



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:05 am BST

PDB ID : 5CZA  
Title : Yeast 20S proteasome beta5-D166N mutant  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-07-31  
Resolution : 2.50 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

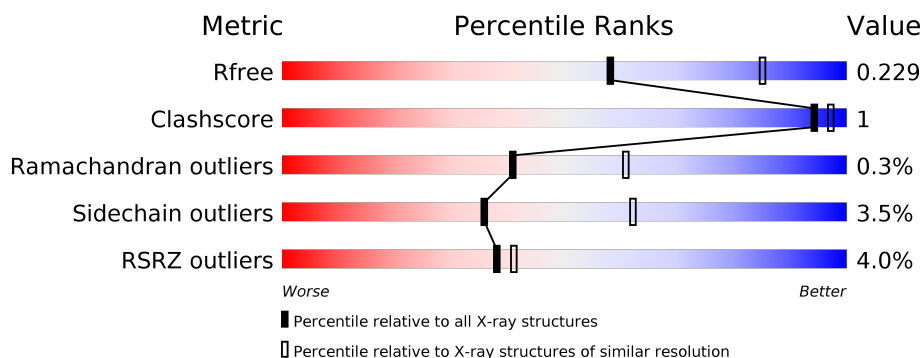
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>7%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>6%</div> <div>97%</div> <div>•</div> </div>
2	B	258	<div> <div>4%</div> <div>87%</div> <div>7% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>87%</div> <div>7% • 5%</div> </div>
3	C	254	<div> <div>9%</div> <div>87%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>13%</div> <div>87%</div> <div>6% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
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 50531 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
			1644	1045	281	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	281	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	168	ASN	ASP	engineered mutation	UNP P30656
Y	168	ASN	ASP	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	229	Total	C	N	O	S	0	0	0
			1790	1133	306	344	7			
13	a	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	42	Total O 42 42	0	0
17	B	39	Total O 39 39	0	0
17	C	31	Total O 31 31	0	0
17	D	39	Total O 39 39	0	0
17	E	29	Total O 29 29	0	0
17	F	45	Total O 45 45	0	0
17	G	52	Total O 52 52	0	0
17	H	55	Total O 55 55	0	0
17	I	47	Total O 47 47	0	0

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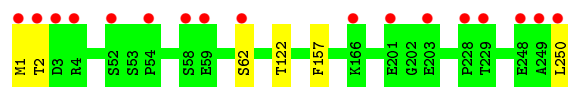
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	51	Total O 51 51	0	0
17	K	50	Total O 50 50	0	0
17	L	56	Total O 56 56	0	0
17	M	62	Total O 62 62	0	0
17	N	50	Total O 50 50	0	0
17	O	23	Total O 23 23	0	0
17	P	30	Total O 30 30	0	0
17	Q	28	Total O 28 28	0	0
17	R	23	Total O 23 23	0	0
17	S	21	Total O 21 21	0	0
17	T	33	Total O 33 33	0	0
17	U	52	Total O 52 52	0	0
17	V	35	Total O 35 35	0	0
17	W	45	Total O 45 45	0	0
17	X	29	Total O 29 29	0	0
17	Y	61	Total O 61 61	0	0
17	Z	56	Total O 56 56	0	0
17	a	67	Total O 67 67	0	0
17	b	47	Total O 47 47	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 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.

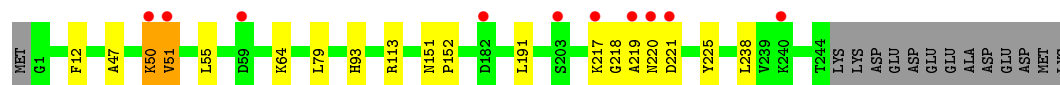
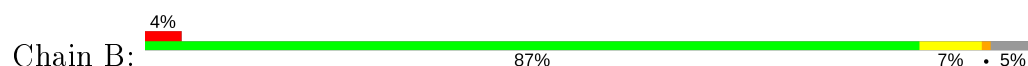
- Molecule 1: Proteasome subunit alpha type-2



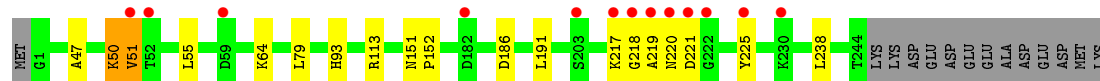
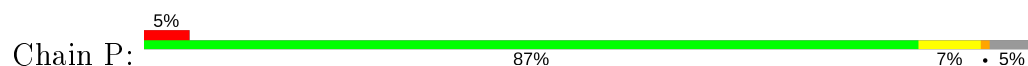
- Molecule 1: Proteasome subunit alpha type-2



