



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:59 AM UTC

PDB ID : 3EI7 / pdb_00003ei7
Title : Crystal structure of apo-LL-diaminopimelate aminotransferase from *Arabidopsis thaliana* (no PLP)
Authors : Watanabe, N.; Clay, M.D.; van Belkum, M.J.; Cherney, M.M.; Vederas, J.C.; James, M.N.G.
Deposited on : 2008-09-15
Resolution : 1.99 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

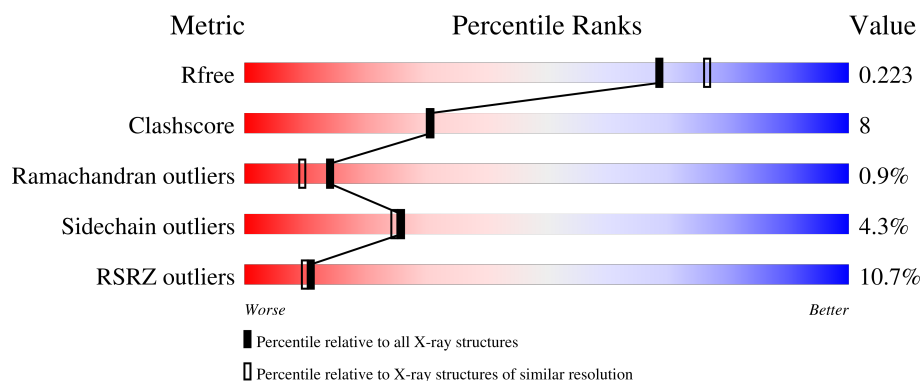
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	432	11% 78% 15% • 5%
1	B	432	9% 80% 13% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6977 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 LL-diaminopimelate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3184	2027	536	605	16			
1	B	409	Total	C	N	O	S	0	0	0
			3154	2009	527	602	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP Q93ZN9
A	428	HIS	-	expression tag	UNP Q93ZN9
A	429	HIS	-	expression tag	UNP Q93ZN9
A	430	HIS	-	expression tag	UNP Q93ZN9
A	431	HIS	-	expression tag	UNP Q93ZN9
A	432	HIS	-	expression tag	UNP Q93ZN9
B	427	HIS	-	expression tag	UNP Q93ZN9
B	428	HIS	-	expression tag	UNP Q93ZN9
B	429	HIS	-	expression tag	UNP Q93ZN9
B	430	HIS	-	expression tag	UNP Q93ZN9
B	431	HIS	-	expression tag	UNP Q93ZN9
B	432	HIS	-	expression tag	UNP Q93ZN9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

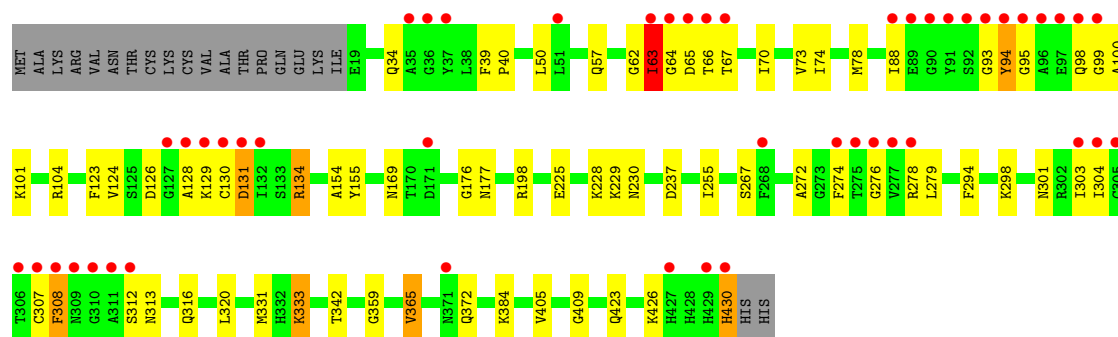
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	326	Total	O	0	0
			326	326		
3	B	303	Total	O	0	0
			303	303		

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.

