



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 09:14 PM BST

PDB ID : 4YA3
Title : Yeast 20S proteasome beta2-H116N mutant in complex with Ac-PAE-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-17
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

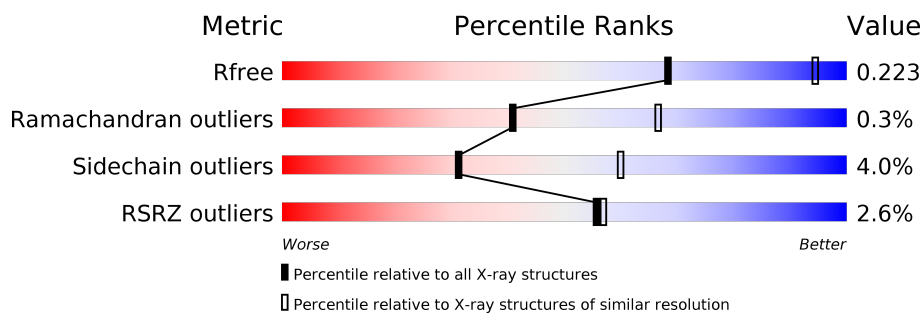
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>4%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>3%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>3%</div> <div>90%</div> <div>5%</div> </div>
2	P	258	<div> <div>5%</div> <div>90%</div> <div>5%</div> </div>
3	C	254	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>6%</div> </div>
3	Q	254	<div> <div>8%</div> <div>89%</div> <div>6%</div> <div>6%</div> </div>
4	D	260	<div> <div>%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
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 49911 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	297	333	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	297	333	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	ASN	HIS	conflict	UNP P25043
V	116	ASN	HIS	conflict	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	20	Total	O	0	0
			20	20		
18	B	16	Total	O	0	0
			16	16		
18	C	15	Total	O	0	0
			15	15		
18	D	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	E	9	Total O 9 9	0	0
18	F	12	Total O 12 12	0	0
18	G	29	Total O 29 29	0	0
18	H	27	Total O 27 27	0	0
18	I	13	Total O 13 13	0	0
18	J	21	Total O 21 21	0	0
18	K	20	Total O 20 20	0	0
18	L	30	Total O 30 30	0	0
18	M	23	Total O 23 23	0	0
18	N	17	Total O 17 17	0	0
18	O	11	Total O 11 11	0	0
18	P	8	Total O 8 8	0	0
18	Q	9	Total O 9 9	0	0
18	R	9	Total O 9 9	0	0
18	S	10	Total O 10 10	0	0
18	T	19	Total O 19 19	0	0
18	U	29	Total O 29 29	0	0
18	V	21	Total O 21 21	0	0
18	W	14	Total O 14 14	0	0
18	X	16	Total O 16 16	0	0
18	Y	21	Total O 21 21	0	0

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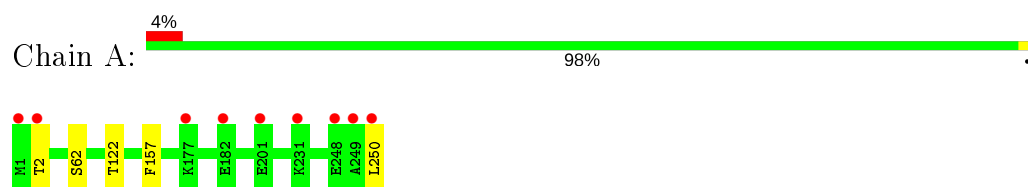
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	Z	18	Total 18	O 18	0	0
18	a	26	Total 26	O 26	0	0
18	b	14	Total 14	O 14	0	0
18	d	1	Total 1	O 1	0	0

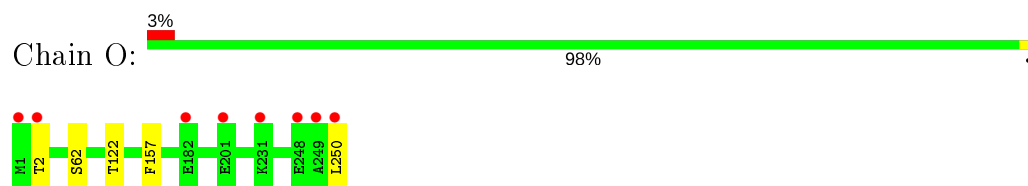
3 Residue-property plots [i](#)

