



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:27 AM GMT

PDB ID : 3UNF
Title : Mouse 20S immunoproteasome in complex with PR-957
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary 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>

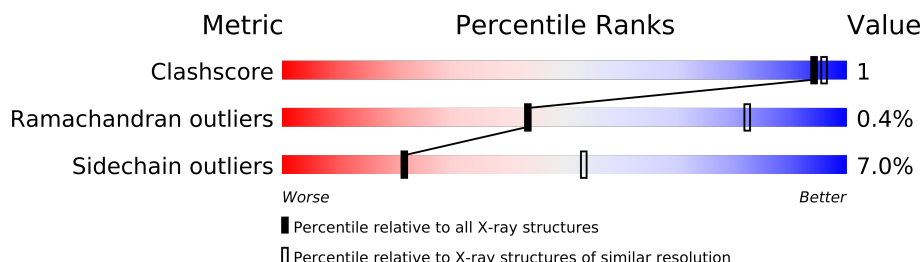
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)







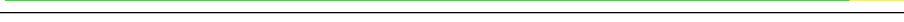

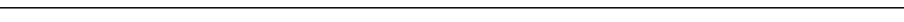


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	234	
1	O	234	
2	B	261	
2	P	261	
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	

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Mol	Chain	Length	Quality of chain
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	199	
14	b	199	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49805 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 subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			
1	O	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	P	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			
3	Q	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	R	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	S	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			
8	V	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			

- 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
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			
11	Y	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			
14	b	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	Q	4	Total 4	Cl 4	0	0
15	D	1	Total 1	Cl 1	0	0
15	a	4	Total 4	Cl 4	0	0
15	E	1	Total 1	Cl 1	0	0
15	H	1	Total 1	Cl 1	0	0
15	I	1	Total 1	Cl 1	0	0
15	V	4	Total 4	Cl 4	0	0
15	W	1	Total 1	Cl 1	0	0
15	Z	1	Total 1	Cl 1	0	0
15	A	3	Total 3	Cl 3	0	0
15	N	1	Total 1	Cl 1	0	0
15	U	1	Total 1	Cl 1	0	0
15	X	3	Total 3	Cl 3	0	0
15	O	2	Total 2	Cl 2	0	0
15	R	3	Total 3	Cl 3	0	0
15	L	2	Total 2	Cl 2	0	0
15	S	2	Total 2	Cl 2	0	0
15	M	4	Total 4	Cl 4	0	0

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

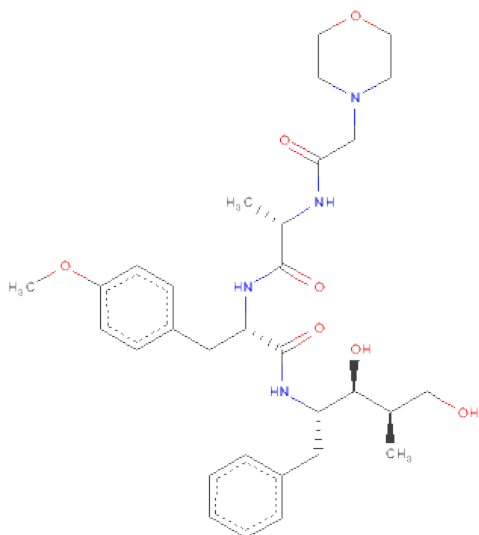
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total K 1 1	0	0
16	b	1	Total K 1 1	0	0
16	B	1	Total K 1 1	0	0
16	I	1	Total K 1 1	0	0
16	Z	3	Total K 3 3	0	0
16	a	1	Total K 1 1	0	0
16	X	1	Total K 1 1	0	0
16	L	1	Total K 1 1	0	0
16	S	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0

- Molecule 17 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: $C_{31}H_{44}N_4O_7$).



