wwPDB X-ray Structure Validation Summary Report (i)

Dec 7, 2023 – 10:34 pm GMT

PDB ID	:	2JKR
Title	:	AP2 CLATHRIN ADAPTOR CORE with Dileucine peptide RM(phosphoS)QIKRLLSE
Authors	:	Owen, D.J.; McCoy, A.J.; Kelly, B.T.; Evans, P.R.
Deposited on	:	2008-08-29
Resolution	:	2.98 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 (i)) were used in the production of this report:

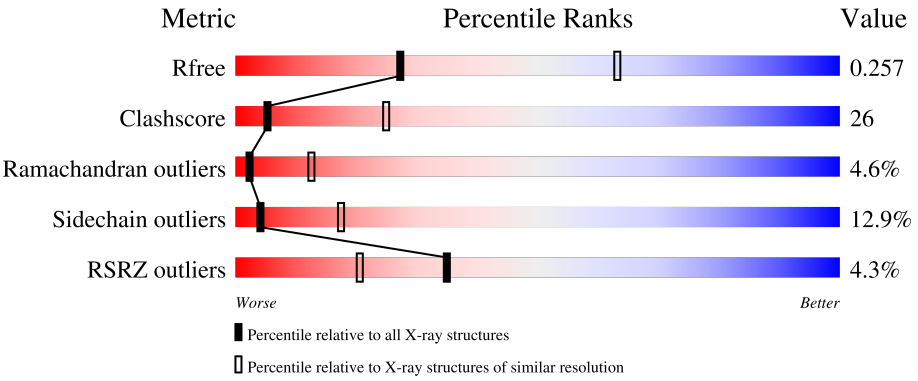
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	623	4% 51% 40% 8%
1	L	623	4% 53% 38% 8%
2	B	591	5% 39% 45% 12%
2	E	591	5% 40% 45% 11%
3	I	142	55% 40% 5%

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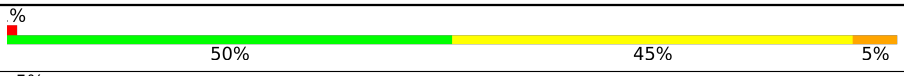
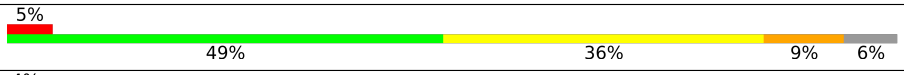
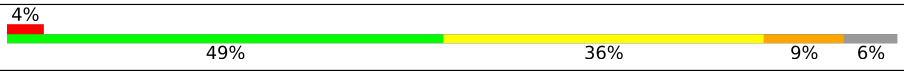
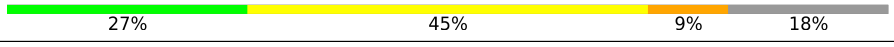
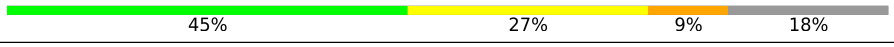
Mol	Chain	Length	Quality of chain
3	S	142	
4	M	435	
4	U	435	
5	P	11	
5	Q	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	1624	-	-	X	-
6	SO4	A	1625	-	-	X	-
6	SO4	E	1587	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28120 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 AP-2 COMPLEX SUBUNIT ALPHA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			
1	L	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			

- Molecule 2 is a protein called AP-2 COMPLEX SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			
2	E	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			

- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT SIGMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			
3	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

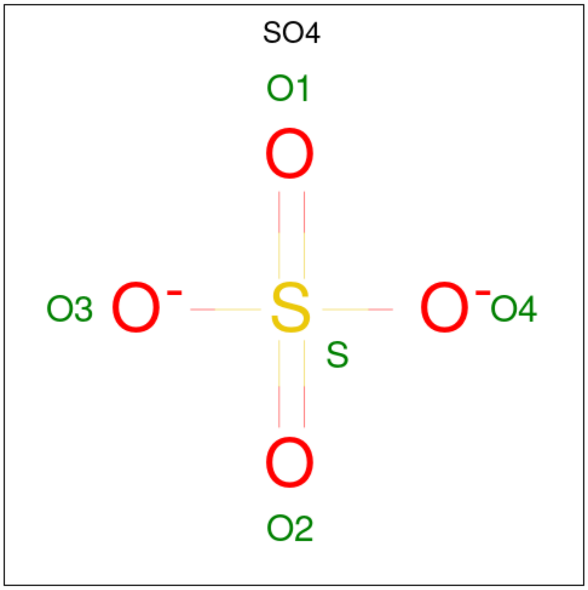
- Molecule 4 is a protein called AP-2 COMPLEX SUBUNIT MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			
4	U	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			

- Molecule 5 is a protein called CD4 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total 73	C 46	N 14	O 12	S 1	0	0	0
5	Q	9	Total 73	C 46	N 14	O 12	S 1	0	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0
6	M	1	Total O S 5 4 1	0	0
6	M	1	Total O S 5 4 1	0	0
6	M	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

