Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 01:26 am GMT

PDB ID	:	4U4C
Title	:	The molecular architecture of the TRAMP complex reveals the organization and interplay of its two catalytic activities
Authors	:	Falk, S.; Weir, J.R.; Hentschel, J.; Reichelt, P.; Bonneau, F.; Conti, E.
Deposited on	:	2014-07-23
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

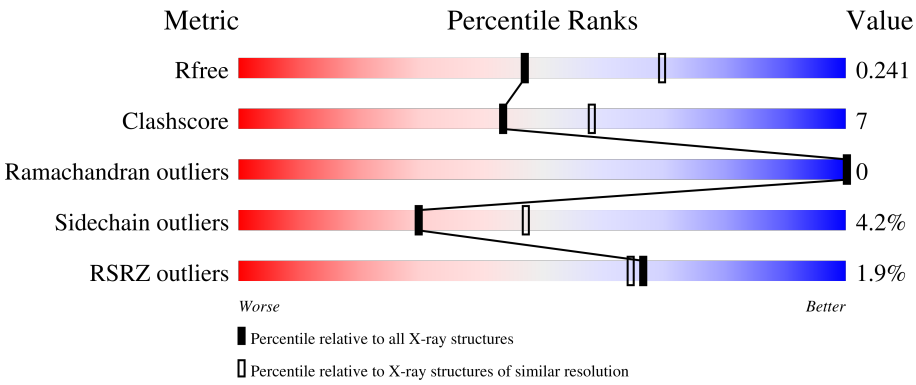
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	998	2% 76% 15% • 7%
2	B	116	3% 42% 6% 52%

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
3	SO4	A	1102	-	-	X	-
5	CL	A	1110	-	-	-	X
5	CL	A	1111	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8023 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 ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	924	7301	4659	1248	1352	42	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	expression tag	UNP P47047
A	77	ALA	-	expression tag	UNP P47047
A	78	ALA	-	expression tag	UNP P47047
A	79	SER	-	expression tag	UNP P47047
A	80	MET	-	expression tag	UNP P47047

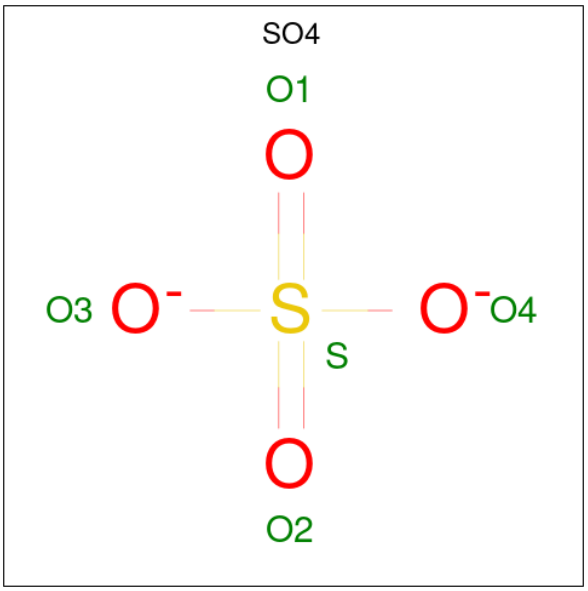
- Molecule 2 is a protein called Protein AIR2,Poly(A) RNA polymerase protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	56	423	263	71	89	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

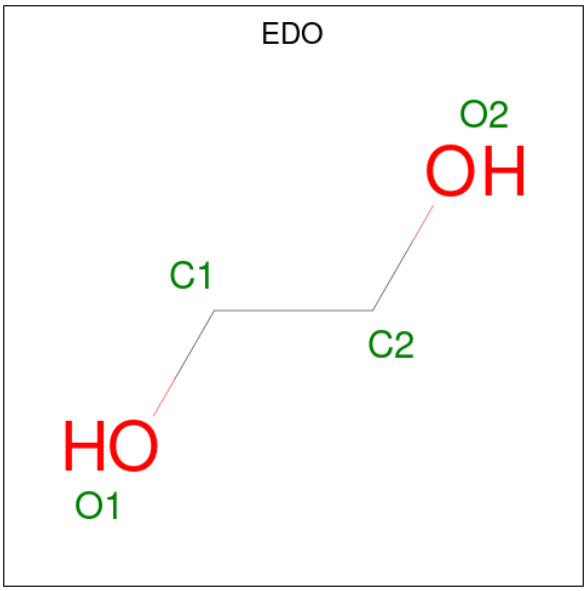
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q12476
B	-2	ALA	-	expression tag	UNP Q12476
B	-1	ALA	-	expression tag	UNP Q12476
B	0	SER	-	expression tag	UNP Q12476

