Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:36 am BST

PDB ID	:	6FKV
Title	:	Structure and function of aldehyde dehydrogenase from Thermus thermophilus: An enzyme with an evolutionarily-distinct C-terminal arm (Recombinant protein with shortened C-terminal, ADH508)
Authors	:	Hayes, K.A.; Noor, M.R.; Djeghader, A.; Soulimane, T.
Deposited on	:	2018-01-24
Resolution	:	2.90 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 ⓘ symbol.

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

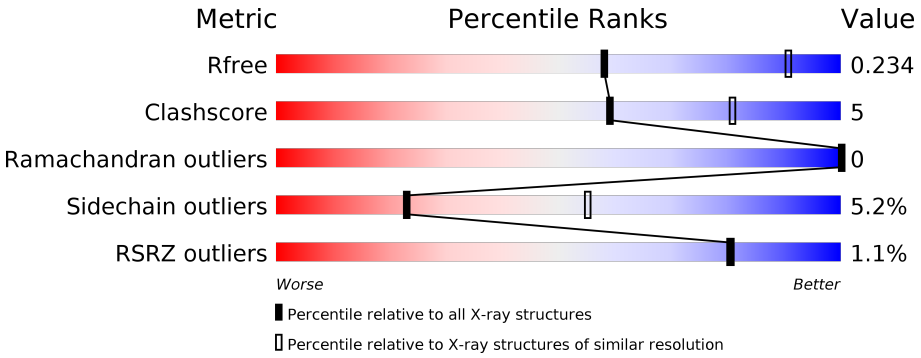
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	517	% 80% 16%
1	B	517	% 82% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7994 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.

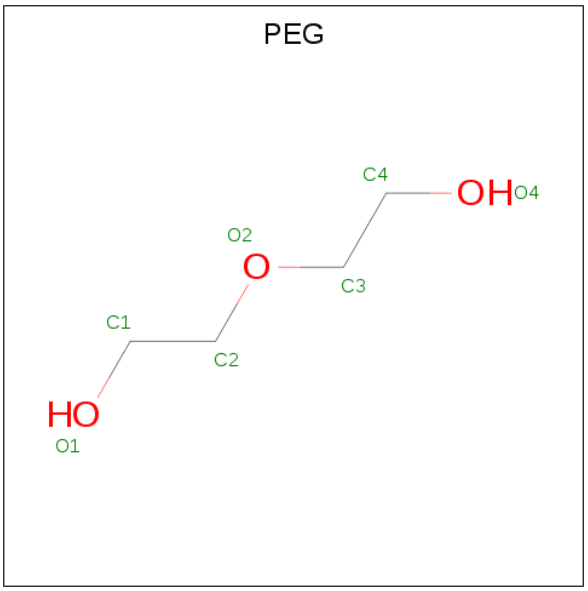
- Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3946	2530	692	717	7			
1	B	505	Total	C	N	O	S	0	0	0
			3954	2536	693	718	7			

There are 14 discrepancies between the modelled and reference sequences:

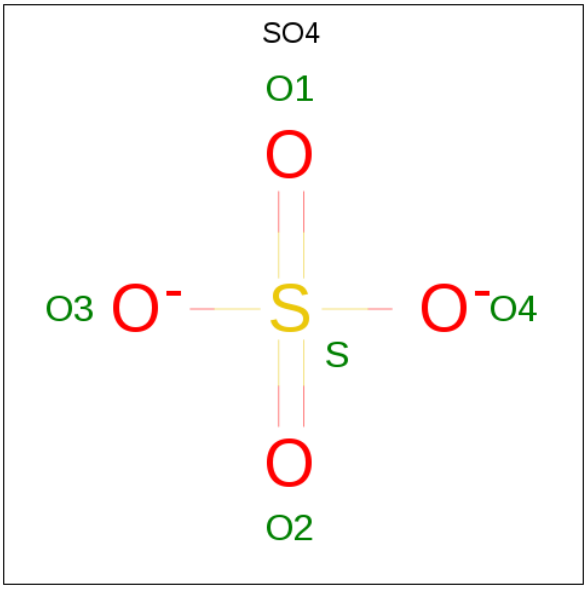
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q72KD3
A	-4	HIS	-	expression tag	UNP Q72KD3
A	-3	HIS	-	expression tag	UNP Q72KD3
A	-2	HIS	-	expression tag	UNP Q72KD3
A	-1	HIS	-	expression tag	UNP Q72KD3
A	0	HIS	-	expression tag	UNP Q72KD3
A	1	HIS	-	expression tag	UNP Q72KD3
B	-5	MET	-	expression tag	UNP Q72KD3
B	-4	HIS	-	expression tag	UNP Q72KD3
B	-3	HIS	-	expression tag	UNP Q72KD3
B	-2	HIS	-	expression tag	UNP Q72KD3
B	-1	HIS	-	expression tag	UNP Q72KD3
B	0	HIS	-	expression tag	UNP Q72KD3
B	1	HIS	-	expression tag	UNP Q72KD3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

