



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:34 PM GMT

PDB ID : 3EEG  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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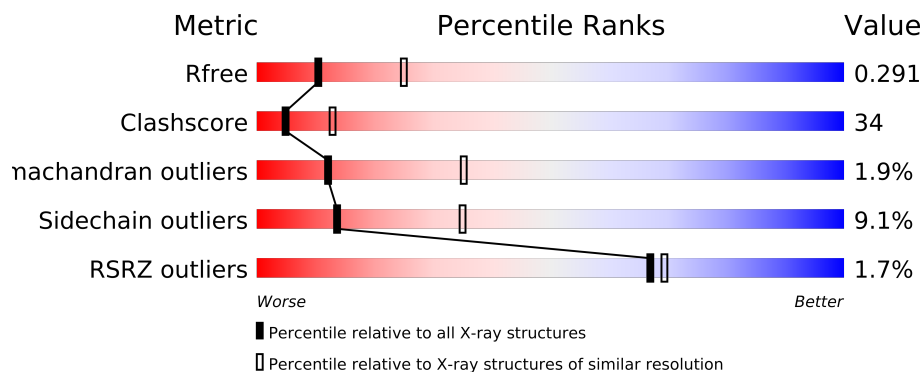
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2193 (2.80-2.76)
Clashscore	79885	2751 (2.80-2.76)
Ramachandran outliers	78287	2699 (2.80-2.76)
Sidechain outliers	78261	2701 (2.80-2.76)
RSRZ outliers	66119	2196 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	325	
1	B	325	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4170 atoms, of which 0 are hydrogen and 0 are deuterium.