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

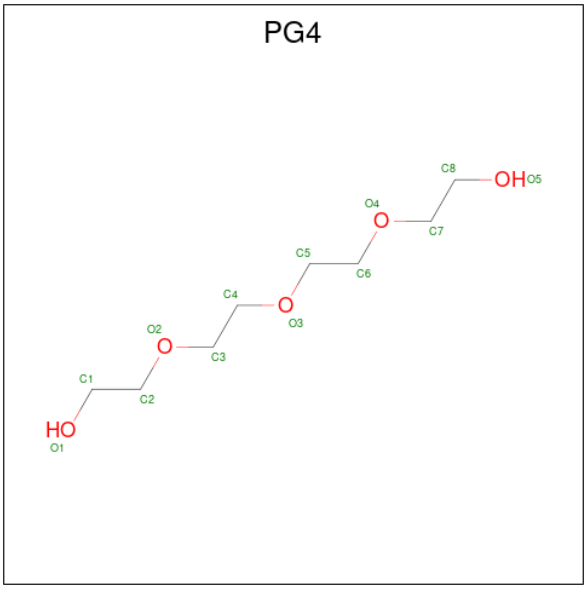


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

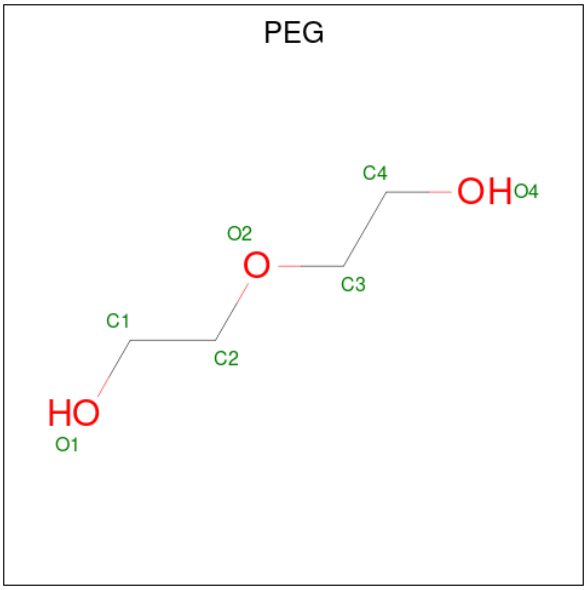
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	13	8	5	0	0
			Total	C	O		
6	A	1	13	8	5	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	7	4	3	0	0

- Molecule 8 is water.

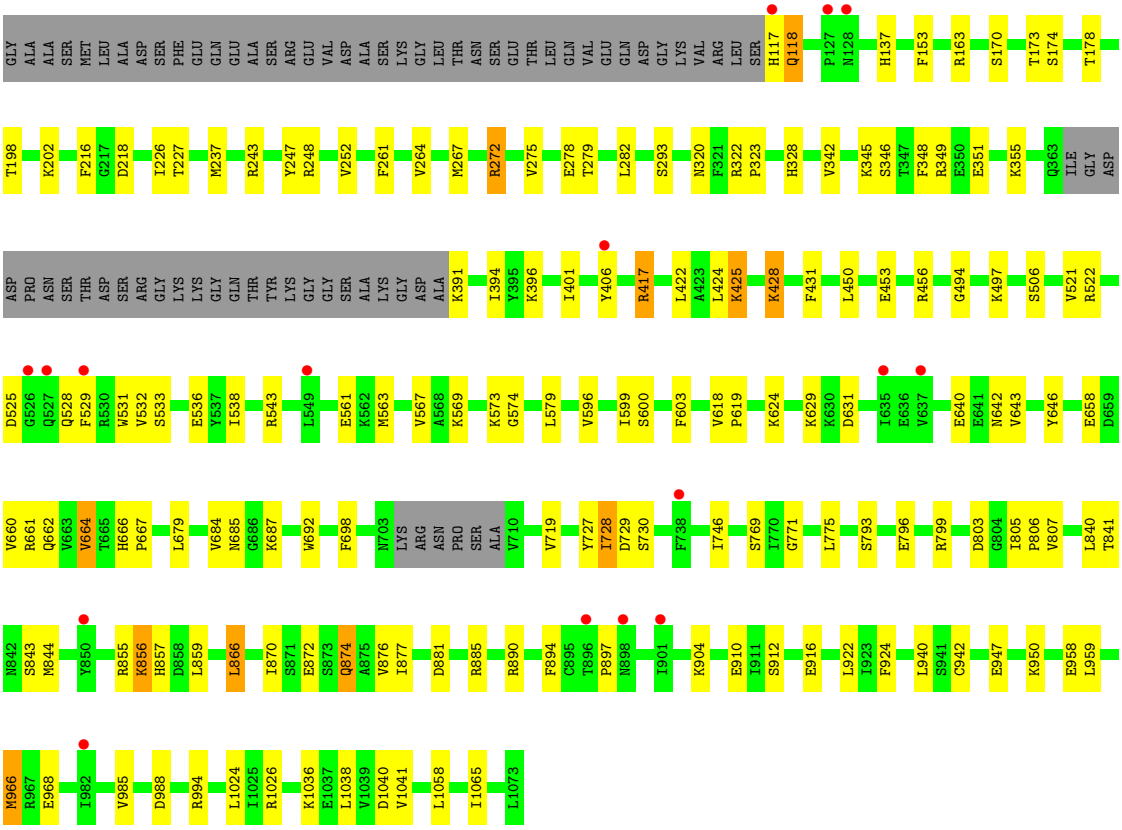
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	202	202	202	0	0
			Total	O		
8	B	19	19	19	0	0

