



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:48 PM UTC

PDB ID : 3VMK / pdb_00003vmk
Title : 3-isopropylmalate dehydrogenase from Shewanella benthica DB21 MT-2
Authors : Nagae, T.; Watanabe, N.
Deposited on : 2011-12-13
Resolution : 1.48 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

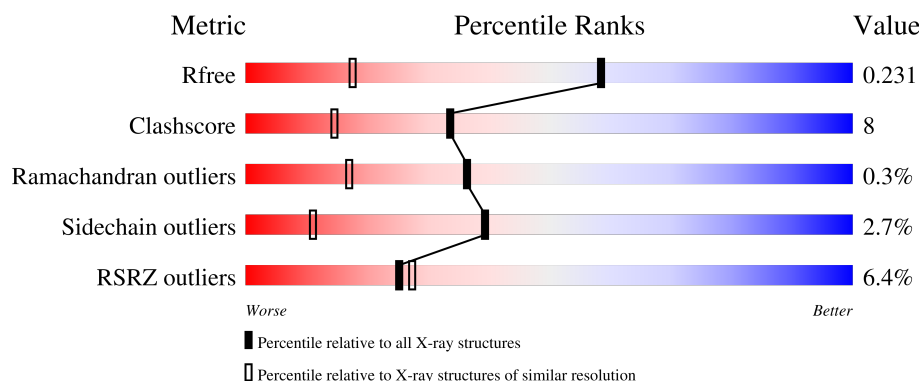
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	375	5% 78% 17% ...
1	B	375	7% 79% 17% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6391 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.

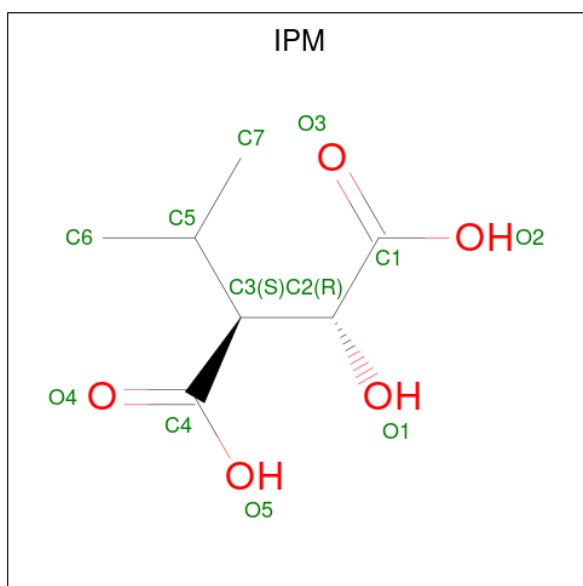
- Molecule 1 is a protein called 3-isopropylmalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	7	0
			2832	1778	490	543	21			
1	B	368	Total	C	N	O	S	0	8	0
			2822	1772	487	541	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP D2YZL2
A	-9	ARG	-	expression tag	UNP D2YZL2
A	-8	GLY	-	expression tag	UNP D2YZL2
A	-7	SER	-	expression tag	UNP D2YZL2
A	-6	HIS	-	expression tag	UNP D2YZL2
A	-5	HIS	-	expression tag	UNP D2YZL2
A	-4	HIS	-	expression tag	UNP D2YZL2
A	-3	HIS	-	expression tag	UNP D2YZL2
A	-2	HIS	-	expression tag	UNP D2YZL2
A	-1	HIS	-	expression tag	UNP D2YZL2
A	0	GLY	-	expression tag	UNP D2YZL2
A	1	SER	-	expression tag	UNP D2YZL2
B	-10	MET	-	expression tag	UNP D2YZL2
B	-9	ARG	-	expression tag	UNP D2YZL2
B	-8	GLY	-	expression tag	UNP D2YZL2
B	-7	SER	-	expression tag	UNP D2YZL2
B	-6	HIS	-	expression tag	UNP D2YZL2
B	-5	HIS	-	expression tag	UNP D2YZL2
B	-4	HIS	-	expression tag	UNP D2YZL2
B	-3	HIS	-	expression tag	UNP D2YZL2
B	-2	HIS	-	expression tag	UNP D2YZL2
B	-1	HIS	-	expression tag	UNP D2YZL2
B	0	GLY	-	expression tag	UNP D2YZL2
B	1	SER	-	expression tag	UNP D2YZL2

