (96%)	6 (4%)	32	62
10	X	173/175 (99%)	167 (96%)	6 (4%)	32	62
11	K	171/171 (100%)	165 (96%)	6 (4%)	32	62
11	Y	171/171 (100%)	166 (97%)	5 (3%)	37	66
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	78
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	78
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	69
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	73
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	73
All	All	5324/5544 (96%)	5183 (97%)	141 (3%)	40	68

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	20	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN

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Mol	Chain	Res	Type
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	23	ARG
10	J	25	ILE
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	35	ILE
11	K	49	THR
11	K	107	LYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	107	LYS
14	N	119	VAL
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU

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Mol	Chain	Res	Type
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	68	LEU
8	V	196	ARG

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	23	ARG
10	X	25	ILE
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	35	ILE
11	Y	107	LYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	107	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	176	GLN
2	B	232	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	165	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN

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Mol	Chain	Res	Type
6	F	123	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	66	HIS
8	H	91	GLN
9	I	44	HIS
9	I	63	ASN
9	I	203	GLN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	208	ASN
11	K	209	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	79	HIS
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	194	ASN
13	M	213	GLN
14	N	141	ASN
2	P	176	GLN
2	P	232	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	165	GLN
5	S	184	ASN

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Mol	Chain	Res	Type
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
8	V	66	HIS
9	W	44	HIS
9	W	63	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	108	ASN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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%)	-0.72	0 100 100	50, 68, 109, 143	0
1	O	250/250 (100%)	-0.69	0 100 100	53, 75, 121, 153	0
2	B	244/258 (94%)	-0.64	0 100 100	46, 73, 118, 187	0
2	P	244/258 (94%)	-0.63	1 (0%) 88 76	56, 74, 116, 183	0
3	C	240/254 (94%)	-0.65	0 100 100	53, 76, 135, 158	0
3	Q	240/254 (94%)	-0.55	2 (0%) 82 65	58, 89, 159, 191	0
4	D	235/260 (90%)	-0.67	0 100 100	59, 80, 111, 143	0
4	R	235/260 (90%)	-0.59	0 100 100	63, 86, 127, 159	0
5	E	231/234 (98%)	-0.69	0 100 100	54, 81, 116, 149	0
5	S	231/234 (98%)	-0.59	0 100 100	59, 88, 130, 163	0
6	F	243/288 (84%)	-0.66	0 100 100	49, 75, 126, 152	0
6	T	243/288 (84%)	-0.61	1 (0%) 88 76	55, 84, 140, 169	0
7	G	241/252 (95%)	-0.74	0 100 100	49, 68, 103, 154	0
7	U	241/252 (95%)	-0.66	0 100 100	51, 72, 111, 155	0
8	H	226/232 (97%)	-0.69	1 (0%) 88 76	44, 64, 98, 173	0
8	V	226/232 (97%)	-0.74	1 (0%) 88 76	47, 67, 98, 188	0
9	I	204/205 (99%)	-0.81	0 100 100	42, 63, 92, 129	0
9	W	204/205 (99%)	-0.81	0 100 100	45, 63, 97, 123	0
10	J	195/198 (98%)	-0.79	0 100 100	44, 63, 92, 130	0
10	X	195/198 (98%)	-0.76	1 (0%) 87 73	47, 65, 91, 144	0
11	K	212/212 (100%)	-0.65	0 100 100	45, 66, 97, 116	0
11	Y	212/212 (100%)	-0.70	0 100 100	49, 66, 96, 109	0
12	L	222/222 (100%)	-0.70	0 100 100	48, 66, 107, 145	0
12	Z	222/222 (100%)	-0.69	0 100 100	38, 68, 114, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
13	M	233/246 (94%)	-0.83	0	100	100	41, 64, 90, 112	0
13	a	233/246 (94%)	-0.82	0	100	100	45, 64, 89, 111	0
14	N	196/196 (100%)	-0.83	0	100	100	42, 58, 89, 116	0
14	b	196/196 (100%)	-0.83	0	100	100	44, 61, 92, 119	0
All	All	6344/6614 (95%)	-0.70	7 (0%)	92	86	38, 71, 118, 191	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	223	ILE	3.5
10	X	1	MET	3.3
3	Q	205	ALA	2.9
8	H	223	ILE	2.8
3	Q	50	LEU	2.7
6	T	178	HIS	2.5
2	P	219	ALA	2.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	H	301	1/1	0.95	0.07	58,58,58,58	0
15	MG	G	301	1/1	0.98	0.04	66,66,66,66	0
15	MG	K	301	1/1	0.98	0.09	59,59,59,59	0
15	MG	N	201	1/1	0.98	0.03	54,54,54,54	0
15	MG	V	301	1/1	0.99	0.07	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	Y	301	1/1	0.99	0.05	74,74,74,74	0
16	CL	G	302	1/1	0.99	0.05	46,46,46,46	0
16	CL	U	301	1/1	0.99	0.11	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.