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 96.3 (38.95-2.78)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16798 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.48	0/2045	0.73	0/2748
1	B	0.42	0/2103	0.67	1/2826 (0.0%)
All	All	0.45	0/4148	0.70	1/5574 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	MSE	N-CA-C	-5.61	95.86	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2029	0	2048	130	0
1	B	2085	0	2107	152	0
2	A	39	0	0	3	0
2	B	17	0	0	2	0
All	All	4170	0	4155	281	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (281) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:105:ILE:H	1:A:105:ILE:HD12	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:H	1:B:194:ILE:HD13	1.48	0.78
1:A:117:ASN:O	1:A:120:GLU:HG2	1.84	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:H	1:A:194:ILE:HD13	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:119:LEU:C	1:A:121:MSE:H	1.92	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:170:ASP:CB	1:B:175:MSE:HE3	2.24	0.66
1:A:105:ILE:CD1	1:A:105:ILE:H	2.08	0.66
1:A:194:ILE:CD1	1:A:194:ILE:H	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:A:262:ASN:HD22	1:A:262:ASN:C	1.99	0.65
1:B:177:PRO:HA	1:B:213:ASN:ND2	2.12	0.64
1:A:103:SER:O	1:A:107:ILE:HG13	1.97	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:B:156:GLU:HG3	1:B:191:VAL:HG13	1.80	0.63
1:A:107:ILE:HD12	2:A:361:HOH:O	1.98	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: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:A:145:ARG:NH1	1:A:172:THR:HG22	2.15	0.61
1:B:13:ARG:HH11	1:B:13:ARG:HG2	1.65	0.61
1:B:176:LEU:HB2	1:B:179:GLN:HG3	1.82	0.60
1:A:177:PRO:HA	1:A:213:ASN:ND2	2.15	0.60
1:A:10:THR:HG22	1:A:228:THR:HG22	1.82	0.60
1:B:114:THR:HG21	1:B:119:LEU:CA	2.31	0.60
1:B:119:LEU:HD22	1:B:121:MSE:HE3	1.84	0.60
1:B:33:LYS:HB2	1:B:33:LYS:HZ2	1.67	0.60
1:A:49:VAL:HG21	1:A:80:ASP:HB3	1.82	0.59
1:B:242:GLU:CD	1:B:242:GLU:H	2.04	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:B:229:ILE:CD1	1:B:241:LEU:HD23	2.33	0.58
1:B:188:MSE:HG3	1:B:220:ASN:O	2.03	0.58
1:A:244:VAL:HG12	1:A:248:MSE:HE2	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(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:230:ASN:H	1:A:242:GLU:CD	2.07	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: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: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:A:8:PHE:CD2	1:A:226:GLU:HG3	2.40	0.56
1:B:229:ILE:HD12	1:B:241:LEU:HD23	1.87	0.56
1:A:103:SER:OG	1:A:106:HIS:HB2	2.05	0.56
1:A:10:THR:O	1:A:10:THR:HG23	2.05	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:B:249:GLU:HG3	1:B:263:HIS:NE2	2.20	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:49:VAL:HG21	1:B:80:ASP:CG	2.27	0.55
1:B:69:THR:HB	1:B:93:ARG:HG3	1.87	0.55
1:A:115:ARG:C	1:A:117:ASN:H	2.10	0.55
1:A:69:THR:HB	1:A:93:ARG:CG	2.36	0.55
1:B:144:GLY:HA3	1:B:175:MSE:HE2	1.89	0.55
1:A:191:VAL:HG12	1:A:193:ASN:H	1.71	0.55
1:B:12:LEU:HD22	1:B:28:LYS:HD2	1.87	0.55
1:B:114:THR:CG2	1:B:115:ARG:N	2.70	0.55
1:A:121:MSE:HA	2:A:324:HOH:O	2.06	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:B:245:VAL:CG2	1:B:261:ILE:HG13	2.36	0.54
1:A:48:PRO:HG3	1:A:58:VAL:HG21	1.87	0.54
1:B:194:ILE:HD13	1:B:194:ILE:N	2.21	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:3:LYS:HE3	1:B:223:ARG:HD3	1.89	0.54
1:A:198:ILE:HG23	1:A:223:ARG:HB2	1.88	0.54
1:B:121:MSE:O	1:B:124:ALA:HB3	2.07	0.54
1:A:177:PRO:HA	1:A:213:ASN:HD22	1.71	0.54
1:A:119:LEU:C	1:A:121:MSE:N	2.59	0.54
1:B:269:ILE:HA	1:B:272:LEU:HD23	1.88	0.54
1:A:145:ARG:HH11	1:A:172:THR:CG2	2.20	0.53
1:A:43:ILE:O	1:A:43:ILE:HG13	2.08	0.53
1:B:25:THR:O	1:B:29:ILE:HD13	2.08	0.53
1:A:156:GLU:HG2	1:A:191:VAL:HG13	1.91	0.53
1:A:26:GLU:O	1:A:30:ILE:HG12	2.09	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:CG2	1:B:10:THR:O	2.57	0.52
1:B:159:ILE:C	1:B:161:ALA:H	2.10	0.52
1:A:114:THR:HB	1:A:118:ILE:CG2	2.38	0.52
1:A:242:GLU:CD	1:A:242:GLU:H	2.13	0.52
1:B:63:LYS:HD3	1:B:90:PHE:CD1	2.44	0.52
1:B:227:CYS:SG	1:B:241:LEU:HD13	2.50	0.52
1:A:115:ARG:C	1:A:117:ASN:N	2.62	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: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:B:170:ASP:OD1	1:B:175:MSE:HG3	2.10	0.51
1:A:132:VAL:O	1:A:133:VAL:HG13	2.09	0.51
1:A:43:ILE:HD12	1:A:43:ILE:C	2.31	0.51
1:B:75:ARG:HG2	2:B:327:HOH:O	2.10	0.51
1:A:38:LEU:HD11	1:A:266:LEU:HA	1.91	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:214:SER:O	1:A:218:LEU:HG	2.11	0.51
1:A:245:VAL:HA	1:A:248:MSE:HE3	1.91	0.51
1:B:159:ILE:HB	1:B:193:ASN:ND2	2.26	0.50
1:B:67:ARG:HB3	1:B:68:PRO:HD3	1.93	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:249:GLU:HG3	1:B:263:HIS:CE1	2.47	0.49
1:A:273:VAL:HG12	1:A:279:MSE:CE	2.42	0.49
1:A:9:ASP:CG	1:A:11:THR:HG22	2.31	0.49
1:B:126:VAL:O	1:B:130:LYS:HB2	2.11	0.49
1:A:120:GLU:C	1:A:122:ALA:H	2.13	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: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: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:115:ARG:O	1:A:118:ILE:HG23	2.14	0.48
1:A:114:THR:HB	1:A:118:ILE:HG21	1.94	0.48
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.78	0.48
1:A:105:ILE:HD12	1:A:105:ILE:N	2.15	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:A:180:TYR:CE2	1:A:217:ALA:HB2	2.49	0.48
1:B:115:ARG:O	1:B:117:ASN:N	2.46	0.48
1:B:198:ILE:HG13	1:B:198:ILE:O	2.14	0.48
1:B:114:THR:HG22	1:B:115:ARG:H	1.79	0.48
1:B:114:THR:CG2	1:B:115:ARG:H	2.27	0.47
1:B:11:THR:CG2	1:B:229:ILE: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:38:LEU:HD13	1:B:269:ILE:HD12	1.96	0.46
1:A:194:ILE:CD1	1:A:194:ILE:N	2.68	0.46
1:A:131:LYS:HG3	2:A:335:HOH:O	2.14	0.46
1:B:240:ALA:O	1:B:244:VAL:HG23	2.14	0.46
1:B:148:GLN:NE2	1:B:186:TYR:CE1	2.83	0.46
1:B:115:ARG:O	1:B:116:GLU:C	2.54	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
1:B:62:THR:HB	1:B:91:ALA:CA	2.45	0.46
1:B:119:LEU:HA	1:B:121:MSE:HE3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:THR:O	1:A:215:LEU:HG	2.15	0.45
1:A:4:ARG:HG2	1:A:4:ARG:HH11	1.81	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:A:67:ARG:HB3	1:A:68:PRO:CD	2.47	0.45
1:B:33:LYS:CB	1:B:33:LYS:NZ	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:114:THR:CG2	1:A:118:ILE:HG12	2.47	0.45
1:A:40:VAL:CG2	1:A:43:ILE:HG22	2.47	0.45
1:B:114:THR:HG21	1:B:119:LEU:HA	1.98	0.45
1:B:23:LEU:HG	1:B:24:ASN:N	2.32	0.45
1:A:191:VAL:HB	1:A:194:ILE:CG2	2.33	0.45
1:A:118:ILE:O	1:A:121:MSE:HB3	2.17	0.45
1:B:29:ILE:N	1:B:29:ILE:HD12	2.32	0.45
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:29:ILE:HA	1:B:32:ALA:HB3	1.98	0.44
1:B:75:ARG:HB3	1:B:77:LYS:HD2	1.99	0.44
1:A:262:ASN:ND2	1:A:262:ASN:C	2.69	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:193:ASN:N	1:A:193:ASN:OD1	2.50	0.44
1:B:96:ILE:HB	1:B:133:VAL:HG21	1.99	0.44
1:B:17:GLN:C	1:B:17:GLN:OE1	2.56	0.44
1:B:229:ILE:O	1:B:230:ASN:HB2	2.18	0.43
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: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:A:24:ASN:CG	1:A:27:GLU:HG3	2.35	0.43
1:B:114:THR:HA	1:B:118:ILE:HD12	2.00	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:A:119:LEU:O	1:A:121:MSE:N	2.52	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:272:LEU:O	1:B:276:LEU:HB2	2.19	0.42
1:B:119:LEU:HA	1:B:119:LEU:HD22	1.76	0.42
1:B:43:ILE:HG13	1:B:43:ILE:O	2.19	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: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:99:GLY:HA2	1:A:138:PHE:CE1	2.55	0.42
1:A:249:GLU:OE2	1:A:252:LYS:HD3	2.20	0.42
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.84	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:B:138:PHE:CE2	1:B:158:VAL:HG21	2.55	0.41
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.36	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:261:ILE:HG21	1:B:266:LEU:HD21	2.02	0.41
1:B:39:GLY:HA3	1:B:260:GLY:O	2.21	0.41
1:B:3:LYS:CE	1:B:223:ARG:HD3	2.50	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: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:138:PHE:CD2	1:A:158:VAL:HG21	2.56	0.40
1:A:137:GLU:HA	1:A:165:VAL:O	2.22	0.40
1:A:67:ARG:HB3	1:A:68:PRO:HD3	2.04	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%)	21	55
1	B	269/325 (83%)	235 (87%)	27 (10%)	7 (3%)	8	25
All	All	530/650 (82%)	471 (89%)	49 (9%)	10 (2%)	12	35