- Molecule 2 is 3-ISOPROPYLMALIC ACID (CCD ID: IPM) (formula: $C_7H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	B	1	Total	C	O	0	0
			12	7	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

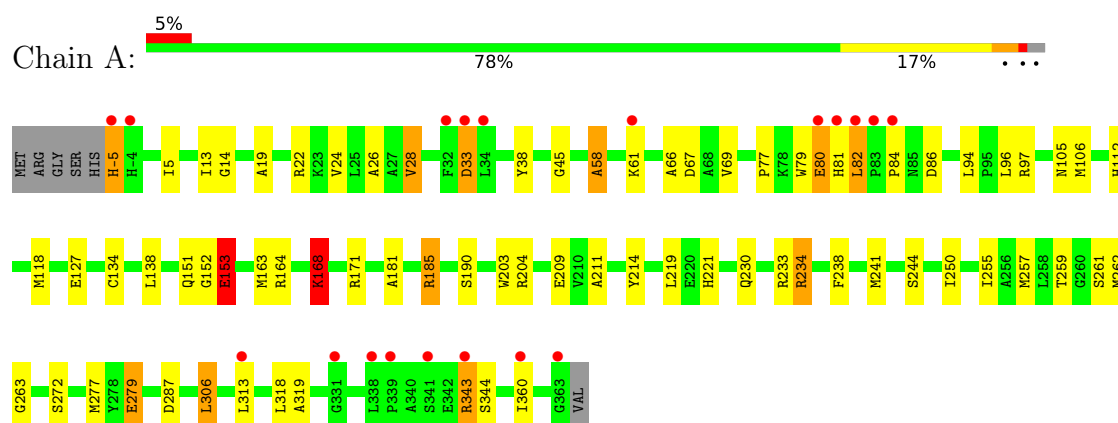
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	375	Total 375	O 375	0	0
5	B	334	Total 334	O 334	0	0

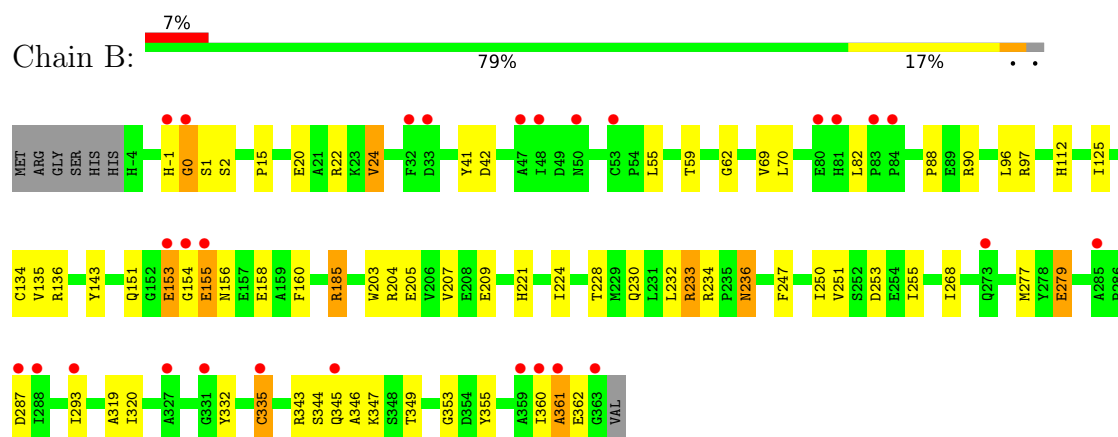
3 Residue-property plots [i](#)

