



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 AM UTC

PDB ID : 4YA5 / pdb_00004ya5
Title : Yeast 20S proteasome beta2-H114D mutant in complex with Ac-PAE-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-17
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

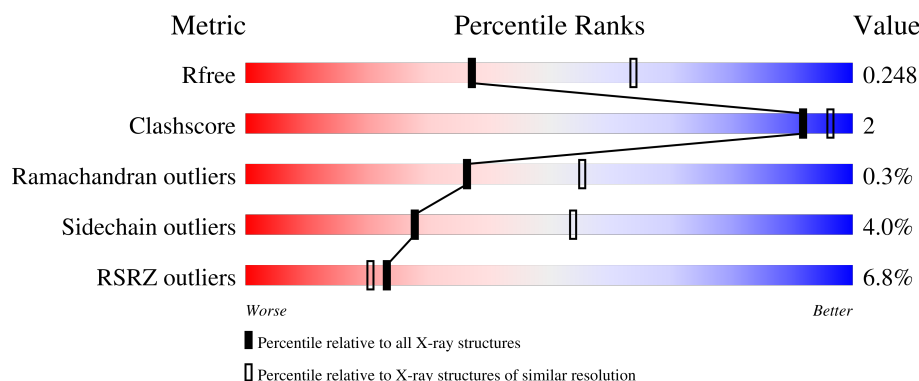
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	4% 97% .
1	O	250	8% 96% .
2	B	258	11% 84% 9% • 5%
2	P	258	11% 85% 8% • 5%
3	C	254	12% 85% 8% • 6%

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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	
15	c	5	
15	d	5	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50389 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
			1717	1080	296	334	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	296	334	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	114	ASP	HIS	engineered mutation	UNP P25043
V	114	ASP	HIS	engineered mutation	UNP P25043

- 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			
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	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

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

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

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

- Molecule 15 is a protein called Ac-PAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			28	18	3	7			
15	d	5	Total	C	N	O	0	0	0
			28	18	3	7			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	37	Total	O	0	0
			37	37		
18	B	27	Total	O	0	0
			27	27		
18	C	25	Total	O	0	0
			25	25		
18	D	27	Total	O	0	0
			27	27		
18	E	17	Total	O	0	0
			17	17		
18	F	32	Total	O	0	0
			32	32		

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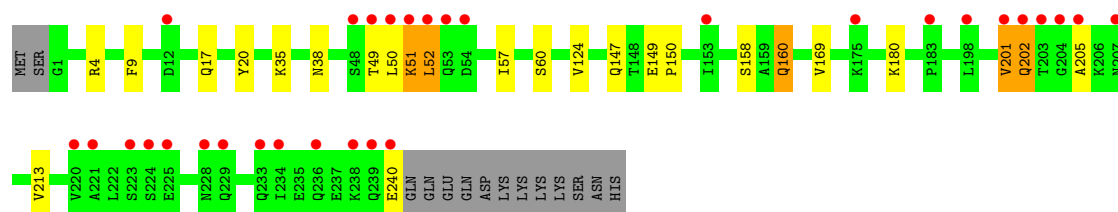
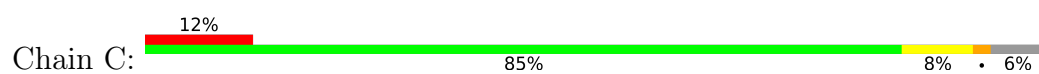
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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18	H	50	Total 50	O 50	0	0
18	I	39	Total 39	O 39	0	0
18	J	42	Total 42	O 42	0	0
18	K	41	Total 41	O 41	0	0
18	L	40	Total 40	O 40	0	0
18	M	50	Total 50	O 50	0	0
18	N	41	Total 41	O 41	0	0
18	O	26	Total 26	O 26	0	0
18	P	26	Total 26	O 26	0	0
18	Q	13	Total 13	O 13	0	0
18	R	18	Total 18	O 18	0	0
18	S	15	Total 15	O 15	0	0
18	T	28	Total 28	O 28	0	0
18	U	40	Total 40	O 40	0	0
18	V	38	Total 38	O 38	0	0
18	W	42	Total 42	O 42	0	0
18	X	37	Total 37	O 37	0	0
18	Y	36	Total 36	O 36	0	0
18	Z	40	Total 40	O 40	0	0
18	a	41	Total 41	O 41	0	0

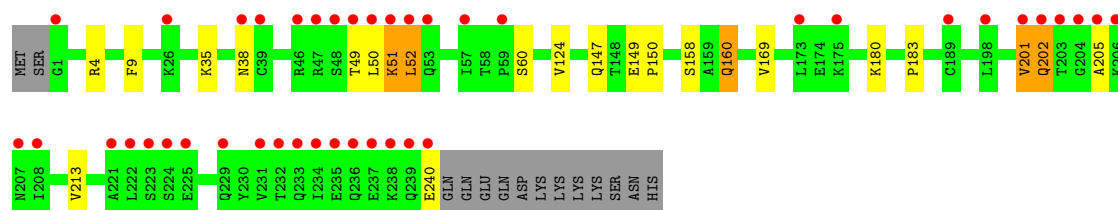
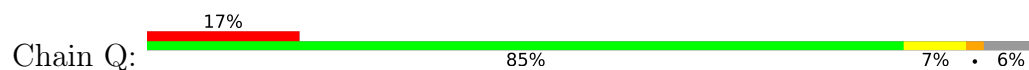
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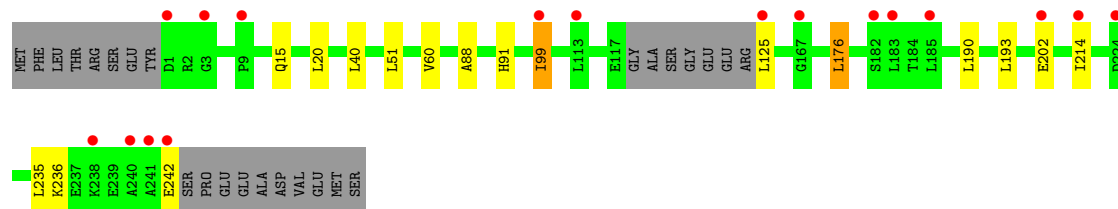
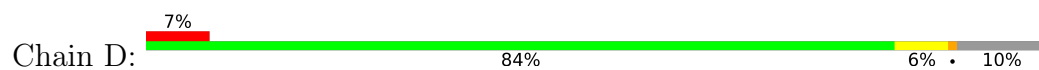
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	38	Total 38	O 38	0	0
18	c	3	Total 3	O 3	0	0
18	d	2	Total 2	O 2	0	0