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

- Molecule 18 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	1	Total	I	0	0
			1	1		
18	H	1	Total	I	0	0
			1	1		
18	b	1	Total	I	0	0
			1	1		
18	V	1	Total	I	0	0
			1	1		
18	N	1	Total	I	0	0
			1	1		
18	Y	1	Total	I	0	0
			1	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	43	Total	O	0	0
			43	43		
19	B	42	Total	O	0	0
			42	42		
19	C	29	Total	O	0	0
			29	29		
19	D	24	Total	O	0	0
			24	24		
19	E	39	Total	O	0	0
			39	39		
19	F	37	Total	O	0	0
			37	37		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	G	44	Total 44	O 44	0	0
19	H	40	Total 40	O 40	0	0
19	I	25	Total 25	O 25	0	0
19	J	28	Total 28	O 28	0	0
19	K	32	Total 32	O 32	0	0
19	L	43	Total 43	O 43	0	0
19	M	50	Total 50	O 50	0	0
19	N	29	Total 29	O 29	0	0
19	O	44	Total 44	O 44	0	0
19	P	38	Total 38	O 38	0	0
19	Q	13	Total 13	O 13	0	0
19	R	24	Total 24	O 24	0	0
19	S	40	Total 40	O 40	0	0
19	T	32	Total 32	O 32	0	0
19	U	38	Total 38	O 38	0	0
19	V	39	Total 39	O 39	0	0
19	W	39	Total 39	O 39	0	0
19	X	20	Total 20	O 20	0	0
19	Y	36	Total 36	O 36	0	0
19	Z	49	Total 49	O 49	0	0
19	a	35	Total 35	O 35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	b	33	Total	O	0	0
			33	33		

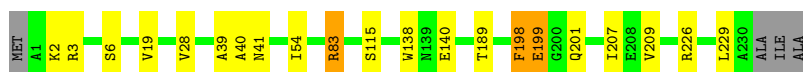
3 Residue-property plots

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 subunit alpha type-2

Chain A: 



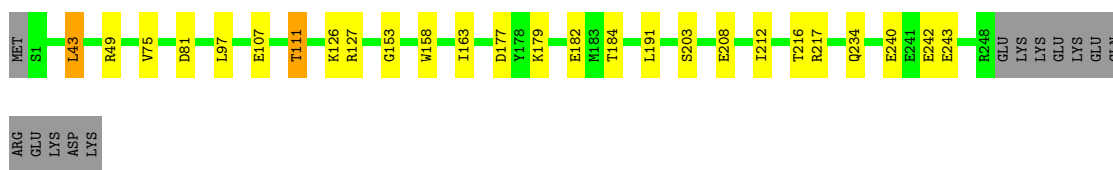
- Molecule 1: Proteasome subunit alpha type-2

Chain O: 



- Molecule 2: Proteasome subunit alpha type-4

Chain B: 



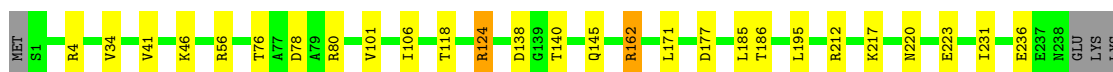
- Molecule 2: Proteasome subunit alpha type-4

Chain P: 



- Molecule 3: Proteasome subunit alpha type-7

Chain C: 



LYS
GLN
LYS
LYS
ALA
SER

• Molecule 3: Proteasome subunit alpha type-7

Chain Q:

MET SI R4 V34 V41 K46 R56 T76 A77 D78 A79 R80 V101 I106 R124 D138 G139 T140 Q145 R162 L171 D177 L185 T186 L195 R212 K217 N220 E223 I231 E236 E237 N238 GLU LYS LYS LYS GLN

LYS
LYS
ALA
SER

• Molecule 4: Proteasome subunit alpha type-5

Chain D:

MET PHE LEU THR ARG SER GLU TYR D1 R12 T28 H65 V92 H99 A112 E118 R127 E140 V176 L183 K201 E228 V229 I233

• Molecule 4: Proteasome subunit alpha type-5

Chain R:

MET PHE LEU THR ARG SER GLU TYR D1 R12 T28 H65 V92 H99 A112 E118 R127 E140 V176 L183 K201 E228 V229 I233

• Molecule 5: Proteasome subunit alpha type-1

Chain E:

MET PHE ARG N1 V7 L35 R98 C153 R154 Q163 C179 N180 L184 T204 K205 N206 V226 Q238 ARG LYS ALA GLN PRO SER GLN ALA ALA GLU GLU PRO PRO ALA GLU LYS ASP ASP PRO PRO MET MET HIS

• Molecule 5: Proteasome subunit alpha type-1

Chain S:

MET PHE ARG N1 V7 L35 R98 C153 R154 Q163 C179 N180 L184 T204 K205 N206 V226 Q238 ARG LYS ALA GLN PRO SER GLN ALA ALA GLU GLU PRO PRO ALA GLU LYS ASP ASP PRO PRO MET MET HIS

