



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 07:14 PM EDT

PDB ID : 3AH3
Title : Crystal structure of LR5-1, 3-isopropylmalate dehydrogenase created by directed evolution
Authors : Tomita, T.; Suzuki, Y.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2010-04-13
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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), 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

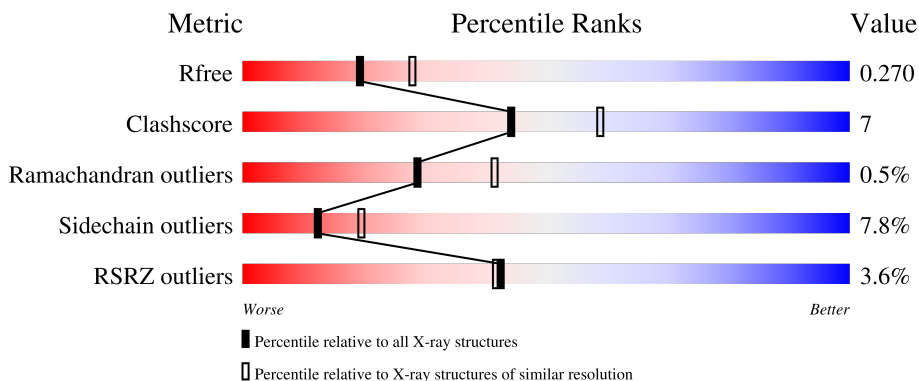
1 Overall quality at a glance i

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 $\leq 5\%$. 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	334	 81% 14% .
1	B	334	 % 83% 14% .
1	C	334	 3% 85% 13% .
1	D	334	 10% 84% 14% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10518 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 Homoisocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2534	1605	441	479	9	0	4	0
1	B	333	2528	1601	441	477	9	0	3	0
1	C	333	2544	1609	450	476	9	0	5	0
1	D	333	2537	1607	444	477	9	0	4	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	TYR	HIS	SEE REMARK 999	UNP Q72IW9
A	57	VAL	GLU	SEE REMARK 999	UNP Q72IW9
A	72	ILE	SER	SEE REMARK 999	UNP Q72IW9
A	85	MET	ARG	SEE REMARK 999	UNP Q72IW9
A	86	ALA	TYR	SEE REMARK 999	UNP Q72IW9
A	208	THR	MET	SEE REMARK 999	UNP Q72IW9
A	217	TYR	PHE	SEE REMARK 999	UNP Q72IW9
A	238	MET	VAL	SEE REMARK 999	UNP Q72IW9
A	310	MET	ARG	SEE REMARK 999	UNP Q72IW9
B	15	TYR	HIS	SEE REMARK 999	UNP Q72IW9
B	57	VAL	GLU	SEE REMARK 999	UNP Q72IW9
B	72	ILE	SER	SEE REMARK 999	UNP Q72IW9
B	85	MET	ARG	SEE REMARK 999	UNP Q72IW9
B	86	ALA	TYR	SEE REMARK 999	UNP Q72IW9
B	208	THR	MET	SEE REMARK 999	UNP Q72IW9
B	217	TYR	PHE	SEE REMARK 999	UNP Q72IW9
B	238	MET	VAL	SEE REMARK 999	UNP Q72IW9
B	310	MET	ARG	SEE REMARK 999	UNP Q72IW9
C	15	TYR	HIS	SEE REMARK 999	UNP Q72IW9
C	57	VAL	GLU	SEE REMARK 999	UNP Q72IW9
C	72	ILE	SER	SEE REMARK 999	UNP Q72IW9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	85	MET	ARG	SEE REMARK 999	UNP Q72IW9
C	86	ALA	TYR	SEE REMARK 999	UNP Q72IW9
C	208	THR	MET	SEE REMARK 999	UNP Q72IW9
C	217	TYR	PHE	SEE REMARK 999	UNP Q72IW9
C	238	MET	VAL	SEE REMARK 999	UNP Q72IW9
C	310	MET	ARG	SEE REMARK 999	UNP Q72IW9
D	15	TYR	HIS	SEE REMARK 999	UNP Q72IW9
D	57	VAL	GLU	SEE REMARK 999	UNP Q72IW9
D	72	ILE	SER	SEE REMARK 999	UNP Q72IW9
D	85	MET	ARG	SEE REMARK 999	UNP Q72IW9
D	86	ALA	TYR	SEE REMARK 999	UNP Q72IW9
D	208	THR	MET	SEE REMARK 999	UNP Q72IW9
D	217	TYR	PHE	SEE REMARK 999	UNP Q72IW9
D	238	MET	VAL	SEE REMARK 999	UNP Q72IW9
D	310	MET	ARG	SEE REMARK 999	UNP Q72IW9

