wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 11:42 pm GMT

PDB ID	:	4Y8K
Title	:	Yeast 20S proteasome in complex with H-APLL-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-16
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49865 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	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 subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	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	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	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 H-APLL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			32	23	4	5			
15	d	5	Total	C	N	O	0	0	0
			32	23	4	5			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	5	Total C N O 32 23 4 5	0	0	0
15	f	5	Total C N O 32 23 4 5	0	0	0

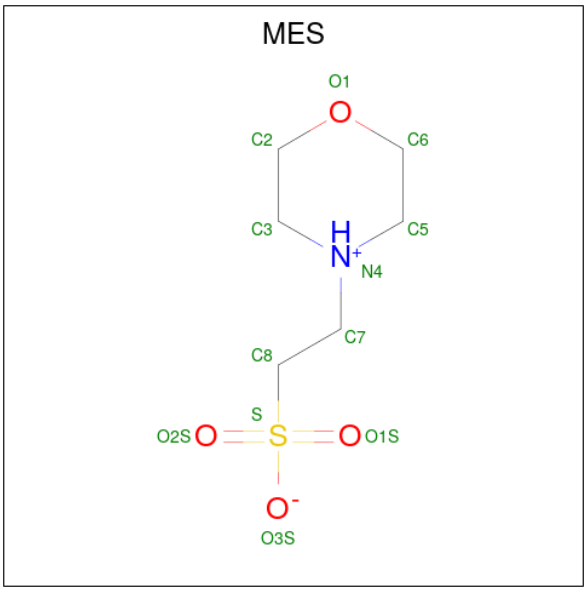
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	Y	1	Total C N O S 12 6 1 4 1	0	0
18	c	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	17	Total O 17 17	0	0
19	B	20	Total O 20 20	0	0
19	C	15	Total O 15 15	0	0
19	D	3	Total O 3 3	0	0
19	E	5	Total O 5 5	0	0
19	F	17	Total O 17 17	0	0
19	G	27	Total O 27 27	0	0
19	H	16	Total O 16 16	0	0
19	I	18	Total O 18 18	0	0
19	J	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	18	Total O 18 18	0	0
19	L	24	Total O 24 24	0	0
19	M	20	Total O 20 20	0	0
19	N	19	Total O 19 19	0	0
19	O	10	Total O 10 10	0	0
19	P	10	Total O 10 10	0	0
19	Q	9	Total O 9 9	0	0
19	R	8	Total O 8 8	0	0
19	S	5	Total O 5 5	0	0
19	T	11	Total O 11 11	0	0
19	U	18	Total O 18 18	0	0
19	V	19	Total O 19 19	0	0
19	W	12	Total O 12 12	0	0
19	X	16	Total O 16 16	0	0
19	Y	20	Total O 20 20	0	0
19	Z	15	Total O 15 15	0	0
19	a	24	Total O 24 24	0	0
19	b	15	Total O 15 15	0	0
19	d	2	Total O 2 2	0	0
19	f	3	Total O 3 3	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.56Å 300.72Å 145.43Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.60) 98.6 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.236 0.214 , 0.238	Depositor DCC
R_{free} test set	16129 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49865	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality (i)

3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: POL, MES, CL, MG, DCL

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	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.28	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.46	0/2634
7	U	0.28	0/1945	0.46	0/2634
8	H	0.26	0/1715	0.46	0/2326
8	V	0.26	0/1715	0.46	0/2326
9	I	0.28	0/1611	0.48	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.58	4/1681 (0.2%)	0.56	0/2274
11	Y	0.58	4/1681 (0.2%)	0.57	0/2274
12	L	0.28	0/1795	0.53	1/2420 (0.0%)
12	Z	0.28	0/1795	0.53	1/2420 (0.0%)
13	M	0.28	0/1828	0.51	0/2480
13	a	0.28	0/1855	0.51	0/2514
14	N	0.34	0/1541	0.51	1/2087 (0.0%)
14	b	0.33	0/1541	0.50	1/2087 (0.0%)
15	c	1.82	1/20 (5.0%)	1.39	0/27
15	d	1.58	1/20 (5.0%)	1.09	0/27
15	e	1.72	1/20 (5.0%)	1.38	0/27
15	f	1.60	1/20 (5.0%)	1.12	0/27