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.

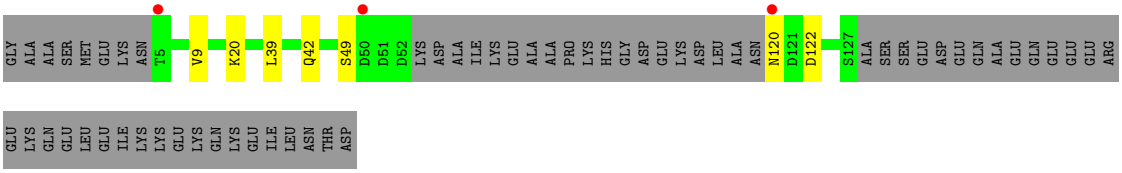
• Molecule 1: ATP-dependent RNA helicase DOB1

Chain A: 2% 76% 15% 7%



• Molecule 2: Protein AIR2,Poly(A) RNA polymerase protein 2

Chain B: 3% 42% 6% 52%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	156.18Å 166.77Å 131.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.40 49.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.70-2.40) 99.6 (49.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.204 , 0.240 0.209 , 0.241	Depositor DCC
R_{free} test set	3354 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8023	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, EDO, PEG, PG4, 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	0.45	0/7443	0.55	0/10062
2	B	0.42	0/431	0.52	0/589
All	All	0.44	0/7874	0.55	0/10651

There are no bond length outliers.

There are no bond angle outliers.

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	7301	0	7282	103	0
2	B	423	0	397	3	0
3	A	35	0	0	2	0
4	A	8	0	12	0	0
5	A	2	0	0	0	0
6	A	26	0	36	3	0
7	A	7	0	10	2	0
8	A	202	0	0	3	0
8	B	19	0	0	0	0
All	All	8023	0	7737	104	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 7.