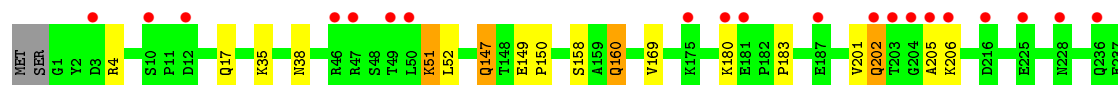
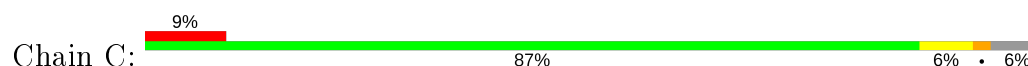
- Molecule 2: Proteasome subunit alpha type-3

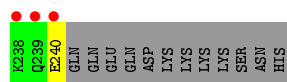


- Molecule 2: Proteasome subunit alpha type-3

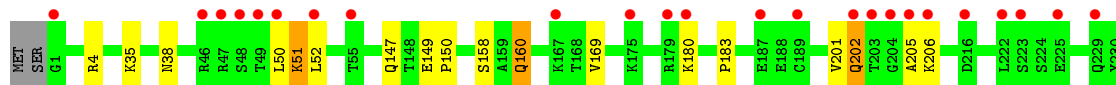
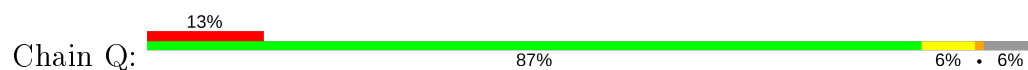


- Molecule 3: Proteasome subunit alpha type-4

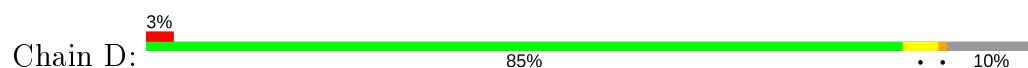




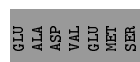
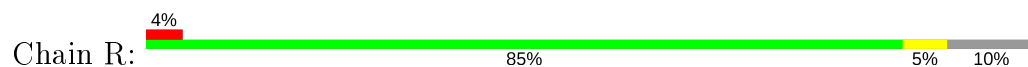
• Molecule 3: Proteasome subunit alpha type-4



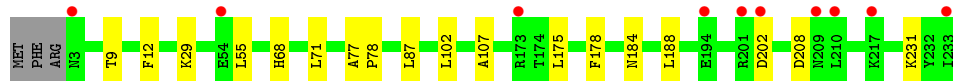
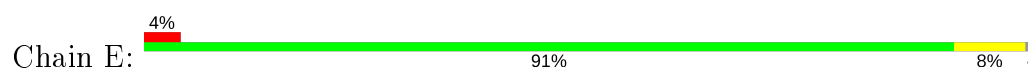
• Molecule 4: Proteasome subunit alpha type-5



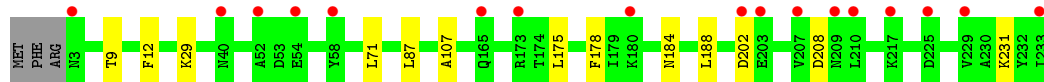
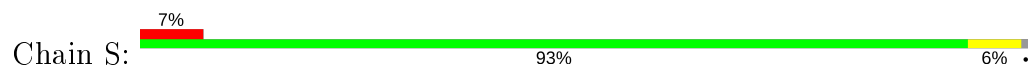
• Molecule 4: Proteasome subunit alpha type-5



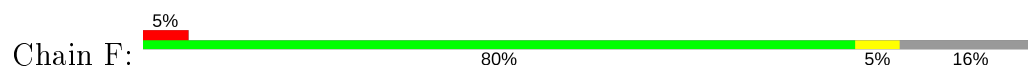
• Molecule 5: Proteasome subunit alpha type-6