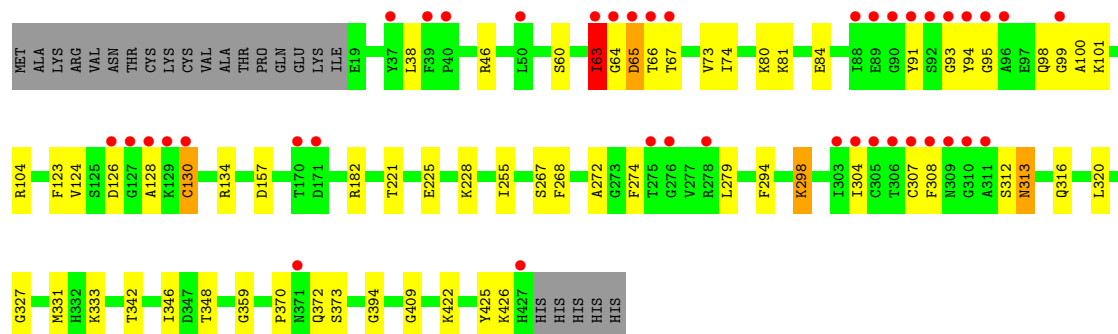
- Molecule 1: LL-diaminopimelate aminotransferase

Chain A: 



- Molecule 1: LL-diaminopimelate aminotransferase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.10Å 103.10Å 171.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 1.99 38.72 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.72-1.99) 99.9 (38.72-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.189 , 0.229 0.186 , 0.223	Depositor DCC
R_{free} test set	3680 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4

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	1.02	3/3263 (0.1%)	0.98	1/4422 (0.0%)
1	B	0.98	1/3230 (0.0%)	0.96	2/4377 (0.0%)
All	All	1.00	4/6493 (0.1%)	0.97	3/8799 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	ILE	CA-CB	5.63	1.59	1.53
1	A	73	VAL	CA-CB	5.37	1.61	1.54
1	A	255	ILE	CA-CB	5.10	1.59	1.53
1	A	63	ILE	CA-C	5.10	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	LYS	N-CA-C	6.10	118.44	111.11
1	A	131	ASP	N-CA-C	5.35	119.06	112.54
1	B	91	TYR	N-CA-C	5.31	116.90	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3184	0	3092	59	0
1	B	3154	0	3071	53	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	326	0	0	12	0
3	B	303	0	0	13	0
All	All	6977	0	6163	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 8.

