



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:56 AM UTC

PDB ID : 3EEG / pdb_00003eeg
Title : Crystal structure of a 2-isopropylmalate synthase from *Cytophaga hutchinsonii*
Authors : Sugadev, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2008-09-04
Resolution : 2.78 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

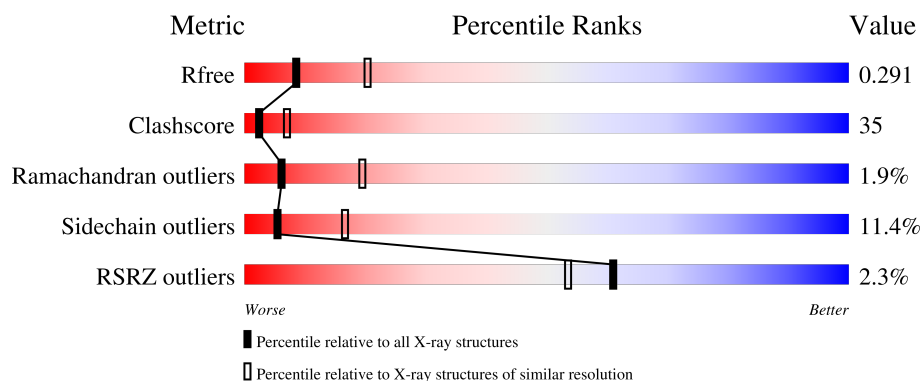
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	325	3% 43% 33% 6% 18%
1	B	325	3% 36% 38% 10% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4170 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 2-isopropylmalate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	Se	0	0	0
			2029	1267	358	391	5	8			
1	B	273	Total	C	N	O	S	Se	0	0	0
			2085	1301	371	400	5	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q11NN9
A	0	SER	-	expression tag	UNP Q11NN9
A	1	LEU	-	expression tag	UNP Q11NN9
A	316	GLU	-	expression tag	UNP Q11NN9
A	317	GLY	-	expression tag	UNP Q11NN9
A	318	HIS	-	expression tag	UNP Q11NN9
A	319	HIS	-	expression tag	UNP Q11NN9
A	320	HIS	-	expression tag	UNP Q11NN9
A	321	HIS	-	expression tag	UNP Q11NN9
A	322	HIS	-	expression tag	UNP Q11NN9
A	323	HIS	-	expression tag	UNP Q11NN9
B	-1	MSE	-	expression tag	UNP Q11NN9
B	0	SER	-	expression tag	UNP Q11NN9
B	1	LEU	-	expression tag	UNP Q11NN9
B	316	GLU	-	expression tag	UNP Q11NN9
B	317	GLY	-	expression tag	UNP Q11NN9
B	318	HIS	-	expression tag	UNP Q11NN9
B	319	HIS	-	expression tag	UNP Q11NN9
B	320	HIS	-	expression tag	UNP Q11NN9
B	321	HIS	-	expression tag	UNP Q11NN9
B	322	HIS	-	expression tag	UNP Q11NN9
B	323	HIS	-	expression tag	UNP Q11NN9

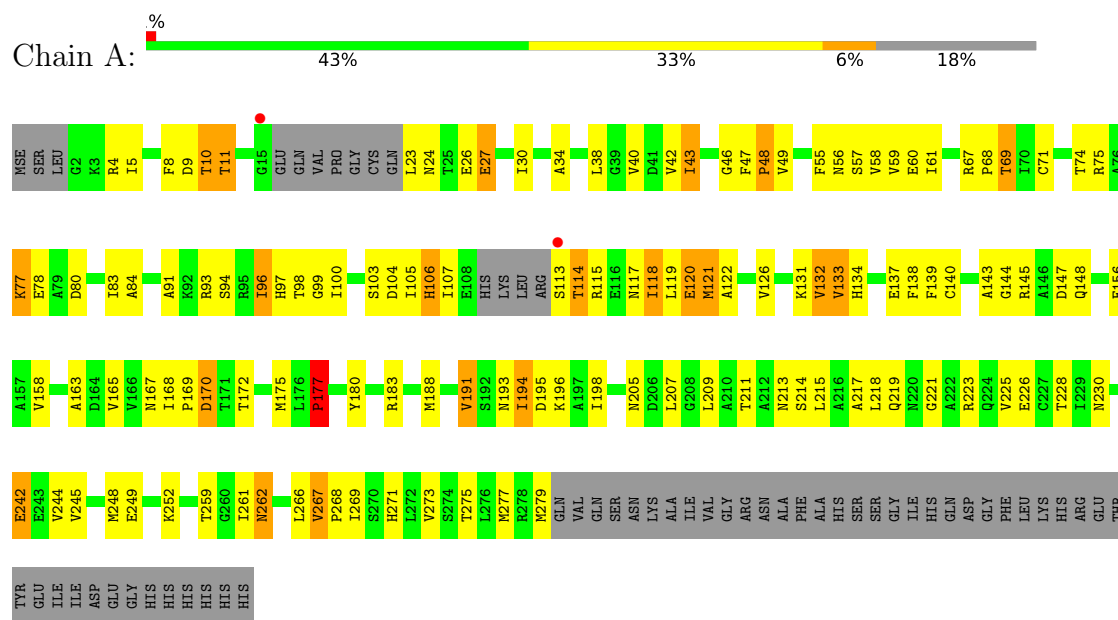
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total 39	O 39	0	0
2	B	17	Total 17	O 17	0	0

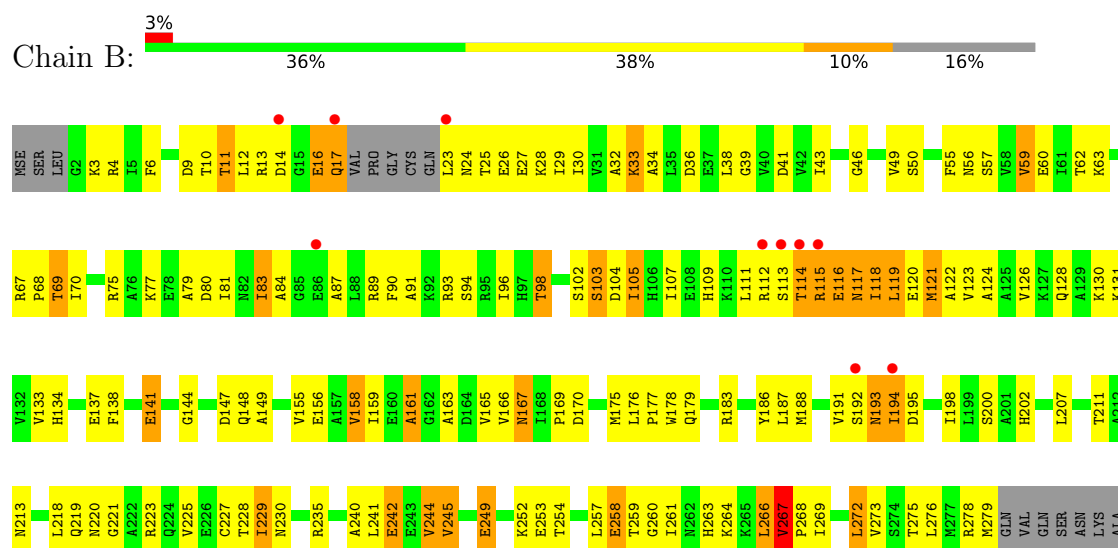
3 Residue-property plots [i](#)

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: 2-isopropylmalate synthase



• Molecule 1: 2-isopropylmalate synthase