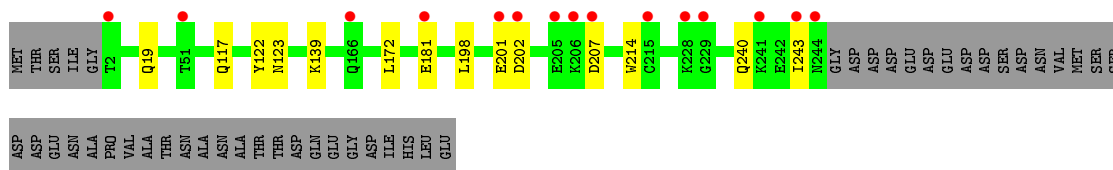


• Molecule 5: Proteasome subunit alpha type-6

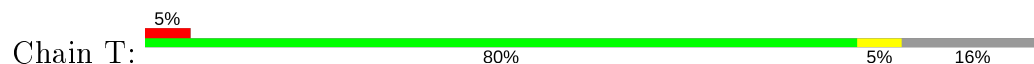


• Molecule 6: Probable proteasome subunit alpha type-7

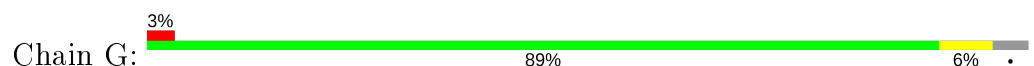




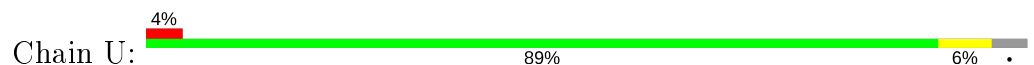
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1



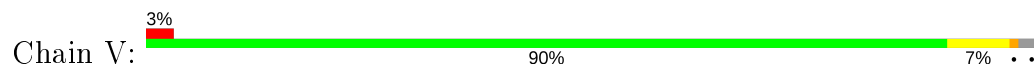
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2

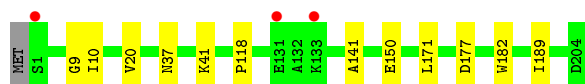


- Molecule 8: Proteasome subunit beta type-2

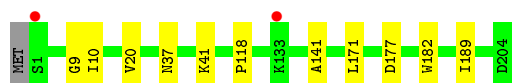


- Molecule 9: Proteasome subunit beta type-3





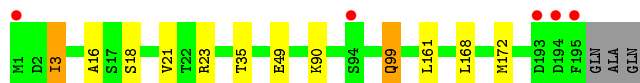
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



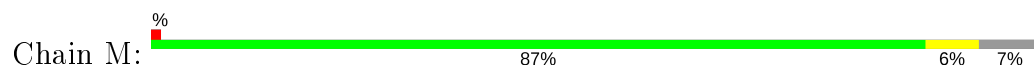
- Molecule 12: Proteasome subunit beta type-6



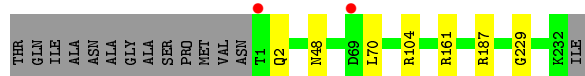
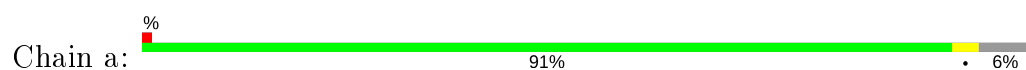
- Molecule 12: Proteasome subunit beta type-6



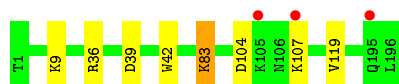
- Molecule 13: Proteasome subunit beta type-7



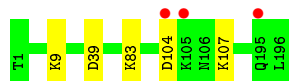
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.77Å 301.43Å 144.14Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.50) 97.5 (15.00-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.206 , 0.224 0.214 , 0.229	Depositor DCC
$R_{free}$ test set	17654 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.26	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.47	0/2433
5	S	0.26	0/1800	0.47	0/2433
6	F	0.26	0/1932	0.45	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.26	0/1750	0.48	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.48	0/2174
9	W	0.26	0/1611	0.48	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.31	0/1681	0.49	0/2274
11	Y	0.30	0/1681	0.49	0/2274
12	L	0.26	0/1795	0.48	0/2420
12	Z	0.29	0/1795	0.48	0/2420
13	M	0.27	0/1821	0.50	0/2470
13	a	0.27	0/1846	0.50	0/2503
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50221	0.48	0/67907

