



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:24 AM GMT

PDB ID : 3UN4
Title : Yeast 20S proteasome in complex with PR-957 (morpholine)
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

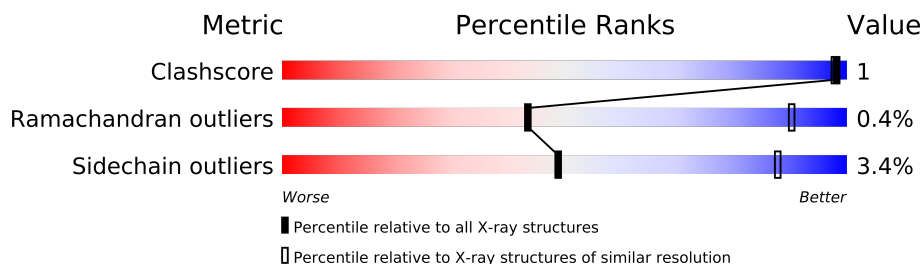
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	258	
2	P	258	
3	C	254	
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	

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Mol	Chain	Length	Quality of chain
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51112 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

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

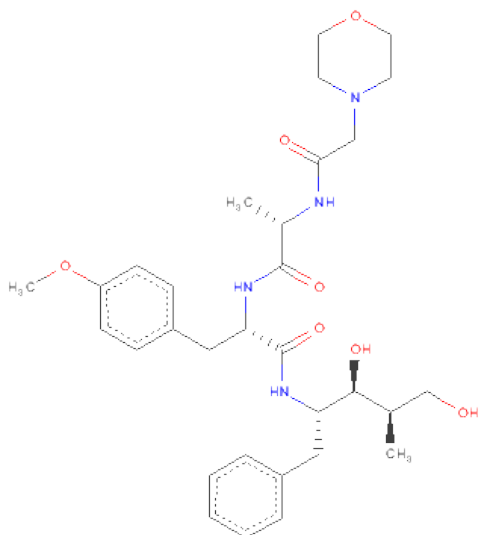
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is 1,2,4-TRIDEOXY-4-METHYL-2-{[N-(MORPHOLIN-4-YLACETYL)-L-ALANYL-O-METHYL-L-TYROSYL]AMINO}-1-PHENYL-D-XYLITOL (three-letter code: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	23	Total	O	0	0
			23	23		
16	F	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	61	Total O 61 61	0	0
16	H	49	Total O 49 49	0	0
16	I	62	Total O 62 62	0	0
16	J	54	Total O 54 54	0	0
16	K	46	Total O 46 46	0	0
16	L	55	Total O 55 55	0	0
16	M	72	Total O 72 72	0	0
16	N	51	Total O 51 51	0	0
16	O	32	Total O 32 32	0	0
16	P	30	Total O 30 30	0	0
16	Q	30	Total O 30 30	0	0
16	R	27	Total O 27 27	0	0
16	S	20	Total O 20 20	0	0
16	T	41	Total O 41 41	0	0
16	U	61	Total O 61 61	0	0
16	V	45	Total O 45 45	0	0
16	W	57	Total O 57 57	0	0
16	X	52	Total O 52 52	0	0
16	Y	49	Total O 49 49	0	0
16	Z	50	Total O 50 50	0	0
16	a	75	Total O 75 75	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	58	Total	O	0	0
			58	58		

3 Residue-property plots

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

Note EDS failed to run properly.