ILE	VAL	GLY	ARG	ASN	ALA	PHE	ALA	HIS	SER	SER	GLY	ILE	HIS	GLN	ASP	GLY	PHE	LEU	LYS	HIS	ARG	GLU	THR	TYR	GLU	ILE	ILE	ASP	GLU	GLY	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.67Å 118.67Å 154.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.95 – 2.78 38.95 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.95-2.78) 96.2 (38.95-2.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.298 0.243 , 0.291	Depositor DCC
R_{free} test set	655 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

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	0.59	0/2045	1.10	19/2748 (0.7%)
1	B	0.53	1/2103 (0.0%)	1.06	12/2826 (0.4%)
All	All	0.56	1/4148 (0.0%)	1.08	31/5574 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	VAL	CA-CB	5.11	1.56	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	MSE	N-CA-C	-13.20	95.86	112.88
1	A	121	MSE	N-CA-C	-9.00	102.85	112.93
1	B	104	ASP	N-CA-C	-7.06	103.92	112.54
1	A	27	GLU	N-CA-C	-7.02	103.39	112.23
1	B	235	ARG	CB-CA-C	-6.76	108.03	117.23
1	A	47	PHE	CA-C-N	6.59	128.08	119.84
1	A	47	PHE	C-N-CA	6.59	128.08	119.84
1	A	169	PRO	N-CA-C	6.30	120.86	111.41
1	B	161	ALA	N-CA-C	-6.29	104.35	114.09
1	B	46	GLY	N-CA-C	6.26	118.58	110.45
1	A	170	ASP	N-CA-C	-6.06	100.50	109.11
1	A	114	THR	N-CA-C	6.06	123.70	110.80
1	B	109	HIS	N-CA-C	6.00	120.73	113.41
1	A	104	ASP	N-CA-C	-5.97	104.86	111.36
1	B	193	ASN	N-CA-C	5.88	119.71	111.30
1	A	11	THR	N-CA-C	5.86	119.90	112.87
1	B	117	ASN	N-CA-C	5.85	118.88	111.69
1	B	34	ALA	N-CA-C	-5.83	104.93	111.28
1	A	132	VAL	N-CA-C	5.77	118.70	113.10
1	A	83	ILE	N-CA-C	-5.77	105.11	110.53
1	A	113	SER	CA-C-N	-5.71	110.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SER	C-N-CA	-5.71	110.63	121.54
1	B	83	ILE	N-CA-C	-5.59	105.07	110.72
1	B	114	THR	N-CA-C	5.47	118.62	110.14
1	B	103	SER	N-CA-C	5.35	118.39	110.48
1	A	191	VAL	N-CA-C	-5.30	101.90	108.89
1	A	55	PHE	N-CA-C	-5.20	105.30	110.97
1	A	168	ILE	CA-C-N	5.15	125.13	120.03
1	A	168	ILE	C-N-CA	5.15	125.13	120.03
1	A	147	ASP	N-CA-C	-5.11	102.35	109.96
1	A	205	ASN	N-CA-C	5.05	118.28	112.57

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	2029	0	2048	134	0
1	B	2085	0	2107	157	0
2	A	39	0	0	3	0
2	B	17	0	0	2	0
All	All	4170	0	4155	290	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 35.