• Molecule 6: Proteasome subunit alpha type-3

Chain F:

MET SI D17 V30 S34 I37 R65 L66 D83 R99 T123 R129 C133 M181 E203 V204 K205 S214 W215 V216 E225 D230 K244 GLU GLU ASP GLU SER ASP ASP ASP ASN MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T:

MET SI D17 V30 S34 I37 R65 L66 D83 T123 R129 C133 W161 M181 E203 V204 K205 S214 W215 V216 E225 D230 K244 GLU GLU ASP GLU SER ASP ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G: 



- Molecule 7: Proteasome subunit alpha type-6

Chain U: 



- Molecule 8: Proteasome subunit beta type-10

Chain H: 



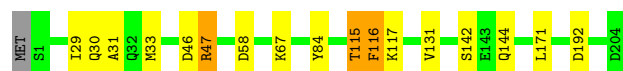
- Molecule 8: Proteasome subunit beta type-10

Chain V: 



- Molecule 9: Proteasome subunit beta type-3

Chain I: 



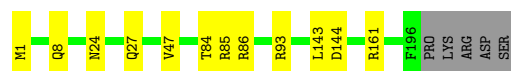
- Molecule 9: Proteasome subunit beta type-3

Chain W: 



- Molecule 10: Proteasome subunit beta type-2

Chain J: 



- Molecule 10: Proteasome subunit beta type-2

Chain X: 



- Molecule 11: Proteasome subunit beta type-8

Chain K: 



- Molecule 11: Proteasome subunit beta type-8

Chain Y:



- Molecule 12: Proteasome subunit beta type-1

Chain L:



- Molecule 12: Proteasome subunit beta type-1

Chain Z:



- Molecule 13: Proteasome subunit beta type-4

Chain M:



- Molecule 13: Proteasome subunit beta type-4

Chain a:



- Molecule 14: Proteasome subunit beta type-9

Chain N:



- Molecule 14: Proteasome subunit beta type-9

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	117.30Å 194.60Å 157.70Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.1 (15.00-2.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.235 , 0.275	Depositor
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.520	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 145087 reflections (0.001%)	Xtriage
Total number of atoms	49805	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: K, IOD, 04C, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	1/1840 (0.1%)	0.50	0/2491
1	O	0.39	1/1840 (0.1%)	0.50	0/2491
2	B	0.37	1/1980 (0.1%)	0.51	1/2667 (0.0%)
2	P	0.37	1/1980 (0.1%)	0.51	0/2667
3	C	0.34	0/1903	0.51	0/2569
3	Q	0.34	0/1903	0.51	0/2569
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	0/1805	0.47	0/2437
5	E	0.38	0/1907	0.51	0/2578
5	S	0.37	0/1907	0.51	0/2578
6	F	0.38	0/1938	0.49	0/2608
6	T	0.38	0/1938	0.49	0/2608
7	G	0.37	1/1924 (0.1%)	0.49	0/2600
7	U	0.37	1/1924 (0.1%)	0.49	0/2600
8	H	0.36	1/1645 (0.1%)	0.53	0/2235
8	V	0.37	1/1645 (0.1%)	0.53	0/2235
9	I	0.34	0/1621	0.50	0/2185
9	W	0.34	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.50	0/2167
10	X	0.33	0/1602	0.49	0/2167
11	K	0.43	1/1597 (0.1%)	0.55	0/2151
11	Y	0.43	1/1597 (0.1%)	0.55	0/2151
12	L	0.32	0/1685	0.49	0/2271
12	Z	0.32	0/1685	0.50	0/2271
13	M	0.40	0/1718	0.50	0/2325
13	a	0.40	1/1718 (0.1%)	0.50	0/2325
14	N	0.37	0/1526	0.51	0/2071
14	b	0.37	0/1526	0.51	1/2071 (0.0%)
All	All	0.37	12/49382 (0.0%)	0.50	2/66710 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
14	N	0	2
14	b	0	1
All	All	0	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	1	THR	C-N	5.77	1.47	1.34
8	H	1	THR	C-N	5.51	1.46	1.34
11	Y	104	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.04	1.47	1.41
1	A	138	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1	THR	C-N-CA	5.78	136.14	121.70
2	B	43	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
14	N	1	THR	Mainchain,Peptide
11	Y	1	THR	Peptide
14	b	1	THR	Peptide