- Molecule 2 is SULFATE ION (three-letter code: 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		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

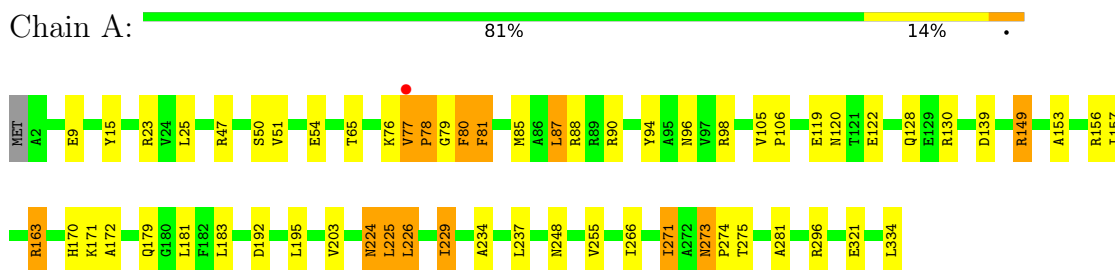
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total 115	O 115	0	0
4	B	85	Total 85	O 85	0	0
4	C	63	Total 63	O 63	0	0
4	D	48	Total 48	O 48	0	0

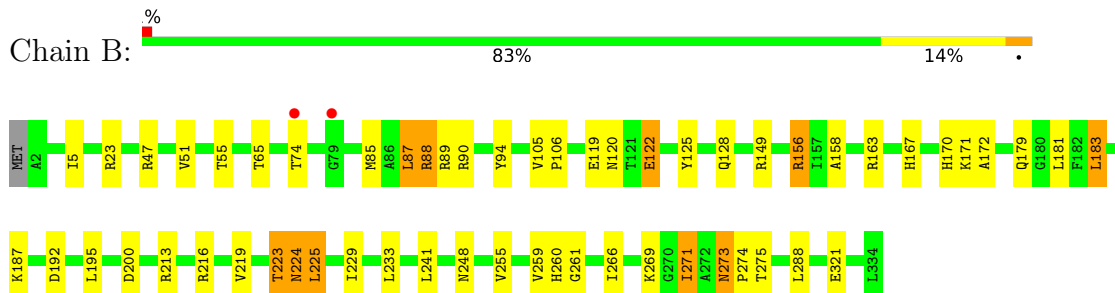
3 Residue-property plots

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.

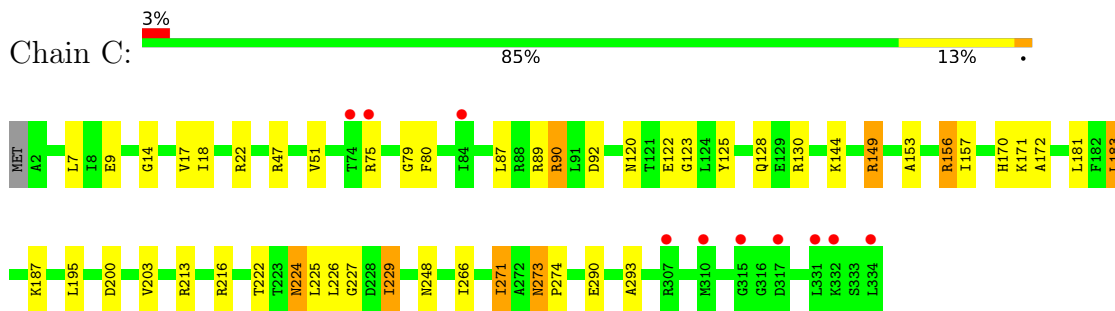
- Molecule 1: Homoisocitrate dehydrogenase