All (290) 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:103:SER:HB3	1:B:105:ILE:HG12	1.35	1.08
1:B:114:THR:HG23	1:B:118:ILE:HB	1.46	0.97
1:B:94:SER:H	1:B:134:HIS:HD2	1.13	0.96
1:B:170:ASP:HB2	1:B:175:MSE:HE3	1.45	0.96
1:A:9:ASP:OD1	1:A:11:THR:HG22	1.70	0.92
1:A:191:VAL:HB	1:A:194:ILE:HG23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HD12	1:A:105:ILE:H	1.33	0.90
1:A:24:ASN:OD1	1:A:27:GLU:HG3	1.72	0.88
1:B:263:HIS:HA	1:B:266:LEU:HD23	1.56	0.88
1:A:74:THR:HG21	1:A:84:ALA:HB2	1.55	0.86
1:A:188:MSE:HE2	1:A:221:GLY:HA3	1.56	0.83
1:A:94:SER:H	1:A:134:HIS:HD2	1.25	0.82
1:B:94:SER:H	1:B:134:HIS:CD2	1.97	0.82
1:A:148:GLN:HE21	1:A:183:ARG:HD2	1.44	0.81
1:A:267:VAL:HG13	1:A:268:PRO:HD3	1.62	0.81
1:B:267:VAL:HG13	1:B:268:PRO:HD3	1.64	0.80
1:B:194:ILE:HD13	1:B:194:ILE:H	1.48	0.78
1:A:117:ASN:O	1:A:120:GLU:HG2	1.84	0.78
1:A:119:LEU:C	1:A:121:MSE:H	1.92	0.78
1:A:191:VAL:CB	1:A:194:ILE:HG23	2.13	0.78
1:A:267:VAL:HG13	1:A:268:PRO:CD	2.15	0.77
1:A:145:ARG:HH11	1:A:172:THR:HG22	1.51	0.76
1:A:194:ILE:HD13	1:A:194:ILE:H	1.51	0.76
1:B:191:VAL:HB	1:B:194:ILE:HG23	1.68	0.75
1:A:194:ILE:HD13	1:A:194:ILE:N	2.02	0.75
1:B:124:ALA:O	1:B:128:GLN:HG3	1.87	0.75
1:A:115:ARG:H	1:A:118:ILE:HG23	1.54	0.73
1:B:245:VAL:HG21	1:B:261:ILE:HG13	1.71	0.72
1:A:170:ASP:HB2	1:A:175:MSE:HE3	1.71	0.71
1:B:10:THR:HG22	1:B:10:THR:O	1.89	0.70
1:B:119:LEU:HD13	1:B:119:LEU:O	1.93	0.69
1:B:267:VAL:HG13	1:B:268:PRO:CD	2.22	0.69
1:A:57:SER:O	1:A:61:ILE:HG12	1.92	0.69
1:A:262:ASN:C	1:A:262:ASN:HD22	1.99	0.69
1:A:74:THR:CG2	1:A:84:ALA:HB2	2.21	0.69
1:B:33:LYS:HB2	1:B:33:LYS:NZ	2.07	0.69
1:B:6:PHE:HA	1:B:41:ASP:OD2	1.91	0.69
1:B:114:THR:HG23	1:B:118:ILE:CB	2.21	0.69
1:A:188:MSE:HE2	1:A:221:GLY:CA	2.23	0.68
1:B:128:GLN:O	1:B:131:LYS:HG2	1.92	0.68
1:B:114:THR:HG22	1:B:115:ARG:N	2.08	0.68
1:B:114:THR:HG21	1:B:119:LEU:N	2.09	0.68
1:A:170:ASP:CB	1:A:175:MSE:HE3	2.24	0.68
1:B:102:SER:HB3	1:B:141:GLU:O	1.93	0.68
1:A:94:SER:H	1:A:134:HIS:CD2	2.10	0.67
1:B:9:ASP:OD1	1:B:11:THR:HG23	1.95	0.67
1:B:56:ASN:O	1:B:59:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:CB	1:B:175:MSE:HE3	2.24	0.66
1:A:105:ILE:H	1:A:105:ILE:CD1	2.08	0.66
1:A:194:ILE:H	1:A:194:ILE:CD1	2.08	0.66
1:B:188:MSE:HE2	1:B:221:GLY:CA	2.26	0.66
1:B:188:MSE:HE2	1:B:221:GLY:HA3	1.78	0.66
1:B:62:THR:HG22	1:B:70:ILE:HG21	1.78	0.65
1:B:27:GLU:HA	1:B:30:ILE:HD12	1.78	0.65
1:B:242:GLU:CD	1:B:242:GLU:H	2.04	0.65