All (104) 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)
1:A:349:ARG:NH1	2:B:122:ASP:OD2	2.20	0.74
1:A:870:ILE:O	1:A:874:GLN:NE2	2.20	0.73
1:A:658:GLU:OE2	1:A:662:GLN:NE2	2.20	0.73
1:A:525:ASP:HB2	1:A:528:GLN:HB3	1.72	0.72
1:A:1036:LYS:HZ3	6:A:1113:PG4:H41	1.59	0.67
1:A:243:ARG:HD2	1:A:275:VAL:HG13	1.79	0.62
1:A:596:VAL:HG23	1:A:599:ILE:HG22	1.80	0.62
1:A:872:GLU:HA	1:A:877:ILE:HD11	1.83	0.61
1:A:985:VAL:HG13	1:A:988:ASP:HB2	1.83	0.61
1:A:692:TRP:CG	1:A:805:ILE:HD12	2.37	0.58
1:A:248:ARG:NH2	1:A:1040:ASP:OD2	2.38	0.57
1:A:561:GLU:H	1:A:561:GLU:CD	2.07	0.57
1:A:890:ARG:HD3	1:A:897:PRO:HA	1.86	0.56
1:A:1036:LYS:NZ	6:A:1113:PG4:H41	2.19	0.56
1:A:730:SER:HB3	1:A:746:ILE:HD13	1.88	0.56
1:A:904:LYS:HG2	1:A:924:PHE:CD2	2.40	0.56
1:A:275:VAL:O	1:A:279:THR:HG23	2.06	0.55
1:A:685:ASN:O	1:A:687:LYS:HG3	2.07	0.55
1:A:247:TYR:OH	1:A:278:GLU:OE2	2.23	0.55
1:A:894:PHE:HE1	1:A:904:LYS:HE2	1.72	0.55
1:A:771:GLY:HA2	1:A:807:VAL:HA	1.88	0.55
1:A:569:LYS:HG2	1:A:573:LYS:HE2	1.90	0.54
1:A:624:LYS:HB3	1:A:866:LEU:HD21	1.90	0.54
2:B:39:LEU:O	2:B:42:GLN:NE2	2.36	0.53
1:A:117:HIS:CE1	1:A:320:ASN:HB2	2.44	0.53
1:A:679:LEU:HD23	1:A:805:ILE:HD13	1.90	0.53
1:A:640:GLU:HB2	1:A:643:VAL:HG23	1.90	0.53
1:A:775:LEU:HD22	1:A:793:SER:HB3	1.91	0.53
1:A:904:LYS:HG2	1:A:924:PHE:CE2	2.44	0.52
1:A:401:ILE:HG23	1:A:406:TYR:HB2	1.91	0.52
1:A:391:LYS:O	1:A:425:LYS:NZ	2.40	0.52
1:A:968:GLU:HG3	8:A:1292:HOH:O	2.08	0.52
1:A:855:ARG:NH2	1:A:859:LEU:HD11	2.25	0.52
1:A:264:VAL:HG12	1:A:293:SER:HB2	1.93	0.51
1:A:643:VAL:HG22	1:A:840:LEU:HD21	1.93	0.51
1:A:348:PHE:CE2	1:A:569:LYS:HE3	2.45	0.50
1:A:922:LEU:HD11	1:A:966:MET:HG3	1.94	0.50
1:A:646:TYR:CE1	1:A:841:THR:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:CZ	1:A:282:LEU:HD11	2.47	0.50
1:A:394:ILE:HG21	1:A:422:LEU:HD22	1.95	0.49
1:A:660:VAL:O	1:A:664:VAL:HG13	2.12	0.48
1:A:1038:LEU:HA	1:A:1041:VAL:HG22	1.93	0.48
1:A:351:GLU:H	1:A:351:GLU:CD	2.17	0.48
1:A:904:LYS:HA	1:A:924:PHE:HE2	1.77	0.48
1:A:428:LYS:H	1:A:428:LYS:HG3	1.45	0.48
1:A:796:GLU:OE2	1:A:799:ARG:NH1	2.46	0.48
1:A:881:ASP:OD2	1:A:885:ARG:NE	2.40	0.48
1:A:698:PHE:HB3	1:A:719:VAL:HG13	1.96	0.47
1:A:646:TYR:HE1	1:A:841:THR:HG22	1.79	0.47
1:A:538:ILE:HD11	1:A:574:GLY:C	2.34	0.47
1:A:856:LYS:HE3	1:A:857:HIS:NE2	2.30	0.47