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: 3-isopropylmalate dehydrogenase



- Molecule 1: 3-isopropylmalate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.97Å 59.21Å 119.78Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	25.77 – 1.48 25.77 – 1.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.77-1.48) 97.9 (25.77-1.48)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.193 , 0.232 (Not available) , 0.231	Depositor DCC
R_{free} test set	5928 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6391	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: CL, MG, IPM

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	1.73	28/2907 (1.0%)	1.49	19/3925 (0.5%)
1	B	1.72	23/2899 (0.8%)	1.48	15/3914 (0.4%)
All	All	1.72	51/5806 (0.9%)	1.48	34/7839 (0.4%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	GLY	N-CA	8.66	1.58	1.45
1	B	155	GLU	C-O	8.33	1.34	1.24
1	B	268	ILE	CA-CB	-8.15	1.44	1.54
1	A	13	ILE	CA-C	7.82	1.61	1.52
1	A	28	VAL	CA-CB	7.70	1.64	1.54
1	B	0	GLY	N-CA	7.31	1.55	1.45
1	A	306	LEU	CA-CB	7.07	1.64	1.53
1	B	24	VAL	CA-CB	6.94	1.63	1.54
1	B	209	GLU	C-O	6.94	1.32	1.24
1	A	181	ALA	CA-CB	-6.93	1.42	1.53
1	B	203	TRP	C-O	6.53	1.31	1.24
1	B	205	GLU	C-O	6.33	1.31	1.24
1	A	219	LEU	CA-C	-6.27	1.45	1.52
1	B	70	LEU	CA-C	-6.25	1.45	1.52
1	A	106	MET	SD-CE	-6.17	1.64	1.79
1	A	58	ALA	CA-C	6.15	1.61	1.52
1	B	0	GLY	CA-C	6.13	1.60	1.51
1	A	66	ALA	N-CA	-6.13	1.38	1.45
1	B	2	SER	N-CA	6.12	1.53	1.46
1	A	45	GLY	N-CA	6.10	1.53	1.45
1	B	135	VAL	N-CA	6.07	1.53	1.46
1	A	5	ILE	CA-CB	-6.06	1.46	1.54
1	A	263	GLY	C-O	6.04	1.30	1.24
1	A	234	ARG	CA-C	5.98	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	ALA	CA-CB	-5.91	1.44	1.53
1	B	153	GLU	CA-C	5.68	1.59	1.52
1	A	211	ALA	CA-C	5.67	1.60	1.52
1	A	259	THR	CA-CB	5.66	1.63	1.53
1	A	313	LEU	CA-C	-5.56	1.47	1.53
1	A	66	ALA	CA-CB	5.51	1.62	1.53
1	B	207	VAL	C-O	5.47	1.30	1.24
1	B	59	THR	C-O	5.46	1.30	1.24
1	B	233	ARG	CA-C	-5.46	1.45	1.52
1	B	320	ILE	CA-CB	5.44	1.60	1.54