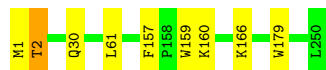
- Molecule 1: Proteasome component Y7

Chain A: 



- Molecule 1: Proteasome component Y7

Chain O: 



- Molecule 2: Proteasome component Y13

Chain B: 



- Molecule 2: Proteasome component Y13

Chain P: 



- Molecule 3: Proteasome component PRE6

Chain C: 



- Molecule 3: Proteasome component PRE6

Chain Q: 



- Molecule 4: Proteasome component PUP2

Chain D: 



- Molecule 4: Proteasome component PUP2

Chain R: 



- Molecule 5: Proteasome component PRE5

Chain E: 



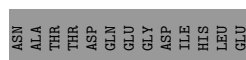
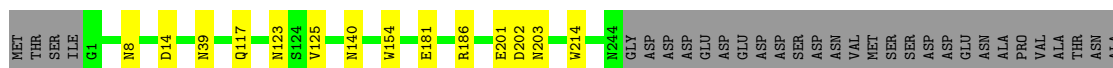
- Molecule 5: Proteasome component PRE5

Chain S: 



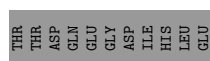
- Molecule 6: Proteasome component C1

Chain F: 



- Molecule 6: Proteasome component C1

Chain T: 



- Molecule 7: Proteasome component C7-alpha

Chain G: 



- Molecule 7: Proteasome component C7-alpha

Chain U:



- Molecule 8: Proteasome component PUP1

Chain H:



- Molecule 8: Proteasome component PUP1

Chain V:



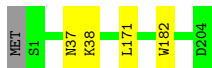
- Molecule 9: Proteasome component PUP3

Chain I:



- Molecule 9: Proteasome component PUP3

Chain W:



- Molecule 10: Proteasome component C11

Chain J:



- Molecule 10: Proteasome component C11

Chain X:



- Molecule 11: Proteasome component PRE2

Chain K:



- Molecule 11: Proteasome component PRE2

Chain Y:



- Molecule 12: Proteasome component C5

Chain L:



- Molecule 12: Proteasome component C5

Chain Z:



- Molecule 13: Proteasome component PRE4

Chain M:



- Molecule 13: Proteasome component PRE4

Chain a:



- Molecule 14: Proteasome component PRE3

Chain N:



- Molecule 14: Proteasome component PRE3

Chain b:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.41Å 300.78Å 143.82Å 90.00° 112.75° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40	Depositor
% Data completeness (in resolution range)	98.3 (15.00-3.40)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.179 , 0.219	Depositor
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.786	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 141633 reflections	Xtriage
Total number of atoms	51112	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	2/1952 (0.1%)	0.48	0/2642
1	O	0.36	2/1952 (0.1%)	0.48	0/2642
2	B	0.33	0/1934	0.48	0/2618
2	P	0.33	0/1934	0.48	0/2618
3	C	0.34	0/1919	0.49	0/2598
3	Q	0.33	0/1919	0.49	0/2598
4	D	0.36	0/1886	0.50	0/2541
4	R	0.35	0/1886	0.50	0/2541
5	E	0.31	0/1823	0.48	0/2463
5	S	0.30	0/1823	0.48	0/2463
6	F	0.41	1/1936 (0.1%)	0.47	0/2614
6	T	0.40	0/1936	0.47	0/2614
7	G	0.34	0/1959	0.48	0/2652
7	U	0.34	0/1959	0.48	0/2652
8	H	0.46	1/1715 (0.1%)	0.48	0/2326
8	V	0.46	2/1715 (0.1%)	0.49	0/2326
9	I	0.35	1/1611 (0.1%)	0.49	0/2174
9	W	0.34	0/1611	0.49	0/2174
10	J	0.31	0/1613	0.48	0/2173
10	X	0.31	0/1613	0.48	0/2173
11	K	0.52	3/1681 (0.2%)	0.52	1/2274 (0.0%)
11	Y	0.52	3/1681 (0.2%)	0.52	1/2274 (0.0%)
12	L	0.36	0/1795	0.50	0/2420
12	Z	0.36	0/1795	0.50	0/2420
13	M	0.36	1/1855 (0.1%)	0.50	0/2514
13	a	0.36	0/1855	0.50	0/2514
14	N	0.43	1/1541 (0.1%)	0.49	1/2087 (0.0%)
14	b	0.43	1/1541 (0.1%)	0.51	1/2087 (0.0%)
All	All	0.38	18/50440 (0.0%)	0.49	4/68192 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	b	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1	THR	C-N	6.64	1.49	1.34
14	N	1	THR	C-N	6.25	1.48	1.34
8	V	1	THR	C-N	5.61	1.47	1.34
11	K	1	THR	C-N	5.37	1.46	1.34
8	H	1	THR	C-N	5.34	1.46	1.34
11	Y	1	THR	C-N	5.12	1.45	1.34
6	F	154	TRP	CD2-CE2	5.07	1.47	1.41
13	M	219	TRP	CD2-CE2	5.05	1.47	1.41
1	O	159	TRP	CD2-CE2	5.04	1.47	1.41
8	V	142	TRP	CD2-CE2	5.04	1.47	1.41
1	A	159	TRP	CD2-CE2	5.04	1.47	1.41
11	Y	146	TRP	CD2-CE2	5.02	1.47	1.41
11	Y	58	TRP	CD2-CE2	5.02	1.47	1.41
1	A	179	TRP	CD2-CE2	5.02	1.47	1.41
1	O	179	TRP	CD2-CE2	5.01	1.47	1.41
9	I	182	TRP	CD2-CE2	5.01	1.47	1.41
11	K	58	TRP	CD2-CE2	5.01	1.47	1.41
11	K	146	TRP	CD2-CE2	5.00	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1	THR	N-CA-C	6.01	127.24	111.00
11	Y	4	LEU	CA-CB-CG	5.22	127.30	115.30
11	K	4	LEU	CA-CB-CG	5.21	127.27	115.30
14	N	1	THR	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	b	1	THR	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	0	2	0
1	O	1915	0	0	2	0
2	B	1904	0	0	0	0
2	P	1904	0	0	2	0
3	C	1890	0	0	0	0
3	Q	1890	0	0	1	0
4	D	1861	0	0	0	0
4	R	1861	0	0	0	0
5	E	1795	0	0	0	0
5	S	1795	0	0	1	0
6	F	1896	0	0	2	0
6	T	1896	0	0	2	0
7	G	1921	0	0	0	0
7	U	1921	0	0	0	0
8	H	1684	0	0	2	0
8	V	1684	0	0	1	0
9	I	1581	0	0	2	0
9	W	1581	0	0	1	0
10	J	1585	0	0	3	0
10	X	1585	0	0	3	0
11	K	1644	0	0	2	0
11	Y	1644	0	0	2	0
12	L	1757	0	0	0	0
12	Z	1757	0	0	2	0
13	M	1824	0	0	2	0
13	a	1824	0	0	0	0
14	N	1512	0	0	1	0
14	b	1512	0	0	0	0
15	H	42	0	0	0	0
15	K	42	0	0	0	0
15	N	42	0	0	0	0
15	V	42	0	0	0	0
15	Y	42	0	0	0	0
15	b	42	0	0	0	0
16	A	56	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	38	0	0	0	0
16	C	42	0	0	0	0
16	D	38	0	0	0	0
16	E	23	0	0	0	0
16	F	48	0	0	0	0
16	G	61	0	0	0	0
16	H	49	0	0	0	0
16	I	62	0	0	0	0
16	J	54	0	0	1	0
16	K	46	0	0	0	0
16	L	55	0	0	0	0
16	M	72	0	0	0	0
16	N	51	0	0	0	0
16	O	32	0	0	0	0
16	P	30	0	0	0	0
16	Q	30	0	0	0	0
16	R	27	0	0	0	0
16	S	20	0	0	0	0
16	T	41	0	0	0	0
16	U	61	0	0	0	0
16	V	45	0	0	0	0
16	W	57	0	0	0	0
16	X	52	0	0	1	0
16	Y	49	0	0	0	0
16	Z	50	0	0	0	0
16	a	75	0	0	0	0
16	b	58	0	0	0	0
All	All	51112	0	0	26	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:73:ARG:NH2	11:K:104:TYR:O	2.27	0.67
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.28	0.67
10:J:139:TYR:CD1	16:J:228:HOH:O	2.53	0.56
10:J:25:ILE:O	10:X:139:TYR:OH	2.23	0.56
10:J:139:TYR:OH	10:X:25:ILE:O	2.24	0.55
14:N:1:THR:CG2	14:N:2:SER:N	2.70	0.55
6:F:8:ASN:ND2	6:F:125:VAL:O	2.43	0.52
6:T:8:ASN:ND2	6:T:125:VAL:O	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:206:PRO:O	8:H:209:THR:OG1	2.34	0.46
8:V:206:PRO:O	8:V:209:THR:OG1	2.35	0.45
9:I:37:ASN:ND2	9:I:37:ASN:N	2.64	0.45
6:F:14:ASP:N	6:F:14:ASP:OD2	2.51	0.44
6:T:14:ASP:N	6:T:14:ASP:OD2	2.50	0.44
5:S:92:ASN:ND2	12:Z:70:ASN:ND2	2.67	0.43
1:A:1:MET:SD	1:A:2:THR:N	2.93	0.42
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.37	0.42
11:K:209:ASN:O	9:W:38:LYS:NZ	2.53	0.42
13:M:1:THR:N	13:M:107:MET:O	2.53	0.41
13:M:48:ASN:ND2	13:M:48:ASN:N	2.68	0.41
11:Y:10:GLY:O	11:Y:179:HIS:NE2	2.54	0.41
1:O:160:LYS:N	2:P:55:LEU:O	2.53	0.41
8:H:174:ASP:OD2	8:H:188:ARG:NH1	2.54	0.41
12:Z:48:ASP:OD2	12:Z:84:LEU:N	2.54	0.41
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.54	0.41
10:X:142:SER:N	16:X:211:HOH:O	2.54	0.40
1:O:1:MET:SD	1:O:2:THR:N	2.95	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%)	7 (3%)	2 (1%)	27	81
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	27	81
2	B	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	27	81
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	27	81
3	C	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	18	72
3	Q	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	18	72
4	D	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	18	72
4	R	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	18	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	43	90
5	S	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	43	90
6	F	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
6	T	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
7	U	241/252 (96%)	231 (96%)	10 (4%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	210 (96%)	10 (4%)	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	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	38	87
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	38	87
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	38	87
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	38	87
12	L	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	7 (4%)	1 (0%)	38	87
All	All	6312/6588 (96%)	6042 (96%)	243 (4%)	27 (0%)	43	90