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	11	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	6	0
11	K	1644	0	1597	6	0
11	Y	1644	0	1597	6	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	2	0
13	M	1790	0	1793	4	0
13	a	1815	0	1821	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	42	0	0	0	0
17	B	39	0	0	1	0
17	C	31	0	0	0	0
17	D	39	0	0	0	0
17	E	29	0	0	0	0
17	F	45	0	0	0	0
17	G	52	0	0	0	0
17	H	55	0	0	0	0
17	I	47	0	0	0	0
17	J	51	0	0	0	0
17	K	50	0	0	0	0
17	L	56	0	0	0	0
17	M	62	0	0	0	0
17	N	50	0	0	0	0
17	O	23	0	0	0	0
17	P	30	0	0	1	0
17	Q	28	0	0	0	0
17	R	23	0	0	0	0
17	S	21	0	0	0	0
17	T	33	0	0	0	0
17	U	52	0	0	0	0
17	V	35	0	0	0	0
17	W	45	0	0	0	0
17	X	29	0	0	0	0
17	Y	61	0	0	0	0
17	Z	56	0	0	0	0
17	a	67	0	0	0	0
17	b	47	0	0	0	0
All	All	50531	0	49084	118	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 (118) 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)
8:V:52:THR:O	8:V:56:THR:OG1	2.04	0.75
8:H:52:THR:O	8:H:56:THR:OG1	2.05	0.73
8:V:80:LEU:HD13	8:V:119:THR:HG21	1.86	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.55	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.55
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.43	0.54
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.89	0.54
2:P:217:LYS:C	2:P:219:ALA:H	2.13	0.52
2:P:93:HIS:HB3	17:P:301:HOH:O	2.08	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.41	0.51
2:B:93:HIS:HB3	17:B:301:HOH:O	2.10	0.51
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.93	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.94	0.50
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.94	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
2:B:217:LYS:C	2:B:219:ALA:H	2.13	0.50
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.94	0.50
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.12	0.49
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.94	0.49
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.78	0.48
3:C:51:LYS:O	3:C:52:LEU:HB2	2.12	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
2:B:12:PHE:H	3:C:17:GLN:HE22	1.60	0.47
8:V:3:ILE:HG21	8:V:44:ALA:HB3	1.95	0.47
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.49	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.98	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.98	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.98	0.46
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.45
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.51	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.99	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.45
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.51	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.53	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.44
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.99	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.00	0.44
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.53	0.43
8:H:43:CYS:SG	8:H:56:THR:HG23	2.58	0.43
8:H:196:ARG:NH2	9:I:150:GLU:OE2	2.51	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.43
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.00	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.43
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.87	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.43
10:J:49:GLU:HB2	10:J:99:GLN:HB3	2.00	0.43
5:S:12:PHE:H	6:T:19:GLN:HE22	1.66	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.43
8:H:43:CYS:SG	8:H:56:THR:CG2	3.07	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.01	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.42
8:H:3:ILE:HD11	8:H:127:LEU:HB3	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.42
10:X:49:GLU:HB2	10:X:99:GLN:HB3	2.00	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
8:V:43:CYS:SG	8:V:56:THR:HG23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.42
5:E:12:PHE:H	6:F:19:GLN:HE22	1.67	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.42
8:V:43:CYS:SG	8:V:56:THR:CG2	3.08	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.02	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.41
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.01	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.01	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
2:P:219:ALA:HB2	2:P:225:TYR:HB2	2.01	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.03	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.40
5:E:68:HIS:HE1	5:E:102:LEU:O	2.04	0.40
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.40
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
3:C:147:GLN:NE2	3:C:160:GLN:OE1	2.55	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.95	0.40
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.03	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.04	0.40
10:X:168:LEU:O	10:X:172:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	34	54
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	54
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	16
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	16
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	21
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	21
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	227/246 (92%)	221 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	230/246 (94%)	223 (97%)	6 (3%)	1 (0%)	34	54
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6279/6614 (95%)	6135 (98%)	127 (2%)	17 (0%)	41	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO
13	a	229	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%)	205 (98%)	4 (2%)	57	80
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	80
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	63
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	49
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	50
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	50
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	54
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	46
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	46
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	47
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	47
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	77
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	77
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	82
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	82
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	76
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	76
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	43
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	43
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	65
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	71
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	67
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	68
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	67
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	67
All	All	5315/5540 (96%)	5128 (96%)	187 (4%)	36	62