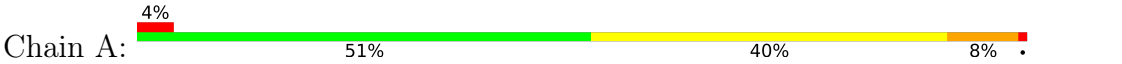
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	3	Total O 3 3	0	0
7	E	3	Total O 3 3	0	0
7	I	2	Total O 2 2	0	0
7	L	3	Total O 3 3	0	0
7	M	3	Total O 3 3	0	0
7	S	1	Total O 1 1	0	0
7	U	1	Total O 1 1	0	0

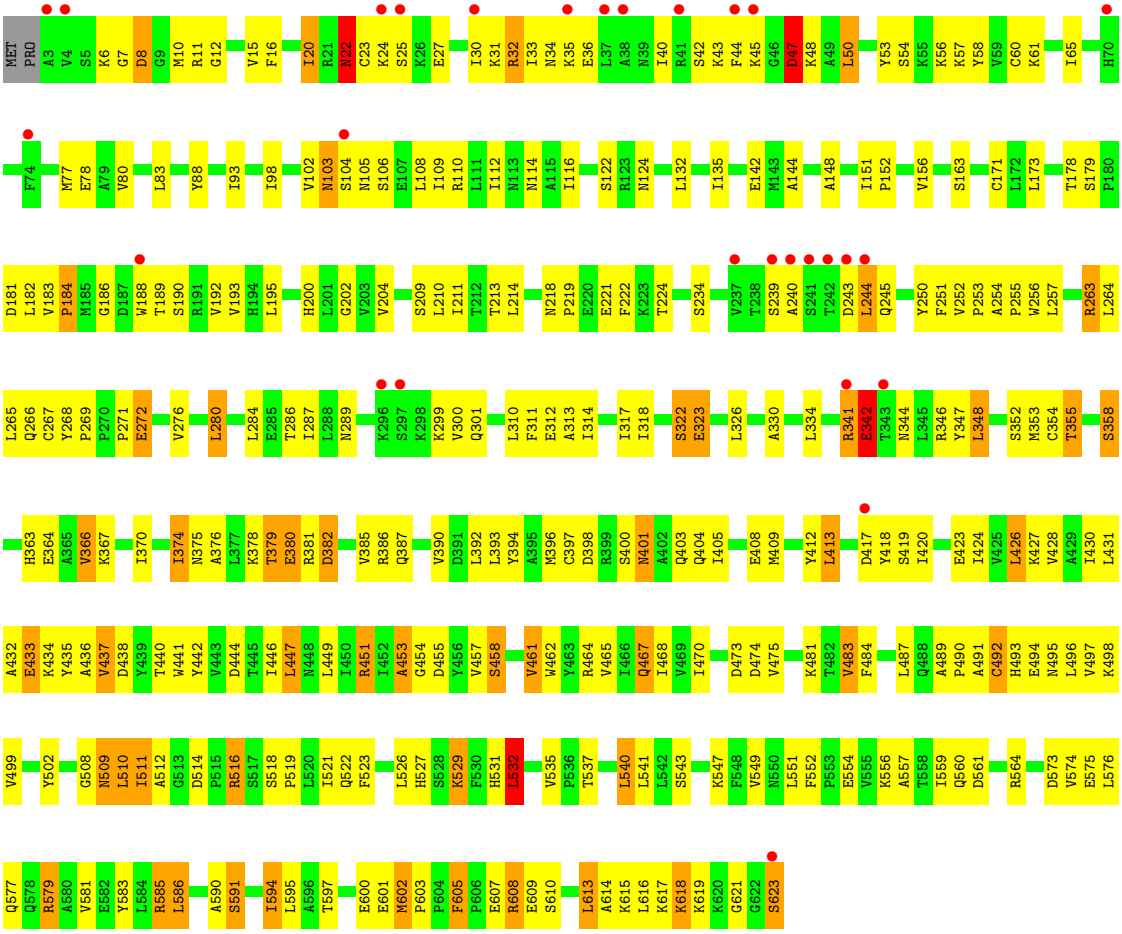
3 Residue-property plots (i)

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: AP-2 COMPLEX SUBUNIT ALPHA-2

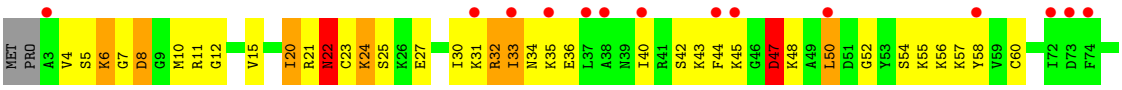
Chain A:

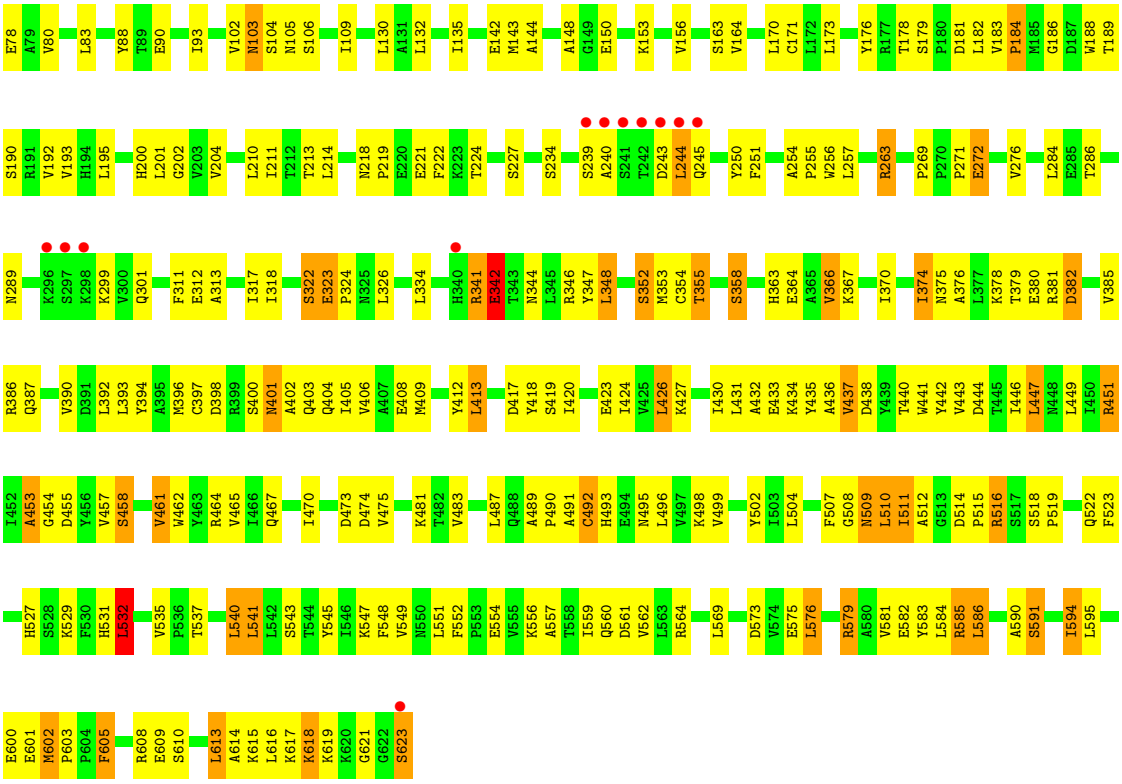




• Molecule 1: AP-2 COMPLEX SUBUNIT ALPHA-2

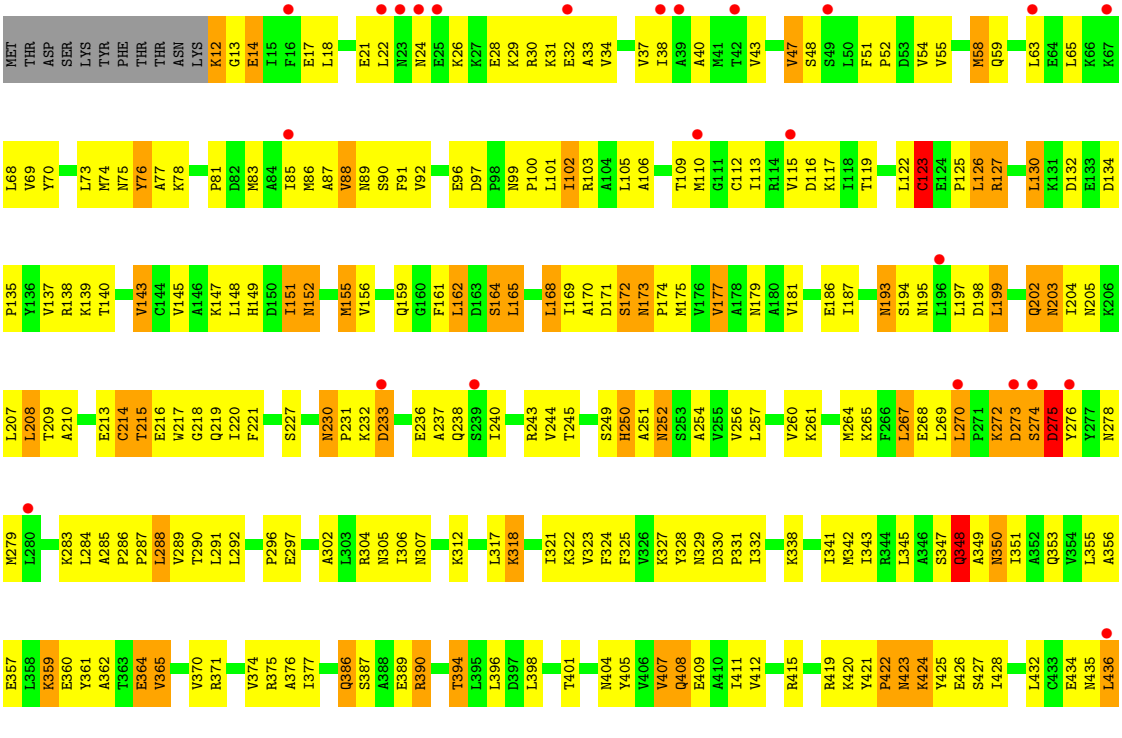
Chain L:

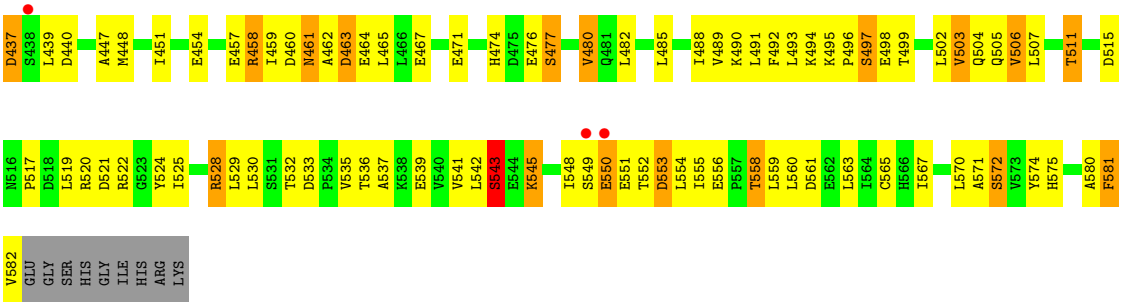




• Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1

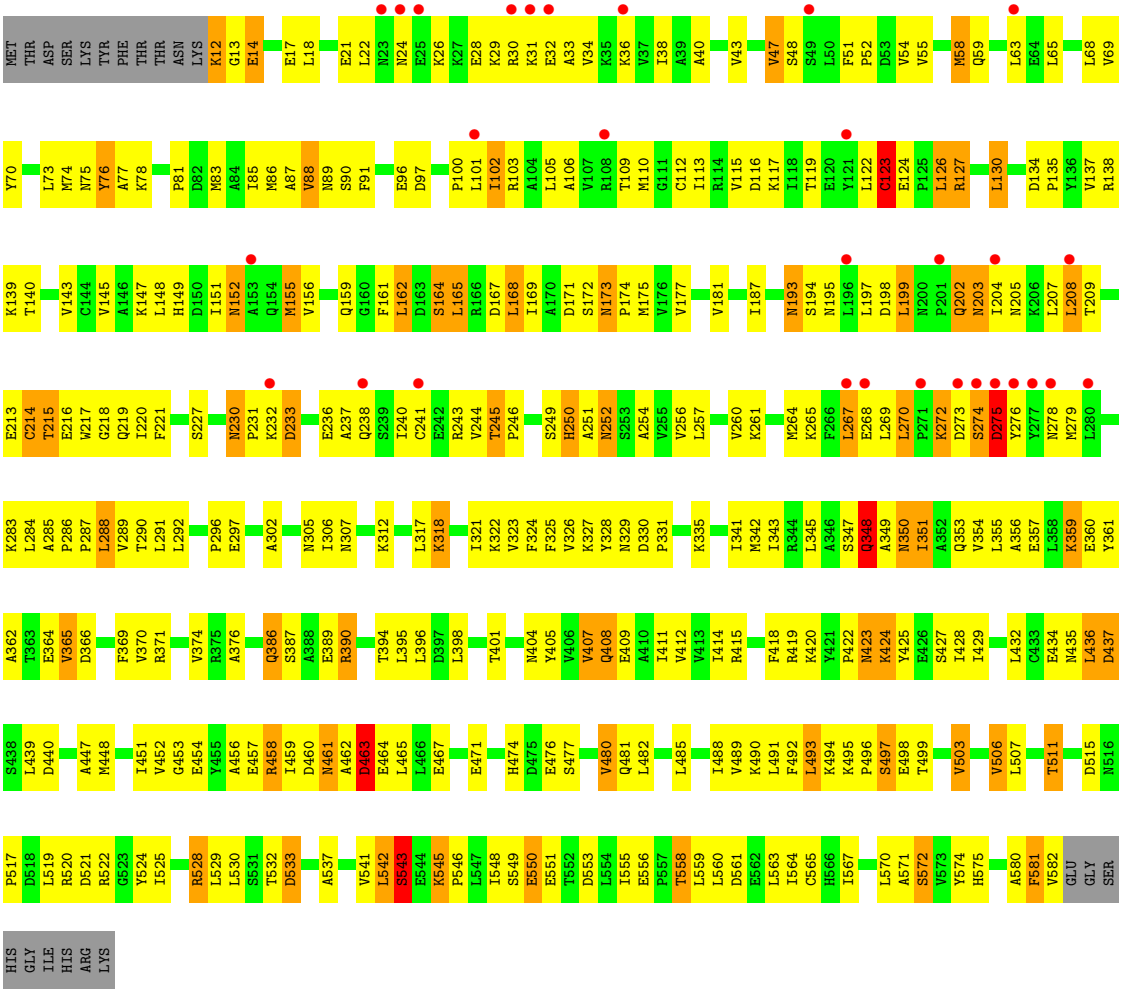
Chain B:





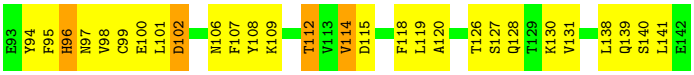
• Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1

Chain E:



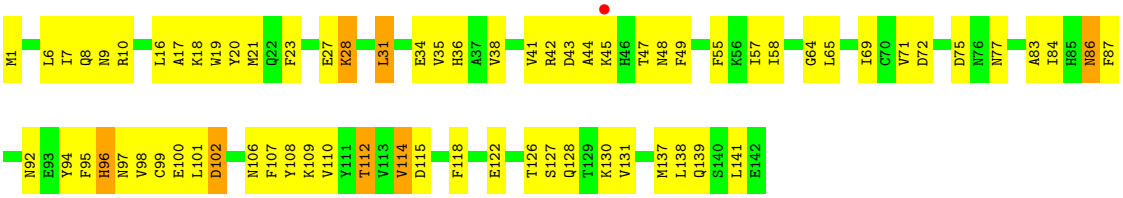
• Molecule 3: AP-2 COMPLEX SUBUNIT SIGMA-1

Chain I:



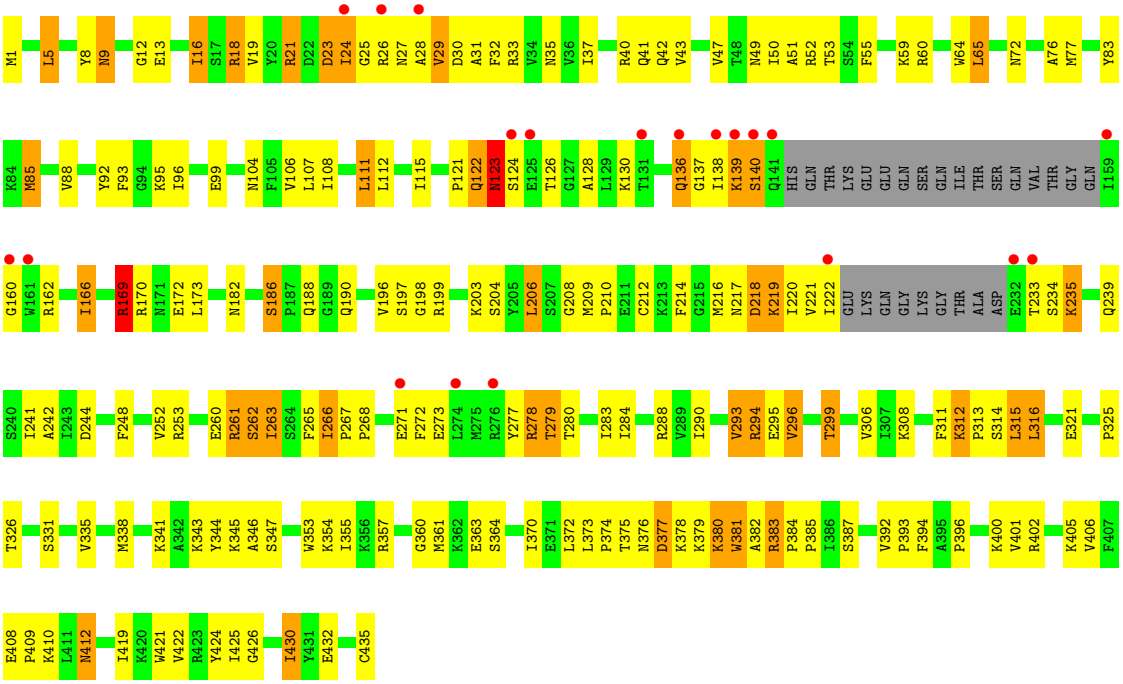
• Molecule 3: AP-2 COMPLEX SUBUNIT SIGMA-1

Chain S:



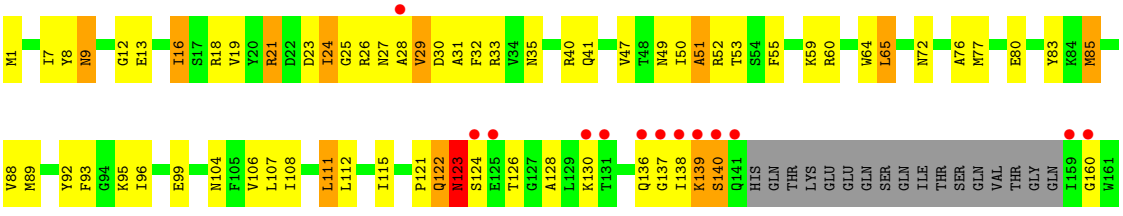
• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1