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	166	LYS
3	C	203	THR
4	D	122	GLU
5	E	201	ARG
1	O	166	LYS
3	Q	203	THR
4	R	122	GLU
5	S	201	ARG

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Mol	Chain	Res	Type
14	b	2	SER
1	A	2	THR
2	B	221	ASP
4	D	121	GLY
11	K	39	PRO
1	O	2	THR
2	P	221	ASP
4	R	121	GLY
11	Y	39	PRO
2	B	51	VAL
3	C	183	PRO
2	P	51	VAL
3	Q	183	PRO
10	J	9	VAL
10	X	9	VAL
4	D	118	GLY
4	R	118	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	78	95
1	O	209/209 (100%)	206 (99%)	3 (1%)	78	95
2	B	203/216 (94%)	193 (95%)	10 (5%)	35	79
2	P	203/216 (94%)	193 (95%)	10 (5%)	35	79
3	C	213/226 (94%)	204 (96%)	9 (4%)	40	83
3	Q	213/226 (94%)	204 (96%)	9 (4%)	40	83
4	D	198/215 (92%)	190 (96%)	8 (4%)	42	84
4	R	198/215 (92%)	190 (96%)	8 (4%)	42	84
5	E	192/193 (100%)	183 (95%)	9 (5%)	36	81
5	S	192/193 (100%)	183 (95%)	9 (5%)	36	81
6	F	201/239 (84%)	191 (95%)	10 (5%)	34	79
6	T	201/239 (84%)	191 (95%)	10 (5%)	34	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	207/210 (99%)	198 (96%)	9 (4%)	40	83
7	U	207/210 (99%)	198 (96%)	9 (4%)	40	83
8	H	181/190 (95%)	177 (98%)	4 (2%)	64	93
8	V	181/190 (95%)	177 (98%)	4 (2%)	64	93
9	I	172/173 (99%)	169 (98%)	3 (2%)	73	94
9	W	172/173 (99%)	169 (98%)	3 (2%)	73	94
10	J	175/175 (100%)	172 (98%)	3 (2%)	73	94
10	X	175/175 (100%)	172 (98%)	3 (2%)	73	94
11	K	169/169 (100%)	161 (95%)	8 (5%)	36	81
11	Y	169/169 (100%)	161 (95%)	8 (5%)	36	81
12	L	185/185 (100%)	180 (97%)	5 (3%)	57	91
12	Z	185/185 (100%)	180 (97%)	5 (3%)	57	91
13	M	199/199 (100%)	191 (96%)	8 (4%)	42	84
13	a	199/199 (100%)	191 (96%)	8 (4%)	42	84
14	N	162/162 (100%)	160 (99%)	2 (1%)	82	95
14	b	162/162 (100%)	160 (99%)	2 (1%)	82	95
All	All	5332/5522 (97%)	5150 (97%)	182 (3%)	49	88