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE

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Mol	Chain	Res	Type
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
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	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
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	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP

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Mol	Chain	Res	Type
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	128	CYS
11	K	131	SER
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG

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Mol	Chain	Res	Type
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
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	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP

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Mol	Chain	Res	Type
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	80	LEU
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS
11	Y	131	SER
11	Y	140	LEU
11	Y	148	LEU

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Mol	Chain	Res	Type
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	130	SER
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN

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Mol	Chain	Res	Type
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	22	GLN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	95	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
4	R	15	GLN
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	22	GLN
8	V	116	HIS
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 10 ligands modelled in this entry, 10 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.05	17 (6%) 17 17	32, 45, 81, 116	0
1	O	250/250 (100%)	0.09	14 (5%) 24 25	37, 53, 99, 128	0
2	B	244/258 (94%)	0.08	10 (4%) 37 40	31, 51, 91, 143	0
2	P	244/258 (94%)	0.14	13 (5%) 26 28	37, 54, 98, 145	0
3	C	240/254 (94%)	0.25	23 (9%) 8 7	31, 56, 118, 148	0
3	Q	240/254 (94%)	0.55	32 (13%) 3 2	40, 69, 151, 186	0
4	D	235/260 (90%)	0.04	8 (3%) 45 48	38, 57, 89, 131	0
4	R	235/260 (90%)	0.17	11 (4%) 31 33	39, 60, 103, 143	0
5	E	231/234 (98%)	0.06	10 (4%) 35 38	38, 57, 93, 136	0
5	S	231/234 (98%)	0.30	17 (7%) 14 15	44, 68, 108, 151	0
6	F	243/288 (84%)	-0.05	15 (6%) 20 21	34, 50, 103, 132	0
6	T	243/288 (84%)	0.13	13 (5%) 26 28	39, 63, 118, 149	0
7	G	241/252 (95%)	-0.17	8 (3%) 46 50	26, 46, 80, 131	0
7	U	241/252 (95%)	-0.05	9 (3%) 41 45	37, 51, 81, 126	0
8	H	226/232 (97%)	0.06	10 (4%) 34 37	28, 44, 77, 137	0
8	V	226/232 (97%)	0.11	8 (3%) 44 47	35, 49, 80, 153	0
9	I	204/205 (99%)	-0.36	3 (1%) 73 75	28, 40, 69, 92	0
9	W	204/205 (99%)	-0.31	2 (0%) 82 84	31, 42, 73, 95	0