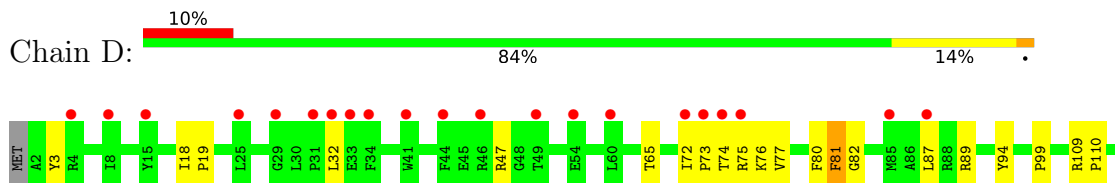
- Molecule 1: Homoisocitrate dehydrogenase

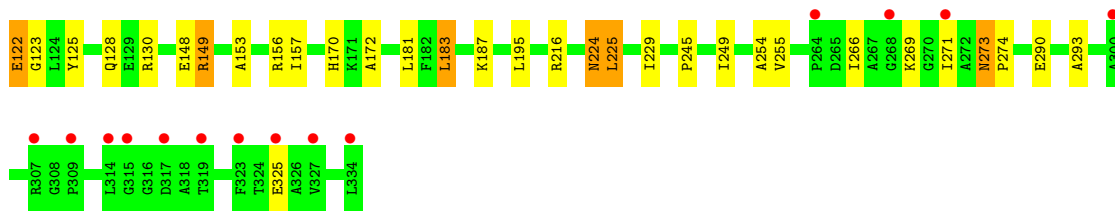


- Molecule 1: Homoisocitrate dehydrogenase



- Molecule 1: Homoisocitrate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.33Å 61.74Å 170.05Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	49.78 – 2.40 49.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.78-2.40) 99.2 (49.78-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.216 , 0.267 0.221 , 0.270	Depositor DCC
R_{free} test set	3406 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10518	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

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	0.41	0/2587	0.56	0/3513
1	B	0.39	0/2578	0.54	0/3501
1	C	0.37	0/2599	0.55	0/3527
1	D	0.35	0/2590	0.52	0/3517
All	All	0.38	0/10354	0.54	0/14058