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

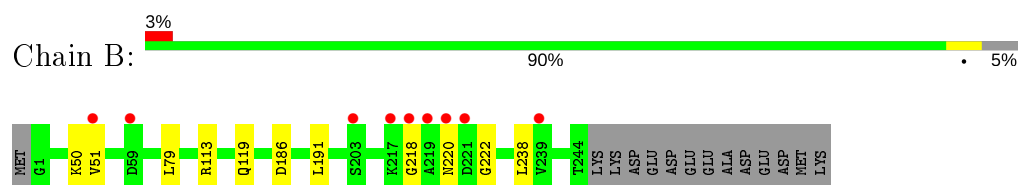
- Molecule 1: Proteasome subunit alpha type-2



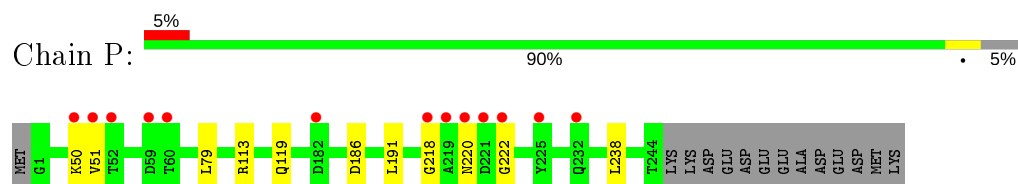
- Molecule 1: Proteasome subunit alpha type-2



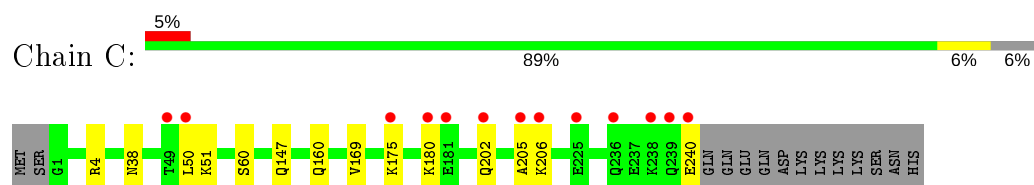
- Molecule 2: Proteasome subunit alpha type-3



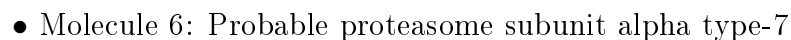
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-4



- Molecule 3: Proteasome subunit alpha type-4







- Molecule 10: Proteasome subunit beta type-4



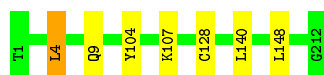
- Molecule 10: Proteasome subunit beta type-4



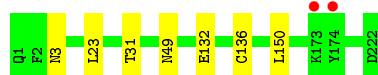
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



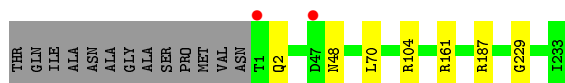
- Molecule 12: Proteasome subunit beta type-6



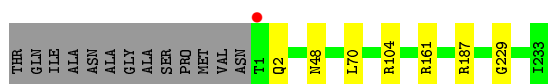
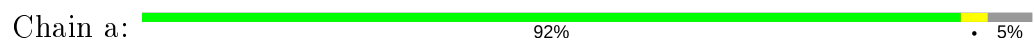
- Molecule 12: Proteasome subunit beta type-6



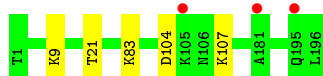
- Molecule 13: Proteasome subunit beta type-7



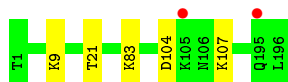
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



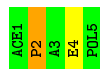
- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: Ac-PAE-ep