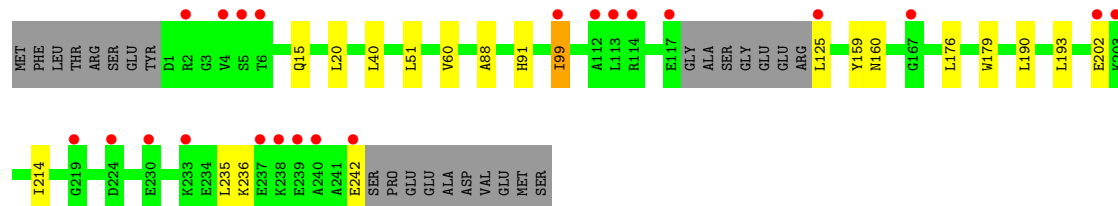
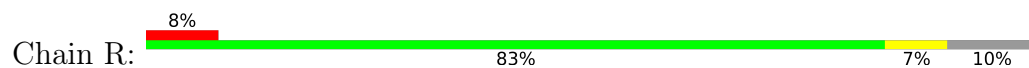
• Molecule 3: Proteasome subunit alpha type-4



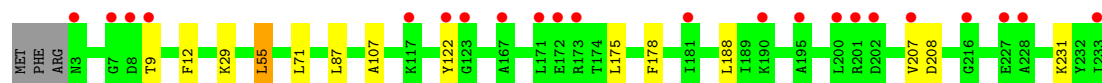
• Molecule 4: Proteasome subunit alpha type-5



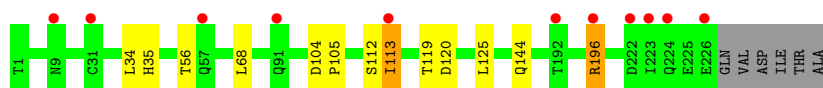
• Molecule 4: Proteasome subunit alpha type-5



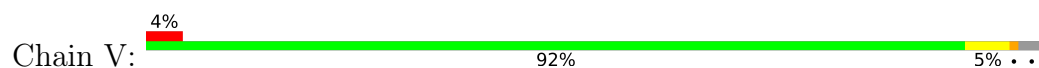
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit beta type-2



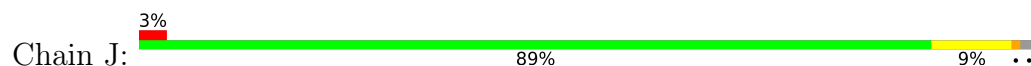
- Molecule 9: Proteasome subunit beta type-3



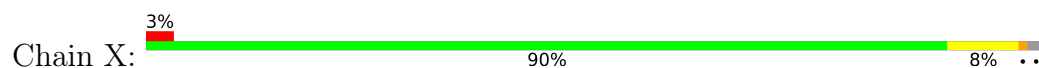
- Molecule 9: Proteasome subunit beta type-3



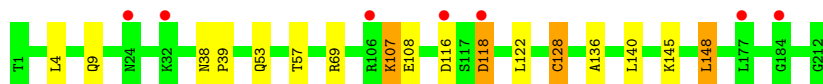
- Molecule 10: Proteasome subunit beta type-4



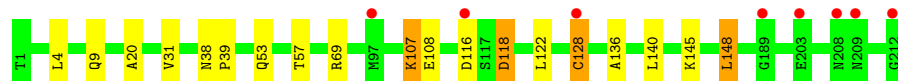
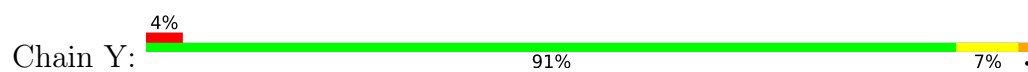
- Molecule 10: Proteasome subunit beta type-4



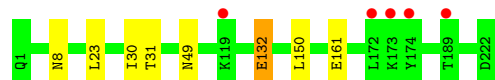
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



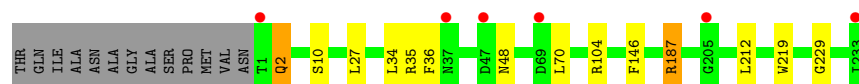
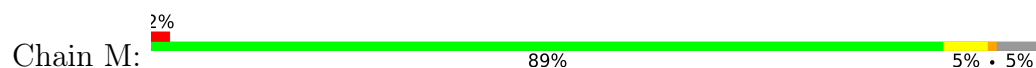
- Molecule 12: Proteasome subunit beta type-6