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%)	204 (94%)	13 (6%)	27	59
1	B	223/258 (86%)	196 (88%)	27 (12%)	7	20
All	All	440/516 (85%)	400 (91%)	40 (9%)	14	35

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	43	ILE
1	A	69	THR
1	A	106	HIS
1	A	113	SER
1	A	118	ILE
1	A	133	VAL

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Mol	Chain	Res	Type
1	A	160	GLU
1	A	194	ILE
1	A	196	LYS
1	A	207	LEU
1	A	262	ASN
1	A	267	VAL
1	B	11	THR
1	B	16	GLU
1	B	26	GLU
1	B	33	LYS
1	B	47	PHE
1	B	69	THR
1	B	98	THR
1	B	105	ILE
1	B	112	ARG
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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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

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Mol	Chain	Res	Type
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	230	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/325 (82%)	-0.23	1 (0%) 90 92	9, 24, 45, 50	0
1	B	273/325 (84%)	0.12	8 (2%) 49 52	16, 37, 56, 78	0
All	All	540/650 (83%)	-0.05	9 (1%) 67 69	9, 31, 53, 78	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	MSE	4.3
1	B	113	SER	3.2
1	B	148	GLN	3.2
1	B	194	ILE	2.5
1	B	112	ARG	2.3
1	A	253	GLU	2.3
1	B	276	LEU	2.1
1	B	178	TRP	2.1
1	B	90	PHE	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.