- Molecule 15: Ac-PAE-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.50Å 301.36Å 145.84Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.70) 96.9 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.220 0.205 , 0.223	Depositor DCC
R_{free} test set	14322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49911	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POL, GAU, ACE, 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	0.29	0/1952	0.47	0/2642
1	O	0.29	0/1952	0.47	0/2642
2	B	0.29	0/1934	0.50	0/2618
2	P	0.29	0/1934	0.51	0/2618
3	C	0.29	0/1910	0.52	0/2586
3	Q	0.29	0/1910	0.51	0/2586
4	D	0.28	0/1837	0.49	0/2475
4	R	0.28	0/1837	0.49	0/2475
5	E	0.28	0/1800	0.48	0/2433
5	S	0.28	0/1800	0.48	0/2433
6	F	0.29	0/1932	0.46	0/2609
6	T	0.28	0/1932	0.46	0/2609
7	G	0.29	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.30	0/1747	0.49	0/2369
8	V	0.28	0/1747	0.48	0/2369
9	I	0.30	0/1611	0.49	0/2174
9	W	0.31	0/1611	0.49	0/2174
10	J	0.30	0/1589	0.50	0/2142
10	X	0.28	0/1589	0.49	0/2142
11	K	0.29	0/1681	0.51	1/2274 (0.0%)
11	Y	0.27	0/1681	0.51	1/2274 (0.0%)
12	L	0.29	0/1795	0.50	0/2420
12	Z	0.29	0/1795	0.50	0/2420
13	M	0.29	0/1855	0.51	0/2514
13	a	0.29	0/1855	0.51	0/2514
14	N	0.35	0/1541	0.51	0/2087
14	b	0.34	0/1541	0.50	0/2087
15	c	2.69	1/13 (7.7%)	1.44	0/18
15	d	2.62	1/13 (7.7%)	1.34	0/18
All	All	0.30	2/50284 (0.0%)	0.49	2/67990 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	2	PRO	CA-C	-7.67	1.37	1.52
15	c	2	PRO	CA-C	-7.31	1.38	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.18	127.20	115.30
11	Y	4	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	238 (96%)	9 (4%)	1 (0%)	34	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	23
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	23
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	43
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	43
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	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%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	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%)	29	54
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	54
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%)	224 (97%)	6 (3%)	1 (0%)	34	60
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	60
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%)	6140 (98%)	130 (2%)	18 (0%)	41	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR

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Mol	Chain	Res	Type
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

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	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	200 (94%)	12 (6%)	20	44
3	Q	212/226 (94%)	200 (94%)	12 (6%)	20	44
4	D	194/215 (90%)	181 (93%)	13 (7%)	16	37
4	R	194/215 (90%)	181 (93%)	13 (7%)	16	37
5	E	190/193 (98%)	178 (94%)	12 (6%)	18	40
5	S	190/193 (98%)	178 (94%)	12 (6%)	18	40
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	206/210 (98%)	194 (94%)	12 (6%)	20	43
7	U	206/210 (98%)	194 (94%)	12 (6%)	20	43
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	79
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	88
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	78
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	59
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	59
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	62
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
15	c	1/1 (100%)	0	1 (100%)	0	0
15	d	1/1 (100%)	0	1 (100%)	0	0
All	All	5322/5542 (96%)	5107 (96%)	215 (4%)	31	60

All (215) 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
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
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	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
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
6	F	240	GLN
7	G	13	GLU

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Mol	Chain	Res	Type
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	178	LYS
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	192	ASP
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	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
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	21	THR
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	79	LEU
2	P	113	ARG
2	P	119	GLN
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	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
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

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Mol	Chain	Res	Type
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
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	13	GLU
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	178	LYS
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	113	ILE
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG

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Mol	Chain	Res	Type
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	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
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	21	THR
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
15	c	2	PRO
15	d	2	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) 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
2	B	176	GLN

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Mol	Chain	Res	Type
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	114	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
10	J	147	HIS
11	K	85	ASN
11	K	176	ASN

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Mol	Chain	Res	Type
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	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
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
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	30	ASN

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Mol	Chain	Res	Type
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	66	HIS
8	V	114	HIS
8	V	165	ASN
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	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	5,8,8	1.52	1 (20%)	5,9,9	1.67	2 (40%)
15	GAU	d	4	15,14	5,8,8	1.46	1 (20%)	5,9,9	1.66	2 (40%)