1	A	151	GLN	CA-C	-5.39	1.46	1.52
1	A	19	ALA	CA-CB	5.36	1.62	1.53
1	A	279	GLU	CA-C	-5.35	1.46	1.52
1	A	164	ARG	CZ-NH1	5.33	1.40	1.32
1	A	38	TYR	CE1-CZ	5.25	1.50	1.38
1	B	251	VAL	C-O	5.23	1.30	1.24
1	B	22	ARG	N-CA	5.21	1.52	1.46
1	B	125	ILE	CA-CB	5.20	1.61	1.54
1	A	203	TRP	CA-C	5.18	1.59	1.52
1	B	346	ALA	N-CA	5.17	1.52	1.45
1	A	38	TYR	C-O	5.16	1.30	1.24
1	A	261	SER	CB-OG	5.14	1.52	1.42
1	A	272	SER	N-CA	5.10	1.53	1.46
1	A	214	TYR	CA-CB	5.09	1.59	1.53
1	B	250	ILE	C-O	5.07	1.29	1.24
1	B	247	PHE	N-CA	5.03	1.52	1.46
1	A	94	LEU	C-O	-5.01	1.19	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASN	N-CA-C	-7.90	103.21	112.92
1	B	0	GLY	CA-C-N	7.11	135.13	121.54
1	B	0	GLY	C-N-CA	7.11	135.13	121.54
1	B	0	GLY	N-CA-C	6.63	128.90	113.18
1	B	55	LEU	O-C-N	6.33	126.55	121.17
1	A	22	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	A	26	ALA	N-CA-C	-6.13	104.59	111.28
1	B	233	ARG	N-CA-CB	6.03	119.37	110.33
1	A	190	SER	O-C-N	-5.97	116.41	123.22
1	A	-5	HIS	CA-C-N	-5.85	114.64	122.72
1	A	-5	HIS	C-N-CA	-5.85	114.64	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	CA-C-N	-5.82	112.59	119.05
1	A	14	GLY	C-N-CA	-5.82	112.59	119.05
1	A	153	GLU	N-CA-C	5.80	116.75	108.74
1	B	319	ALA	N-CA-C	5.78	118.05	111.11
1	A	33	ASP	N-CA-C	5.76	123.07	110.80
1	A	152	GLY	CA-C-N	-5.72	113.02	122.11
1	A	152	GLY	C-N-CA	-5.72	113.02	122.11
1	B	279	GLU	CA-C-N	-5.70	113.89	119.76
1	B	279	GLU	C-N-CA	-5.70	113.89	119.76
1	A	344	SER	N-CA-C	5.69	120.06	113.18
1	A	153	GLU	N-CA-CB	5.66	120.67	111.21
1	B	143	TYR	O-C-N	5.41	128.32	122.15
1	A	22	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	A	28	VAL	O-C-N	5.28	126.99	121.87
1	A	209	GLU	O-C-N	-5.23	116.68	122.07
1	B	42	ASP	CA-C-N	-5.21	115.69	122.51
1	B	42	ASP	C-N-CA	-5.21	115.69	122.51
1	B	97	ARG	O-C-N	5.19	127.62	122.12
1	B	136	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	168	LYS	O-C-N	5.18	127.61	122.12
1	B	136	ARG	NH1-CZ-NH2	-5.17	112.59	119.30
1	A	241	MET	O-C-N	-5.10	117.22	123.19
1	A	185	ARG	NE-CZ-NH2	-5.01	114.69	119.20

