



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:55 AM GMT

PDB ID : 4FSH  
Title : Crystal Structure of Shikimate Dehydrogenase (aroE) Clinical Variant v2356  
from Helicobacter pylori in Complex with Shikimate  
Authors : Cheng, W.C.; Chen, T.J.; Wang, W.C.  
Deposited on : 2012-06-27  
Resolution : 2.85 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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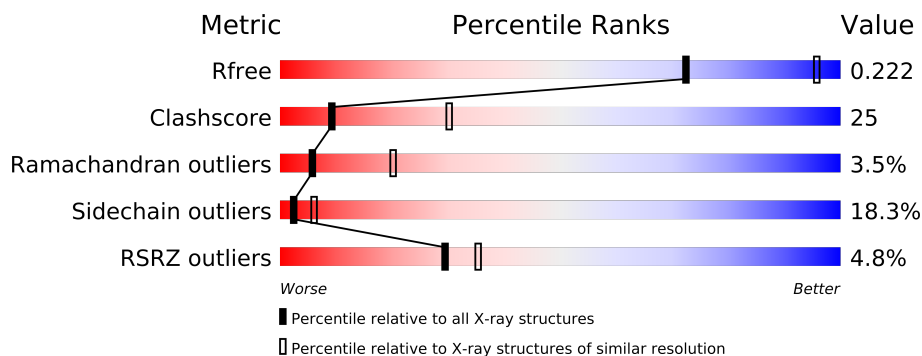
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.85 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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	271	
1	B	271	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4150 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 Shikimate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2036	1330	337	359	10			
1	B	263	Total	C	N	O	S	0	0	0
			2061	1345	341	365	10			

There are 52 discrepancies between the modelled and reference sequences:

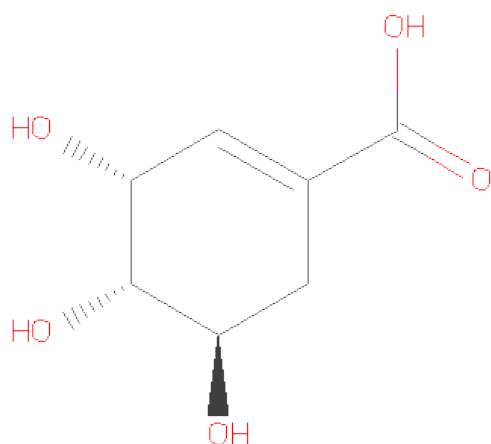
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	LYS	GLU	CONFLICT	UNP P56119
A	34	GLY	ARG	CONFLICT	UNP P56119
A	40	ARG	HIS	CONFLICT	UNP P56119
A	52	ASN	SER	CONFLICT	UNP P56119
A	87	ALA	GLY	CONFLICT	UNP P56119
A	88	SER	ALA	CONFLICT	UNP P56119
A	89	ILE	VAL	CONFLICT	UNP P56119
A	115	HIS	GLN	CONFLICT	UNP P56119
A	116	GLN	LYS	CONFLICT	UNP P56119
A	126	SER	ALA	CONFLICT	UNP P56119
A	136	GLY	GLU	CONFLICT	UNP P56119
A	143	LYS	GLN	CONFLICT	UNP P56119
A	151	PRO	SER	CONFLICT	UNP P56119
A	185	ASN	HIS	CONFLICT	UNP P56119
A	202	ALA	GLY	CONFLICT	UNP P56119
A	218	ALA	SER	CONFLICT	UNP P56119
A	225	ILE	THR	CONFLICT	UNP P56119
A	239	SER	ALA	CONFLICT	UNP P56119
A	264	LEU	-	EXPRESSION TAG	UNP P56119
A	265	GLU	-	EXPRESSION TAG	UNP P56119
A	266	HIS	-	EXPRESSION TAG	UNP P56119
A	267	HIS	-	EXPRESSION TAG	UNP P56119
A	268	HIS	-	EXPRESSION TAG	UNP P56119
A	269	HIS	-	EXPRESSION TAG	UNP P56119
A	270	HIS	-	EXPRESSION TAG	UNP P56119