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	-	0/5/7/7	-
15	GAU	d	4	15,14	-	2/5/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	GAU	C-CA	2.94	1.57	1.52
15	d	4	GAU	C-CA	2.65	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	GAU	CB-CA-N	-2.79	100.94	109.03
15	c	4	GAU	CB-CA-N	-2.72	101.12	109.03
15	c	4	GAU	CG-CB-CA	-2.31	107.90	112.74
15	d	4	GAU	CG-CB-CA	-2.10	108.33	112.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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%)	-0.31	9 (3%) 42 42	40, 53, 88, 130	0
1	O	250/250 (100%)	-0.22	8 (3%) 47 48	46, 63, 107, 134	0
2	B	244/258 (94%)	-0.18	9 (3%) 41 41	41, 59, 101, 151	0
2	P	244/258 (94%)	-0.04	13 (5%) 26 25	49, 66, 110, 158	0
3	C	240/254 (94%)	-0.08	13 (5%) 25 24	42, 64, 126, 151	0
3	Q	240/254 (94%)	0.15	20 (8%) 11 9	50, 77, 151, 174	0
4	D	235/260 (90%)	-0.25	2 (0%) 84 85	49, 67, 98, 139	0
4	R	235/260 (90%)	-0.13	6 (2%) 56 57	51, 71, 110, 139	0
5	E	231/234 (98%)	-0.06	11 (4%) 30 28	50, 70, 109, 157	0
5	S	231/234 (98%)	0.07	11 (4%) 30 28	53, 77, 120, 166	0
6	F	243/288 (84%)	-0.32	5 (2%) 63 65	44, 61, 109, 137	0
6	T	243/288 (84%)	-0.11	8 (3%) 46 46	48, 72, 126, 156	0
7	G	241/252 (95%)	-0.41	3 (1%) 79 80	36, 55, 87, 137	0
7	U	241/252 (95%)	-0.29	5 (2%) 63 65	44, 59, 91, 133	0
8	H	226/232 (97%)	-0.27	6 (2%) 54 55	38, 53, 86, 149	0
8	V	226/232 (97%)	-0.22	9 (3%) 38 37	44, 56, 89, 170	0
9	I	204/205 (99%)	-0.59	2 (0%) 82 83	39, 51, 79, 106	0
9	W	204/205 (99%)	-0.46	3 (1%) 73 76	43, 55, 84, 109	0
10	J	195/198 (98%)	-0.46	2 (1%) 82 83	41, 55, 78, 133	0
10	X	195/198 (98%)	-0.41	2 (1%) 82 83	42, 57, 80, 143	0
11	K	212/212 (100%)	-0.43	2 (0%) 84 85	39, 57, 79, 100	0
11	Y	212/212 (100%)	-0.42	0 100 100	43, 56, 79, 99	0
12	L	222/222 (100%)	-0.42	2 (0%) 84 85	41, 56, 90, 123	0
12	Z	222/222 (100%)	-0.42	4 (1%) 68 70	36, 55, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.49	2 (0%) 84 85	39, 54, 75, 96	0
13	a	233/246 (94%)	-0.44	1 (0%) 92 93	39, 54, 74, 93	0
14	N	196/196 (100%)	-0.52	3 (1%) 73 76	37, 49, 76, 104	0
14	b	196/196 (100%)	-0.50	2 (1%) 82 83	39, 51, 76, 111	0
15	c	2/5 (40%)	-0.64	0 100 100	60, 60, 60, 63	0
15	d	2/5 (40%)	-1.01	0 100 100	54, 54, 54, 59	0
All	All	6348/6624 (95%)	-0.29	163 (2%) 56 57	36, 60, 104, 174	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	218	GLY	7.0
10	X	1	MET	6.5
3	Q	49	THR	6.5
3	Q	50	LEU	6.4
3	Q	206	LYS	6.3
3	C	50	LEU	6.1
3	C	206	LYS	6.1
2	B	51	VAL	5.9
8	V	224	GLN	5.5
9	W	1	SER	5.5
2	P	51	VAL	5.4
3	C	49	THR	5.2
3	Q	239	GLN	5.1
2	P	59	ASP	5.1
5	S	202	ASP	4.9
5	E	202	ASP	4.8
10	J	1	MET	4.7
12	L	174	TYR	4.6
2	P	221	ASP	4.4
2	B	218	GLY	4.3
8	V	226	GLU	4.3
3	Q	236	GLN	4.3
10	X	194	ASP	4.3
1	A	1	MET	4.2
8	V	221	CYS	4.1
2	B	220	ASN	3.9
8	H	226	GLU	3.8
1	O	1	MET	3.8
5	S	227	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
12	Z	174	TYR	3.7
1	A	2	THR	3.7
3	Q	48	SER	3.7