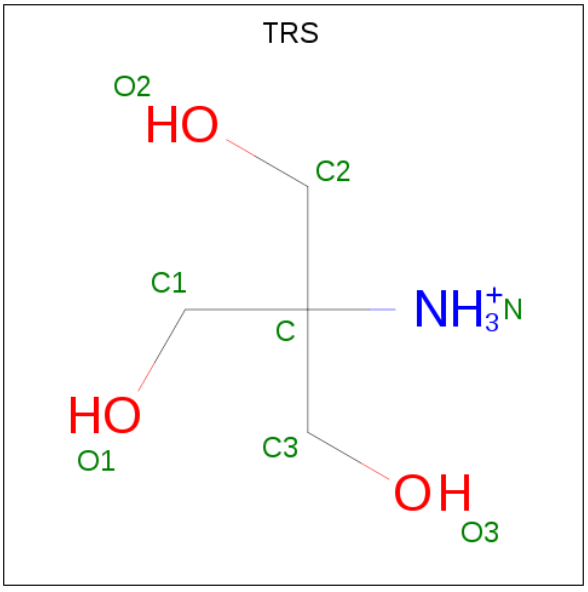


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is water.

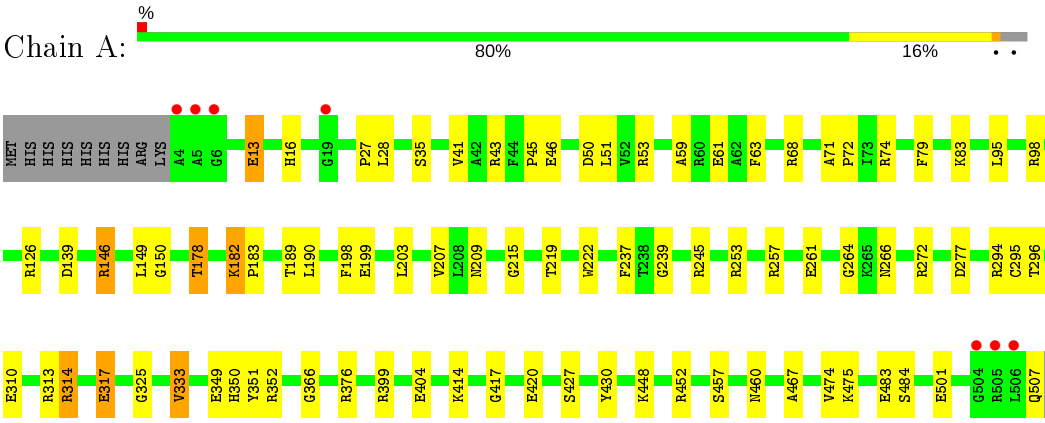
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

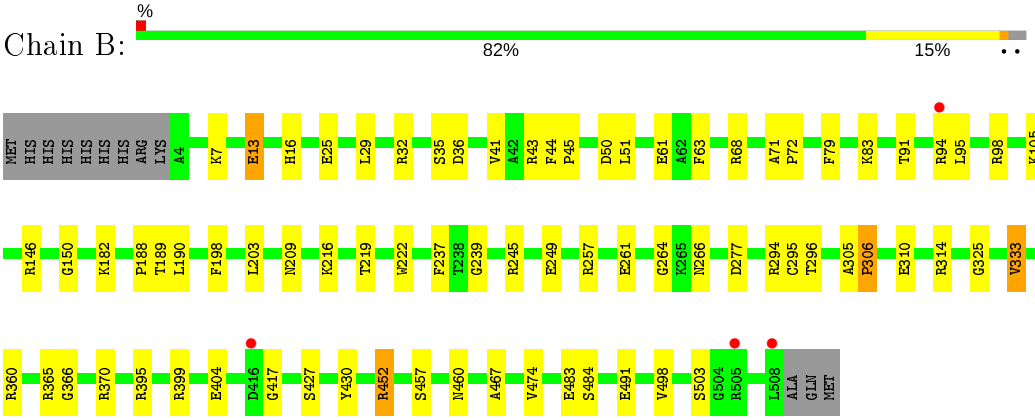
- Molecule 1: Aldehyde dehydrogenase

Chain A:



- Molecule 1: Aldehyde dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.19Å 105.19Å 314.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.90 48.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.04-2.90) 97.7 (48.04-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.190 , 0.229 0.201 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	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	7994	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, PEG, SO4, 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	0.54	0/4049	0.78	1/5500 (0.0%)
1	B	0.54	0/4057	0.76	0/5511
All	All	0.54	0/8106	0.77	1/11011 (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
1	A	0	10
1	B	0	13
All	All	0	23

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ASP	CB-CG-OD1	6.83	124.45	118.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain
1	A	146	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	352	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	376	ARG	Sidechain
1	A	399	ARG	Sidechain
1	A	417	GLY	Peptide
1	A	68	ARG	Sidechain
1	A	74	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	146	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	257	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	360	ARG	Sidechain
1	B	365	ARG	Sidechain
1	B	370	ARG	Sidechain
1	B	399	ARG	Sidechain
1	B	417	GLY	Peptide
1	B	452	ARG	Sidechain
1	B	68	ARG	Sidechain
1	B	94	ARG	Sidechain

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	3946	0	3896	43	0
1	B	3954	0	3907	34	0
2	A	14	0	20	4	0
2	B	21	0	30	3	0
3	A	20	0	0	2	0
3	B	10	0	0	0	0
4	A	4	0	0	0	0
5	B	8	0	12	2	0
6	A	7	0	0	0	0
6	B	10	0	0	0	0
All	All	7994	0	7865	74	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 5.