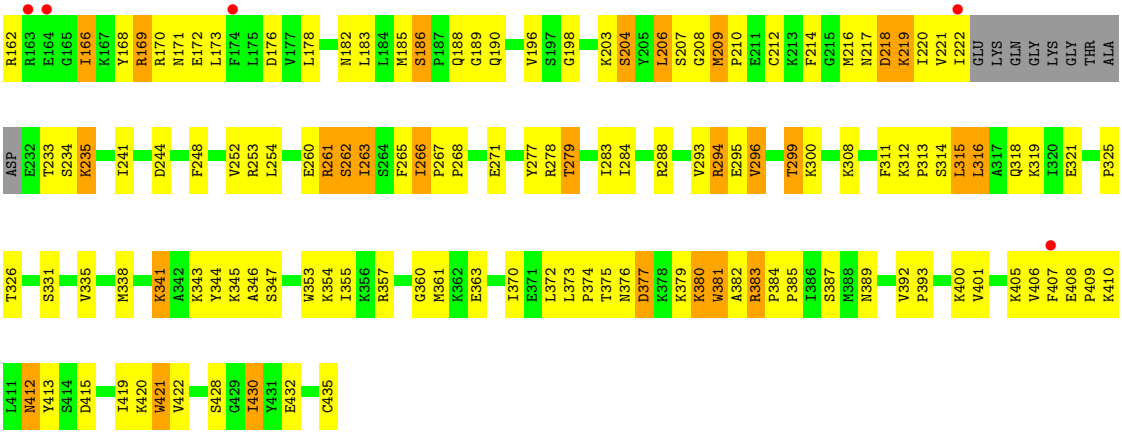
Chain M:



• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1

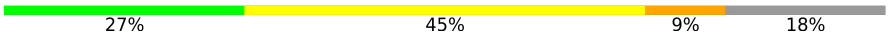
Chain U:

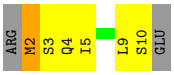




• Molecule 5: CD4 PEPTIDE

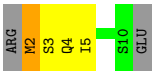
Chain P:





• Molecule 5: CD4 PEPTIDE

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.90Å 169.90Å 321.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.95 – 2.98 50.96 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.95-2.98) 99.9 (50.96-2.98)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.199 , 0.260 0.196 , 0.257	Depositor DCC
R_{free} test set	4819 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28120	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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.

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: SO4, SEP

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	0.50	0/4970	0.69	1/6734 (0.0%)
1	L	0.49	0/4970	0.69	2/6734 (0.0%)
2	B	0.46	0/4597	0.66	0/6236
2	E	0.46	0/4597	0.67	0/6236
3	I	0.52	0/1224	0.66	0/1650
3	S	0.50	0/1224	0.67	0/1650
4	M	0.54	0/3353	0.72	0/4513
4	U	0.55	0/3353	0.72	0/4513
5	P	0.40	0/65	0.61	0/82
5	Q	0.41	0/65	0.68	0/82
All	All	0.50	0/28418	0.69	3/38430 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	586	LEU	CA-CB-CG	5.97	129.03	115.30
1	L	586	LEU	CA-CB-CG	5.79	128.62	115.30
1	L	540	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	4885	0	4999	251	0
1	L	4885	0	4999	245	0
2	B	4527	0	4646	310	0
2	E	4527	0	4646	306	0
3	I	1200	0	1195	58	0
3	S	1200	0	1195	69	0
4	M	3288	0	3382	180	0
4	U	3288	0	3382	176	0
5	P	73	0	83	8	0
5	Q	73	0	83	5	0
6	A	35	0	0	7	0
6	B	20	0	0	2	0
6	E	25	0	0	2	0
6	L	40	0	0	1	0
6	M	15	0	0	1	0
6	U	20	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	E	3	0	0	0	0
7	I	2	0	0	0	0
7	L	3	0	0	1	0
7	M	3	0	0	0	0
7	S	1	0	0	0	0
7	U	1	0	0	0	0
All	All	28120	0	28610	1501	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 26.