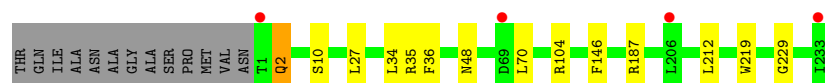
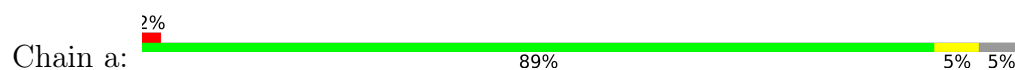
- Molecule 12: Proteasome subunit beta type-6



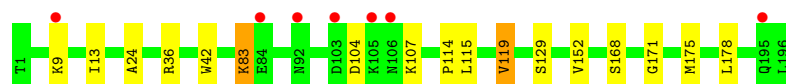
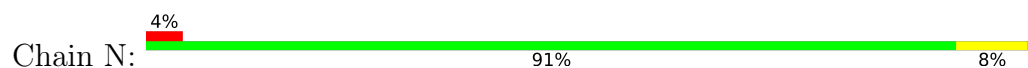
- Molecule 13: Proteasome subunit beta type-7



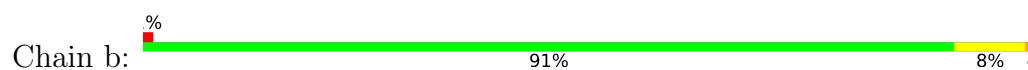
- Molecule 13: Proteasome subunit beta type-7



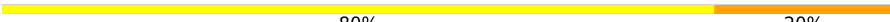
- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1

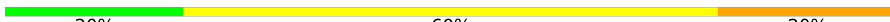


- Molecule 15: Ac-PAE-ep

Chain c:  80% 20%

ACE1	P2	A3	E4	POL5
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- Molecule 15: Ac-PAE-ep

Chain d:  20% 60% 20%

ACE1	P2	A3	E4	POL5
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.71Å 301.32Å 145.93Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (15.00-2.50) 95.5 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.226 , 0.242 0.232 , 0.248	Depositor DCC
R_{free} test set	17789 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50389	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: POL, GAU, CL, ACE, MG

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	0.43	0/1952	0.69	0/2642
1	O	0.42	0/1952	0.68	0/2642
2	B	0.43	0/1934	0.68	0/2618
2	P	0.43	0/1934	0.68	0/2618
3	C	0.43	0/1910	0.70	1/2586 (0.0%)
3	Q	0.43	0/1910	0.70	1/2586 (0.0%)
4	D	0.42	0/1837	0.68	0/2475
4	R	0.42	0/1837	0.68	0/2475
5	E	0.42	0/1800	0.65	0/2433
5	S	0.42	0/1800	0.65	0/2433
6	F	0.42	0/1932	0.69	0/2609
6	T	0.42	0/1932	0.69	0/2609
7	G	0.42	0/1945	0.68	0/2634
7	U	0.42	0/1945	0.68	0/2634
8	H	0.41	0/1747	0.65	0/2369
8	V	0.41	0/1747	0.65	0/2369
9	I	0.43	0/1611	0.70	1/2174 (0.0%)
9	W	0.43	0/1611	0.70	1/2174 (0.0%)
10	J	0.44	1/1589 (0.1%)	0.66	0/2142
10	X	0.44	1/1589 (0.1%)	0.66	0/2142
11	K	0.40	0/1681	0.67	0/2274
11	Y	0.40	0/1681	0.67	0/2274
12	L	0.41	0/1795	0.69	1/2420 (0.0%)
12	Z	0.41	0/1795	0.69	0/2420
13	M	0.43	0/1855	0.68	1/2514 (0.0%)
13	a	0.43	0/1855	0.68	1/2514 (0.0%)
14	N	0.44	0/1541	0.69	0/2087
14	b	0.41	0/1541	0.67	0/2087
15	c	4.01	2/13 (15.4%)	1.05	0/18
15	d	2.90	2/13 (15.4%)	0.97	0/18
All	All	0.43	6/50284 (0.0%)	0.68	7/67990 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	1	ACE	C-N	-11.28	1.32	1.43
15	d	1	ACE	C-N	-7.94	1.35	1.43
15	c	2	PRO	CA-C	-6.74	1.38	1.52
15	d	2	PRO	CA-C	-6.06	1.40	1.52
10	J	2	ASP	CA-C	6.00	1.55	1.52
10	X	2	ASP	CA-C	5.24	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.76	116.88	110.53
3	C	201	VAL	N-CA-C	6.63	116.76	110.53
9	W	126	ILE	N-CA-C	5.45	117.45	112.43
13	a	10	SER	N-CA-C	5.31	117.73	110.24
13	M	10	SER	N-CA-C	5.20	117.57	110.24
9	I	126	ILE	CB-CA-C	-5.19	105.32	111.65
12	L	132	GLU	CA-CB-CG	5.06	124.23	114.10

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	4	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	6	0
8	H	1717	0	1716	9	0
8	V	1717	0	1716	8	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	9	0
11	K	1644	0	1595	8	0
11	Y	1644	0	1595	9	0
12	L	1757	0	1711	1	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	9	0
13	a	1824	0	1832	7	0
14	N	1512	0	1478	11	0
14	b	1512	0	1478	11	0
15	c	28	0	26	4	0
15	d	28	0	26	1	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
18	A	37	0	0	0	0
18	B	27	0	0	2	0
18	C	25	0	0	0	0
18	D	27	0	0	1	0
18	E	17	0	0	0	0
18	F	32	0	0	0	0
18	G	52	0	0	0	0
18	H	50	0	0	0	0
18	I	39	0	0	0	0
18	J	42	0	0	0	0
18	K	41	0	0	0	0
18	L	40	0	0	0	0
18	M	50	0	0	1	0
18	N	41	0	0	1	0
18	O	26	0	0	0	0
18	P	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	13	0	0	0	0
18	R	18	0	0	0	0
18	S	15	0	0	0	0
18	T	28	0	0	1	0
18	U	40	0	0	0	0
18	V	38	0	0	0	0
18	W	42	0	0	0	0
18	X	37	0	0	0	0
18	Y	36	0	0	0	0
18	Z	40	0	0	1	0
18	a	41	0	0	1	0
18	b	38	0	0	0	0
18	c	3	0	0	1	0
18	d	2	0	0	0	0
All	All	50389	0	49170	161	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 2.