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.32	12/50247 (0.0%)	0.49	4/67942 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	104	TYR	CE1-CZ	-11.75	1.23	1.38
11	Y	104	TYR	CE1-CZ	-10.68	1.24	1.38
11	Y	104	TYR	CG-CD2	-9.77	1.26	1.39
11	K	104	TYR	CG-CD2	-9.32	1.27	1.39
11	Y	104	TYR	CG-CD1	-9.27	1.27	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	173	LYS	CD-CE-NZ	8.49	131.24	111.70
12	L	173	LYS	CD-CE-NZ	8.01	130.12	111.70
14	N	1	THR	N-CA-C	5.18	124.98	111.00
14	b	1	THR	N-CA-C	5.14	124.89	111.00

There are no chirality outliers.

There are no planarity outliers.

3.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1684	0	1688	3	0
8	V	1684	0	1688	6	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	3	0
11	K	1644	0	1592	29	0
11	Y	1644	0	1592	37	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	7	0
13	M	1797	0	1800	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	1	0
14	b	1512	0	1478	0	0
15	c	32	0	41	0	0
15	d	32	0	41	0	0
15	e	32	0	41	0	0
15	f	32	0	41	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	Y	12	0	13	0	0
18	c	12	0	13	0	0
19	A	17	0	0	0	0
19	B	20	0	0	0	0
19	C	15	0	0	0	0
19	D	3	0	0	0	0
19	E	5	0	0	0	0
19	F	17	0	0	0	0
19	G	27	0	0	0	0
19	H	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	18	0	0	0	0
19	J	17	0	0	0	0
19	K	18	0	0	0	0
19	L	24	0	0	0	0
19	M	20	0	0	0	0
19	N	19	0	0	0	0
19	O	10	0	0	0	0
19	P	10	0	0	0	0
19	Q	9	0	0	0	0
19	R	8	0	0	0	0
19	S	5	0	0	0	0
19	T	11	0	0	0	0
19	U	18	0	0	0	0
19	V	19	0	0	0	0
19	W	12	0	0	0	0
19	X	16	0	0	0	0
19	Y	20	0	0	0	0
19	Z	15	0	0	1	0
19	a	24	0	0	0	0
19	b	15	0	0	0	0
19	d	2	0	0	0	0
19	f	3	0	0	0	0
All	All	49865	0	49214	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 141 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:104:TYR:CE2	11:K:182:GLU:HG2	1.74	1.22
11:Y:40:PHE:CD1	11:Y:73:ARG:NH2	2.27	1.01
11:K:104:TYR:HE2	11:K:182:GLU:HG2	1.10	1.01
11:Y:104:TYR:CE1	11:Y:110:PRO:HD3	1.96	1.01
11:Y:104:TYR:HE1	11:Y:110:PRO:HD3	1.29	0.92

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	39
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	19	39
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	4 (2%)	1 (0%)	29	52
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	228/246 (93%)	222 (97%)	5 (2%)	1 (0%)	34	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	a	231/246 (94%)	225 (97%)	5 (2%)	1 (0%)	34 57
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100 100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100 100
15	c	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
15	d	2/5 (40%)	2 (100%)	0	0	100 100
15	e	2/5 (40%)	2 (100%)	0	0	100 100
15	f	2/5 (40%)	2 (100%)	0	0	100 100
All	All	6281/6634 (95%)	6109 (97%)	159 (2%)	13 (0%)	47 71