1:A:103:SER:O	1:A:107:ILE:HG13	1.97	0.64
1:B:177:PRO:HA	1:B:213:ASN:ND2	2.12	0.64
1:B:69:THR:HB	1:B:93:ARG:CG	2.27	0.64
1:A:115:ARG:H	1:A:118:ILE:CG2	2.11	0.64
1:B:79:ALA:O	1:B:83:ILE:HG13	1.98	0.64
1:B:114:THR:CG2	1:B:119:LEU:N	2.61	0.63
1:A:107:ILE:HD12	2:A:361:HOH:O	1.98	0.63
1:B:156:GLU:HG3	1:B:191:VAL:HG13	1.80	0.63
1:A:230:ASN:H	1:A:242:GLU:CD	2.07	0.63
1:B:155:VAL:HG22	1:B:166:VAL:HG11	1.80	0.63
1:B:123:VAL:HG13	1:B:161:ALA:HB2	1.81	0.62
1:B:191:VAL:HB	1:B:194:ILE:CG2	2.30	0.62
1:B:126:VAL:HG21	1:B:158:VAL:HG22	1.81	0.62
1:B:62:THR:CG2	1:B:91:ALA:HB2	2.30	0.61
1:A:145:ARG:NH1	1:A:172:THR:HG22	2.15	0.61
1:A:191:VAL:CG1	1:A:194:ILE:HG23	2.31	0.61
1:B:11:THR:HG22	1:B:228:THR:HA	1.83	0.61
1:B:13:ARG:HG2	1:B:13:ARG:HH11	1.65	0.61
1:A:177:PRO:HA	1:A:213:ASN:ND2	2.15	0.60
1:B:176:LEU:HB2	1:B:179:GLN:HG3	1.82	0.60
1:A:119:LEU:C	1:A:121:MSE:N	2.59	0.60
1:B:49:VAL:HG21	1:B:80:ASP:CG	2.27	0.60
1:A:10:THR:HG22	1:A:228:THR:HG22	1.82	0.60
1:A:115:ARG:C	1:A:117:ASN:H	2.10	0.60
1:B:114:THR:HG21	1:B:119:LEU:CA	2.31	0.60
1:B:33:LYS:HB2	1:B:33:LYS:HZ2	1.67	0.60
1:B:119:LEU:HD22	1:B:121:MSE:HE3	1.84	0.60
1:A:49:VAL:HG21	1:A:80:ASP:HB3	1.82	0.59
1:A:114:THR:HB	1:A:118:ILE:HG12	1.83	0.59
1:A:118:ILE:HG13	1:A:118:ILE:O	2.00	0.59
1:A:244:VAL:HG12	1:A:248:MSE:HE2	1.84	0.58
1:B:188:MSE:HG3	1:B:220:ASN:O	2.03	0.58
1:B:229:ILE:CD1	1:B:241:LEU:HD23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:O	1:B:273:VAL:HG23	2.04	0.58
1:B:3:LYS:HB3	1:B:257:LEU:HD23	1.86	0.58
1:A:10:THR:HG22	1:A:228:THR:CG2	2.33	0.58
1:A:271:HIS:O	1:A:275:THR:HG22	2.04	0.58
1:B:24:ASN:O	1:B:28:LYS:HG2	2.03	0.58
1:B:218:LEU:HD21	1:B:225:VAL:HG22	1.86	0.57
1:A:191:VAL:O	1:A:194:ILE:HD12	2.04	0.57
1:B:177:PRO:HA	1:B:213:ASN:HD22	1.69	0.57
1:B:94:SER:N	1:B:134:HIS:HD2	1.94	0.57
1:A:114:THR:CB	1:A:118:ILE:HG12	2.35	0.57
1:A:139:PHE:CB	1:A:167:ASN:HB3	2.35	0.57
1:A:242:GLU:CD	1:A:242:GLU:H	2.13	0.57
1:B:111:LEU:O	1:B:113:SER:N	2.38	0.56
1:B:167:ASN:HD22	1:B:200:SER:HB3	1.70	0.56
1:A:158:VAL:HG12	1:A:163:ALA:HB3	1.86	0.56
1:B:123:VAL:HG13	1:B:161:ALA:CB	2.35	0.56
1:A:115:ARG:C	1:A:117:ASN:N	2.62	0.56
1:B:4:ARG:HH21	1:B:260:GLY:H	1.53	0.56
1:B:138:PHE:CD2	1:B:158:VAL:HG21	2.39	0.56
1:B:159:ILE:C	1:B:161:ALA:H	2.10	0.56
1:A:8:PHE:CD2	1:A:226:GLU:HG3	2.40	0.56
1:A:10:THR:HG23	1:A:10:THR:O	2.05	0.56
1:A:43:ILE:C	1:A:43:ILE:HD12	2.31	0.56