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	2832	0	2814	53	0
1	B	2822	0	2811	43	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	375	0	0	5	0
5	B	334	0	0	3	0
All	All	6391	0	5643	87	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 (87) 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:B:185:ARG:HG3	1:B:185:ARG:HH11	1.09	1.10
1:B:185:ARG:HG3	1:B:185:ARG:NH1	1.80	0.94
1:A:69:VAL:HG11	1:A:277[B]:MET:HE3	1.49	0.91
1:A:127:GLU:HG2	5:A:766:HOH:O	1.75	0.86
1:A:171:ARG:NH1	1:B:155:GLU:CD	2.38	0.81
1:B:361:ALA:O	1:B:362:GLU:HG3	1.83	0.78
5:A:525:HOH:O	1:B:158:GLU:HG3	1.86	0.76
1:B:-1:HIS:O	1:B:1:SER:N	2.18	0.75
1:A:112:HIS:HD2	5:A:622:HOH:O	1.68	0.75
1:A:171:ARG:NH1	1:B:155:GLU:OE1	2.21	0.73
1:A:77:PRO:HA	1:A:80:GLU:CG	2.19	0.73
1:B:230:GLN:HE22	1:B:233:ARG:HH11	1.35	0.71
1:B:96:LEU:HD13	1:B:277[B]:MET:HE1	1.71	0.70
1:B:69:VAL:HG11	1:B:277[B]:MET:HE3	1.70	0.70
1:A:171:ARG:HH12	1:B:155:GLU:CD	1.99	0.70
1:A:84:PRO:HB3	5:B:695:HOH:O	1.91	0.70
1:B:112:HIS:HD2	5:B:619:HOH:O	1.76	0.69
1:B:344:SER:OG	1:B:345:GLN:OE1	2.10	0.67
1:B:151:GLN:OE1	1:B:158:GLU:OE1	2.12	0.67
1:B:185:ARG:NH1	1:B:185:ARG:CG	2.57	0.66
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.11	0.66
1:A:69:VAL:HG11	1:A:277[B]:MET:CE	2.23	0.65
1:A:343:ARG:NE	1:A:343:ARG:HA	2.12	0.65
1:A:-5:HIS:HD2	1:A:67:ASP:OD1	1.78	0.65
1:A:24:VAL:HG13	1:A:360:ILE:HD12	1.79	0.64
1:A:168:LYS:NZ	1:B:155:GLU:HB3	2.12	0.64
1:A:230:GLN:HE21	1:A:234:ARG:HE	1.46	0.64
1:A:81:HIS:CE1	1:A:82:LEU:HD13	2.33	0.63
1:A:153:GLU:CA	1:A:153:GLU:OE2	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD13	1:A:277[B]:MET:HE1	1.80	0.61
1:B:230:GLN:HE21	1:B:234:ARG:HE	1.48	0.60
1:A:77:PRO:HA	1:A:80:GLU:HG2	1.82	0.59
1:A:343:ARG:HA	1:A:343:ARG:HE	1.67	0.59
1:B:332:TYR:CD2	1:B:347:LYS:HG3	2.37	0.58
1:A:230:GLN:HE22	1:A:233:ARG:HH11	1.50	0.58
1:A:28:VAL:HG23	1:A:360:ILE:HD13	1.87	0.56
1:A:168:LYS:HB2	1:A:168:LYS:HZ2	1.73	0.53
1:B:151:GLN:HG2	1:B:158:GLU:HG2	1.91	0.52
1:A:257:MET:HE2	1:A:262[A]:MET:HE1	1.92	0.51
1:B:230:GLN:NE2	1:B:234:ARG:HE	2.09	0.51
1:A:134[B]:CYS:SG	1:A:255:ILE:HD12	2.51	0.50
1:B:277[A]:MET:HE2	1:B:279:GLU:OE2	2.12	0.50
1:B:185:ARG:HH11	1:B:185:ARG:CG	1.95	0.49