The worst 5 of 1501 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)
2:B:434:GLU:HG3	2:B:435:ASN:HD22	1.19	1.08
2:E:434:GLU:HG3	2:E:435:ASN:HD22	1.17	1.08
1:L:579:ARG:HG2	1:L:579:ARG:HH11	1.16	1.07
1:L:516:ARG:HG3	1:L:516:ARG:HH11	1.14	1.05
1:A:516:ARG:HG3	1:A:516:ARG:HH11	1.15	1.04

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	619/623 (99%)	532 (86%)	64 (10%)	23 (4%)	3 17
1	L	619/623 (99%)	534 (86%)	63 (10%)	22 (4%)	3 17
2	B	569/591 (96%)	469 (82%)	67 (12%)	33 (6%)	1 8
2	E	569/591 (96%)	469 (82%)	68 (12%)	32 (6%)	2 9
3	I	140/142 (99%)	119 (85%)	19 (14%)	2 (1%)	11 41
3	S	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	11 41
4	M	403/435 (93%)	321 (80%)	58 (14%)	24 (6%)	1 7
4	U	403/435 (93%)	325 (81%)	55 (14%)	23 (6%)	1 9
5	P	6/11 (54%)	4 (67%)	2 (33%)	0	100 100
5	Q	6/11 (54%)	5 (83%)	1 (17%)	0	100 100
All	All	3474/3604 (96%)	2896 (83%)	417 (12%)	161 (5%)	2 12

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	47	ASP
1	A	240	ALA
1	A	453	ALA
1	A	492	CYS

5.3.2 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	542/544 (100%)	474 (88%)	68 (12%)	4 18
1	L	542/544 (100%)	476 (88%)	66 (12%)	5 20
2	B	514/532 (97%)	438 (85%)	76 (15%)	3 13
2	E	514/532 (97%)	440 (86%)	74 (14%)	3 14
3	I	131/131 (100%)	124 (95%)	7 (5%)	22 56
3	S	131/131 (100%)	123 (94%)	8 (6%)	18 51
4	M	364/387 (94%)	312 (86%)	52 (14%)	3 14
4	U	364/387 (94%)	316 (87%)	48 (13%)	4 16
5	P	8/10 (80%)	7 (88%)	1 (12%)	4 18
5	Q	8/10 (80%)	7 (88%)	1 (12%)	4 18
All	All	3118/3208 (97%)	2717 (87%)	401 (13%)	4 17

5 of 401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	47	ASP
1	L	591	SER
4	U	430	ILE
1	L	163	SER
1	L	409	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	200	HIS
4	M	72	ASN
1	L	319	HIS
1	L	509	ASN
4	M	182	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
5	SEP	Q	3	5	4,5,10	0.56	0	0,5,14	-	-
5	SEP	P	3	5	4,5,10	0.63	0	0,5,14	-	-

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
5	SEP	Q	3	5	-	2/2/4/10	-
5	SEP	P	3	5	-	2/2/4/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	3	SEP	N-CA-CB-OG
5	P	3	SEP	C-CA-CB-OG
5	Q	3	SEP	N-CA-CB-OG
5	Q	3	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	3	SEP	1	0
5	P	3	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
6	SO4	B	1583	-	4,4,4	0.18	0	6,6,6	0.24	0
6	SO4	E	1583	-	4,4,4	0.18	0	6,6,6	0.25	0
6	SO4	L	1631	-	4,4,4	0.17	0	6,6,6	0.18	0
6	SO4	A	1625	-	4,4,4	0.13	0	6,6,6	0.20	0
6	SO4	B	1585	-	4,4,4	0.18	0	6,6,6	0.11	0
6	SO4	M	1436	-	4,4,4	0.17	0	6,6,6	0.27	0
6	SO4	A	1624	-	4,4,4	0.18	0	6,6,6	0.16	0
6	SO4	L	1624	-	4,4,4	0.13	0	6,6,6	0.26	0
6	SO4	B	1584	-	4,4,4	0.18	0	6,6,6	0.14	0
6	SO4	E	1584	-	4,4,4	0.16	0	6,6,6	0.22	0
6	SO4	A	1629	-	4,4,4	0.11	0	6,6,6	0.19	0
6	SO4	E	1585	-	4,4,4	0.19	0	6,6,6	0.18	0
6	SO4	B	1586	-	4,4,4	0.19	0	6,6,6	0.07	0
6	SO4	U	1439	-	4,4,4	0.15	0	6,6,6	0.18	0
6	SO4	L	1628	-	4,4,4	0.10	0	6,6,6	0.19	0
6	SO4	M	1438	-	4,4,4	0.15	0	6,6,6	0.29	0
6	SO4	A	1628	-	4,4,4	0.13	0	6,6,6	0.20	0
6	SO4	A	1626	-	4,4,4	0.13	0	6,6,6	0.36	0
6	SO4	U	1437	-	4,4,4	0.16	0	6,6,6	0.15	0
6	SO4	A	1630	-	4,4,4	0.12	0	6,6,6	0.17	0
6	SO4	L	1625	-	4,4,4	0.13	0	6,6,6	0.27	0
6	SO4	L	1629	-	4,4,4	0.17	0	6,6,6	0.23	0
6	SO4	U	1438	-	4,4,4	0.22	0	6,6,6	0.36	0
6	SO4	L	1626	-	4,4,4	0.15	0	6,6,6	0.34	0
6	SO4	A	1627	-	4,4,4	0.27	0	6,6,6	0.19	0
6	SO4	E	1587	-	4,4,4	0.12	0	6,6,6	0.28	0
6	SO4	L	1630	-	4,4,4	0.17	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	U	1436	-	4,4,4	0.13	0	6,6,6	0.27	0
6	SO4	E	1586	-	4,4,4	0.14	0	6,6,6	0.14	0
6	SO4	L	1627	-	4,4,4	0.12	0	6,6,6	0.26	0
6	SO4	M	1437	-	4,4,4	0.12	0	6,6,6	0.46	0