All (161) 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:H:112:SER:OG	8:H:120:ASP:OD1	2.01	0.75
8:V:112:SER:OG	8:V:120:ASP:OD1	2.02	0.74
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.70	0.74
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.71	0.73
11:Y:116:ASP:OD2	11:Y:118:ASP:OD1	2.15	0.66
14:N:129:SER:OG	15:c:5:POL:H11	1.98	0.64
14:N:168:SER:HB3	15:c:5:POL:H33	1.80	0.64
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.46	0.63
13:M:2:GLN:HB3	18:N:326:HOH:O	1.99	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.62
11:Y:118:ASP:OD1	11:Y:118:ASP:N	2.33	0.61
5:S:12:PHE:H	6:T:19:GLN:HE22	1.47	0.61
8:H:113:ILE:CG1	8:H:119:THR:HG22	2.32	0.60
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.59
14:b:152:VAL:HA	14:b:175:MET:HE1	1.84	0.59
11:K:118:ASP:N	11:K:118:ASP:OD1	2.35	0.58
2:P:93:HIS:HB3	18:P:301:HOH:O	2.03	0.58
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:113:ILE:CG1	8:V:119:THR:HG22	2.33	0.58
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.86	0.58
11:K:116:ASP:OD2	11:K:118:ASP:OD1	2.23	0.56
2:B:221:ASP:O	2:B:223:GLU:N	2.39	0.56
6:T:215:CYS:HB3	18:T:302:HOH:O	2.03	0.56
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.88	0.56
2:P:221:ASP:O	2:P:223:GLU:N	2.39	0.56
2:P:217:LYS:C	2:P:219:ALA:H	2.16	0.54
13:a:35:ARG:HH12	14:b:114:PRO:HB3	1.74	0.53
2:B:93:HIS:HB3	18:B:301:HOH:O	2.08	0.53
13:M:35:ARG:HH12	14:N:114:PRO:HB3	1.74	0.53
2:B:217:LYS:C	2:B:219:ALA:H	2.15	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.76	0.51
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.46	0.51
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.76	0.51
15:d:3:ALA:C	15:d:4:GAU:HG2	2.36	0.50
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.94	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.94	0.49
7:U:68:ARG:HH12	14:b:36:ARG:HH22	1.61	0.49
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.12	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.48
12:Z:179:GLU:HG3	18:Z:427:HOH:O	2.12	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.96	0.48
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.96	0.48
11:K:53:GLN:O	11:K:57:THR:HG23	2.14	0.48
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.96	0.48
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.95	0.48
15:c:3:ALA:C	15:c:4:GAU:HG2	2.39	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.47
3:C:9:PHE:H	4:D:15:GLN:HE22	1.61	0.47
15:c:5:POL:H12	18:c:101:HOH:O	2.13	0.47
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.47
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.47
13:M:35:ARG:NH1	14:N:114:PRO:HB3	2.30	0.47
13:a:35:ARG:HD3	13:a:36:PHE:CZ	2.50	0.47
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.50	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.50	0.46
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.46
13:a:35:ARG:NH1	14:b:114:PRO:HB3	2.30	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.46
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.98	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.97	0.46
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.46	0.46
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.46	0.46
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.98	0.45
7:U:23:PHE:O	7:U:26:THR:HB	2.16	0.45
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.57	0.45
1:O:12:PHE:H	2:P:20:GLN:HE22	1.65	0.45
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.99	0.45
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.52	0.45
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.57	0.45
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.99	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
14:N:24:ALA:HB3	13:a:146:PHE:HE2	1.81	0.44
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.65	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.44
7:G:23:PHE:O	7:G:26:THR:HB	2.18	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.53	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.53	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.44
2:P:113:ARG:NE	18:P:301:HOH:O	2.36	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.00	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.43
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.53	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.48	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.43
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.43
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.33	0.43
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.43
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.99	0.43
2:B:217:LYS:C	2:B:219:ALA:N	2.77	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.43
2:B:3:ARG:CB	5:E:122:TYR:OH	2.67	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.49	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.42
2:B:113:ARG:NE	18:B:301:HOH:O	2.36	0.42
13:M:146:PHE:HE2	14:b:24:ALA:HB3	1.84	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
10:J:91:SER:HG	10:J:98:TYR:H	1.65	0.42
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.42
10:J:25:ILE:O	10:X:139:TYR:OH	2.37	0.42
13:M:2:GLN:NE2	18:M:301:HOH:O	2.53	0.42
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.34	0.42
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.55	0.42
2:P:217:LYS:C	2:P:219:ALA:N	2.77	0.42
2:P:3:ARG:HB3	5:S:122:TYR:OH	2.20	0.41
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.03	0.41
4:D:99:ILE:HG23	18:D:314:HOH:O	2.21	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
13:M:187:ARG:HA	14:b:26:ILE:HB	2.01	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
14:b:1:THR:CG2	14:b:3:ILE:HG23	2.50	0.41
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.02	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
10:X:1:MET:CB	10:X:34:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:CB	10:J:34:LYS:HE3	2.51	0.41
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.03	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.04	0.40
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.40
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.04	0.40
13:a:2:GLN:NE2	18:a:302:HOH:O	2.55	0.40
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.04	0.40
9:I:170:LEU:C	9:I:170:LEU:HD23	2.46	0.40
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.57	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.04	0.40
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.03	0.40
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.52	0.40
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.40
9:W:170:LEU:C	9:W:170:LEU:HD23	2.46	0.40
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	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	49
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	49
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	13
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	13
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	18
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%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	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%)	189 (98%)	3 (2%)	1 (0%)	24	43
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
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	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30	49
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	30	49
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6288/6624 (95%)	6148 (98%)	121 (2%)	19 (0%)	36	55