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	LEU
1	A	157	PHE
2	B	55	LEU
2	B	65	LEU
2	B	69	ASN
2	B	119	GLN
2	B	149	THR
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
3	C	4	ARG
3	C	19	GLU

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Mol	Chain	Res	Type
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	20	LEU
4	D	68	CYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	198	GLN
5	E	208	ASP
5	E	227	GLU
5	E	231	LYS
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	140	ASN
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	202	ASP
6	F	203	ASN
6	F	214	TRP
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	154	TYR
7	G	166	GLN
7	G	186	ASN
7	G	201	MET
7	G	221	LYS

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Mol	Chain	Res	Type
7	G	235	ARG
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	71	GLU
10	J	78	GLN
10	J	127	GLU
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	69	ARG
11	K	73	ARG
11	K	100	MET
11	K	104	TYR
11	K	107	LYS
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	109	THR
12	L	150	LEU
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	171	GLN
13	M	226	LYS
14	N	119	VAL
14	N	149	GLU
1	O	30	GLN
1	O	61	LEU
1	O	157	PHE
2	P	55	LEU
2	P	65	LEU
2	P	69	ASN
2	P	119	GLN
2	P	149	THR

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Mol	Chain	Res	Type
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	206	LYS
4	R	20	LEU
4	R	68	CYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR
5	S	29	LYS
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	198	GLN
5	S	208	ASP
5	S	227	GLU
5	S	231	LYS
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	140	ASN
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	214	TRP
7	U	68	ARG

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Mol	Chain	Res	Type
7	U	83	ASN
7	U	115	LEU
7	U	154	TYR
7	U	166	GLN
7	U	186	ASN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	71	GLU
10	X	78	GLN
10	X	127	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	69	ARG
11	Y	73	ARG
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	109	THR
12	Z	150	LEU
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	171	GLN
13	a	226	LYS
14	b	119	VAL
14	b	149	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	04C	H	301	8	44,44,44	1.25	3 (6%)	58,58,58	0.96	6 (10%)
15	04C	K	301	11	44,44,44	1.18	2 (4%)	58,58,58	1.30	6 (10%)
15	04C	N	201	14	44,44,44	1.33	2 (4%)	58,58,58	1.28	4 (6%)
15	04C	V	301	8	44,44,44	1.31	3 (6%)	58,58,58	0.88	3 (5%)
15	04C	Y	301	11	44,44,44	1.27	2 (4%)	58,58,58	1.21	6 (10%)
15	04C	b	201	14	44,44,44	1.40	4 (9%)	58,58,58	1.63	9 (15%)