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:74:ILE:HD13	1:A:274:PHE:CZ	2.01	0.95
1:A:333:LYS:HB2	1:A:333:LYS:HZ3	1.32	0.91
1:A:313:ASN:HB3	3:A:697:HOH:O	1.72	0.90
1:A:430:HIS:H	1:A:430:HIS:CD2	1.92	0.85
1:B:74:ILE:HD13	1:B:274:PHE:CZ	2.15	0.81
1:A:333:LYS:HB2	1:A:333:LYS:NZ	1.95	0.81
1:B:313:ASN:HB3	3:B:672:HOH:O	1.82	0.79
1:B:80:LYS:O	1:B:84:GLU:HG3	1.85	0.76
1:B:46:ARG:HH22	1:B:60:SER:HB2	1.52	0.75
1:A:130:CYS:HB3	3:A:642:HOH:O	1.85	0.74
1:A:228:LYS:HD3	3:A:640:HOH:O	1.85	0.74
1:A:94:TYR:HD2	1:B:65:ASP:HB2	1.55	0.71
1:A:129:LYS:HB3	1:B:307:CYS:O	1.89	0.71
1:A:126:ASP:H	1:A:308:PHE:HZ	1.39	0.70
1:A:74:ILE:CD1	1:A:274:PHE:CZ	2.74	0.68
1:B:221:THR:O	1:B:225:GLU:HG3	1.94	0.68
1:B:126:ASP:HB2	1:B:308:PHE:HZ	1.59	0.68
1:A:100:ALA:H	1:A:316:GLN:HE22	1.42	0.67
1:A:225:GLU:CD	3:A:696:HOH:O	2.38	0.66
1:A:94:TYR:CD2	1:B:65:ASP:HB2	2.33	0.64
1:B:74:ILE:CD1	1:B:274:PHE:CZ	2.81	0.64
1:A:225:GLU:OE2	3:A:696:HOH:O	2.15	0.64
1:A:228:LYS:HE3	3:A:618:HOH:O	1.98	0.62
1:A:95:GLY:HA3	3:A:576:HOH:O	1.99	0.62
1:A:278:ARG:HH22	1:B:95:GLY:H	1.45	0.62
1:B:126:ASP:HB2	1:B:308:PHE:CZ	2.34	0.61
1:A:313:ASN:CB	3:A:697:HOH:O	2.37	0.61
1:B:99:GLY:HA3	1:B:124:VAL:HB	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:HG21	1:B:409:GLY:HA2	1.82	0.60
1:B:66:THR:CG2	3:B:478:HOH:O	2.50	0.60
1:B:225:GLU:CG	3:B:581:HOH:O	2.50	0.59
1:A:278:ARG:NH1	1:B:312:SER:HA	2.18	0.59
1:B:98:GLN:HG2	1:B:104:ARG:HD3	1.87	0.57
1:B:228:LYS:HE3	3:B:601:HOH:O	2.04	0.57
1:A:225:GLU:CG	3:A:696:HOH:O	2.52	0.57
1:B:128:ALA:CB	1:B:267:SER:HB2	2.36	0.55
1:A:70:ILE:HD11	1:A:276:GLY:HA3	1.88	0.55
1:A:342:THR:HG21	1:A:359:GLY:HA2	1.88	0.55
1:B:348:THR:HG23	1:B:422:LYS:HG3	1.88	0.55
1:B:272:ALA:HB1	1:B:274:PHE:CZ	2.40	0.55
1:A:128:ALA:CB	1:A:267:SER:HB2	2.37	0.54
1:A:74:ILE:HD13	1:A:274:PHE:HZ	1.68	0.53
1:B:372:GLN:HB3	3:B:622:HOH:O	2.09	0.52
1:A:423:GLN:O	1:A:426:LYS:HG2	2.09	0.52
1:B:46:ARG:NH2	1:B:60:SER:HB2	2.22	0.52
1:A:128:ALA:HA	1:A:131:ASP:OD1	2.09	0.52
1:B:313:ASN:ND2	3:B:672:HOH:O	2.31	0.51
1:B:126:ASP:CB	1:B:308:PHE:HZ	2.22	0.51
1:B:342:THR:HG21	1:B:359:GLY:HA2	1.92	0.51
1:B:294:PHE:CZ	1:B:298:LYS:HE2	2.46	0.51
1:B:66:THR:HG23	3:B:478:HOH:O	2.08	0.50
1:B:128:ALA:HB3	1:B:267:SER:HB2	1.91	0.50
1:A:98:GLN:HG2	1:A:104:ARG:HD3	1.94	0.50
1:A:128:ALA:HB2	1:A:267:SER:HB2	1.94	0.49
1:B:225:GLU:HG3	3:B:581:HOH:O	2.11	0.49