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Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	EXPRESSION TAG	UNP P56119
B	32	LYS	GLU	CONFLICT	UNP P56119
B	34	GLY	ARG	CONFLICT	UNP P56119
B	40	ARG	HIS	CONFLICT	UNP P56119
B	52	ASN	SER	CONFLICT	UNP P56119
B	87	ALA	GLY	CONFLICT	UNP P56119
B	88	SER	ALA	CONFLICT	UNP P56119
B	89	ILE	VAL	CONFLICT	UNP P56119
B	115	HIS	GLN	CONFLICT	UNP P56119
B	116	GLN	LYS	CONFLICT	UNP P56119
B	126	SER	ALA	CONFLICT	UNP P56119
B	136	GLY	GLU	CONFLICT	UNP P56119
B	143	LYS	GLN	CONFLICT	UNP P56119
B	151	PRO	SER	CONFLICT	UNP P56119
B	185	ASN	HIS	CONFLICT	UNP P56119
B	202	ALA	GLY	CONFLICT	UNP P56119
B	218	ALA	SER	CONFLICT	UNP P56119
B	225	ILE	THR	CONFLICT	UNP P56119
B	239	SER	ALA	CONFLICT	UNP P56119
B	264	LEU	-	EXPRESSION TAG	UNP P56119
B	265	GLU	-	EXPRESSION TAG	UNP P56119
B	266	HIS	-	EXPRESSION TAG	UNP P56119
B	267	HIS	-	EXPRESSION TAG	UNP P56119
B	268	HIS	-	EXPRESSION TAG	UNP P56119
B	269	HIS	-	EXPRESSION TAG	UNP P56119
B	270	HIS	-	EXPRESSION TAG	UNP P56119
B	271	HIS	-	EXPRESSION TAG	UNP P56119

- Molecule 2 is (3R,4S,5R)-3,4,5-TRIHYDROXYCYCLOHEX-1-ENE-1-CARBOXYLIC ACID (three-letter code: SKM) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	22	Total	O	0	0
			22	22		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.12Å 71.87Å 176.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 25.49 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.85) 99.6 (25.49-2.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.99 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.214 , 0.260 0.212 , 0.222	Depositor DCC
$R_{free}$ test set	988 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19323 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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 ⓘ

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

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	0.86	5/2082 (0.2%)	0.63	0/2800
1	B	0.87	1/2108 (0.0%)	0.65	0/2838
All	All	0.86	6/4190 (0.1%)	0.64	0/5638

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	TYR	CG-CD2	14.42	1.57	1.39
1	A	118	TYR	CE1-CZ	10.29	1.51	1.38
1	A	118	TYR	CE2-CZ	9.38	1.50	1.38
1	A	135	CYS	CB-SG	-7.39	1.69	1.82
1	A	118	TYR	CG-CD1	6.93	1.48	1.39
1	B	85	GLU	CG-CD	5.07	1.59	1.51

There are no bond angle outliers.

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	2036	0	2091	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2061	0	2114	61	0
2	A	12	0	9	0	0
3	A	19	0	0	10	0
3	B	22	0	0	2	0
All	All	4150	0	4214	207	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 25.