All (74) 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:277:ASP:OD1	1:A:314:ARG:NH1	1.97	0.97
1:B:277:ASP:OD1	1:B:314:ARG:NH1	2.00	0.94
1:A:59:ALA:HB1	1:A:178:THR:HG23	1.51	0.91
1:A:59:ALA:O	1:A:178:THR:HG21	1.87	0.74
1:A:261:GLU:OE2	1:A:483:GLU:HG3	1.94	0.68
1:A:501:GLU:OE1	1:A:507:GLN:NE2	2.27	0.67
1:B:261:GLU:OE2	1:B:483:GLU:HG3	1.95	0.66
1:A:95:LEU:HD23	1:A:190:LEU:HD23	1.80	0.63
1:B:294:ARG:HH12	5:B:704:TRS:H11	1.69	0.57
1:A:59:ALA:HB1	1:A:178:THR:CG2	2.29	0.57
1:B:294:ARG:HH22	5:B:704:TRS:H12	1.68	0.56
1:B:95:LEU:HD23	1:B:190:LEU:HD23	1.86	0.56
1:A:414:LYS:HD3	2:A:601:PEG:C1	2.35	0.56
1:A:79:PHE:CE2	1:A:83:LYS:HE2	2.42	0.55
1:B:198:PHE:CD1	1:B:203:LEU:HD22	2.42	0.55
1:B:474:VAL:HG23	2:B:701:PEG:H11	1.89	0.55
1:B:79:PHE:CE2	1:B:83:LYS:HE2	2.41	0.54
1:A:257:ARG:NH2	1:B:491:GLU:OE1	2.39	0.54
1:B:351:TYR:CE2	1:B:366:GLY:HA2	2.45	0.52
1:A:149:LEU:O	2:B:701:PEG:H41	2.10	0.52
1:A:198:PHE:CD1	1:A:203:LEU:HD22	2.45	0.52
1:B:7:LYS:HE2	1:B:36:ASP:OD2	2.11	0.51
1:A:294:ARG:NH1	3:A:604:SO4:O3	2.43	0.51
1:B:7:LYS:CE	1:B:36:ASP:OD2	2.59	0.51
1:B:7:LYS:NZ	1:B:36:ASP:OD2	2.43	0.51
1:A:16:HIS:CD2	1:A:51:LEU:CD2	2.95	0.50
1:A:414:LYS:HD3	2:A:601:PEG:H12	1.93	0.50
1:B:237:PHE:CZ	1:B:239:GLY:HA3	2.47	0.50
1:A:237:PHE:CZ	1:A:239:GLY:HA3	2.47	0.49
1:B:305:ALA:HB3	1:B:306:PRO:HD3	1.95	0.49
1:B:266:ASN:ND2	1:B:296:THR:HA	2.28	0.49
1:B:29:LEU:O	1:B:43:ARG:HG2	2.12	0.48
1:A:253:ARG:HB3	1:B:249:GLU:HB2	1.95	0.48
1:A:414:LYS:HD3	2:A:601:PEG:H11	1.95	0.48
1:A:95:LEU:HD21	1:A:189:THR:HG22	1.96	0.47
1:A:41:VAL:HG13	1:A:98:ARG:NH1	2.29	0.47
1:A:13:GLU:HA	1:A:43:ARG:O	2.14	0.47
1:B:16:HIS:CD2	1:B:51:LEU:CD2	2.96	0.47
1:B:41:VAL:HG13	1:B:98:ARG:NH1	2.28	0.47
1:B:16:HIS:CD2	1:B:51:LEU:HD21	2.49	0.47
1:A:16:HIS:CD2	1:A:51:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:HA	1:B:43:ARG:O	2.15	0.47
1:B:95:LEU:HD21	1:B:189:THR:HG22	1.97	0.46
1:B:63:PHE:CE2	1:B:150:GLY:HA2	2.51	0.46
1:A:457:SER:HB3	1:A:460:ASN:HB3	1.98	0.46
1:A:351:TYR:CE2	1:A:366:GLY:HA2	2.51	0.46
1:A:27:PRO:HG2	1:A:46:GLU:HB3	1.98	0.46
1:A:266:ASN:ND2	1:A:296:THR:HA	2.31	0.44
1:A:53:ARG:NH2	3:A:606:SO4:O4	2.39	0.44
1:A:325:GLY:N	1:A:333:VAL:HG21	2.33	0.44
1:B:219:THR:HA	1:B:222:TRP:CD1	2.52	0.43
1:B:325:GLY:N	1:B:333:VAL:HG21	2.33	0.43
1:A:448:LYS:HD2	1:B:498:VAL:HG11	2.00	0.43
1:A:71:ALA:N	1:A:72:PRO:CD	2.81	0.43
1:B:467:ALA:O	1:B:484:SER:HB3	2.18	0.43
1:A:178:THR:OG1	1:A:207:VAL:HA	2.19	0.42
1:A:215:GLY:HA3	2:A:602:PEG:H22	2.01	0.42
1:B:44:PHE:CE1	1:B:188:PRO:HG3	2.53	0.42
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.84	0.42
1:B:139:ASP:CB	1:B:503:SER:HB3	2.50	0.42
1:A:264:GLY:HA2	1:A:430:TYR:CG	2.55	0.42
1:A:149:LEU:O	2:B:701:PEG:H22	2.19	0.42
1:B:264:GLY:HA2	1:B:430:TYR:CG	2.55	0.42
1:B:457:SER:HB3	1:B:460:ASN:HB3	2.02	0.42
1:A:313:ARG:NH1	1:A:317:GLU:OE1	2.52	0.42
1:A:219:THR:HA	1:A:222:TRP:CD1	2.54	0.41
1:A:474:VAL:HG22	1:A:475:LYS:N	2.35	0.41
1:A:182:LYS:HE3	1:A:183:PRO:O	2.20	0.41
1:A:305:ALA:HB3	1:A:306:PRO:HD3	2.03	0.41
1:A:467:ALA:O	1:A:484:SER:HB3	2.20	0.41
1:A:63:PHE:CE2	1:A:150:GLY:HA2	2.55	0.41
1:B:16:HIS:CE1	1:B:45:PRO:HG2	2.55	0.41
1:B:71:ALA:N	1:B:72:PRO:CD	2.83	0.41
1:A:16:HIS:CE1	1:A:45:PRO:HG2	2.56	0.41

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	502/517 (97%)	481 (96%)	21 (4%)	0	100	100
1	B	503/517 (97%)	484 (96%)	19 (4%)	0	100	100
All	All	1005/1034 (97%)	965 (96%)	40 (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	402/414 (97%)	380 (94%)	22 (6%)	21	53
1	B	403/414 (97%)	383 (95%)	20 (5%)	24	57
All	All	805/828 (97%)	763 (95%)	42 (5%)	23	55

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	28	LEU
1	A	35	SER
1	A	61	GLU
1	A	105	LYS
1	A	123	SER
1	A	139	ASP
1	A	178	THR

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Mol	Chain	Res	Type
1	A	182	LYS
1	A	199	GLU
1	A	209	ASN
1	A	295	CYS
1	A	310	GLU
1	A	314	ARG
1	A	317	GLU
1	A	333	VAL
1	A	349	GLU
1	A	350	HIS
1	A	404	GLU
1	A	420	GLU
1	A	427	SER
1	A	452	ARG
1	B	13	GLU
1	B	25	GLU
1	B	35	SER
1	B	50	ASP
1	B	61	GLU
1	B	91	THR
1	B	105	LYS
1	B	182	LYS
1	B	209	ASN
1	B	216	LYS
1	B	295	CYS
1	B	306	PRO
1	B	310	GLU
1	B	333	VAL
1	B	349	GLU
1	B	350	HIS
1	B	395	ARG
1	B	404	GLU
1	B	427	SER
1	B	452	ARG