1:B:225:GLU:HG2	3:B:581:HOH:O	2.10	0.49
1:A:365:VAL:HG22	1:A:405:VAL:HB	1.95	0.48
1:B:130:CYS:O	1:B:134:ARG:HG3	2.14	0.47
1:B:228:LYS:HB2	1:B:228:LYS:HE2	1.65	0.47
1:B:333:LYS:HE2	3:B:493:HOH:O	2.15	0.47
1:B:425:TYR:OH	3:B:674:HOH:O	2.20	0.47
1:A:74:ILE:HG22	1:A:78:MET:HE2	1.95	0.47
1:A:155:TYR:OH	1:A:237:ASP:OD2	2.32	0.47
1:A:228:LYS:HE3	3:A:590:HOH:O	2.15	0.47
1:A:278:ARG:HH11	1:B:312:SER:HA	1.78	0.47
1:A:129:LYS:HE3	1:A:154:ALA:HB2	1.97	0.46
1:A:67:THR:HG21	1:A:409:GLY:HA2	1.98	0.46
1:A:313:ASN:HB3	3:A:586:HOH:O	2.15	0.46
1:B:63:ILE:HA	3:B:650:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:CYS:O	1:B:130:CYS:HB3	2.16	0.45
1:B:100:ALA:H	1:B:316:GLN:HE22	1.65	0.45
1:A:74:ILE:HD13	1:A:274:PHE:CE1	2.52	0.44
1:B:327:GLY:O	1:B:331:MET:HG3	2.16	0.44
1:A:62:GLY:O	1:A:63:ILE:C	2.60	0.44
1:B:346:ILE:HD11	1:B:359:GLY:HA3	1.99	0.44
1:A:272:ALA:HB1	1:A:274:PHE:CZ	2.52	0.44
1:A:301:ASN:O	1:A:304:ILE:HG12	2.18	0.44
1:A:229:LYS:HG3	1:A:230:ASN:N	2.31	0.43
1:A:294:PHE:CZ	1:A:298:LYS:HE2	2.53	0.43
1:B:370:PRO:O	1:B:372:GLN:HG3	2.17	0.43
1:A:372:GLN:HG3	3:A:496:HOH:O	2.17	0.43
1:A:98:GLN:HG3	1:A:123:PHE:CD2	2.53	0.43
1:A:176:GLY:O	1:A:177:ASN:CB	2.66	0.43
1:B:73:VAL:HG13	1:B:74:ILE:HG13	2.01	0.43
1:B:98:GLN:HG2	1:B:98:GLN:O	2.17	0.43
1:A:70:ILE:CD1	1:A:276:GLY:HA3	2.49	0.43
1:A:63:ILE:HD11	1:B:94:TYR:CE2	2.54	0.42
1:A:134:ARG:HH11	1:A:307:CYS:HB3	1.84	0.42
1:A:272:ALA:HA	1:A:331:MET:HG2	2.00	0.42
1:B:348:THR:HG23	1:B:422:LYS:HE2	2.00	0.42
1:A:198:ARG:HG3	1:A:230:ASN:HB3	2.02	0.42
1:B:38:LEU:HD13	1:B:394:GLY:HA3	2.01	0.42
1:B:294:PHE:HZ	1:B:298:LYS:HE2	1.84	0.42
1:A:63:ILE:O	1:A:65:ASP:N	2.53	0.42
1:A:99:GLY:HA3	1:A:124:VAL:HB	2.02	0.42
1:A:94:TYR:HB3	1:A:95:GLY:H	1.67	0.42
1:B:98:GLN:HG3	1:B:123:PHE:HA	2.03	0.41
1:A:228:LYS:HE2	1:A:228:LYS:HB2	1.51	0.41
1:B:342:THR:CG2	1:B:359:GLY:HA2	2.50	0.41
1:B:81:LYS:HA	1:B:81:LYS:HD3	1.74	0.41
1:B:182:ARG:HG3	3:B:623:HOH:O	2.21	0.41
1:A:169:ASN:OD1	1:A:169:ASN:C	2.64	0.41
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.80	0.40
1:A:39:PHE:N	1:A:40:PRO:HD2	2.36	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	410/432 (95%)	399 (97%)	7 (2%)	4 (1%)	12	8
1	B	407/432 (94%)	395 (97%)	9 (2%)	3 (1%)	18	14
All	All	817/864 (95%)	794 (97%)	16 (2%)	7 (1%)	14	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	64	GLY
1	A	93	GLY
1	B	64	GLY
1	B	93	GLY
1	A	94	TYR
1	B	63	ILE