1:A:985:VAL:HG21	8:A:1335:HOH:O	2.15	0.47
1:A:431:PHE:HB3	1:A:497:LYS:HG3	1.97	0.47
1:A:453:GLU:HA	1:A:456:ARG:HB2	1.96	0.46
1:A:506:SER:O	1:A:543:ARG:HD2	2.15	0.46
1:A:431:PHE:O	1:A:497:LYS:HE2	2.16	0.46
1:A:618:VAL:HB	1:A:619:PRO:HD3	1.96	0.46
1:A:1038:LEU:HA	1:A:1038:LEU:HD23	1.76	0.45
1:A:173:THR:O	3:A:1102:SO4:S	2.74	0.45
1:A:355:LYS:HE3	1:A:355:LYS:HB2	1.70	0.45
1:A:563:MET:HE2	1:A:567:VAL:HB	1.99	0.45
1:A:252:VAL:N	8:A:1367:HOH:O	2.50	0.45
1:A:267:MET:HB2	1:A:267:MET:HE3	1.87	0.45
1:A:727:TYR:CE2	1:A:729:ASP:HB2	2.51	0.44
1:A:805:ILE:HA	1:A:806:PRO:HD3	1.89	0.44
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.87	0.44
1:A:916:GLU:H	1:A:916:GLU:CD	2.21	0.44
1:A:117:HIS:CG	1:A:118:GLN:H	2.36	0.44
1:A:843:SER:OG	1:A:844:MET:N	2.51	0.44
1:A:538:ILE:HD11	1:A:574:GLY:O	2.18	0.44
1:A:855:ARG:HA	1:A:855:ARG:HD2	1.76	0.44
1:A:198:THR:OG1	1:A:261:PHE:HA	2.19	0.43
1:A:600:SER:O	1:A:603:PHE:HB3	2.18	0.43
1:A:198:THR:HA	1:A:237:MET:O	2.18	0.43
1:A:942:CYS:HA	1:A:994:ARG:O	2.19	0.43
1:A:874:GLN:HB3	1:A:876:VAL:HG12	2.00	0.43
1:A:1024:LEU:HD23	1:A:1024:LEU:HA	1.92	0.43
1:A:521:VAL:HG23	1:A:531:TRP:CZ3	2.54	0.43
1:A:174:SER:OG	1:A:323:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:GLU:HB2	1:A:1041:VAL:CG1	2.49	0.42
1:A:728:ILE:O	1:A:728:ILE:HG13	2.19	0.42
1:A:958:GLU:O	1:A:959:LEU:HD23	2.20	0.42
1:A:532:VAL:HG13	1:A:536:GLU:HB2	2.00	0.42
1:A:216:PHE:O	1:A:218:ASP:N	2.48	0.42
1:A:950:LYS:O	2:B:20:LYS:HB3	2.20	0.42
1:A:328:HIS:HB2	1:A:342:VAL:HB	2.01	0.42
1:A:417:ARG:HE	1:A:417:ARG:H	1.68	0.42
1:A:599:ILE:HD12	1:A:599:ILE:HA	1.86	0.42
1:A:272:ARG:HE	1:A:272:ARG:HB3	1.69	0.41
1:A:494:GLY:HA2	7:A:1114:PEG:H21	2.01	0.41
1:A:1036:LYS:HZ1	6:A:1113:PG4:H21	1.85	0.41
1:A:137:HIS:CE1	1:A:163:ARG:HG3	2.55	0.41
1:A:856:LYS:HE3	1:A:857:HIS:CD2	2.55	0.41
1:A:178:THR:N	3:A:1102:SO4:O4	2.50	0.41
1:A:345:LYS:O	1:A:346:SER:HB2	2.20	0.41
1:A:1058:LEU:HA	1:A:1058:LEU:HD23	1.80	0.41
1:A:563:MET:HE3	1:A:563:MET:HA	2.02	0.41
1:A:666:HIS:CG	1:A:667:PRO:HD2	2.55	0.41
1:A:881:ASP:O	1:A:885:ARG:HG3	2.21	0.40
1:A:226:ILE:HG12	1:A:227:THR:N	2.37	0.40
1:A:692:TRP:CD1	1:A:805:ILE:HD12	2.56	0.40
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.84	0.40
1:A:494:GLY:CA	7:A:1114:PEG:H21	2.52	0.40
1:A:692:TRP:CE2	1:A:805:ILE:HB	2.56	0.40