8	V	222	ASP	3.7
2	P	219	ALA	3.7
7	U	242	GLN	3.6
1	A	249	ALA	3.6
2	B	221	ASP	3.6
1	O	2	THR	3.5
3	Q	187	GLU	3.5
9	I	1	SER	3.5
13	a	1	THR	3.4
2	P	220	ASN	3.4
2	B	219	ALA	3.4
10	J	194	ASP	3.3
6	T	244	ASN	3.3
1	O	231	LYS	3.3
3	Q	240	GLU	3.3
3	Q	202	GLN	3.3
5	E	122	TYR	3.2
7	U	222	ASP	3.2
5	S	180	LYS	3.2
2	B	59	ASP	3.2
8	H	224	GLN	3.2
3	C	238	LYS	3.2
6	F	244	ASN	3.1
6	F	205	GLU	3.1
3	C	202	GLN	3.1
6	T	243	ILE	3.1
8	V	223	ILE	3.1
1	O	201	GLU	3.1
6	T	230	ASP	3.0
13	M	47	ASP	3.0
3	C	236	GLN	3.0
8	H	223	ILE	3.0
2	P	222	GLY	2.9
9	W	133	LYS	2.9
3	C	239	GLN	2.9
4	R	125	LEU	2.9
8	V	225	GLU	2.9
14	N	105	LYS	2.9
4	R	242	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
8	H	222	ASP	2.8
3	Q	205	ALA	2.8
3	C	180	LYS	2.8
3	C	240	GLU	2.8
6	F	215	CYS	2.8
6	T	215	CYS	2.8
14	b	195	GLN	2.7
3	Q	229	GLN	2.7
4	R	230	GLU	2.7
5	S	173	ARG	2.7
9	I	133	LYS	2.7
5	E	123	GLY	2.7
8	H	198	GLU	2.6
8	V	91	GLN	2.6
1	O	250	LEU	2.6
2	P	60	THR	2.6
3	C	205	ALA	2.6
3	C	225	GLU	2.6
8	H	221	CYS	2.6
12	L	173	LYS	2.6
3	Q	47	ARG	2.6
5	E	217	LYS	2.5
6	T	204	LYS	2.5
14	N	195	GLN	2.5
1	A	201	GLU	2.5
7	U	3	TYR	2.5
4	R	217	GLN	2.5
12	Z	1	GLN	2.5
11	K	23	GLY	2.5
2	P	182	ASP	2.5
5	S	194	GLU	2.5
3	Q	225	GLU	2.4
5	S	54	GLU	2.4
6	T	205	GLU	2.4
7	G	188	GLU	2.4
5	S	58	TYR	2.4
12	Z	165	ASN	2.4
1	O	248	GLU	2.4
3	Q	180	LYS	2.4
4	R	241	ALA	2.4
2	B	203	SER	2.4
5	S	30	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
8	V	145	ASP	2.4
4	D	242	GLU	2.4
5	S	201	ARG	2.4
6	T	241	LYS	2.4
5	E	173	ARG	2.3
14	N	181	ALA	2.3
1	O	249	ALA	2.3
6	T	181	GLU	2.3
11	K	212	GLY	2.3
3	Q	237	GLU	2.2
2	P	225	TYR	2.2
7	U	181	LYS	2.2
6	F	2	THR	2.2
7	U	2	GLY	2.2
1	O	182	GLU	2.2
3	C	181	GLU	2.2
7	G	230	GLU	2.2
1	A	231	LYS	2.2
7	G	179	LYS	2.2
3	Q	203	THR	2.2
9	W	192	ASP	2.2
3	Q	216	ASP	2.1
14	b	105	LYS	2.1
5	S	233	ILE	2.1
2	P	232	GLN	2.1
4	D	125	LEU	2.1
5	E	233	ILE	2.1
1	A	182	GLU	2.1
5	E	54	GLU	2.1
3	Q	223	SER	2.1
3	C	175	LYS	2.1
1	A	177	LYS	2.1
5	E	194	GLU	2.1
6	F	181	GLU	2.1
13	M	1	THR	2.1
1	A	250	LEU	2.1
4	R	226	GLU	2.1
5	E	117	LYS	2.1
5	E	207	VAL	2.1
2	B	217	LYS	2.1
2	P	50	LYS	2.1
2	P	52	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	232	THR	2.1
5	S	187	GLU	2.1
12	Z	210	ASP	2.1
3	Q	181	GLU	2.0
8	V	9	ASN	2.0
2	B	239	VAL	2.0
5	E	227	GLU	2.0
1	A	248	GLU	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	0.96	0.15	53,61,64,64	0
15	GAU	c	4	9/9	0.97	0.12	57,66,71,72	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	N	201	1/1	0.93	0.12	53,53,53,53	0
16	MG	G	301	1/1	0.95	0.10	51,51,51,51	0
17	CL	U	301	1/1	0.95	0.27	30,30,30,30	0
16	MG	Z	301	1/1	0.96	0.30	60,60,60,60	0
16	MG	I	301	1/1	0.96	0.38	67,67,67,67	0
17	CL	G	302	1/1	0.97	0.19	30,30,30,30	0
16	MG	V	301	1/1	0.98	0.05	67,67,67,67	0
16	MG	Y	301	1/1	0.99	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	K	301	1/1	0.99	0.07	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.