10	J	195/198 (98%)	-0.20	5 (2%) 56 59	29, 44, 70, 122	0
10	X	195/198 (98%)	-0.16	5 (2%) 56 59	31, 46, 69, 131	0
11	K	212/212 (100%)	-0.28	1 (0%) 91 91	26, 43, 67, 85	0
11	Y	212/212 (100%)	-0.24	3 (1%) 75 77	32, 45, 69, 89	0
12	L	222/222 (100%)	-0.24	4 (1%) 68 71	28, 45, 77, 111	0
12	Z	222/222 (100%)	-0.28	2 (0%) 84 86	29, 44, 78, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	229/246 (93%)	-0.34	3 (1%)	77 79	26, 44, 67, 84	0
13	a	232/246 (94%)	-0.33	2 (0%)	84 86	27, 45, 65, 83	0
14	N	196/196 (100%)	-0.36	3 (1%)	73 75	28, 39, 66, 93	0
14	b	196/196 (100%)	-0.30	3 (1%)	73 75	28, 40, 68, 98	0
All	All	6339/6614 (95%)	-0.05	254 (4%)	38 41	26, 49, 95, 186	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	223	ILE	9.9
3	Q	50	LEU	9.8
8	V	224	GLN	9.6
8	V	226	GLU	8.9
2	B	221	ASP	8.8
2	P	219	ALA	8.2
2	B	51	VAL	7.4
8	H	223	ILE	6.9
3	Q	49	THR	6.8
8	H	222	ASP	6.7
8	V	222	ASP	6.6
2	B	219	ALA	6.4
2	P	51	VAL	6.3
5	S	202	ASP	6.2
10	X	194	ASP	6.1
7	U	242	GLN	6.1
8	H	224	GLN	6.1
1	O	2	THR	6.0
8	V	221	CYS	5.9
2	P	221	ASP	5.8
3	Q	239	GLN	5.7
12	L	174	TYR	5.7
3	Q	205	ALA	5.4
1	A	2	THR	5.4
8	H	221	CYS	5.4
1	O	249	ALA	5.4
3	Q	236	GLN	5.4
10	X	1	MET	5.4
2	B	220	ASN	5.3
6	F	2	THR	5.1
4	D	242	GLU	5.0
3	C	49	THR	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	238	LYS	4.9
4	R	241	ALA	4.9
3	Q	240	GLU	4.8
9	I	1	SER	4.8
1	A	1	MET	4.7
5	S	210	LEU	4.7
3	Q	204	GLY	4.6
3	Q	48	SER	4.6
1	O	53	SER	4.6
7	U	222	ASP	4.6
3	Q	206	LYS	4.5
1	O	1	MET	4.5
14	b	105	LYS	4.5
10	J	1	MET	4.5
6	F	244	ASN	4.3
14	b	195	GLN	4.3
1	O	52	SER	4.3
4	R	1	ASP	4.3
3	C	236	GLN	4.3
14	N	105	LYS	4.3
9	W	1	SER	4.3
3	C	238	LYS	4.2
3	C	50	LEU	4.2
2	P	222	GLY	4.2
2	P	220	ASN	4.2
8	H	225	GLU	4.2
1	O	250	LEU	4.2
4	R	125	LEU	4.2
2	P	52	THR	4.2
10	J	193	ASP	4.2
10	J	194	ASP	4.1
6	F	205	GLU	4.0
5	E	233	ILE	4.0
9	W	133	LYS	4.0
4	D	241	ALA	4.0
3	Q	202	GLN	3.8
11	Y	212	GLY	3.8
6	F	202	ASP	3.8
3	C	202	GLN	3.8
8	V	225	GLU	3.8
2	P	59	ASP	3.8
6	T	244	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
3	Q	187	GLU	3.7
6	T	206	LYS	3.6
8	H	226	GLU	3.6
5	E	202	ASP	3.6
5	S	173	ARG	3.6
3	Q	223	SER	3.6
3	C	203	THR	3.6
1	A	229	THR	3.5
14	N	195	GLN	3.5
12	Z	174	TYR	3.5
6	T	243	ILE	3.4
3	C	206	LYS	3.4
13	a	1	THR	3.4
4	D	1	ASP	3.4
10	X	195	PHE	3.3
2	P	218	GLY	3.3
3	Q	1	GLY	3.3
3	Q	234	ILE	3.3
5	S	233	ILE	3.3
5	E	194	GLU	3.3
1	O	229	THR	3.3
1	A	203	GLU	3.3
4	D	125	LEU	3.2
3	C	240	GLU	3.2
10	X	193	ASP	3.2
6	F	51	THR	3.2
7	G	2	GLY	3.2
3	C	205	ALA	3.2
3	C	239	GLN	3.2
3	Q	47	ARG	3.1
2	P	217	LYS	3.1
5	E	201	ARG	3.1
5	E	173	ARG	3.1
3	C	204	GLY	3.1
1	O	203	GLU	3.0
14	b	104	ASP	3.0
6	F	243	ILE	3.0
1	O	201	GLU	3.0
2	P	182	ASP	3.0
7	U	183	ASP	3.0
3	Q	225	GLU	3.0
3	Q	167	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	54	GLU	3.0
4	R	238	LYS	3.0
4	R	242	GLU	2.9
6	T	181	GLU	2.9