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	2534	0	2604	42	0
1	B	2528	0	2598	38	0
1	C	2544	0	2630	40	0
1	D	2537	0	2613	19	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	16	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	24	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
4	A	115	0	0	4	0
4	B	85	0	0	6	0
4	C	63	0	0	1	0
4	D	48	0	0	0	0
All	All	10518	0	10511	137	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 (137) 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:C:203:VAL:HG21	1:C:226:LEU:HD21	1.33	1.11
1:C:90[A]:ARG:HH11	1:C:90[A]:ARG:HG3	0.97	1.10
1:C:90[B]:ARG:CG	1:C:90[B]:ARG:HH11	1.69	1.04
1:A:78:PRO:HB2	1:A:79:GLY:HA2	1.40	1.01
1:A:78:PRO:HB2	1:A:79:GLY:CA	1.92	0.99
1:C:90[B]:ARG:HH11	1:C:90[B]:ARG:HG3	1.28	0.95
1:C:90[A]:ARG:HG3	1:C:90[A]:ARG:NH1	1.70	0.89
1:A:156:ARG:HD2	4:A:363:HOH:O	1.72	0.89
1:C:203:VAL:CG2	1:C:226:LEU:HD21	2.05	0.85
1:A:224:ASN:O	1:A:225:LEU:HB2	1.79	0.80
1:A:170:HIS:HD2	1:A:172:ALA:H	1.25	0.80
1:D:170:HIS:HD2	1:D:172:ALA:H	1.28	0.79
1:B:224:ASN:O	1:B:225:LEU:HB2	1.84	0.78
1:B:170:HIS:HD2	1:B:172:ALA:H	1.29	0.77
1:A:229:ILE:HD12	1:C:229:ILE:HD12	1.67	0.77
1:C:170:HIS:HD2	1:C:172:ALA:H	1.32	0.76
1:B:88:ARG:HH11	1:B:88:ARG:CG	1.99	0.75
1:C:222:THR:OG1	1:C:226:LEU:HD22	1.87	0.75
1:A:171:LYS:H	1:A:179:GLN:HE21	1.32	0.75
1:C:224:ASN:HD22	1:C:224:ASN:C	1.91	0.73
1:C:203:VAL:HG21	1:C:226:LEU:CD2	2.16	0.73
1:C:90[B]:ARG:HG3	1:C:90[B]:ARG:NH1	1.99	0.72
1:B:88:ARG:HH11	1:B:88:ARG:HG2	1.54	0.72
1:C:90[A]:ARG:HH11	1:C:90[A]:ARG:CG	1.86	0.70
1:B:171:LYS:H	1:B:179:GLN:HE21	1.38	0.70
1:B:23:ARG:NH2	1:B:321:GLU:OE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90[B]:ARG:HH11	1:C:90[B]:ARG:HG2	1.53	0.67
1:B:88:ARG:HB3	1:B:122:GLU:HG3	1.80	0.64
1:A:296:ARG:HD2	1:A:334:LEU:O	1.96	0.64
1:C:273:ASN:HD22	1:C:274:PRO:HD2	1.62	0.64
1:B:163:ARG:NH1	4:B:382:HOH:O	2.30	0.64
1:D:224:ASN:O	1:D:225:LEU:HB2	1.96	0.63
1:A:9:GLU:OE2	1:A:15[A]:TYR:HD2	1.80	0.63
1:A:88:ARG:HB3	1:A:122:GLU:HG3	1.79	0.63
1:A:23:ARG:NH2	1:A:321:GLU:OE2	2.32	0.63
1:B:266:ILE:HB	1:B:271:ILE:HD11	1.82	0.62
1:D:89:ARG:HA	1:D:123:GLY:HA2	1.82	0.61
1:D:170:HIS:CD2	1:D:172:ALA:H	2.16	0.60
1:A:170:HIS:CD2	1:A:172:ALA:H	2.15	0.60
1:D:153:ALA:O	1:D:157:ILE:HG12	2.02	0.60