1:A:103:SER:OG	1:A:106:HIS:HB2	2.05	0.56
1:B:229:ILE:HD12	1:B:241:LEU:HD23	1.87	0.56
1:B:147:ASP:OD1	1:B:149:ALA:HB3	2.06	0.56
1:A:170:ASP:HA	1:A:175:MSE:CE	2.35	0.56
1:A:126:VAL:HG21	1:A:158:VAL:HG13	1.88	0.56
1:A:158:VAL:HG12	1:A:163:ALA:CB	2.36	0.56
1:B:36:ASP:OD1	1:B:68:PRO:HD3	2.06	0.56
1:B:249:GLU:HG3	1:B:263:HIS:NE2	2.20	0.56
1:B:69:THR:HB	1:B:93:ARG:HG3	1.87	0.55
1:A:69:THR:HB	1:A:93:ARG:CG	2.36	0.55
1:A:191:VAL:HG12	1:A:193:ASN:H	1.71	0.55
1:B:144:GLY:HA3	1:B:175:MSE:HE2	1.89	0.55
1:B:12:LEU:HD22	1:B:28:LYS:HD2	1.87	0.55
1:A:121:MSE:HA	2:A:324:HOH:O	2.06	0.55
1:B:114:THR:CG2	1:B:115:ARG:N	2.70	0.55
1:B:23:LEU:HG	1:B:24:ASN:H	1.71	0.55
1:B:176:LEU:HD13	1:B:178:TRP:CH2	2.42	0.55
1:A:48:PRO:HG3	1:A:58:VAL:HG21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:CG2	1:B:261:ILE:HG13	2.36	0.54
1:A:198:ILE:HG23	1:A:223:ARG:HB2	1.88	0.54
1:B:3:LYS:HE3	1:B:223:ARG:HD3	1.89	0.54
1:B:194:ILE:HD13	1:B:194:ILE:N	2.21	0.54
1:A:177:PRO:HA	1:A:213:ASN:HD22	1.71	0.54
1:B:121:MSE:O	1:B:124:ALA:HB3	2.07	0.54
1:A:9:ASP:CG	1:A:11:THR:HG22	2.31	0.54
1:B:269:ILE:HA	1:B:272:LEU:HD23	1.88	0.54
1:A:120:GLU:C	1:A:122:ALA:H	2.13	0.54
1:A:145:ARG:HH11	1:A:172:THR:CG2	2.20	0.53
1:A:43:ILE:HG13	1:A:43:ILE:O	2.08	0.53
1:B:25:THR:O	1:B:29:ILE:HD13	2.08	0.53
1:A:26:GLU:O	1:A:30:ILE:HG12	2.09	0.53
1:A:156:GLU:HG2	1:A:191:VAL:HG13	1.91	0.53
1:A:249:GLU:O	1:A:252:LYS:HG3	2.08	0.53
1:A:122:ALA:HB1	1:A:138:PHE:CZ	2.44	0.52
1:B:98:THR:O	1:B:138:PHE:HA	2.09	0.52
1:B:10:THR:O	1:B:10:THR:CG2	2.57	0.52
1:A:114:THR:HB	1:A:118:ILE:CG2	2.38	0.52
1:B:63:LYS:HD3	1:B:90:PHE:CD1	2.44	0.52
1:A:138:PHE:HB3	1:A:158:VAL:HG11	1.92	0.52
1:B:89:ARG:HG3	1:B:90:PHE:CD2	2.45	0.52
1:B:137:GLU:HG3	1:B:165:VAL:HB	1.91	0.52
1:B:227:CYS:SG	1:B:241:LEU:HD13	2.50	0.52
1:B:10:THR:HG22	1:B:14:ASP:H	1.75	0.52
1:A:91:ALA:HB3	1:A:94:SER:HB3	1.90	0.51
1:A:132:VAL:O	1:A:133:VAL:HG13	2.09	0.51
1:B:170:ASP:OD1	1:B:175:MSE:HG3	2.10	0.51
1:A:38:LEU:HD11	1:A:266:LEU:HA	1.91	0.51
1:B:75:ARG:HG2	2:B:327:HOH:O	2.10	0.51
1:A:71:CYS:SG	1:A:97:HIS:HB2	2.50	0.51
1:B:279:MSE:HG2	2:B:334:HOH:O	2.10	0.51
1:A:24:ASN:CG	1:A:27:GLU:HG3	2.35	0.51
1:A:214:SER:O	1:A:218:LEU:HG	2.11	0.51
1:B:115:ARG:O	1:B:116:GLU:C	2.54	0.51
1:A:245:VAL:HA	1:A:248:MSE:HE3	1.91	0.51
1:B:67:ARG:HB3	1:B:68:PRO:HD3	1.93	0.50
1:B:159:ILE:HB	1:B:193:ASN:ND2	2.26	0.50
1:A:209:LEU:HD21	1:B:211:THR:HG22	1.92	0.50