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 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 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	605	-	4,4,4	0.51	0	6,6,6	0.45	0
5	TRS	B	704	-	7,7,7	0.45	0	9,9,9	0.95	0
3	SO4	A	604	-	4,4,4	0.49	0	6,6,6	0.83	0
3	SO4	B	706	-	4,4,4	0.33	0	6,6,6	1.17	1 (16%)
2	PEG	B	701	-	6,6,6	1.10	0	5,5,5	1.86	1 (20%)
3	SO4	A	603	-	4,4,4	0.69	0	6,6,6	0.87	0
3	SO4	A	606	-	4,4,4	0.48	0	6,6,6	0.65	0
3	SO4	B	705	-	4,4,4	0.41	0	6,6,6	0.54	0
2	PEG	A	602	-	6,6,6	0.69	0	5,5,5	0.95	0
2	PEG	B	702	-	6,6,6	0.61	0	5,5,5	0.54	0
2	PEG	B	703	-	6,6,6	0.73	0	5,5,5	0.58	0
2	PEG	A	601	-	6,6,6	0.80	0	5,5,5	0.88	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
5	TRS	B	704	-	-	3/9/9/9	-
2	PEG	B	701	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	602	-	-	1/4/4/4	-
2	PEG	B	702	-	-	1/4/4/4	-
2	PEG	A	601	-	-	1/4/4/4	-
2	PEG	B	703	-	-	3/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	PEG	O2-C2-C1	3.36	124.82	110.07
3	B	706	SO4	O4-S-O3	2.34	119.06	109.06

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	PEG	C4-C3-O2-C2
2	A	602	PEG	C1-C2-O2-C3
2	A	601	PEG	O2-C3-C4-O4
2	B	703	PEG	O2-C3-C4-O4
2	B	702	PEG	O1-C1-C2-O2
5	B	704	TRS	C1-C-C3-O3
2	B	703	PEG	O1-C1-C2-O2
2	B	701	PEG	O1-C1-C2-O2
5	B	704	TRS	C2-C-C3-O3
5	B	704	TRS	N-C-C3-O3
2	B	703	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	704	TRS	2	0
3	A	604	SO4	1	0
2	B	701	PEG	3	0
3	A	606	SO4	1	0
2	A	602	PEG	1	0
2	A	601	PEG	3	0

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

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	504/517 (97%)	-0.19	7 (1%) 75 75	37, 54, 76, 113	0
1	B	505/517 (97%)	-0.16	4 (0%) 86 86	38, 55, 79, 97	0
All	All	1009/1034 (97%)	-0.18	11 (1%) 80 80	37, 55, 78, 113	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	2.9
1	A	505	ARG	2.9
1	A	506	LEU	2.6
1	A	504	GLY	2.5
1	A	6	GLY	2.4
1	B	508	LEU	2.4
1	B	505	ARG	2.2
1	A	5	ALA	2.2
1	B	94	ARG	2.2
1	A	19	GLY	2.2
1	B	416	ASP	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	PEG	B	701	7/7	0.75	0.28	61,72,77,81	0
2	PEG	A	601	7/7	0.79	0.33	57,62,70,70	0
2	PEG	B	702	7/7	0.83	0.24	56,67,69,69	0
5	TRS	B	704	8/8	0.83	0.28	62,89,93,106	0
2	PEG	A	602	7/7	0.88	0.24	53,68,76,76	0
4	CL	A	609	1/1	0.89	0.14	67,67,67,67	0
2	PEG	B	703	7/7	0.89	0.21	54,66,72,74	0
3	SO4	A	606	5/5	0.90	0.25	77,96,101,107	0
4	CL	A	610	1/1	0.92	0.13	66,66,66,66	0
3	SO4	A	605	5/5	0.92	0.16	84,101,109,118	0
4	CL	A	608	1/1	0.93	0.13	60,60,60,60	0
3	SO4	B	705	5/5	0.94	0.17	60,68,73,75	0
4	CL	A	607	1/1	0.94	0.37	63,63,63,63	0
3	SO4	A	604	5/5	0.95	0.17	66,68,86,93	0
3	SO4	B	706	5/5	0.95	0.16	78,80,85,85	0
3	SO4	A	603	5/5	0.98	0.12	55,64,71,72	0

6.5 Other polymers

There are no such residues in this entry.