1:A:171:LYS:H	1:A:179:GLN:NE2	2.01	0.59
1:A:203:VAL:HG21	1:A:226:LEU:HG	1.85	0.58
1:A:120:ASN:HD21	1:A:248:ASN:ND2	2.02	0.57
1:A:266:ILE:HB	1:A:271:ILE:HD11	1.86	0.56
1:C:90[B]:ARG:CG	1:C:90[B]:ARG:NH1	2.42	0.56
1:B:224:ASN:O	1:B:224:ASN:ND2	2.39	0.56
1:B:273:ASN:ND2	1:B:275:THR:H	2.03	0.55
1:B:156:ARG:HD2	4:B:356:HOH:O	2.07	0.54
1:B:65:THR:HB	1:B:255:VAL:HG22	1.90	0.53
1:C:120:ASN:HD21	1:C:248:ASN:HD22	1.57	0.53
1:C:156:ARG:HD2	4:C:364:HOH:O	2.09	0.53
1:B:120:ASN:HD21	1:B:248:ASN:ND2	2.07	0.53
1:A:153:ALA:O	1:A:157:ILE:HG12	2.09	0.53
1:A:273:ASN:ND2	1:A:275:THR:H	2.07	0.53
1:A:23:ARG:HH22	1:A:321:GLU:CD	2.13	0.52
1:A:50:SER:OG	1:A:81:PHE:HB3	2.10	0.52
1:B:170:HIS:CD2	1:B:172:ALA:H	2.17	0.51
1:A:23:ARG:HD2	4:A:451:HOH:O	2.09	0.51
1:B:88:ARG:CG	1:B:88:ARG:NH1	2.69	0.51
1:C:92:ASP:OD2	1:C:149:ARG:NH2	2.41	0.51
1:A:78:PRO:HB2	1:A:79:GLY:HA3	1.87	0.50
1:A:163:ARG:HD2	4:A:454:HOH:O	2.12	0.49
1:A:78:PRO:CB	1:A:79:GLY:CA	2.71	0.49
1:C:224:ASN:C	1:C:224:ASN:ND2	2.65	0.49
1:C:90[A]:ARG:NH1	1:C:90[A]:ARG:CG	2.53	0.49
1:B:51:VAL:HG11	1:B:87:LEU:HG	1.95	0.48
1:B:105:VAL:HB	1:B:106:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HD21	1:A:248:ASN:HD22	1.59	0.48
1:D:273:ASN:HD22	1:D:274:PRO:HD2	1.79	0.48
1:A:163:ARG:HG3	4:A:355:HOH:O	2.13	0.48
1:A:273:ASN:HD22	1:A:274:PRO:N	2.12	0.47
1:A:157:ILE:HD12	3:A:337:EDO:H11	1.97	0.47
1:B:23:ARG:HH22	1:B:321:GLU:CD	2.17	0.47
1:B:23:ARG:HD2	4:B:343:HOH:O	2.15	0.47
1:B:167:HIS:HD2	4:B:360:HOH:O	1.97	0.46
1:C:183:LEU:HD22	1:C:187:LYS:CD	2.46	0.46
1:D:249:ILE:HG23	1:D:254:ALA:HB2	1.97	0.46
1:C:183:LEU:HD22	1:C:187:LYS:HD2	1.96	0.46
1:C:51:VAL:HG11	1:C:87:LEU:HG	1.98	0.46
1:B:85:MET:O	1:B:89:ARG:HG3	2.15	0.46
1:B:269:LYS:HB2	1:B:271:ILE:HD12	1.98	0.45
1:A:94:TYR:O	1:A:119:GLU:HA	2.16	0.45
1:D:81:PHE:HA	1:D:82:GLY:HA3	1.83	0.45
1:C:170:HIS:CD2	1:C:172:ALA:H	2.21	0.44
1:D:65:THR:HB	1:D:255:VAL:HG22	1.98	0.44
1:D:183:LEU:HD22	1:D:187:LYS:HD2	1.99	0.44
1:A:105:VAL:HB	1:A:106:PRO:HD2	1.98	0.44
1:C:90[B]:ARG:NH1	1:C:90[B]:ARG:HG2	2.24	0.44
1:B:260:HIS:HD2	1:B:261:GLY:O	2.01	0.44
1:C:89:ARG:HA	1:C:123:GLY:HA2	2.00	0.44
1:C:89:ARG:HG2	1:C:122:GLU:O	2.18	0.44
1:C:290:GLU:HB3	1:C:293:ALA:HB3	1.99	0.44
1:B:213:ARG:HD2	1:B:216:ARG:HH11	1.82	0.44
1:B:273:ASN:HD22	1:B:274:PRO:N	2.16	0.43