All (207) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:LEU:C	1:A:148:ASN:HD22	1.47	1.17
1:A:50:ILE:HD11	1:A:72:ALA:HA	1.25	1.14
1:A:113:LEU:HA	1:A:114:LYS:CB	1.74	1.13
1:A:113:LEU:CA	1:A:114:LYS:HB3	1.91	1.00
1:A:147:LEU:C	1:A:148:ASN:ND2	2.16	0.98
1:A:113:LEU:HA	1:A:114:LYS:HB3	0.99	0.98
1:A:176:ILE:HD12	1:A:176:ILE:N	1.81	0.94
1:A:90:ASN:ND2	1:A:105:ASP:OD2	2.01	0.94
1:A:72:ALA:HB1	1:A:89:ILE:HD11	1.49	0.91
1:A:72:ALA:CB	1:A:89:ILE:HD11	2.01	0.90
1:A:113:LEU:HB3	1:A:114:LYS:HE3	1.54	0.90
1:A:203:LYS:O	1:A:204:LEU:HD23	1.70	0.88
1:A:50:ILE:CD1	1:A:72:ALA:HA	2.04	0.88
1:B:10:GLY:HA3	1:B:13:ILE:HD13	1.64	0.80
1:A:141:GLY:O	1:A:142:LEU:HD12	1.81	0.80
1:A:120:ASN:HB2	1:A:143:LYS:O	1.82	0.79
1:A:109:PHE:O	1:A:112:SER:HB3	1.83	0.79
1:A:44:LEU:CD2	1:A:45:PRO:HD2	2.15	0.77
1:B:166:MET:HA	1:B:166:MET:CE	2.14	0.77
1:A:147:LEU:HD12	1:A:148:ASN:N	2.00	0.76
1:A:176:ILE:N	1:A:176:ILE:CD1	2.49	0.76
1:A:168:PRO:HD3	3:A:615:HOH:O	1.85	0.75
1:A:111:LEU:C	1:A:113:LEU:H	1.92	0.73
1:A:148:ASN:N	1:A:148:ASN:ND2	2.36	0.72
1:A:175:LEU:C	1:A:176:ILE:HD12	2.09	0.72
1:A:115:HIS:O	1:A:115:HIS:HD2	1.73	0.71
1:A:203:LYS:C	1:A:204:LEU:HD23	2.11	0.71
1:A:147:LEU:C	1:A:147:LEU:HD12	2.12	0.69
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.57	0.69
1:A:113:LEU:CA	1:A:114:LYS:CB	2.58	0.69
1:B:105:ASP:HA	1:B:237:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:LEU:HD21	1:B:246:SER:HB2	1.74	0.68
1:A:222:GLU:HG2	3:A:609:HOH:O	1.91	0.68
1:A:110:TYR:CZ	1:A:140:GLN:HG2	2.28	0.68
1:B:10:GLY:HA2	1:B:65:THR:HG22	1.73	0.67
1:A:144:VAL:O	1:A:162:CYS:HB2	1.94	0.67
1:B:116:GLN:HE21	1:B:118:TYR:H	1.40	0.67
1:A:185:ASN:OD1	1:A:185:ASN:N	2.27	0.67
1:A:115:HIS:O	1:A:115:HIS:CD2	2.48	0.66
1:A:44:LEU:HD23	1:A:45:PRO:HD2	1.77	0.66
1:A:174:ASP:OD1	1:A:174:ASP:N	2.27	0.66
1:A:138:LYS:O	1:A:141:GLY:N	2.25	0.66
1:B:10:GLY:O	1:B:68:PHE:HE2	1.78	0.66
1:A:56:HIS:HE1	3:A:606:HOH:O	1.77	0.66
1:B:116:GLN:NE2	1:B:118:TYR:H	1.94	0.65
1:B:32:LYS:HG3	3:B:314:HOH:O	1.96	0.65
1:A:151:PRO:O	1:A:154:LEU:HB3	1.96	0.65
1:B:166:MET:HA	1:B:166:MET:HE3	1.78	0.65
1:A:44:LEU:HD22	1:A:45:PRO:HD2	1.79	0.64
1:A:122:LEU:HA	1:A:145:SER:O	1.97	0.64
1:B:212:PHE:HD1	1:B:212:PHE:H	1.45	0.64
1:A:196:LYS:HG2	1:A:197:GLY:N	2.13	0.64
1:A:72:ALA:C	1:A:89:ILE:HD11	2.18	0.64
1:A:9:PHE:O	1:A:65:THR:HG22	1.97	0.64
1:A:21:ILE:HB	1:A:259:MET:HG2	1.81	0.63
1:B:10:GLY:CA	1:B:13:ILE:HD13	2.28	0.63
1:A:149:ARG:N	1:A:149:ARG:HD2	2.13	0.63
1:A:72:ALA:CB	1:A:89:ILE:CD1	2.76	0.63
1:A:67:PRO:HD2	1:A:68:PHE:CE2	2.35	0.62
1:A:113:LEU:HA	1:A:114:LYS:CG	2.29	0.62
1:B:10:GLY:HA3	1:B:13:ILE:CD1	2.29	0.62
1:A:177:ILE:O	1:A:178:ASN:HB3	2.01	0.61
1:A:113:LEU:CB	1:A:114:LYS:HG2	2.30	0.61
1:B:172:ALA:HB2	1:B:201:GLU:OE1	2.01	0.61
1:A:149:ARG:HH22	1:A:180:THR:HG23	1.65	0.61
1:A:73:PHE:N	1:A:89:ILE:CD1	2.65	0.60
1:A:124:LEU:N	1:A:124:LEU:HD23	2.17	0.59
1:A:95:GLU:O	1:A:98:GLU:HB2	2.02	0.59
1:B:13:ILE:HG13	1:B:13:ILE:O	2.01	0.59
1:A:169:PRO:C	1:A:171:SER:H	2.05	0.59
1:A:217:LEU:O	1:A:217:LEU:HD23	2.01	0.59
1:A:166:MET:HB3	1:B:184:LEU:HD13	1.85	0.59