1:A:69:VAL:CG1	1:A:277[B]:MET:HE3	2.32	0.49
1:A:-5:HIS:CD2	1:A:67:ASP:OD1	2.64	0.49
1:A:257:MET:HE2	1:A:262[A]:MET:CE	2.43	0.49
1:B:20:GLU:OE2	1:B:353:GLY:HA3	2.13	0.49
1:A:58:ALA:HA	1:A:61:LYS:HE3	1.95	0.48
1:A:257:MET:CE	1:A:262[A]:MET:CE	2.92	0.48
1:B:293:ILE:HG23	1:B:335[A]:CYS:HB3	1.96	0.48
1:B:355:TYR:C	1:B:355:TYR:CD2	2.91	0.48
1:B:24:VAL:HG13	1:B:360:ILE:CD1	2.43	0.47
1:A:257:MET:CE	1:A:262[A]:MET:HE1	2.44	0.47
1:A:230:GLN:NE2	1:A:233:ARG:HH11	2.12	0.47
1:B:134[B]:CYS:SG	1:B:255:ILE:HD12	2.54	0.47
1:A:97:ARG:HD3	1:A:138:LEU:HG	1.97	0.47
1:A:171:ARG:NH1	1:B:155:GLU:OE2	2.47	0.47
1:B:335[B]:CYS:SG	1:B:343:ARG:HD2	2.55	0.47
1:A:79:TRP:O	1:A:82:LEU:HB2	2.16	0.46
1:A:28:VAL:CG2	1:A:360:ILE:HD13	2.46	0.46
1:A:250:ILE:HG23	1:B:228:THR:HG21	1.97	0.46
1:B:343:ARG:HG2	1:B:343:ARG:HH11	1.81	0.45
1:A:171:ARG:NH2	1:B:155:GLU:OE2	2.49	0.45
1:B:41:TYR:CZ	1:B:62:GLY:HA3	2.52	0.45
1:B:224:ILE:O	1:B:228:THR:HG23	2.16	0.45
1:A:277[A]:MET:HE2	1:A:279:GLU:OE2	2.17	0.45
1:A:306:LEU:C	1:A:306:LEU:HD23	2.42	0.45
1:B:236:ASN:ND2	5:B:565:HOH:O	2.50	0.44
1:A:168:LYS:HG3	5:A:549:HOH:O	2.17	0.44
1:A:24:VAL:HG13	1:A:360:ILE:CD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD2	1:A:287:ASP:N	2.51	0.43
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.43
1:B:335[B]:CYS:SG	1:B:343:ARG:CD	3.07	0.43
1:A:230:GLN:NE2	1:A:234:ARG:HE	2.16	0.42
1:A:84:PRO:C	1:A:86:ASP:H	2.28	0.41
1:B:20:GLU:HG3	1:B:349:THR:HG22	2.03	0.41
1:B:232:LEU:HA	1:B:232:LEU:HD23	1.83	0.41
1:A:230:GLN:HE22	1:A:233:ARG:HE	1.68	0.41
1:B:204:ARG:HG3	1:B:221:HIS:CE1	2.56	0.41
1:A:244:SER:OG	5:A:747:HOH:O	1.94	0.41
1:A:163:MET:O	1:B:160:PHE:HA	2.20	0.40
1:B:232:LEU:H	1:B:232:LEU:HG	1.82	0.40
1:A:168:LYS:HZ3	1:B:155:GLU:HB3	1.82	0.40
1:A:105:ASN:HB2	1:A:138:LEU:HD22	2.01	0.40
1:A:118:MET:HE3	1:A:118:MET:HB3	1.89	0.40
1:A:204:ARG:HG3	1:A:221:HIS:CE1	2.56	0.40
1:A:185:ARG:NH2	1:A:238:PHE:O	2.50	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	374/375 (100%)	360 (96%)	14 (4%)	0	100	100
1	B	374/375 (100%)	357 (96%)	15 (4%)	2 (0%)	24	8
All	All	748/750 (100%)	717 (96%)	29 (4%)	2 (0%)	36	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	GLY