1:D:99:PRO:HG2	1:D:245:PRO:HG2	1.99	0.43
1:D:109:ARG:HA	1:D:110:PRO:HD3	1.79	0.43
1:B:55:THR:OG1	4:B:395:HOH:O	2.16	0.43
1:B:273:ASN:HD22	1:B:273:ASN:C	2.21	0.43
1:C:9:GLU:HA	1:C:18:ILE:HG13	2.00	0.43
1:B:241:LEU:HD22	1:B:259:VAL:HG11	2.01	0.42
1:D:290:GLU:HB3	1:D:293:ALA:HB3	2.01	0.42
1:A:229:ILE:HD13	1:A:229:ILE:O	2.19	0.42
1:A:234:ALA:HA	1:A:237:LEU:HD12	2.01	0.42
1:B:183:LEU:HD22	1:B:187:LYS:HD2	2.00	0.42
1:C:153:ALA:O	1:C:157:ILE:HG12	2.19	0.42
1:B:233:LEU:C	1:B:233:LEU:HD23	2.40	0.42
1:A:25:LEU:HD21	1:A:281:ALA:HB1	2.02	0.42
1:C:7:LEU:HD11	1:C:22:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:HD21	1:C:248:ASN:ND2	2.17	0.42
1:A:79:GLY:HA3	1:A:80:PHE:HA	1.73	0.42
1:C:171:LYS:HG3	1:C:203:VAL:HG12	2.00	0.42
1:B:158:ALA:HA	1:B:219:VAL:HG21	2.00	0.42
1:D:3:TYR:HB2	1:D:32:LEU:HD23	2.01	0.42
1:D:72:ILE:O	1:D:74:THR:N	2.53	0.42
1:A:96:ASN:HD21	1:A:98:ARG:HG3	1.83	0.42
1:A:273:ASN:HD22	1:A:273:ASN:C	2.23	0.42
1:B:223:THR:CG2	4:B:351:HOH:O	2.68	0.41
2:A:335:SO4:O3	1:C:144:LYS:NZ	2.47	0.41
1:B:5:ILE:HD11	1:B:288:LEU:HD11	2.03	0.41
1:A:51:VAL:HG11	1:A:87:LEU:HG	2.01	0.41
1:A:81:PHE:CD1	1:A:81:PHE:N	2.88	0.41
1:A:130:ARG:NH2	1:A:139:ASP:OD1	2.54	0.41
1:B:105:VAL:O	1:C:213[B]:ARG:HD2	2.21	0.41
1:D:18:ILE:HB	1:D:19:PRO:HD3	2.03	0.41
1:C:14:GLY:HA2	1:C:17:VAL:HG22	2.02	0.41
1:C:266:ILE:HB	1:C:271:ILE:HD11	2.01	0.41
1:D:266:ILE:HA	1:D:269:LYS:HD2	2.01	0.41
1:A:65:THR:HB	1:A:255:VAL:HG22	2.03	0.41
1:B:94:TYR:O	1:B:119:GLU:HA	2.20	0.41
1:B:120:ASN:HD21	1:B:248:ASN:HD22	1.68	0.41
1:A:77:VAL:HG12	1:A:80:PHE:HB2	2.03	0.40
1:C:273:ASN:HD22	1:C:274:PRO:CD	2.31	0.40
1:D:122:GLU:H	1:D:122:GLU:HG2	1.66	0.40
1:A:149:ARG:H	1:A:149:ARG:HG3	1.65	0.40
1:B:171:LYS:H	1:B:179:GLN:NE2	2.12	0.40
1:C:222:THR:HG21	1:C:227:GLY:HA2	2.03	0.40
1:D:94:TYR:CD1	1:D:149:ARG:HD3	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	335/334 (100%)	323 (96%)	10 (3%)	2 (1%)	25	36
1	B	334/334 (100%)	322 (96%)	11 (3%)	1 (0%)	41	55
1	C	336/334 (101%)	323 (96%)	12 (4%)	1 (0%)	41	55
1	D	335/334 (100%)	317 (95%)	15 (4%)	3 (1%)	17	25
All	All	1340/1336 (100%)	1285 (96%)	48 (4%)	7 (0%)	29	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	D	73	PRO
1	A	225	LEU
1	C	79	GLY
1	B	225	LEU
1	D	80	PHE
1	D	225	LEU