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	04C	H	301	8	-	0/44/52/52	0/3/3/3
15	04C	K	301	11	-	0/44/52/52	0/3/3/3
15	04C	N	201	14	-	0/44/52/52	0/3/3/3
15	04C	V	301	8	-	0/44/52/52	0/3/3/3
15	04C	Y	301	11	-	0/44/52/52	0/3/3/3
15	04C	b	201	14	-	0/44/52/52	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	04C	C12-C10	3.97	1.57	1.53
15	b	201	04C	C12-C10	3.73	1.57	1.53
15	b	201	04C	C10-C9	3.68	1.60	1.53
15	N	201	04C	C10-C9	3.51	1.60	1.53
15	K	301	04C	C12-C10	3.47	1.57	1.53
15	V	301	04C	C12-C10	3.26	1.57	1.53
15	H	301	04C	C12-C10	3.21	1.56	1.53
15	Y	301	04C	C10-C9	3.15	1.59	1.53
15	N	201	04C	C12-C10	3.15	1.56	1.53
15	K	301	04C	C10-C9	3.10	1.59	1.53
15	V	301	04C	C10-C9	2.98	1.59	1.53
15	H	301	04C	C10-C9	2.88	1.59	1.53
15	b	201	04C	C9-C8	2.43	1.58	1.53
15	b	201	04C	C7-C8	2.25	1.59	1.53
15	V	301	04C	C9-C8	2.13	1.57	1.53
15	H	301	04C	C9-C8	2.10	1.57	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	201	04C	C11-C10-C12	-5.46	102.74	109.94
15	b	201	04C	C10-C9-C8	5.29	122.26	113.38
15	N	201	04C	C11-C10-C12	-4.95	103.41	109.94
15	K	301	04C	C11-C10-C12	-4.03	104.62	109.94
15	Y	301	04C	C6-C7-C8	4.00	120.88	113.46
15	b	201	04C	C12-C10-C9	3.93	116.84	110.81
15	b	201	04C	C30-N31-C32	3.92	116.64	110.99
15	b	201	04C	C30-N31-C36	3.79	116.45	110.99
15	b	201	04C	C35-C36-N31	-3.75	104.55	110.04
15	K	301	04C	C12-C10-C9	3.67	116.43	110.81
15	K	301	04C	C6-C7-C8	3.62	120.17	113.46
15	N	201	04C	C10-C9-C8	3.43	119.14	113.38
15	Y	301	04C	C10-C9-C8	3.43	119.14	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	201	04C	C6-C7-C8	3.38	119.72	113.46
15	N	201	04C	C12-C10-C9	3.18	115.69	110.81
15	K	301	04C	C30-N31-C36	3.16	115.54	110.99
15	Y	301	04C	C7-C8-C9	-3.07	104.26	110.99
15	K	301	04C	C10-C9-C8	2.90	118.25	113.38
15	V	301	04C	C11-C10-C12	-2.74	106.32	109.94
15	K	301	04C	C7-C8-C9	-2.70	105.08	110.99
15	Y	301	04C	C12-C10-C9	2.59	114.78	110.81
15	H	301	04C	C11-C10-C12	-2.56	106.57	109.94
15	Y	301	04C	C7-C8-N22	-2.54	107.24	110.20
15	H	301	04C	C32-N31-C36	2.54	115.17	108.86
15	Y	301	04C	C30-N31-C32	2.52	114.63	110.99
15	V	301	04C	C6-C7-C8	2.45	118.01	113.46
15	b	201	04C	C33-O34-C35	2.40	118.09	109.90
15	H	301	04C	C7-C8-N22	-2.32	107.50	110.20
15	H	301	04C	C10-C9-C8	2.30	117.25	113.38
15	H	301	04C	C6-C7-C8	2.30	117.73	113.46
15	b	201	04C	C33-C32-N31	-2.22	106.78	110.04
15	V	301	04C	C10-C9-C8	2.17	117.03	113.38
15	H	301	04C	C35-C36-N31	2.14	113.17	110.04
15	b	201	04C	C29-C30-N31	-2.12	107.75	113.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.