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN

3.3.2 Protein sidechains (i)

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%)	67 85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67 85
2	B	203/216 (94%)	197 (97%)	6 (3%)	41 67
2	P	203/216 (94%)	197 (97%)	6 (3%)	41 67
3	C	212/226 (94%)	204 (96%)	8 (4%)	33 59
3	Q	212/226 (94%)	205 (97%)	7 (3%)	38 64
4	D	194/215 (90%)	184 (95%)	10 (5%)	23 46
4	R	194/215 (90%)	184 (95%)	10 (5%)	23 46
5	E	190/193 (98%)	183 (96%)	7 (4%)	34 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	S	190/193 (98%)	183 (96%)	7 (4%)	34 60
6	F	201/239 (84%)	191 (95%)	10 (5%)	24 47
6	T	201/239 (84%)	191 (95%)	10 (5%)	24 47
7	G	206/210 (98%)	198 (96%)	8 (4%)	32 58
7	U	206/210 (98%)	198 (96%)	8 (4%)	32 58
8	H	181/190 (95%)	176 (97%)	5 (3%)	43 69
8	V	181/190 (95%)	176 (97%)	5 (3%)	43 69
9	I	172/173 (99%)	168 (98%)	4 (2%)	50 75
9	W	172/173 (99%)	168 (98%)	4 (2%)	50 75
10	J	173/175 (99%)	168 (97%)	5 (3%)	42 68
10	X	173/175 (99%)	168 (97%)	5 (3%)	42 68
11	K	169/169 (100%)	160 (95%)	9 (5%)	22 45
11	Y	169/169 (100%)	157 (93%)	12 (7%)	14 29
12	L	185/185 (100%)	179 (97%)	6 (3%)	39 65
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39 65
13	M	196/208 (94%)	190 (97%)	6 (3%)	40 66
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 67
14	N	162/162 (100%)	160 (99%)	2 (1%)	71 87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71 87
15	c	2/2 (100%)	1 (50%)	1 (50%)	0 0
15	d	2/2 (100%)	2 (100%)	0	100 100
15	e	2/2 (100%)	2 (100%)	0	100 100
15	f	2/2 (100%)	2 (100%)	0	100 100
All	All	5317/5548 (96%)	5136 (97%)	181 (3%)	37 63

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	9	THR
8	V	68	LEU
5	S	184	ASN
6	T	214	TRP
10	X	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	117	GLN
12	Z	70	ASN
6	T	240	GLN
9	W	37	ASN
13	a	108	ASN

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

4 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	DCL	c	4	11,15	7,7,7	0.65	0	6,8,8	1.00	1 (16%)
15	DCL	e	4	11,15	7,7,7	0.48	0	6,8,8	0.90	0
15	DCL	d	4	14,15	7,7,7	0.64	0	6,8,8	1.30	1 (16%)
15	DCL	f	4	14,15	7,7,7	0.69	0	6,8,8	1.28	1 (16%)

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	DCL	c	4	11,15	-	3/6/6/6	-
15	DCL	e	4	11,15	-	2/6/6/6	-
15	DCL	d	4	14,15	-	3/6/6/6	-
15	DCL	f	4	14,15	-	3/6/6/6	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	4	DCL	CB-CA-C	-2.55	107.60	111.79
15	f	4	DCL	CB-CA-C	-2.48	107.73	111.79
15	c	4	DCL	O-C-CA	-2.09	103.27	111.52

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	DCL	N-CA-CB-CG
15	c	4	DCL	C-CA-CB-CG
15	d	4	DCL	N-CA-CB-CG
15	d	4	DCL	C-CA-CB-CG
15	e	4	DCL	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
18	MES	c	101	-	12,12,12	2.22	1 (8%)	14,16,16	1.22	2 (14%)
18	MES	Y	301	-	12,12,12	2.21	1 (8%)	14,16,16	1.24	2 (14%)