1:A:144:GLY:HA3	1:A:175:MSE:CE	2.41	0.50
1:B:122:ALA:HB1	1:B:138:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:N	1:A:134:HIS:HD2	2.04	0.50
1:B:155:VAL:O	1:B:159:ILE:HG13	2.11	0.50
1:A:34:ALA:HB1	1:A:269:ILE:HG23	1.93	0.50
1:B:105:ILE:HD13	1:B:105:ILE:N	2.27	0.50
1:B:194:ILE:H	1:B:194:ILE:CD1	2.22	0.50
1:B:218:LEU:HD21	1:B:225:VAL:CG2	2.42	0.49
1:A:273:VAL:HG12	1:A:279:MSE:CE	2.42	0.49
1:B:249:GLU:HG3	1:B:263:HIS:CE1	2.47	0.49
1:B:126:VAL:O	1:B:130:LYS:HB2	2.11	0.49
1:A:100:ILE:HG22	1:A:138:PHE:HZ	1.78	0.49
1:A:42:VAL:HG22	1:A:69:THR:HG23	1.94	0.49
1:B:17:GLN:C	1:B:17:GLN:OE1	2.56	0.49
1:A:115:ARG:HB2	1:A:118:ILE:HG22	1.95	0.49
1:A:140:CYS:O	1:A:143:ALA:HB2	2.13	0.48
1:A:262:ASN:C	1:A:262:ASN:ND2	2.69	0.48
1:A:115:ARG:O	1:A:117:ASN:N	2.45	0.48
1:B:4:ARG:HH21	1:B:260:GLY:N	2.10	0.48
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.78	0.48
1:A:114:THR:HB	1:A:118:ILE:HG21	1.94	0.48
1:A:115:ARG:O	1:A:118:ILE:HG23	2.14	0.48
1:A:105:ILE:HD12	1:A:105:ILE:N	2.15	0.48
1:A:180:TYR:CE2	1:A:217:ALA:HB2	2.49	0.48
1:B:13:ARG:HG2	1:B:13:ARG:NH1	2.29	0.48
1:B:67:ARG:HB3	1:B:68:PRO:CD	2.43	0.48
1:B:115:ARG:O	1:B:117:ASN:N	2.46	0.48
1:B:114:THR:HG22	1:B:115:ARG:H	1.79	0.48
1:B:11:THR:CG2	1:B:229:ILE:H	2.27	0.47
1:B:114:THR:CG2	1:B:115:ARG:H	2.27	0.47
1:B:24:ASN:OD1	1:B:27:GLU:HG3	2.15	0.47
1:B:218:LEU:HD11	1:B:225:VAL:HG21	1.95	0.47
1:A:23:LEU:HD22	1:A:277:MSE:HE3	1.97	0.47
1:B:198:ILE:O	1:B:198:ILE:HG13	2.14	0.46
1:B:38:LEU:HD13	1:B:269:ILE:HD12	1.96	0.46
1:A:131:LYS:HG3	2:A:335:HOH:O	2.14	0.46
1:A:194:ILE:N	1:A:194:ILE:CD1	2.68	0.46
1:B:148:GLN:NE2	1:B:186:TYR:CE1	2.83	0.46
1:B:240:ALA:O	1:B:244:VAL:HG23	2.14	0.46
1:B:241:LEU:O	1:B:245:VAL:HB	2.15	0.46
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.81	0.46
1:B:25:THR:HG22	1:B:57:SER:CB	2.46	0.46
1:B:169:PRO:HB3	1:B:202:HIS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:HB	1:B:91:ALA:CA	2.45	0.46
1:A:4:ARG:HG2	1:A:4:ARG:HH11	1.81	0.45
1:A:211:THR:O	1:A:215:LEU:HG	2.15	0.45
1:B:119:LEU:HA	1:B:121:MSE:HE3	1.98	0.45
1:A:67:ARG:HB3	1:A:68:PRO:CD	2.47	0.45
1:A:156:GLU:CG	1:A:191:VAL:HG13	2.45	0.45
1:B:62:THR:HB	1:B:91:ALA:HB2	1.97	0.45
1:B:33:LYS:NZ	1:B:33:LYS:CB	2.78	0.45
1:B:167:ASN:ND2	1:B:200:SER:HB3	2.30	0.45
1:B:103:SER:CB	1:B:105:ILE:HG12	2.24	0.45
1:B:116:GLU:O	1:B:120:GLU:HG3	2.17	0.45
1:A:145:ARG:HD2	1:A:172:THR:HG21	1.98	0.45
1:B:62:THR:CG2	1:B:70:ILE:HG21	2.47	0.45