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	1801	0	0	4	0
1	O	1801	0	0	3	0
2	B	1950	0	0	5	0
2	P	1950	0	0	3	0
3	C	1876	0	0	4	0
3	Q	1876	0	0	3	0
4	D	1778	0	0	3	0
4	R	1778	0	0	2	0
5	E	1872	0	0	1	0
5	S	1872	0	0	1	0
6	F	1903	0	0	5	0
6	T	1903	0	0	5	0
7	G	1890	0	0	5	0
7	U	1890	0	0	6	0
8	H	1619	0	0	2	0
8	V	1619	0	0	3	0
9	I	1592	0	0	4	0
9	W	1592	0	0	4	0
10	J	1570	0	0	3	0
10	X	1570	0	0	2	0
11	K	1566	0	0	2	1
11	Y	1566	0	0	3	0
12	L	1654	0	0	1	0
12	Z	1654	0	0	4	0
13	M	1685	0	0	4	1
13	a	1685	0	0	0	0
14	N	1498	0	0	1	0
14	b	1498	0	0	0	0
15	A	3	0	0	0	0
15	D	1	0	0	0	0
15	E	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	L	2	0	0	0	0
15	M	4	0	0	1	0
15	N	1	0	0	0	0
15	O	2	0	0	0	0
15	P	1	0	0	0	0
15	Q	4	0	0	0	0
15	R	3	0	0	0	0
15	S	2	0	0	0	0
15	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	V	4	0	0	0	0
15	W	1	0	0	0	0
15	X	3	0	0	0	0
15	Z	1	0	0	0	0
15	a	4	0	0	0	0
16	B	1	0	0	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	S	1	0	0	0	0
16	X	1	0	0	0	0
16	Z	3	0	0	0	0
16	a	1	0	0	0	0
16	b	1	0	0	0	0
17	H	42	0	0	0	0
17	K	42	0	0	1	0
17	N	42	0	0	0	0
17	V	42	0	0	0	0
17	Y	42	0	0	0	0
17	b	42	0	0	0	0
18	H	1	0	0	0	0
18	K	1	0	0	1	0
18	N	1	0	0	0	0
18	V	1	0	0	0	0
18	Y	1	0	0	0	0
18	b	1	0	0	0	0
19	A	43	0	0	0	0
19	B	42	0	0	1	0
19	C	29	0	0	0	0
19	D	24	0	0	0	0
19	E	39	0	0	0	0
19	F	37	0	0	0	0
19	G	44	0	0	0	0
19	H	40	0	0	0	0
19	I	25	0	0	0	0
19	J	28	0	0	0	0
19	K	32	0	0	0	0
19	L	43	0	0	1	0
19	M	50	0	0	1	0
19	N	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	44	0	0	0	0
19	P	38	0	0	0	0
19	Q	13	0	0	0	0
19	R	24	0	0	0	0
19	S	40	0	0	0	0
19	T	32	0	0	0	0
19	U	38	0	0	0	0
19	V	39	0	0	1	0
19	W	39	0	0	0	0
19	X	20	0	0	0	0
19	Y	36	0	0	0	0
19	Z	49	0	0	3	0
19	a	35	0	0	0	0
19	b	33	0	0	0	0
All	All	49805	0	0	68	1

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.

The worst 5 of 68 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:W:115:THR:O	9:W:116:PHE:CD2	2.46	0.69
9:I:115:THR:O	9:I:116:PHE:CD2	2.46	0.69
2:P:153:GLY:O	3:Q:80:ARG:NH2	2.34	0.60
2:B:153:GLY:O	3:C:80:ARG:NH2	2.36	0.59
1:O:39:ALA:O	1:O:41:ASN:N	2.36	0.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:146:ASP:O	13:M:206:GLN:NE2[2_655]	2.08	0.12

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	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	18	54
1	O	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	18	54
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	43	82
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	43	82
3	C	236/248 (95%)	222 (94%)	14 (6%)	0	100	100
3	Q	236/248 (95%)	221 (94%)	15 (6%)	0	100	100
4	D	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	43	82
4	R	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	43	82
5	E	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
5	S	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
6	F	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	43	82
6	T	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	43	82
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
7	U	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
8	H	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	25	66
8	V	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	25	66
9	I	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	22	63
9	W	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	22	63
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	38	79
10	X	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	38	79
11	K	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
11	Y	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
12	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
12	Z	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
14	b	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
All	All	6188/6446 (96%)	5953 (96%)	213 (3%)	22 (0%)	43	82