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	266/263 (101%)	245 (92%)	21 (8%)	12	19
1	B	265/263 (101%)	245 (92%)	20 (8%)	13	21
1	C	267/263 (102%)	246 (92%)	21 (8%)	12	19
1	D	266/263 (101%)	243 (91%)	23 (9%)	10	16
All	All	1064/1052 (101%)	979 (92%)	85 (8%)	12	18

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	54	GLU
1	A	76	LYS
1	A	77	VAL

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Mol	Chain	Res	Type
1	A	80	PHE
1	A	81	PHE
1	A	85	MET
1	A	87	LEU
1	A	90	ARG
1	A	128	GLN
1	A	149	ARG
1	A	163	ARG
1	A	181	LEU
1	A	183	LEU
1	A	192	ASP
1	A	195	LEU
1	A	224	ASN
1	A	226	LEU
1	A	229	ILE
1	A	271	ILE
1	A	273	ASN
1	B	47	ARG
1	B	74	THR
1	B	87	LEU
1	B	88	ARG
1	B	90	ARG
1	B	122	GLU
1	B	125	TYR
1	B	128	GLN
1	B	149	ARG
1	B	156	ARG
1	B	181	LEU
1	B	183	LEU
1	B	192	ASP
1	B	195	LEU
1	B	200	ASP
1	B	223	THR
1	B	224	ASN
1	B	229	ILE
1	B	271	ILE
1	B	273	ASN
1	C	47	ARG
1	C	75	ARG
1	C	80	PHE
1	C	90[A]	ARG
1	C	90[B]	ARG

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Mol	Chain	Res	Type
1	C	125	TYR
1	C	128[A]	GLN
1	C	128[B]	GLN
1	C	130	ARG
1	C	149	ARG
1	C	156	ARG
1	C	181	LEU
1	C	183	LEU
1	C	195	LEU
1	C	200	ASP
1	C	216	ARG
1	C	224	ASN
1	C	225	LEU
1	C	229	ILE
1	C	271	ILE
1	C	273	ASN
1	D	47	ARG
1	D	75	ARG
1	D	76	LYS
1	D	77	VAL
1	D	81	PHE
1	D	87	LEU
1	D	122	GLU
1	D	125	TYR
1	D	128[A]	GLN
1	D	128[B]	GLN
1	D	130	ARG
1	D	148	GLU
1	D	149	ARG
1	D	156	ARG
1	D	181	LEU
1	D	183	LEU
1	D	195	LEU
1	D	216	ARG
1	D	224	ASN
1	D	229	ILE
1	D	271	ILE
1	D	273	ASN
1	D	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	170	HIS
1	A	179	GLN
1	A	248	ASN
1	A	260	HIS
1	A	273	ASN
1	B	96	ASN
1	B	128	GLN
1	B	167	HIS
1	B	170	HIS
1	B	179	GLN
1	B	224	ASN
1	B	248	ASN
1	B	260	HIS
1	B	273	ASN
1	C	96	ASN
1	C	170	HIS
1	C	199	GLN
1	C	209	GLN
1	C	224	ASN
1	C	248	ASN
1	C	260	HIS
1	C	273	ASN
1	D	96	ASN
1	D	170	HIS
1	D	224	ASN
1	D	248	ASN
1	D	260	HIS
1	D	273	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 monosaccharides in this entry.