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	338/356 (95%)	321 (95%)	17 (5%)	22	20
1	B	335/356 (94%)	323 (96%)	12 (4%)	31	31
All	All	673/712 (94%)	644 (96%)	29 (4%)	26	25

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	50	LEU
1	A	57	GLN
1	A	63	ILE
1	A	66	THR
1	A	88	ILE
1	A	101	LYS
1	A	134	ARG
1	A	279	LEU
1	A	303	ILE
1	A	308	PHE
1	A	312	SER
1	A	320	LEU
1	A	333	LYS
1	A	365	VAL
1	A	384	LYS
1	A	430	HIS
1	B	63	ILE
1	B	65	ASP
1	B	101	LYS
1	B	130	CYS
1	B	157	ASP
1	B	268	PHE
1	B	279	LEU
1	B	298	LYS
1	B	304	ILE
1	B	313	ASN
1	B	320	LEU
1	B	373	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	248	ASN
1	A	429	HIS
1	A	430	HIS
1	B	248	ASN
1	B	301	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	SO4	B	433	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	A	433	-	4,4,4	0.25	0	6,6,6	0.09	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 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	412/432 (95%)	0.50	48 (11%) 9 8	20, 31, 61, 92	0
1	B	409/432 (94%)	0.48	40 (9%) 13 12	21, 32, 62, 88	0
All	All	821/864 (95%)	0.49	88 (10%) 11 10	20, 32, 62, 92	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	GLY	8.1
1	B	94	TYR	7.8
1	A	307	CYS	7.1
1	A	93	GLY	6.8
1	B	92	SER	6.5
1	B	310	GLY	6.4
1	B	99	GLY	6.4
1	B	311	ALA	6.4
1	A	92	SER	6.3
1	A	308	PHE	6.0
1	A	64	GLY	6.0
1	A	94	TYR	5.9
1	A	311	ALA	5.6
1	A	95	GLY	5.6
1	A	306	THR	5.6
1	B	63	ILE	5.5
1	A	63	ILE	5.4
1	A	66	THR	5.4
1	B	91	TYR	5.4
1	A	305	CYS	5.4
1	A	96	ALA	5.2
1	B	93	GLY	5.0
1	B	96	ALA	5.0
1	B	308	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	88	ILE	4.9
1	B	95	GLY	4.8
1	A	88	ILE	4.7
1	A	310	GLY	4.7
1	B	306	THR	4.6
1	B	307	CYS	4.5
1	A	91	TYR	4.5
1	A	128	ALA	4.5
1	B	128	ALA	4.3
1	A	309	ASN	4.1
1	A	97	GLU	4.0
1	A	99	GLY	4.0
1	A	304	ILE	3.9
1	B	37	TYR	3.8
1	A	90	GLY	3.8
1	A	430	HIS	3.8
1	A	98	GLN	3.8
1	B	126	ASP	3.6
1	B	309	ASN	3.6
1	B	65	ASP	3.6
1	B	305	CYS	3.6
1	B	66	THR	3.6
1	A	65	ASP	3.6
1	A	130	CYS	3.5
1	B	304	ILE	3.5
1	B	130	CYS	3.3
1	A	37	TYR	3.3
1	B	89	GLU	3.3
1	B	278	ARG	3.3
1	B	303	ILE	3.2
1	B	127	GLY	3.2
1	B	427	HIS	3.2
1	A	278	ARG	3.1
1	A	274	PHE	3.1
1	A	127	GLY	3.0
1	B	371	ASN	2.9
1	A	275	THR	2.9
1	B	67	THR	2.9
1	B	275	THR	2.9
1	B	276	GLY	2.9
1	A	303	ILE	2.8
1	B	39	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	171	ASP	2.7
1	A	427	HIS	2.7
1	A	312	SER	2.6
1	A	36	GLY	2.6
1	A	268	PHE	2.6
1	B	129	LYS	2.6
1	B	90	GLY	2.5
1	A	429	HIS	2.5
1	A	131	ASP	2.5
1	A	277	VAL	2.4
1	A	371	ASN	2.4
1	A	276	GLY	2.4
1	A	129	LYS	2.4
1	B	50	LEU	2.3
1	A	171	ASP	2.3
1	A	35	ALA	2.3
1	A	132	ILE	2.2
1	A	67	THR	2.2
1	A	51	LEU	2.2
1	B	170	THR	2.1
1	A	89	GLU	2.1
1	B	40	PRO	2.1

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 oligosaccharides 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
2	SO4	A	433	5/5	0.70	0.14	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	433	5/5	0.88	0.09	77,78,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.