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.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1583	SO4	1	0
6	A	1625	SO4	2	0
6	A	1624	SO4	2	0
6	A	1629	SO4	1	0
6	B	1586	SO4	1	0
6	A	1626	SO4	1	0
6	L	1625	SO4	1	0
6	A	1627	SO4	1	0
6	E	1587	SO4	2	0
6	M	1437	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 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	621/623 (99%)	0.10	28 (4%) 33 19	37, 70, 125, 219	0
1	L	621/623 (99%)	0.06	26 (4%) 36 21	36, 70, 127, 220	0
2	B	571/591 (96%)	0.17	27 (4%) 31 18	38, 82, 147, 231	0
2	E	571/591 (96%)	0.20	30 (5%) 26 15	42, 82, 149, 229	0
3	I	142/142 (100%)	-0.30	0 100 100	39, 63, 107, 136	0
3	S	142/142 (100%)	-0.35	1 (0%) 87 74	43, 66, 106, 138	0
4	M	409/435 (94%)	0.16	20 (4%) 29 17	41, 72, 139, 216	0
4	U	409/435 (94%)	0.16	18 (4%) 34 20	40, 72, 140, 216	0
5	P	8/11 (72%)	0.15	0 100 100	62, 87, 119, 121	0
5	Q	8/11 (72%)	0.17	0 100 100	60, 89, 118, 121	0
All	All	3502/3604 (97%)	0.10	150 (4%) 35 20	36, 73, 136, 231	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	240	ALA	9.9
4	M	159	ILE	9.1
1	A	240	ALA	8.8
1	A	241	SER	7.3
1	A	242	THR	7.2

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

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
5	SEP	P	3	6/11	0.91	0.13	70,95,107,128	0
5	SEP	Q	3	6/11	0.95	0.12	71,84,108,126	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, 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
6	SO4	A	1627	5/5	0.72	0.21	101,120,184,186	0
6	SO4	B	1584	5/5	0.82	0.26	123,130,155,171	0
6	SO4	L	1629	5/5	0.83	0.38	118,137,168,169	0
6	SO4	L	1630	5/5	0.83	0.19	126,137,152,172	0
6	SO4	L	1628	5/5	0.84	0.22	123,136,161,174	0
6	SO4	A	1630	5/5	0.86	0.44	164,169,180,186	0
6	SO4	L	1627	5/5	0.87	0.29	101,106,135,154	0
6	SO4	B	1585	5/5	0.89	0.17	95,117,144,156	0
6	SO4	L	1631	5/5	0.89	0.18	111,118,126,128	0
6	SO4	E	1585	5/5	0.90	0.24	100,123,136,157	0
6	SO4	A	1626	5/5	0.90	0.31	112,115,148,158	0
6	SO4	E	1584	5/5	0.90	0.18	105,132,143,151	0
6	SO4	M	1438	5/5	0.90	0.19	75,104,141,151	0
6	SO4	A	1629	5/5	0.91	0.57	117,151,174,187	0
6	SO4	L	1625	5/5	0.91	0.21	110,116,139,144	0
6	SO4	M	1437	5/5	0.92	0.17	90,90,124,130	0
6	SO4	L	1626	5/5	0.93	0.21	87,99,139,170	0
6	SO4	E	1583	5/5	0.93	0.19	72,100,119,132	0
6	SO4	U	1437	5/5	0.93	0.26	92,110,143,154	0
6	SO4	A	1625	5/5	0.94	0.19	87,115,156,158	0
6	SO4	B	1583	5/5	0.95	0.11	51,107,130,133	0
6	SO4	E	1586	5/5	0.95	0.16	93,121,144,157	0
6	SO4	B	1586	5/5	0.95	0.17	126,127,129,137	0
6	SO4	U	1439	5/5	0.95	0.14	88,108,134,139	0
6	SO4	L	1624	5/5	0.96	0.18	57,89,118,119	0
6	SO4	U	1438	5/5	0.96	0.17	64,77,130,145	0
6	SO4	E	1587	5/5	0.96	0.15	93,98,159,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	1628	5/5	0.97	0.13	94,110,133,155	0
6	SO4	M	1436	5/5	0.98	0.16	49,55,73,75	0
6	SO4	A	1624	5/5	0.98	0.14	50,75,94,102	0
6	SO4	U	1436	5/5	0.99	0.14	54,56,72,82	0

6.5 Other polymers (i)

There are no such residues in this entry.