5.6 Ligand geometry

15 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	C	335	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	335	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	D	335	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	338	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	A	336	-	3,3,3	0.47	0	2,2,2	0.34	0
2	SO4	A	335	-	4,4,4	0.15	0	6,6,6	0.11	0
3	EDO	B	337	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	B	336	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	A	338	-	3,3,3	0.47	0	2,2,2	0.37	0
3	EDO	C	337	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	A	337	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	C	336	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	D	336	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	B	339	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	A	339	-	3,3,3	0.48	0	2,2,2	0.39	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
3	EDO	B	338	-	-	1/1/1/1	-
3	EDO	A	336	-	-	0/1/1/1	-
3	EDO	B	337	-	-	1/1/1/1	-
3	EDO	B	336	-	-	1/1/1/1	-
3	EDO	A	338	-	-	0/1/1/1	-
3	EDO	C	337	-	-	1/1/1/1	-
3	EDO	A	337	-	-	1/1/1/1	-
3	EDO	C	336	-	-	1/1/1/1	-
3	EDO	D	336	-	-	0/1/1/1	-
3	EDO	B	339	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	339	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	337	EDO	O1-C1-C2-O2
3	A	337	EDO	O1-C1-C2-O2
3	B	339	EDO	O1-C1-C2-O2
3	B	338	EDO	O1-C1-C2-O2
3	B	336	EDO	O1-C1-C2-O2
3	B	337	EDO	O1-C1-C2-O2
3	C	336	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	335	SO4	1	0
3	A	337	EDO	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 [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	333/334 (99%)	-0.22	1 (0%) 94 93	20, 32, 56, 77	0
1	B	333/334 (99%)	-0.18	2 (0%) 89 88	21, 37, 64, 83	0
1	C	333/334 (99%)	0.13	10 (3%) 50 49	21, 48, 91, 106	0
1	D	333/334 (99%)	0.52	35 (10%) 6 5	32, 64, 111, 127	0
All	All	1332/1336 (99%)	0.06	48 (3%) 42 42	20, 40, 101, 127	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	THR	7.7
1	D	334	LEU	5.6
1	D	72	ILE	5.4
1	C	74	THR	5.2
1	D	32	LEU	4.5
1	D	314	LEU	4.3
1	D	25	LEU	4.1
1	C	75	ARG	3.8
1	B	79	GLY	3.6
1	D	327	VAL	3.6
1	D	73	PRO	3.5
1	D	60	LEU	3.5
1	C	331	LEU	3.5
1	D	49	THR	3.3
1	D	315	GLY	3.3
1	D	15[A]	TYR	3.3
1	C	334	LEU	3.2
1	D	46	ARG	3.0
1	D	54	GLU	3.0
1	D	41	TRP	3.0
1	C	315	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	300	ALA	2.9
1	A	77	VAL	2.7
1	D	87	LEU	2.7
1	C	307	ARG	2.7
1	D	29	GLY	2.6
1	D	323	PHE	2.6
1	C	317	ASP	2.6
1	C	310	MET	2.6
1	D	307	ARG	2.6
1	D	75	ARG	2.6
1	C	332	LYS	2.5
1	D	34	PHE	2.4
1	D	264	PRO	2.4
1	D	325	GLU	2.3
1	D	268	GLY	2.3
1	D	4	ARG	2.2
1	D	33	GLU	2.2
1	D	44	PHE	2.2
1	D	309	PRO	2.2
1	D	319	THR	2.2
1	C	84	ILE	2.1
1	D	8	ILE	2.1
1	B	74	THR	2.1
1	D	31	PRO	2.1
1	D	85	MET	2.0
1	D	271	ILE	2.0
1	D	317	ASP	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
3	EDO	B	339	4/4	0.84	0.27	47,48,49,49	0
3	EDO	B	338	4/4	0.85	0.19	59,59,60,61	0
2	SO4	C	335	5/5	0.86	0.24	78,79,79,79	0
2	SO4	D	335	5/5	0.86	0.24	107,107,108,108	0
3	EDO	A	338	4/4	0.87	0.14	52,52,53,55	0
3	EDO	A	339	4/4	0.88	0.29	42,43,43,44	0
2	SO4	B	335	5/5	0.90	0.17	84,84,85,85	0
3	EDO	A	336	4/4	0.90	0.23	46,46,46,47	0
2	SO4	A	335	5/5	0.92	0.14	71,72,72,72	0
3	EDO	C	336	4/4	0.92	0.22	64,64,64,64	0
3	EDO	D	336	4/4	0.92	0.16	71,72,72,72	0
3	EDO	C	337	4/4	0.93	0.21	39,40,40,42	0
3	EDO	B	336	4/4	0.93	0.29	56,56,56,56	0
3	EDO	B	337	4/4	0.95	0.24	52,52,52,52	0
3	EDO	A	337	4/4	0.95	0.25	46,47,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.