1:A:40:VAL:CG2	1:A:43:ILE:HG22	2.47	0.45
1:A:114:THR:CG2	1:A:118:ILE:HG12	2.47	0.45
1:B:49:VAL:O	1:B:50:SER:C	2.59	0.45
1:B:23:LEU:HG	1:B:24:ASN:N	2.32	0.45
1:B:114:THR:HG21	1:B:119:LEU:HA	1.98	0.45
1:A:118:ILE:O	1:A:121:MSE:HB3	2.17	0.45
1:A:191:VAL:HB	1:A:194:ILE:CG2	2.33	0.45
1:B:29:ILE:N	1:B:29:ILE:HD12	2.32	0.45
1:B:29:ILE:HA	1:B:32:ALA:HB3	1.98	0.44
1:B:59:VAL:CG2	1:B:60:GLU:N	2.80	0.44
1:B:69:THR:HA	1:B:93:ARG:HB3	1.98	0.44
1:B:75:ARG:HB3	1:B:77:LYS:HD2	1.99	0.44
1:B:62:THR:HG21	1:B:91:ALA:HB2	1.99	0.44
1:A:98:THR:O	1:A:138:PHE:HA	2.17	0.44
1:A:259:THR:C	1:A:261:ILE:H	2.24	0.44
1:A:193:ASN:OD1	1:A:193:ASN:N	2.50	0.44
1:B:96:ILE:HB	1:B:133:VAL:HG21	1.99	0.44
1:A:5:ILE:HD12	1:A:223:ARG:HA	1.99	0.43
1:A:56:ASN:O	1:A:60:GLU:HG2	2.17	0.43
1:B:229:ILE:O	1:B:230:ASN:HB2	2.18	0.43
1:A:114:THR:HG21	1:A:118:ILE:HG12	2.00	0.43
1:A:177:PRO:N	1:A:213:ASN:HD21	2.16	0.43
1:B:114:THR:HA	1:B:118:ILE:HD12	2.00	0.43
1:B:178:TRP:O	1:B:179:GLN:C	2.60	0.43
1:A:96:ILE:CG2	1:A:97:HIS:N	2.82	0.43
1:B:81:ILE:O	1:B:84:ALA:HB3	2.19	0.43
1:B:159:ILE:C	1:B:161:ALA:N	2.77	0.43
1:A:119:LEU:O	1:A:121:MSE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:CD	1:A:252:LYS:HD3	2.44	0.42
1:B:55:PHE:CE1	1:B:87:ALA:HB2	2.54	0.42
1:A:191:VAL:HG11	1:A:194:ILE:HG23	1.99	0.42
1:B:9:ASP:HB3	1:B:43:ILE:HG22	2.02	0.42
1:B:89:ARG:HG3	1:B:90:PHE:N	2.34	0.42
1:B:258:GLU:CD	1:B:259:THR:H	2.28	0.42
1:B:272:LEU:O	1:B:276:LEU:HB2	2.19	0.42
1:B:43:ILE:HG13	1:B:43:ILE:O	2.19	0.42
1:B:119:LEU:HD22	1:B:119:LEU:HA	1.76	0.42
1:B:187:LEU:O	1:B:191:VAL:HG23	2.20	0.42
1:A:144:GLY:HA3	1:A:175:MSE:HE2	2.01	0.42
1:A:99:GLY:HA2	1:A:138:PHE:CE1	2.55	0.42
1:B:107:ILE:HA	1:B:111:LEU:HB2	2.02	0.42
1:B:107:ILE:HG12	1:B:119:LEU:HG	2.02	0.42
1:A:75:ARG:HG2	1:A:75:ARG:HH11	1.84	0.42
1:A:249:GLU:OE2	1:A:252:LYS:HD3	2.20	0.42
1:B:11:THR:HG21	1:B:229:ILE:H	1.84	0.41
1:A:177:PRO:CA	1:A:213:ASN:ND2	2.82	0.41
1:A:245:VAL:HG11	1:A:261:ILE:HG21	2.02	0.41
1:B:62:THR:HB	1:B:91:ALA:HA	2.02	0.41
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.36	0.41
1:B:138:PHE:CE2	1:B:158:VAL:HG21	2.55	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.69	0.41
1:B:159:ILE:HB	1:B:193:ASN:HD21	1.85	0.41
1:B:39:GLY:HA3	1:B:260:GLY:O	2.21	0.41
1:B:261:ILE:HG21	1:B:266:LEU:HD21	2.02	0.41
1:A:46:GLY:C	1:A:48:PRO:HD3	2.45	0.41
1:A:218:LEU:HD21	1:A:225:VAL:CG2	2.51	0.41
1:A:273:VAL:HG12	1:A:279:MSE:HE3	2.03	0.41