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	918/998 (92%)	879 (96%)	39 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	52/116 (45%)	50 (96%)	2 (4%)	0	100	100
All	All	970/1114 (87%)	929 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	789/879 (90%)	757 (96%)	32 (4%)	30	48
2	B	48/99 (48%)	45 (94%)	3 (6%)	18	28
All	All	837/978 (86%)	802 (96%)	35 (4%)	30	47

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	153	PHE
1	A	170	SER
1	A	202	LYS
1	A	272	ARG
1	A	322	ARG
1	A	396	LYS
1	A	417	ARG
1	A	425	LYS
1	A	428	LYS
1	A	450	LEU
1	A	522	ARG
1	A	529	PHE
1	A	533	SER
1	A	579	LEU
1	A	629	LYS
1	A	631	ASP
1	A	642	ASN

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Mol	Chain	Res	Type
1	A	661	ARG
1	A	664	VAL
1	A	684	VAL
1	A	728	ILE
1	A	769	SER
1	A	803	ASP
1	A	856	LYS
1	A	866	LEU
1	A	874	GLN
1	A	912	SER
1	A	947	GLU
1	A	966	MET
1	A	1026	ARG
1	A	1065	ILE
2	B	9	VAL
2	B	49	SER
2	B	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	SO4	A	1101	-	4,4,4	0.12	0	6,6,6	0.31	0
3	SO4	A	1103	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	1107	-	4,4,4	0.16	0	6,6,6	0.05	0
4	EDO	A	1109	-	3,3,3	0.51	0	2,2,2	0.30	0
6	PG4	A	1112	-	12,12,12	0.53	0	11,11,11	0.39	0
3	SO4	A	1106	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	A	1105	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	A	1104	-	4,4,4	0.14	0	6,6,6	0.29	0
6	PG4	A	1113	-	12,12,12	0.60	0	11,11,11	0.35	0
4	EDO	A	1108	-	3,3,3	0.46	0	2,2,2	0.34	0
7	PEG	A	1114	-	6,6,6	0.73	0	5,5,5	0.35	0
3	SO4	A	1102	-	4,4,4	0.16	0	6,6,6	0.24	0

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
4	EDO	A	1109	-	-	1/1/1/1	-
6	PG4	A	1112	-	-	4/10/10/10	-
6	PG4	A	1113	-	-	6/10/10/10	-
4	EDO	A	1108	-	-	0/1/1/1	-
7	PEG	A	1114	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1113	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	1113	PG4	O3-C5-C6-O4
6	A	1112	PG4	O2-C3-C4-O3
7	A	1114	PEG	O1-C1-C2-O2
6	A	1112	PG4	O4-C7-C8-O5
7	A	1114	PEG	O2-C3-C4-O4
6	A	1113	PG4	O1-C1-C2-O2
6	A	1113	PG4	O2-C3-C4-O3
6	A	1113	PG4	C8-C7-O4-C6
6	A	1112	PG4	C5-C6-O4-C7
7	A	1114	PEG	C4-C3-O2-C2
6	A	1113	PG4	C6-C5-O3-C4
4	A	1109	EDO	O1-C1-C2-O2
6	A	1112	PG4	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1113	PG4	3	0
7	A	1114	PEG	2	0
3	A	1102	SO4	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	924/998 (92%)	-0.03	16 (1%)	70	68	38, 57, 103, 270	8 (0%)
2	B	56/116 (48%)	-0.04	3 (5%)	25	24	39, 51, 173, 286	0
All	All	980/1114 (87%)	-0.04	19 (1%)	66	64	38, 57, 105, 286	8 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	637	VAL	3.8
1	A	406	TYR	3.8
1	A	850	TYR	3.5
1	A	117	HIS	3.2
1	A	901	ILE	3.2
1	A	529	PHE	3.0
1	A	635	ILE	3.0
1	A	527	GLN	2.6
1	A	982	ILE	2.4
1	A	549	LEU	2.4
1	A	128	ASN	2.4
1	A	896	THR	2.4
1	A	127	PRO	2.4
2	B	5	THR	2.3
2	B	50	ASP	2.3
2	B	120	ASN	2.3
1	A	898	ASN	2.3
1	A	526	GLY	2.1
1	A	738	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	1110	1/1	-0.14	0.71	254,254,254,254	0
5	CL	A	1111	1/1	0.41	2.16	179,179,179,179	0
7	PEG	A	1114	7/7	0.73	0.15	61,66,66,69	0
3	SO4	A	1101	5/5	0.76	0.21	105,107,109,113	0
3	SO4	A	1107	5/5	0.77	0.28	125,128,137,142	0
4	EDO	A	1109	4/4	0.79	0.17	56,59,59,60	0
3	SO4	A	1105	5/5	0.83	0.15	130,131,131,135	0
6	PG4	A	1112	13/13	0.86	0.21	53,59,64,67	0
4	EDO	A	1108	4/4	0.88	0.11	72,74,75,76	0
6	PG4	A	1113	13/13	0.89	0.14	49,53,63,67	0
3	SO4	A	1103	5/5	0.90	0.23	108,116,120,121	0
3	SO4	A	1106	5/5	0.96	0.13	57,63,72,76	0
3	SO4	A	1102	5/5	0.97	0.16	48,49,54,59	0
3	SO4	A	1104	5/5	0.99	0.09	49,54,63,65	0

6.5 Other polymers (i)

There are no such residues in this entry.