1:A:114:LYS:NZ	1:A:228:GLN:HE22	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:LEU:HA	1:A:220:ALA:HB3	1.85	0.59
1:A:72:ALA:C	1:A:89:ILE:CD1	2.71	0.59
1:A:176:ILE:C	1:A:177:ILE:HG12	2.23	0.58
1:A:111:LEU:O	1:A:113:LEU:N	2.34	0.58
1:A:167:GLU:HA	3:A:615:HOH:O	2.04	0.58
1:B:155:ASP:O	1:B:159:ARG:HG3	2.04	0.58
1:B:10:GLY:O	1:B:68:PHE:CE2	2.56	0.57
1:A:4:LYS:HD2	1:A:35:PHE:CG	2.40	0.57
1:A:177:ILE:O	1:A:178:ASN:CB	2.53	0.57
1:A:73:PHE:HA	1:A:89:ILE:HD12	1.87	0.57
1:A:235:ILE:HG22	1:A:256:PHE:CD1	2.40	0.56
1:B:166:MET:HE2	1:B:166:MET:HA	1.87	0.56
1:B:191:ASN:OD1	1:B:191:ASN:C	2.43	0.56
1:B:11:ASN:ND2	1:B:45:PRO:HA	2.20	0.56
1:A:196:LYS:CG	1:A:197:GLY:N	2.68	0.56
1:A:146:VAL:HG12	1:A:148:ASN:HD21	1.70	0.56
1:A:8:VAL:HB	1:A:39:TYR:OH	2.06	0.55
1:A:146:VAL:HG21	1:A:157:PHE:CD1	2.41	0.55
1:A:175:LEU:HD21	1:A:204:LEU:HD12	1.89	0.55
1:A:149:ARG:HG3	1:A:190:LEU:HD21	1.89	0.55
1:A:208:LEU:O	1:A:230:GLY:HA3	2.07	0.54
1:A:46:LEU:O	1:A:71:ARG:NH2	2.41	0.54
1:A:65:THR:HA	1:A:69:LYS:HE2	1.89	0.54
1:B:109:PHE:HA	1:B:233:MET:HG3	1.89	0.54
1:B:105:ASP:HA	1:B:237:GLN:HE21	1.72	0.54
1:A:217:LEU:HA	1:A:220:ALA:CB	2.38	0.54
1:A:196:LYS:HG2	1:A:197:GLY:H	1.73	0.53
1:A:213:LEU:HD11	1:A:217:LEU:HD22	1.89	0.53
1:A:111:LEU:C	1:A:113:LEU:N	2.61	0.53
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.19	0.53
1:B:8:VAL:HB	1:B:39:TYR:OH	2.09	0.53
1:A:31:LYS:H	1:A:31:LYS:HD2	1.73	0.52
1:A:124:LEU:HD21	1:A:176:ILE:CG2	2.40	0.52
1:A:247:ALA:O	1:A:248:SER:HB2	2.09	0.52
1:A:4:LYS:HB2	1:A:35:PHE:CD1	2.45	0.52
1:B:234:LEU:CD2	1:B:234:LEU:C	2.78	0.52
1:A:89:ILE:HB	1:A:102:TYR:O	2.10	0.51
1:A:173:PHE:CE2	1:A:198:TYR:OH	2.57	0.51
1:A:26:PHE:CD1	1:A:37:GLY:HA3	2.46	0.51
1:A:124:LEU:HD21	1:A:176:ILE:HG23	1.93	0.51
1:A:127:GLY:HA3	3:A:603:HOH:O	2.11	0.51
1:A:102:TYR:CE1	1:A:244:LYS:HE3	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:ASN:OD1	1:B:193:GLU:N	2.43	0.50
1:A:151:PRO:HD2	1:A:152:ARG:H	1.77	0.50
1:A:217:LEU:O	1:A:220:ALA:HB3	2.11	0.50
1:B:10:GLY:HA2	1:B:65:THR:CG2	2.41	0.50
1:B:234:LEU:HD22	1:B:234:LEU:C	2.32	0.50
1:A:170:LYS:HD2	1:A:170:LYS:N	2.27	0.50
1:A:169:PRO:C	1:A:171:SER:N	2.65	0.50
1:B:213:LEU:HD21	1:B:221:LYS:HD3	1.95	0.49
1:A:190:LEU:HB2	3:A:602:HOH:O	2.12	0.49
1:A:76:CYS:HB2	1:A:79:ILE:HD11	1.95	0.49
1:A:214:THR:O	1:A:215:PRO:C	2.52	0.49
1:A:110:TYR:CE1	1:A:140:GLN:HG2	2.48	0.48
1:A:219:LEU:C	1:A:219:LEU:HD12	2.33	0.48
1:A:146:VAL:CG1	1:A:148:ASN:HD21	2.27	0.48
1:B:154:LEU:CD1	1:B:164:CYS:HB3	2.43	0.48
1:A:120:ASN:ND2	1:A:173:PHE:CE1	2.82	0.48
1:A:219:LEU:O	1:A:220:ALA:C	2.52	0.48
1:A:169:PRO:O	1:A:171:SER:N	2.34	0.48
1:A:219:LEU:HG	1:A:220:ALA:N	2.29	0.47
1:A:227:PHE:CD1	1:A:227:PHE:N	2.82	0.47
1:A:113:LEU:CA	1:A:114:LYS:HG2	2.45	0.47
1:B:154:LEU:HD13	1:B:164:CYS:HB3	1.97	0.46
1:A:147:LEU:C	1:A:147:LEU:CD1	2.81	0.46
1:B:195:LEU:HD12	1:B:195:LEU:HA	1.71	0.46
1:A:113:LEU:HB2	1:A:114:LYS:HG2	1.96	0.46
1:B:86:CYS:O	1:B:87:ALA:C	2.53	0.46
1:A:170:LYS:CD	1:A:170:LYS:N	2.78	0.46
1:A:102:TYR:CD1	1:A:244:LYS:HE3	2.51	0.45
1:B:11:ASN:O	1:B:67:PRO:HD3	2.17	0.45
1:A:175:LEU:CD2	1:A:204:LEU:HD12	2.47	0.45
1:B:165:PHE:CZ	1:B:169:PRO:HB3	2.51	0.45