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN

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Mol	Chain	Res	Type
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
10	J	24	GLY
10	X	24	GLY
13	M	229	GLY
13	a	229	GLY
3	Q	183	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	202 (97%)	7 (3%)	33	61
1	O	209/209 (100%)	202 (97%)	7 (3%)	33	61
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	60
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	60
3	C	212/226 (94%)	199 (94%)	13 (6%)	17	35
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	35
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	28
4	R	194/215 (90%)	180 (93%)	14 (7%)	13	28
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	52
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	52
6	F	201/239 (84%)	193 (96%)	8 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	54
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	50
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	50
8	H	185/190 (97%)	180 (97%)	5 (3%)	39	67
8	V	185/190 (97%)	180 (97%)	5 (3%)	39	67
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	78
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	83
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	65
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	47
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	47
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	62
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	62
13	M	199/208 (96%)	193 (97%)	6 (3%)	36	64
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	64
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	51
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
All	All	5322/5542 (96%)	5111 (96%)	211 (4%)	28	54

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	GLU
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
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
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	68	ARG
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	201	GLU
6	F	207	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	68	LEU
8	H	113	ILE
8	H	144	GLN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	69	ARG
11	K	107	LYS
11	K	118	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	212	LEU
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	59	GLU
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	201	GLU
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
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	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	52	LEU
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL

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Mol	Chain	Res	Type
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
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
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	68	ARG
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	207	ASP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	68	LEU
8	V	113	ILE
8	V	144	GLN
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU

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Mol	Chain	Res	Type
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	69	ARG
11	Y	107	LYS
11	Y	118	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	132	GLU
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	212	LEU
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN

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Mol	Chain	Res	Type
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	86	HIS
8	H	194	ASN
9	I	37	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN

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Mol	Chain	Res	Type
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	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	62	HIS
13	M	102	GLN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	141	ASN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN

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Mol	Chain	Res	Type
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
8	V	86	HIS
8	V	194	ASN
8	V	219	ASN
9	W	37	ASN
9	W	88	GLN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	61	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	135	GLN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN

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Mol	Chain	Res	Type
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	60	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GAU	c	4	15,14	8,8,8	1.35	2 (25%)	8,9,9	1.38	1 (12%)
15	GAU	d	4	15,14	8,8,8	1.31	1 (12%)	8,9,9	1.55	1 (12%)

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	GAU	c	4	15,14	-	2/7/7/7	-
15	GAU	d	4	15,14	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	4	GAU	C-CA	2.70	1.56	1.52
15	c	4	GAU	C-CA	2.67	1.56	1.52
15	c	4	GAU	OE2-CD	-2.39	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	GAU	CG-CB-CA	-3.67	105.04	112.87
15	c	4	GAU	CB-CA-N	-2.34	102.05	109.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	GAU	O-C-CA-CB
15	d	4	GAU	O-C-CA-CB
15	c	4	GAU	O-C-CA-N
15	d	4	GAU	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c	4	GAU	1	0
15	d	4	GAU	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.40	9 (3%) 46 41	31, 43, 77, 114	0
1	O	250/250 (100%)	0.60	19 (7%) 20 17	36, 52, 94, 125	0
2	B	244/258 (94%)	0.64	29 (11%) 9 7	30, 48, 89, 135	0
2	P	244/258 (94%)	0.75	28 (11%) 9 8	37, 54, 99, 145	0
3	C	240/254 (94%)	0.68	31 (12%) 7 6	31, 54, 115, 140	0
3	Q	240/254 (94%)	1.07	42 (17%) 4 3	36, 65, 144, 169	0
4	D	235/260 (90%)	0.69	17 (7%) 21 19	37, 56, 88, 132	0
4	R	235/260 (90%)	0.72	22 (9%) 14 12	40, 60, 99, 134	0
5	E	231/234 (98%)	0.77	22 (9%) 14 12	40, 58, 96, 144	0
5	S	231/234 (98%)	1.07	44 (19%) 3 2	41, 65, 107, 154	0
6	F	243/288 (84%)	0.59	24 (9%) 13 11	32, 50, 100, 130	0
6	T	243/288 (84%)	0.86	33 (13%) 7 5	36, 61, 120, 149	0
7	G	241/252 (95%)	0.38	10 (4%) 41 37	25, 45, 78, 130	0
7	U	241/252 (95%)	0.43	15 (6%) 26 23	34, 49, 81, 124	0
8	H	226/232 (97%)	0.46	11 (4%) 35 31	25, 41, 72, 133	0
8	V	226/232 (97%)	0.51	10 (4%) 39 34	32, 45, 74, 150	0
9	I	204/205 (99%)	0.13	4 (1%) 65 61	26, 39, 66, 90	0
9	W	204/205 (99%)	0.12	3 (1%) 72 68	30, 43, 71, 96	0
10	J	195/198 (98%)	0.27	6 (3%) 51 47	30, 44, 69, 126	0
10	X	195/198 (98%)	0.33	6 (3%) 51 47	30, 45, 70, 132	0
11	K	212/212 (100%)	0.25	7 (3%) 49 45	28, 44, 67, 89	0
11	Y	212/212 (100%)	0.29	8 (3%) 44 39	33, 45, 69, 88	0
12	L	222/222 (100%)	0.32	5 (2%) 61 57	30, 46, 77, 110	0
12	Z	222/222 (100%)	0.37	7 (3%) 50 46	30, 44, 75, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	0.20	6 (2%) 57 52	28, 43, 65, 83	0
13	a	233/246 (94%)	0.22	4 (1%) 69 65	28, 42, 62, 79	0
14	N	196/196 (100%)	0.26	7 (3%) 46 41	28, 39, 65, 94	0
14	b	196/196 (100%)	0.23	2 (1%) 79 76	28, 40, 65, 99	0
15	c	2/5 (40%)	-0.11	0 100 100	52, 52, 52, 54	0
15	d	2/5 (40%)	0.17	0 100 100	44, 44, 44, 51	0
All	All	6348/6624 (95%)	0.50	431 (6%) 23 20	25, 48, 93, 169	0