3	Q	55	THR	2.9
3	Q	179	ARG	2.9
3	C	225	GLU	2.9
2	B	217	LYS	2.9
6	T	205	GLU	2.9
3	C	180	LYS	2.9
3	Q	216	ASP	2.9
13	M	1	THR	2.9
7	G	242	GLN	2.9
7	U	188	GLU	2.8
7	G	179	LYS	2.8
1	O	62	SER	2.8
7	U	2	GLY	2.8
6	T	230	ASP	2.8
1	A	201	GLU	2.8
3	Q	237	GLU	2.8
3	Q	203	THR	2.8
9	I	133	LYS	2.8
2	B	203	SER	2.8
1	A	228	PRO	2.8
2	P	230	LYS	2.8
4	R	201	GLU	2.8
3	Q	229	GLN	2.8
1	A	249	ALA	2.8
5	E	210	LEU	2.7
6	T	229	GLY	2.7
5	S	58	TYR	2.7
2	B	182	ASP	2.7
6	T	235	ALA	2.7
5	S	225	ASP	2.7
6	F	207	ASP	2.7
3	C	175	LYS	2.7
4	R	217	GLN	2.7
6	F	215	CYS	2.7
5	E	3	ASN	2.6
1	A	250	LEU	2.6
3	C	181	GLU	2.6
5	S	229	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	S	180	LYS	2.6
6	F	228	LYS	2.6
3	C	12	ASP	2.6
3	Q	233	GLN	2.5
6	F	229	GLY	2.5
2	P	225	TYR	2.5
3	Q	231	VAL	2.5
7	G	222	ASP	2.5
4	R	224	ASP	2.5
6	F	181	GLU	2.5
12	L	165	ASN	2.4
1	A	166	LYS	2.4
2	B	240	LYS	2.4
11	Y	208	ASN	2.4
3	C	47	ARG	2.4
4	D	217	GLN	2.4
5	S	165	GLN	2.4
4	D	240	ALA	2.4
7	G	68	ARG	2.4
8	H	195	VAL	2.3
3	C	216	ASP	2.3
2	B	50	LYS	2.3
8	H	219	ASN	2.3
3	Q	46	ARG	2.3
7	U	203	ASP	2.3
1	A	59	GLU	2.3
7	G	240	ALA	2.3
1	A	248	GLU	2.3
3	Q	52	LEU	2.3
13	a	69	ASP	2.3
2	P	203	SER	2.3
4	R	230	GLU	2.3
5	S	203	GLU	2.3
6	T	2	THR	2.3
3	C	228	ASN	2.3
2	B	59	ASP	2.3
3	Q	222	LEU	2.3
12	L	172	LEU	2.3
7	U	230	GLU	2.3
1	A	4	ARG	2.3
6	T	166	GLN	2.3
13	M	69	ASP	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	3	ASP	2.2
1	A	58	SER	2.2
3	C	187	GLU	2.2
10	X	94	SER	2.2
8	V	219	ASN	2.2
10	J	135	TYR	2.2
1	A	3	ASP	2.2
8	V	145	ASP	2.2
5	S	207	VAL	2.2
6	F	241	LYS	2.2
5	S	3	ASN	2.2
7	G	241	GLU	2.2
4	R	141	ALA	2.2
5	E	217	LYS	2.2
4	R	54	ASP	2.2
3	C	10	SER	2.2
4	D	201	GLU	2.2
5	S	40	ASN	2.2
11	Y	106	ARG	2.2
7	U	68	ARG	2.1
11	K	212	GLY	2.1
1	A	54	PRO	2.1
5	S	52	ALA	2.1
5	S	217	LYS	2.1
1	O	184	GLU	2.1
8	H	181	GLY	2.1
14	N	107	LYS	2.1
1	O	228	PRO	2.1
1	A	62	SER	2.1
1	O	231	LYS	2.1
8	H	173	VAL	2.1
6	T	180	PRO	2.1
1	A	52	SER	2.1
12	L	173	LYS	2.1
5	S	209	ASN	2.1
1	O	207	ASP	2.1
6	F	201	GLU	2.1
7	G	40	ASP	2.1
5	E	209	ASN	2.0
5	S	54	GLU	2.0
13	M	121	SER	2.0
6	F	166	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	175	LYS	2.0
4	D	224	ASP	2.0
6	F	206	LYS	2.0
6	T	50	ILE	2.0
3	C	46	ARG	2.0
3	Q	189	CYS	2.0
6	T	178	HIS	2.0
10	J	24	GLY	2.0
7	U	153	TYR	2.0
12	Z	106	TYR	2.0
9	I	131	GLU	2.0
3	Q	180	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	MG	Z	301	1/1	0.89	0.21	64,64,64,64	0
15	MG	K	301	1/1	0.93	0.10	41,41,41,41	0
15	MG	I	302	1/1	0.94	0.12	40,40,40,40	0
15	MG	W	301	1/1	0.95	0.20	49,49,49,49	0
15	MG	I	301	1/1	0.95	0.20	46,46,46,46	0
15	MG	G	301	1/1	0.97	0.04	34,34,34,34	0
15	MG	N	201	1/1	0.97	0.07	41,41,41,41	0
15	MG	L	301	1/1	0.98	0.10	41,41,41,41	0
16	CL	U	301	1/1	0.99	0.06	37,37,37,37	0
16	CL	G	302	1/1	0.99	0.05	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.