1:A:149:ARG:HA	1:A:166:MET:HG3	1.98	0.45
1:B:44:LEU:HD11	1:B:53:GLU:HG3	1.99	0.45
1:A:149:ARG:CD	1:A:149:ARG:H	2.28	0.45
1:A:31:LYS:N	1:A:31:LYS:HD2	2.32	0.45
1:A:127:GLY:O	1:A:131:LYS:HG3	2.17	0.45
1:B:235:ILE:HG22	1:B:256:PHE:CD1	2.51	0.45
1:A:22:HIS:HD2	1:A:242:PHE:HD1	1.65	0.45
1:B:254:LYS:O	1:B:255:ALA:C	2.55	0.45
1:A:120:ASN:ND2	1:A:173:PHE:HE1	2.15	0.44
1:B:149:ARG:O	1:B:149:ARG:HG3	2.16	0.44
1:B:89:ILE:HB	1:B:102:TYR:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:LYS:HB3	1:A:139:LYS:HE2	1.51	0.44
1:A:149:ARG:N	1:A:149:ARG:CD	2.75	0.44
1:A:49:HIS:HD2	3:A:614:HOH:O	2.00	0.44
1:B:11:ASN:HA	1:B:43:LEU:HD23	1.99	0.44
1:A:113:LEU:CA	1:A:114:LYS:CG	2.95	0.44
1:A:163:ASP:HB3	1:B:186:ASN:ND2	2.33	0.44
1:A:72:ALA:HB3	1:A:89:ILE:CD1	2.47	0.43
1:A:66:LEU:HA	1:A:67:PRO:HA	1.81	0.43
1:A:118:TYR:HB2	3:A:619:HOH:O	2.19	0.43
1:A:18:SER:N	1:A:19:PRO:CD	2.82	0.43
1:B:1:MET:HE3	1:B:30:GLN:HB2	2.00	0.43
1:B:78:LYS:HB2	1:B:78:LYS:HE2	1.62	0.43
1:B:214:THR:HB	1:B:215:PRO:HD2	2.01	0.43
1:A:143:LYS:HB2	1:A:143:LYS:HE3	1.58	0.43
1:B:184:LEU:N	1:B:184:LEU:CD2	2.83	0.42
1:A:127:GLY:CA	3:A:603:HOH:O	2.66	0.42
1:B:176:ILE:HD12	1:B:198:TYR:HB3	2.00	0.42
1:A:89:ILE:HG12	1:A:89:ILE:O	2.18	0.42
1:B:212:PHE:CD1	1:B:212:PHE:N	2.83	0.42
1:A:182:ALA:O	1:A:183:SER:CB	2.67	0.42
1:B:184:LEU:HD23	1:B:184:LEU:N	2.34	0.42
1:A:179:ALA:HB1	3:A:603:HOH:O	2.20	0.42
1:A:114:LYS:HG3	1:A:115:HIS:N	2.33	0.42
1:A:114:LYS:HZ1	1:A:228:GLN:HE22	1.66	0.42
1:A:151:PRO:O	1:A:154:LEU:CB	2.66	0.42
1:B:231:LYS:O	1:B:234:LEU:HB3	2.20	0.42
1:B:91:THR:HB	1:B:102:TYR:HB2	2.02	0.42
1:B:33:LEU:CD2	1:B:246:SER:HB2	2.46	0.42
1:B:10:GLY:O	1:B:11:ASN:CB	2.66	0.42
1:A:67:PRO:HD2	1:A:68:PHE:CD2	2.55	0.42
1:B:20:LEU:N	3:B:320:HOH:O	2.24	0.41
1:B:183:SER:C	1:B:185:ASN:H	2.24	0.41
1:B:234:LEU:HD22	1:B:234:LEU:O	2.20	0.41
1:A:61:GLY:O	1:A:62:ALA:HB2	2.21	0.41
1:A:217:LEU:HD21	1:A:227:PHE:CD2	2.56	0.41
1:A:124:LEU:HB2	1:A:178:ASN:HA	2.03	0.41
1:A:26:PHE:CG	1:A:37:GLY:HA3	2.56	0.41
1:B:50:ILE:HG12	1:B:50:ILE:H	1.53	0.41
1:B:127:GLY:HA2	1:B:128:GLY:HA2	1.80	0.41
1:A:169:PRO:HB2	1:A:198:TYR:OH	2.21	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.76	0.41
1:A:147:LEU:O	1:A:148:ASN:ND2	2.27	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:ALA:HB1	1:A:89:ILE:CD1	2.35	0.40
1:B:209:ALA:O	1:B:229:ASP:HB2	2.21	0.40
1:B:229:ASP:OD1	1:B:229:ASP:C	2.60	0.40
1:A:176:ILE:HG22	1:A:177:ILE:H	1.85	0.40
1:A:149:ARG:NH2	1:A:180:THR:HG23	2.33	0.40
1:A:180:THR:HG22	1:A:182:ALA:H	1.86	0.40
1:A:199:PHE:CE2	1:A:225:ILE:HG21	2.57	0.40
1:B:131:LYS:HD3	1:B:156:PHE:CG	2.56	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	256/271 (94%)	213 (83%)	27 (10%)	16 (6%)	2	5
1	B	261/271 (96%)	240 (92%)	19 (7%)	2 (1%)	27	66
All	All	517/542 (95%)	453 (88%)	46 (9%)	18 (4%)	6	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA
1	A	112	SER
1	A	151	PRO
1	A	216	PHE
1	A	220	ALA
1	A	113	LEU
1	A	114	LYS
1	A	170	LYS
1	A	177	ILE
1	A	178	ASN
1	A	222	GLU
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	247	ALA
1	A	228	GLN
1	B	11	ASN
1	A	13	ILE
1	A	215	PRO
1	B	151	PRO