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	8.5
10	J	1	MET	8.0
10	X	1	MET	7.4
6	T	243	ILE	7.1
3	Q	49	THR	6.5
6	F	215	CYS	5.8
2	P	219	ALA	5.7
3	Q	205	ALA	5.7
4	D	241	ALA	5.7
13	a	1	THR	5.6
6	T	178	HIS	5.5
8	V	223	ILE	5.4
2	B	219	ALA	5.4
3	Q	50	LEU	5.3
2	P	218	GLY	5.2
5	S	122	TYR	5.1
3	C	205	ALA	4.9
2	P	220	ASN	4.8
2	P	222	GLY	4.7
6	T	14	ASP	4.7
3	Q	236	GLN	4.7
7	U	242	GLN	4.7
1	O	1	MET	4.6
14	b	103	ASP	4.6
1	A	2	THR	4.6
5	S	55	LEU	4.6
3	Q	189	CYS	4.5
1	O	2	THR	4.5
5	S	233	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
6	F	202	ASP	4.3
6	T	205	GLU	4.3
6	T	244	ASN	4.3
3	Q	231	VAL	4.2
8	H	224	GLN	4.2
14	b	195	GLN	4.2
10	X	194	ASP	4.1
5	S	200	LEU	4.1
2	B	221	ASP	4.1
2	P	59	ASP	4.1
3	C	51	LYS	4.1
4	D	240	ALA	4.0
2	P	52	THR	4.0
5	S	204	SER	3.9
3	C	207	ASN	3.9
5	E	233	ILE	3.9
9	W	1	SER	3.9
12	Z	174	TYR	3.9
2	P	55	LEU	3.8
1	A	1	MET	3.8
3	Q	175	LYS	3.8
4	R	113	LEU	3.8
3	Q	206	LYS	3.7
4	D	242	GLU	3.7
6	T	203	ASN	3.7
3	C	201	VAL	3.7
5	S	123	GLY	3.7
3	C	234	ILE	3.7
2	P	51	VAL	3.7
13	M	1	THR	3.7
2	P	244	THR	3.6
5	S	174	THR	3.6
3	Q	204	GLY	3.6
2	P	1	GLY	3.6
3	Q	234	ILE	3.6
6	F	178	HIS	3.5
5	S	52	ALA	3.5
6	T	55	LEU	3.5
10	X	193	ASP	3.5
6	T	204	LYS	3.5
4	D	183	LEU	3.5
5	E	207	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
6	T	202	ASP	3.4
8	V	224	GLN	3.4
5	S	180	LYS	3.4
12	L	174	TYR	3.4
5	S	51	ASN	3.4
12	L	172	LEU	3.4
6	T	182	GLY	3.4
3	Q	238	LYS	3.4
1	O	53	SER	3.4
3	Q	51	LYS	3.3
5	S	202	ASP	3.3
4	R	240	ALA	3.3
2	B	51	VAL	3.3
5	S	231	LYS	3.3
7	U	179	LYS	3.3
2	P	53	SER	3.3
4	R	99	ILE	3.3
3	Q	229	GLN	3.2
5	S	173	ARG	3.2
6	F	244	ASN	3.2
3	C	203	THR	3.2
1	O	250	LEU	3.2
4	R	233	LYS	3.2
3	Q	57	ILE	3.2
2	B	220	ASN	3.2
3	Q	46	ARG	3.2
3	Q	48	SER	3.2
5	S	57	SER	3.2
10	J	195	PHE	3.2
6	F	180	PRO	3.2
10	X	195	PHE	3.1
6	T	53	LYS	3.1
1	A	249	ALA	3.1
5	E	173	ARG	3.1
5	E	228	ALA	3.1
6	T	239	ALA	3.1
3	C	236	GLN	3.1
13	a	69	ASP	3.1
3	C	52	LEU	3.1
5	E	216	GLY	3.1
7	G	239	ILE	3.1
3	C	240	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
6	F	205	GLU	3.1
5	E	202	ASP	3.1
3	Q	207	ASN	3.1
2	B	1	GLY	3.1
8	H	91	GLN	3.0
5	S	58	TYR	3.0
10	J	194	ASP	3.0
3	Q	38	ASN	3.0
3	C	50	LEU	3.0
6	F	241	LYS	3.0
6	T	206	LYS	3.0
4	D	167	GLY	3.0
8	V	91	GLN	3.0
5	E	167	ALA	3.0
8	V	226	GLU	3.0
1	A	53	SER	3.0
2	B	2	SER	3.0
5	S	209	ASN	3.0
3	Q	239	GLN	3.0
3	C	48	SER	3.0
8	H	226	GLU	2.9
3	Q	203	THR	2.9
6	F	2	THR	2.9
4	D	238	LYS	2.9
2	B	222	GLY	2.9
2	P	58	GLN	2.9
3	C	53	GLN	2.9
4	R	239	GLU	2.9
3	Q	26	LYS	2.9
2	B	244	THR	2.9
1	O	61	LEU	2.9
7	U	3	TYR	2.9
3	C	239	GLN	2.9
3	Q	235	GLU	2.9
4	R	5	SER	2.9
9	I	160	GLU	2.9
6	T	2	THR	2.9
5	S	210	LEU	2.9
1	O	241	GLN	2.9
3	Q	237	GLU	2.9
3	C	204	GLY	2.9