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Mol	Chain	Res	Type
1	B	361	ALA

5.3.2 Protein sidechains ⓘ

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	300/298 (101%)	293 (98%)	7 (2%)	44	15
1	B	300/298 (101%)	290 (97%)	10 (3%)	33	7
All	All	600/596 (101%)	583 (97%)	17 (3%)	39	10

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	80	GLU
1	A	82	LEU
1	A	153	GLU
1	A	168	LYS
1	A	318	LEU
1	A	343	ARG
1	B	15	PRO
1	B	82	LEU
1	B	88	PRO
1	B	90	ARG
1	B	153	GLU
1	B	185	ARG
1	B	236	ASN
1	B	253	ASP
1	B	335[A]	CYS
1	B	335[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	-2	HIS
1	A	51	HIS
1	A	81	HIS
1	A	105	ASN
1	A	112	HIS
1	A	151	GLN
1	A	230	GLN
1	B	4	GLN
1	B	112	HIS
1	B	151	GLN
1	B	230	GLN
1	B	236	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	IPM	B	401	3	11,11,11	1.85	4 (36%)	11,15,15	1.82	3 (27%)
2	IPM	A	401	3	11,11,11	2.25	4 (36%)	11,15,15	2.10	4 (36%)

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
2	IPM	B	401	3	-	4/16/16/16	-
2	IPM	A	401	3	-	3/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IPM	C2-C1	-4.64	1.46	1.52
2	B	401	IPM	C2-C1	-3.78	1.47	1.52
2	A	401	IPM	C3-C2	-3.62	1.50	1.54
2	A	401	IPM	O5-C4	-2.67	1.22	1.30
2	B	401	IPM	C3-C2	2.57	1.57	1.54
2	A	401	IPM	O2-C1	-2.39	1.23	1.30
2	B	401	IPM	O2-C1	-2.05	1.24	1.30
2	B	401	IPM	O3-C1	2.01	1.28	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IPM	O2-C1-C2	4.79	126.61	113.31
2	B	401	IPM	O2-C1-O3	-3.82	115.41	124.08
2	B	401	IPM	O2-C1-C2	3.06	121.82	113.31
2	A	401	IPM	O4-C4-C3	-2.86	115.53	122.84
2	A	401	IPM	O2-C1-O3	-2.78	117.77	124.08
2	B	401	IPM	C7-C5-C6	-2.44	103.88	110.58
2	A	401	IPM	O3-C1-C2	-2.30	115.50	121.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	IPM	C2-C3-C4-O4
2	A	401	IPM	C2-C3-C4-O5
2	B	401	IPM	C2-C3-C4-O5
2	B	401	IPM	C1-C2-C3-C4
2	A	401	IPM	C1-C2-C3-C4
2	B	401	IPM	C5-C3-C4-O4
2	B	401	IPM	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	369/375 (98%)	0.26	19 (5%) 33 36	6, 16, 33, 51	7 (1%)
1	B	368/375 (98%)	0.49	28 (7%) 20 21	9, 18, 33, 46	8 (2%)
All	All	737/750 (98%)	0.37	47 (6%) 25 27	6, 17, 33, 51	15 (2%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	5.4
1	B	361	ALA	5.2
1	B	154	GLY	5.2
1	A	84	PRO	5.0
1	B	0	GLY	4.7
1	A	-5	HIS	4.6
1	B	363	GLY	4.5
1	B	293	ILE	4.3
1	A	81	HIS	3.9
1	B	83	PRO	3.8
1	A	83	PRO	3.7
1	B	335[A]	CYS	3.7
1	B	53	CYS	3.7
1	B	287	ASP	3.2
1	A	82	LEU	3.1
1	B	153	GLU	3.1
1	A	343	ARG	2.9
1	B	285	ALA	2.9
1	B	-1	HIS	2.9
1	A	33	ASP	2.9
1	B	331	GLY	2.9
1	B	360	ILE	2.8
1	A	34	LEU	2.8
1	A	339	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	84	PRO	2.8
1	B	155	GLU	2.7
1	A	-4	HIS	2.6
1	B	359	ALA	2.6
1	A	80	GLU	2.6
1	A	313	LEU	2.5
1	B	81	HIS	2.5
1	A	32	PHE	2.5
1	B	327	ALA	2.5
1	A	338	LEU	2.4
1	A	360	ILE	2.3
1	A	341	SER	2.3
1	A	331	GLY	2.2
1	B	345	GLN	2.2
1	B	50	ASN	2.2
1	B	80	GLU	2.2
1	B	273	GLN	2.1
1	B	288	ILE	2.1
1	A	61	LYS	2.0
1	B	47	ALA	2.0
1	B	48	ILE	2.0
1	B	33	ASP	2.0
1	B	32	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IPM	B	401	12/12	0.96	0.05	12,13,14,15	0
3	MG	A	402	1/1	0.96	0.06	7,7,7,7	0
2	IPM	A	401	12/12	0.97	0.05	9,10,11,12	0
3	MG	B	402	1/1	0.99	0.03	12,12,12,12	0
4	CL	B	403	1/1	0.99	0.03	11,11,11,11	0
4	CL	A	403	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.