### 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	220/231 (95%)	170 (77%)	50 (23%)	1	3
1	B	223/231 (96%)	192 (86%)	31 (14%)	5	13
All	All	443/462 (96%)	362 (82%)	81 (18%)	2	6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	LEU
1	A	14	LYS
1	A	17	LYS
1	A	27	LEU
1	A	31	LYS
1	A	44	LEU
1	A	48	SER
1	A	50	ILE
1	A	67	PRO
1	A	89	ILE
1	A	113	LEU
1	A	116	GLN
1	A	117	ASN
1	A	118	TYR
1	A	122	LEU
1	A	124	LEU
1	A	126	SER
1	A	129	SER

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	135	CYS
1	A	139	LYS
1	A	143	LYS
1	A	147	LEU
1	A	148	ASN
1	A	149	ARG
1	A	158	GLN
1	A	159	ARG
1	A	162	CYS
1	A	166	MET
1	A	174	ASP
1	A	176	ILE
1	A	177	ILE
1	A	180	THR
1	A	183	SER
1	A	185	ASN
1	A	194	VAL
1	A	198	TYR
1	A	200	LYS
1	A	204	LEU
1	A	212	PHE
1	A	219	LEU
1	A	227	PHE
1	A	229	ASP
1	A	232	ASP
1	A	237	GLN
1	A	249	GLN
1	A	254	LYS
1	A	257	GLU
1	A	263	PHE
1	B	1	MET
1	B	3	LEU
1	B	17	LYS
1	B	27	LEU
1	B	43	LEU
1	B	47	GLU
1	B	50	ILE
1	B	66	LEU
1	B	71	ARG
1	B	88	SER
1	B	97	ASP