5	E	123	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
6	F	203	ASN	2.8
6	T	241	LYS	2.8
7	U	181	LYS	2.8
5	S	205	LEU	2.8
3	Q	202	GLN	2.8
7	G	179	LYS	2.8
11	Y	208	ASN	2.8
2	B	62	THR	2.8
6	T	15	GLY	2.8
5	S	181	ILE	2.8
14	N	92	ASN	2.8
6	T	215	CYS	2.8
9	I	192	ASP	2.8
5	E	122	TYR	2.8
5	E	181	ILE	2.8
3	Q	223	SER	2.8
5	E	3	ASN	2.8
3	C	49	THR	2.8
5	S	112	CYS	2.8
3	Q	225	GLU	2.8
3	Q	240	GLU	2.8
11	K	116	ASP	2.8
6	T	198	LEU	2.7
5	E	190	LYS	2.7
8	H	222	ASP	2.7
3	Q	224	SER	2.7
6	T	176	VAL	2.7
9	I	1	SER	2.7
2	P	56	LEU	2.7
5	E	200	LEU	2.7
3	C	238	LYS	2.7
7	G	238	ALA	2.7
2	B	59	ASP	2.7
8	H	31	CYS	2.7
6	F	182	GLY	2.7
13	M	233	ILE	2.7
13	a	233	ILE	2.7
4	R	125	LEU	2.7
7	U	206	GLY	2.7
11	Y	212	GLY	2.7
3	C	221	ALA	2.7
5	S	203	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
5	S	170	TYR	2.6
4	R	203	LYS	2.6
6	T	164	GLY	2.6
8	V	221	CYS	2.6
2	B	238	LEU	2.6
8	H	9	ASN	2.6
1	O	248	GLU	2.6
4	R	238	LYS	2.6
3	C	12	ASP	2.6
5	S	53	ASP	2.6
11	K	184	GLY	2.6
11	Y	116	ASP	2.6
13	M	47	ASP	2.6
4	D	214	ILE	2.6
12	Z	132	GLU	2.6
2	P	180	LYS	2.6
2	P	235	LYS	2.6
6	F	204	LYS	2.6
12	Z	173	LYS	2.6
9	W	192	ASP	2.6
10	X	11	ASP	2.6
5	S	54	GLU	2.6
3	Q	53	GLN	2.6
2	P	60	THR	2.6
2	P	62	THR	2.6
3	Q	221	ALA	2.6
3	Q	232	THR	2.6
4	R	112	ALA	2.6
3	Q	201	VAL	2.5
1	A	177	LYS	2.5
2	B	217	LYS	2.5
5	S	121	SER	2.5
2	P	209	ARG	2.5
2	P	221	ASP	2.5
13	M	69	ASP	2.5
8	H	113	ILE	2.5
3	C	233	GLN	2.5
3	C	220	VAL	2.5
6	F	174	LYS	2.5
6	F	179	HIS	2.5
8	V	218	VAL	2.5
4	D	9	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	1	GLY	2.5
4	R	219	GLY	2.5
3	C	225	GLU	2.5
4	D	125	LEU	2.5
5	S	188	LEU	2.5
1	O	184	GLU	2.5
4	D	202	GLU	2.5
7	G	3	TYR	2.5
7	U	230	GLU	2.5
7	U	182	ILE	2.5
2	P	54	THR	2.5
3	Q	208	ILE	2.4
10	J	193	ASP	2.4
6	F	240	GLN	2.4
1	O	204	PHE	2.4
5	S	207	VAL	2.4
1	O	245	ASP	2.4
2	B	234	ILE	2.4
4	D	99	ILE	2.4
5	E	8	ASP	2.4
8	H	57	GLN	2.4
2	B	93	HIS	2.4
8	H	192	THR	2.4
6	F	201	GLU	2.4
9	W	160	GLU	2.4
12	L	173	LYS	2.4
1	O	206	GLY	2.4
6	T	212	ILE	2.4
6	T	236	ILE	2.4
7	G	182	ILE	2.4
1	O	247	LEU	2.4
3	Q	198	LEU	2.4
4	R	6	THR	2.4
6	T	194	LYS	2.4
7	U	180	SER	2.4
6	T	238	PHE	2.4
5	S	227	GLU	2.4
6	F	55	LEU	2.3
6	T	179	HIS	2.3
12	Z	1	GLN	2.3
14	N	103	ASP	2.3
2	B	63	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	R	230	GLU	2.3
3	Q	47	ARG	2.3
5	S	199	SER	2.3
2	B	243	ILE	2.3
4	R	224	ASP	2.3
6	F	177	ASP	2.3
6	F	175	LEU	2.3
4	D	1	ASP	2.3
11	K	118	ASP	2.3
7	U	178	LYS	2.3
2	B	15	GLU	2.3
5	S	3	ASN	2.3
1	O	52	SER	2.3
1	O	209	ILE	2.3
11	K	177	LEU	2.3
13	a	206	LEU	2.3
2	B	180	LYS	2.3
7	U	53	LYS	2.3
14	N	9	LYS	2.3
2	P	57	GLU	2.3
4	R	117	GLU	2.3
1	O	4	ARG	2.3
1	O	249	ALA	2.2
7	G	240	ALA	2.2
11	Y	209	ASN	2.2
5	S	169	THR	2.2
3	Q	233	GLN	2.2
4	D	3	GLY	2.2