1:B:3:LYS:CE	1:B:223:ARG:HD3	2.50	0.41
1:A:77:LYS:O	1:A:78:GLU:C	2.64	0.41
1:A:139:PHE:HB3	1:A:167:ASN:HB3	2.02	0.41
1:B:158:VAL:HG13	1:B:163:ALA:CB	2.51	0.40
1:A:137:GLU:HA	1:A:165:VAL:O	2.22	0.40
1:A:138:PHE:CD2	1:A:158:VAL:HG21	2.56	0.40
1:A:67:ARG:HB3	1:A:68:PRO:HD3	2.04	0.40
1:B:9:ASP:CG	1:B:11:THR:HG23	2.45	0.40
1:A:49:VAL:HG21	1:A:80:ASP:CB	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	261/325 (80%)	236 (90%)	22 (8%)	3 (1%)	11	32
1	B	269/325 (83%)	235 (87%)	27 (10%)	7 (3%)	4	13
All	All	530/650 (82%)	471 (89%)	49 (9%)	10 (2%)	6	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	ARG
1	B	192	SER
1	A	120	GLU
1	B	16	GLU
1	B	116	GLU
1	B	141	GLU
1	A	48	PRO
1	A	177	PRO
1	B	278	ARG
1	B	264	LYS

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	217/258 (84%)	199 (92%)	18 (8%)	10	29
1	B	223/258 (86%)	191 (86%)	32 (14%)	3	10
All	All	440/516 (85%)	390 (89%)	50 (11%)	5	16

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	43	ILE
1	A	59	VAL
1	A	69	THR
1	A	77	LYS
1	A	96	ILE
1	A	106	HIS
1	A	118	ILE
1	A	133	VAL
1	A	177	PRO
1	A	194	ILE
1	A	195	ASP
1	A	196	LYS
1	A	207	LEU
1	A	219	GLN
1	A	242	GLU
1	A	262	ASN
1	A	267	VAL
1	B	11	THR
1	B	16	GLU
1	B	17	GLN
1	B	26	GLU
1	B	33	LYS
1	B	59	VAL
1	B	69	THR
1	B	98	THR
1	B	105	ILE
1	B	115	ARG
1	B	118	ILE
1	B	119	LEU
1	B	158	VAL
1	B	167	ASN
1	B	183	ARG
1	B	194	ILE
1	B	195	ASP
1	B	207	LEU
1	B	219	GLN
1	B	229	ILE
1	B	242	GLU
1	B	244	VAL
1	B	245	VAL
1	B	249	GLU

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Mol	Chain	Res	Type
1	B	252	LYS
1	B	253	GLU
1	B	254	THR
1	B	258	GLU
1	B	266	LEU
1	B	267	VAL
1	B	272	LEU
1	B	275	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	148	GLN
1	A	190	ASN
1	A	202	HIS
1	A	213	ASN
1	A	219	GLN
1	A	238	ASN
1	A	262	ASN
1	A	263	HIS
1	B	134	HIS
1	B	167	ASN
1	B	213	ASN
1	B	224	GLN
1	B	238	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [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	259/325 (79%)	-0.10	2 (0%) 82 77	9, 24, 44, 50	0
1	B	265/325 (81%)	0.38	10 (3%) 44 37	16, 36, 56, 66	0
All	All	524/650 (80%)	0.14	12 (2%) 61 53	9, 30, 52, 66	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ARG	3.0
1	B	114	THR	2.7
1	B	113	SER	2.6
1	B	23	LEU	2.6
1	B	17	GLN	2.5
1	B	194	ILE	2.5
1	B	115	ARG	2.4
1	B	14	ASP	2.3
1	A	113	SER	2.3
1	B	192	SER	2.2
1	A	15	GLY	2.2
1	B	86	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.