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
9	I	30	GLN
6	T	216	VAL
9	W	30	GLN
1	A	40	ALA

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	189/191 (99%)	175 (93%)	14 (7%)	20	50
1	O	189/191 (99%)	174 (92%)	15 (8%)	18	46
2	B	208/221 (94%)	190 (91%)	18 (9%)	15	41
2	P	208/221 (94%)	190 (91%)	18 (9%)	15	41
3	C	202/211 (96%)	178 (88%)	24 (12%)	8	21
3	Q	202/211 (96%)	178 (88%)	24 (12%)	8	21
4	D	195/203 (96%)	186 (95%)	9 (5%)	37	76
4	R	195/203 (96%)	186 (95%)	9 (5%)	37	76
5	E	204/224 (91%)	191 (94%)	13 (6%)	25	59
5	S	204/224 (91%)	191 (94%)	13 (6%)	25	59
6	F	200/211 (95%)	189 (94%)	11 (6%)	30	68
6	T	200/211 (95%)	189 (94%)	11 (6%)	30	68
7	G	207/210 (99%)	197 (95%)	10 (5%)	35	74
7	U	207/210 (99%)	197 (95%)	10 (5%)	35	74
8	H	169/183 (92%)	151 (89%)	18 (11%)	10	28
8	V	169/183 (92%)	151 (89%)	18 (11%)	10	28
9	I	174/175 (99%)	163 (94%)	11 (6%)	25	60
9	W	174/175 (99%)	163 (94%)	11 (6%)	25	60
10	J	166/171 (97%)	158 (95%)	8 (5%)	35	74
10	X	166/171 (97%)	158 (95%)	8 (5%)	35	74
11	K	165/166 (99%)	151 (92%)	14 (8%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	165/166 (99%)	151 (92%)	14 (8%)	15	42
12	L	178/178 (100%)	170 (96%)	8 (4%)	38	77
12	Z	178/178 (100%)	168 (94%)	10 (6%)	30	66
13	M	178/180 (99%)	167 (94%)	11 (6%)	26	61
13	a	178/180 (99%)	167 (94%)	11 (6%)	26	61
14	N	155/155 (100%)	143 (92%)	12 (8%)	18	47
14	b	155/155 (100%)	144 (93%)	11 (7%)	21	52
All	All	5180/5358 (97%)	4816 (93%)	364 (7%)	21	53

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	100	ARG
2	P	179	LYS
12	Z	160	ASN
14	N	20	VAL
1	O	28	VAL

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 ⓘ

Of 66 ligands modelled in this entry, 60 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
17	04C	H	301	8	44,44,44	1.07	2 (4%)	58,58,58	1.07	3 (5%)
17	04C	K	301	11	44,44,44	1.13	2 (4%)	58,58,58	1.07	4 (6%)
17	04C	N	201	14	44,44,44	1.17	3 (6%)	58,58,58	1.30	6 (10%)
17	04C	V	301	8	44,44,44	1.11	3 (6%)	58,58,58	1.08	4 (6%)
17	04C	Y	301	11	44,44,44	1.17	2 (4%)	58,58,58	1.43	8 (13%)
17	04C	b	201	14	44,44,44	1.21	4 (9%)	58,58,58	1.25	8 (13%)

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
17	04C	H	301	8	-	0/44/52/52	0/3/3/3
17	04C	K	301	11	-	0/44/52/52	0/3/3/3
17	04C	N	201	14	-	0/44/52/52	0/3/3/3
17	04C	V	301	8	-	0/44/52/52	0/3/3/3
17	04C	Y	301	11	-	0/44/52/52	0/3/3/3
17	04C	b	201	14	-	0/44/52/52	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	04C	C10-C9	3.16	1.59	1.53
17	K	301	04C	C10-C9	2.97	1.59	1.53
17	b	201	04C	C10-C9	2.86	1.59	1.53
17	Y	301	04C	C10-C9	2.80	1.58	1.53
17	K	301	04C	C12-C10	2.75	1.56	1.53

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	04C	C33-C32-N31	4.47	116.58	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	04C	C11-C10-C12	-4.31	104.25	109.94
17	K	301	04C	C11-C10-C12	-4.26	104.33	109.94
17	Y	301	04C	C32-N31-C36	4.16	119.20	108.86
17	Y	301	04C	C35-C36-N31	4.11	116.06	110.04

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.