7	U	2	GLY	2.2
14	N	195	GLN	2.2
1	O	55	LEU	2.2
2	B	40	SER	2.2
4	D	113	LEU	2.2
2	B	201	ASP	2.2
8	V	145	ASP	2.2
4	R	4	VAL	2.2
11	Y	128	CYS	2.2
2	B	54	THR	2.2
3	C	202	GLN	2.2
7	G	2	GLY	2.2
5	S	175	LEU	2.2
6	F	238	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	162	ALA	2.2
6	T	39	ASN	2.2
11	K	32	LYS	2.2
14	N	105	LYS	2.2
5	S	196	ILE	2.2
1	A	62	SER	2.2
1	O	168	SER	2.2
2	B	7	SER	2.2
3	C	223	SER	2.2
7	U	203	ASP	2.2
4	R	202	GLU	2.2
6	T	242	GLU	2.2
2	P	113	ARG	2.2
2	P	93	HIS	2.2
2	P	204	ALA	2.2
13	M	205	GLY	2.2
3	C	54	ASP	2.2
6	T	207	ASP	2.2
12	Z	26	ASP	2.2
14	N	84	GLU	2.2
6	F	206	LYS	2.2
6	T	200	HIS	2.1
3	Q	173	LEU	2.1
5	E	7	GLY	2.1
5	E	9	THR	2.1
7	G	31	ILE	2.1
7	U	202	ILE	2.1
8	H	223	ILE	2.1
5	E	172	GLU	2.1
5	E	201	ARG	2.1
7	G	68	ARG	2.1
4	D	224	ASP	2.1
1	A	231	LYS	2.1
2	B	231	PRO	2.1
5	S	190	LYS	2.1
12	L	119	LYS	2.1
5	S	178	PHE	2.1
11	Y	97	MET	2.1
11	K	24	ASN	2.1
3	Q	222	LEU	2.1
12	Z	172	LEU	2.1
1	O	191	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	25	ILE	2.1
4	R	242	GLU	2.1
7	U	241	GLU	2.1
11	Y	203	GLU	2.1
6	F	207	ASP	2.1
5	E	117	LYS	2.1
6	T	163	LYS	2.1
10	X	174	MET	2.1
5	S	10	VAL	2.1
5	S	59	GLN	2.1
5	E	195	ALA	2.1
13	M	37	ASN	2.1
5	E	171	LEU	2.1
2	B	52	THR	2.1
11	K	106	ARG	2.1
2	P	223	GLU	2.1
4	R	237	GLU	2.1
5	S	172	GLU	2.1
6	T	187	GLU	2.1
12	Z	161	GLU	2.1
2	B	19	TYR	2.1
6	F	190	LYS	2.1
3	Q	39	CYS	2.1
4	D	182	SER	2.1
2	P	176	GLN	2.1
3	C	229	GLN	2.1
2	B	204	ALA	2.1
3	C	228	ASN	2.1
3	Q	52	LEU	2.1
6	T	29	ASN	2.1
1	A	202	GLY	2.1
11	Y	189	GLY	2.1
1	A	201	GLU	2.1
8	V	215	GLU	2.1
8	V	225	GLU	2.1
12	L	189	THR	2.1
3	C	153	ILE	2.1
5	S	179	ILE	2.1
9	I	191	LYS	2.1
6	T	197	TYR	2.1
2	P	169	SER	2.1
3	C	224	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	183	PRO	2.1
3	Q	59	PRO	2.1
2	P	183	MET	2.1
4	R	2	ARG	2.0
5	E	227	GLU	2.0
6	F	171	GLU	2.0
6	F	187	GLU	2.0
3	C	175	LYS	2.0
7	U	24	LYS	2.0
8	V	94	ILE	2.0
2	B	187	ASP	2.0
10	J	147	HIS	2.0
4	R	114	ARG	2.0
5	S	201	ARG	2.0
8	H	196	ARG	2.0
3	C	198	LEU	2.0
4	D	185	LEU	2.0
5	S	25	LEU	2.0
4	R	167	GLY	2.0
5	S	128	GLY	2.0
14	N	106	ASN	2.0
7	G	40	ASP	2.0
2	B	5	TYR	2.0
5	S	32	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	GAU	d	4	9/9	0.85	0.14	48,52,53,57	0
15	GAU	c	4	9/9	0.87	0.16	56,59,62,63	0

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
16	MG	I	301	1/1	0.91	0.09	63,63,63,63	0
16	MG	K	301	1/1	0.94	0.15	42,42,42,42	0
16	MG	L	301	1/1	0.95	0.11	48,48,48,48	0
16	MG	G	301	1/1	0.97	0.06	43,43,43,43	0
16	MG	N	201	1/1	0.97	0.08	47,47,47,47	0
16	MG	Z	301	1/1	0.97	0.05	50,50,50,50	0
17	CL	G	302	1/1	0.98	0.10	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.08	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.