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
18	MES	c	101	-	-	0/6/14/14	0/1/1/1
18	MES	Y	301	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c	101	MES	C8-S	-7.38	1.67	1.77
18	Y	301	MES	C8-S	-7.33	1.67	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Y	301	MES	O2S-S-C8	2.81	110.30	106.92
18	c	101	MES	O2S-S-C8	2.53	109.96	106.92
18	c	101	MES	O3S-S-C8	2.33	109.53	105.77
18	Y	301	MES	O3S-S-C8	2.32	109.53	105.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.14	6 (2%)	59	53	36, 50, 88, 129	0
1	O	250/250 (100%)	0.01	10 (4%)	38	31	42, 59, 105, 136	0
2	B	244/258 (94%)	-0.07	10 (4%)	37	30	36, 55, 103, 159	0
2	P	244/258 (94%)	0.02	13 (5%)	26	20	41, 60, 109, 159	0
3	C	240/254 (94%)	0.02	16 (6%)	17	13	37, 58, 122, 161	0
3	Q	240/254 (94%)	0.24	21 (8%)	10	7	42, 72, 153, 193	0
4	D	235/260 (90%)	-0.25	3 (1%)	77	73	41, 61, 94, 142	0
4	R	235/260 (90%)	-0.17	8 (3%)	45	38	41, 62, 102, 156	0
5	E	231/234 (98%)	0.06	10 (4%)	35	28	43, 63, 99, 141	0
5	S	231/234 (98%)	0.08	12 (5%)	27	21	48, 73, 115, 155	0
6	F	243/288 (84%)	0.10	13 (5%)	26	20	37, 58, 111, 138	0
6	T	243/288 (84%)	0.15	13 (5%)	26	20	36, 68, 126, 161	0
7	G	241/252 (95%)	0.06	11 (4%)	32	26	37, 54, 96, 150	0
7	U	241/252 (95%)	0.07	9 (3%)	41	34	41, 56, 93, 138	0
8	H	222/232 (95%)	-0.20	4 (1%)	68	64	35, 48, 81, 118	0
8	V	222/232 (95%)	0.08	5 (2%)	60	54	38, 54, 90, 130	0
9	I	204/205 (99%)	-0.55	1 (0%)	91	89	30, 47, 76, 96	0
9	W	204/205 (99%)	-0.46	3 (1%)	73	70	32, 50, 82, 103	0
10	J	195/198 (98%)	-0.38	3 (1%)	73	70	32, 49, 75, 114	0
10	X	195/198 (98%)	-0.38	4 (2%)	63	58	36, 51, 77, 129	0
11	K	212/212 (100%)	-0.17	7 (3%)	46	39	38, 54, 89, 108	0
11	Y	212/212 (100%)	-0.10	9 (4%)	36	29	40, 54, 90, 116	0
12	L	222/222 (100%)	-0.34	4 (1%)	68	64	35, 51, 89, 122	0
12	Z	222/222 (100%)	-0.32	4 (1%)	68	64	33, 52, 89, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	230/246 (93%)	-0.26	4 (1%) 70 66	31, 49, 77, 88	0
13	a	233/246 (94%)	-0.27	3 (1%) 77 73	33, 50, 74, 101	0
14	N	196/196 (100%)	-0.20	1 (0%) 91 89	32, 45, 75, 104	0
14	b	196/196 (100%)	-0.22	4 (2%) 65 60	32, 46, 77, 101	0
15	c	3/5 (60%)	3.56	2 (66%) 0 0	78, 78, 84, 84	0
15	d	3/5 (60%)	-0.12	0 100 100	49, 49, 53, 56	0
15	e	3/5 (60%)	4.08	3 (100%) 0 0	80, 80, 88, 90	0
15	f	3/5 (60%)	-0.15	0 100 100	52, 52, 56, 56	0
All	All	6345/6634 (95%)	-0.11	216 (3%) 45 38	30, 55, 102, 193	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	8.3
3	Q	49	THR	7.8
1	O	1	MET	7.3
3	C	206	LYS	7.1
8	V	222	ASP	6.9

4.2 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	DCL	e	4	8/8	0.62	0.43	77,81,82,83	0
15	DCL	c	4	8/8	0.81	0.28	70,78,79,79	0
15	DCL	d	4	8/8	0.86	0.23	51,56,58,58	0
15	DCL	f	4	8/8	0.93	0.21	50,57,62,62	0

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 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, 95^{th} 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	Z	301	1/1	0.71	0.18	67,67,67,67	0
18	MES	Y	301	12/12	0.79	0.39	76,84,97,106	0
18	MES	c	101	12/12	0.86	0.37	79,86,100,102	0
16	MG	I	302	1/1	0.93	0.07	54,54,54,54	0
16	MG	N	201	1/1	0.96	0.14	46,46,46,46	0
16	MG	I	301	1/1	0.96	0.37	63,63,63,63	0
16	MG	G	301	1/1	0.96	0.07	41,41,41,41	0
16	MG	K	301	1/1	0.96	0.09	56,56,56,56	0
16	MG	L	301	1/1	0.97	0.04	54,54,54,54	0
17	CL	b	201	1/1	0.97	0.23	63,63,63,63	0
17	CL	G	302	1/1	0.99	0.18	30,30,30,30	0
17	CL	N	202	1/1	0.99	0.06	43,43,43,43	0
17	CL	U	301	1/1	0.99	0.23	30,30,30,30	0

4.5 Other polymers (i)

There are no such residues in this entry.