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Mol	Chain	Res	Type
1	B	114	LYS
1	B	116	GLN
1	B	126	SER
1	B	143	LYS
1	B	152	ARG
1	B	158	GLN
1	B	160	LEU
1	B	166	MET
1	B	167	GLU
1	B	171	SER
1	B	175	LEU
1	B	183	SER
1	B	184	LEU
1	B	191	ASN
1	B	206	TYR
1	B	212	PHE
1	B	234	LEU
1	B	248	SER
1	B	254	LYS
1	B	257	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	63	ASN
1	A	115	HIS
1	A	148	ASN
1	A	228	GLN
1	A	237	GLN
1	B	15	HIS
1	B	38	HIS
1	B	63	ASN
1	B	116	GLN
1	B	228	GLN
1	B	237	GLN

### 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 ⓘ

1 ligand is 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	SKM	A	500	-	12,12,12	1.15	2 (16%)	17,17,17	0.72	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
2	SKM	A	500	-	-	0/4/20/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	SKM	C9-C10	2.36	1.53	1.50
2	A	500	SKM	O2-C1	-2.05	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	260/271 (95%)	0.31	22 (8%) 11 13	42, 76, 127, 141	0
1	B	263/271 (97%)	-0.31	3 (1%) 77 84	36, 52, 71, 86	0
All	All	523/542 (96%)	-0.00	25 (4%) 29 35	36, 60, 123, 141	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASN	5.3
1	A	177	ILE	4.0
1	A	118	TYR	3.9
1	A	181	SER	3.4
1	A	170	LYS	3.4
1	A	227	PHE	3.3
1	A	148	ASN	3.2
1	A	224	LYS	2.8
1	A	226	PRO	2.5
1	A	122	LEU	2.5
1	A	182	ALA	2.5
1	A	176	ILE	2.5
1	A	123	ILE	2.4
1	A	175	LEU	2.3
1	A	152	ARG	2.3
1	B	47	GLU	2.2
1	A	213	LEU	2.2
1	B	1	MET	2.2
1	A	149	ARG	2.1
1	A	203	LYS	2.1
1	B	117	ASN	2.1
1	A	193	GLU	2.1
1	A	172	ALA	2.0
1	A	25	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	2.0

## 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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SKM	A	500	12/12	0.20	0.04	67,71,74,77	0

## 6.5 Other polymers

There are no such residues in this entry.