Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 06:09 PM JST

PDB ID	:	8HS9
Title	:	Brucella melitensis 7-alpha-Hydroxysteroid Dehydrogenase mutant:I258M/K262T
Authors	:	Liu, Z.Y.; Zhang, R.Z.
Deposited on	:	2022-12-17
Resolution	:	3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

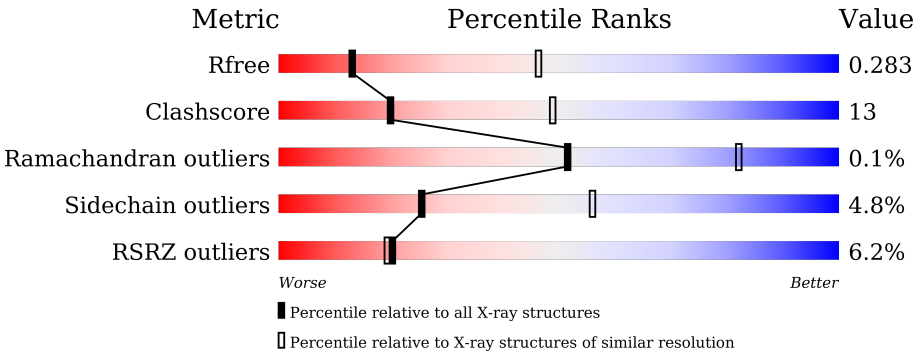
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	251	4% 71% 24% • •
1	B	251	5% 72% 22% • 5%
1	C	251	10% 66% 19% • 13%
1	E	251	5% 72% 23% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6754 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 7-alpha-hydroxysteroid dehydrogenase.

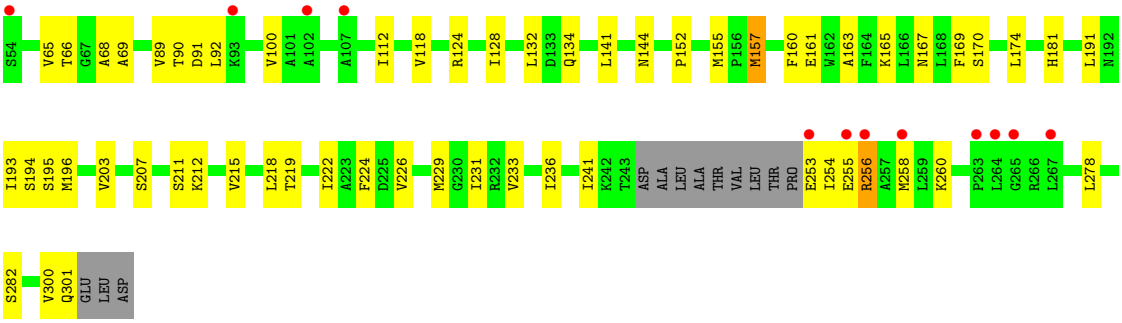
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	239	Total	C	N	O	S	0	0	0
			1718	1080	309	320	9			
1	A	242	Total	C	N	O	S	0	0	0
			1742	1096	312	325	9			
1	B	239	Total	C	N	O	S	0	0	0
			1716	1080	308	319	9			
1	C	219	Total	C	N	O	S	0	0	0
			1578	996	284	290	8			

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: 7-alpha-hydroxysteroid dehydrogenase

Chain E:

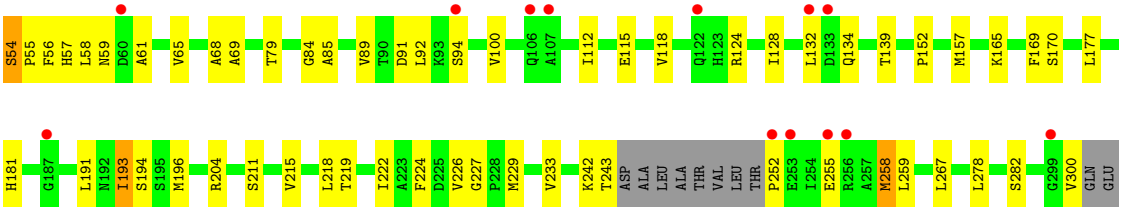


• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain A:

• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

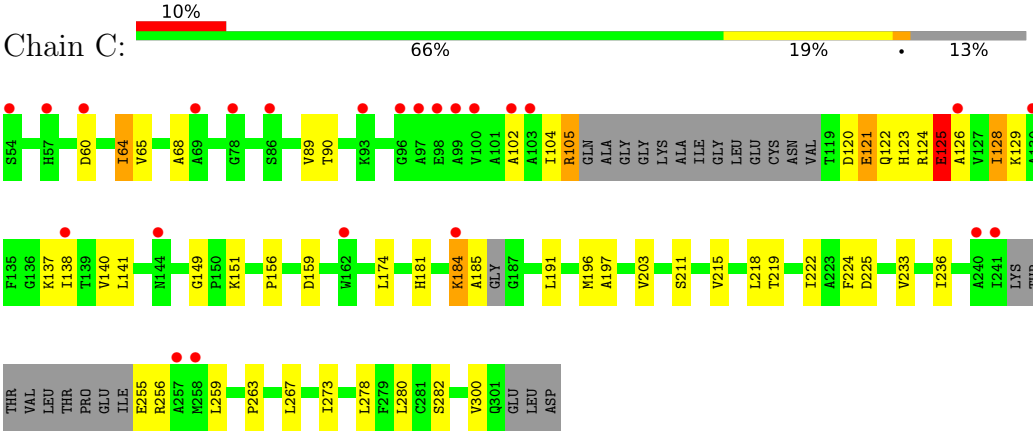
Chain B:



LEU
ASP

• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.77Å 54.81Å 76.50Å 82.94° 70.65° 81.29°	Depositor
Resolution (Å)	23.34 – 3.25 23.34 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.34-3.25) 99.6 (23.34-3.25)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.23Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.240 , 0.285 0.242 , 0.283	Depositor DCC
R_{free} test set	694 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6754	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/1770	0.55	0/2394
1	B	0.43	0/1744	0.56	0/2359
1	C	0.35	0/1602	0.53	0/2164
1	E	0.35	0/1745	0.52	0/2360
All	All	0.37	0/6861	0.54	0/9277

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1742	0	1762	54	0
1	B	1716	0	1737	41	0
1	C	1578	0	1594	45	0
1	E	1718	0	1737	42	0
All	All	6754	0	6830	171	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 13.

All (171) 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:A:241:ILE:CG2	1:A:268:GLY:O	2.20	0.89
1:A:241:ILE:HG22	1:A:268:GLY:O	1.71	0.89
1:C:64:ILE:HD11	1:C:138:ILE:HG23	1.57	0.86
1:A:203:VAL:HG22	1:C:224:PHE:HB3	1.59	0.85
1:A:112:ILE:HD13	1:A:134:GLN:HG3	1.59	0.85
1:C:121:GLU:O	1:C:125:GLU:HB2	1.77	0.84
1:A:203:VAL:CG1	1:C:225:ASP:OD1	2.29	0.81
1:E:157:MET:HA	1:E:157:MET:HE2	1.63	0.79
1:C:64:ILE:HD11	1:C:138:ILE:CG2	2.12	0.79
1:E:152:PRO:O	1:E:155:MET:CE	2.35	0.75
1:A:91:ASP:OD1	1:A:92:LEU:N	2.17	0.75
1:E:241:ILE:HD12	1:E:241:ILE:O	1.86	0.75
1:E:152:PRO:O	1:E:155:MET:HE2	1.87	0.74
1:B:58:LEU:HD12	1:B:58:LEU:O	1.89	0.72
1:A:203:VAL:HG12	1:C:225:ASP:OD1	1.90	0.72
1:C:121:GLU:O	1:C:121:GLU:HG3	1.88	0.71
1:A:203:VAL:HG13	1:C:225:ASP:OD1	1.91	0.70
1:E:152:PRO:O	1:E:155:MET:HB3	1.92	0.70
1:A:219:THR:HG23	1:A:233:VAL:HG12	1.74	0.69
1:A:224:PHE:HB3	1:C:203:VAL:HG22	1.75	0.68
1:B:91:ASP:OD1	1:B:92:LEU:N	2.26	0.68
1:E:157:MET:HA	1:E:157:MET:CE	2.24	0.67
1:C:102:ALA:HA	1:C:105:ARG:HD2	1.76	0.66
1:E:196:MET:HE1	1:E:300:VAL:HA	1.79	0.65
1:E:219:THR:HG23	1:E:233:VAL:HG12	1.79	0.64
1:B:219:THR:HG23	1:B:233:VAL:HG12	1.78	0.64
1:B:118:VAL:O	1:B:124:ARG:NH1	2.29	0.63
1:A:241:ILE:HG23	1:A:268:GLY:O	1.97	0.63
1:E:118:VAL:O	1:E:124:ARG:NH1	2.31	0.62
1:C:68:ALA:HB3	1:C:89:VAL:HG13	1.81	0.62
1:B:118:VAL:HB	1:B:170:SER:HB2	1.83	0.60
1:E:191:LEU:HD11	1:E:236:ILE:HG12	1.83	0.60
1:A:241:ILE:HG23	1:A:268:GLY:C	2.22	0.60
1:B:193:ILE:HG22	1:B:193:ILE:O	2.01	0.59
1:B:54:SER:C	1:B:56:PHE:H	2.05	0.58
1:B:152:PRO:HA	1:B:204:ARG:HD2	1.86	0.58
1:E:152:PRO:O	1:E:155:MET:HE3	2.04	0.58
1:E:112:ILE:HG21	1:E:134:GLN:HG3	1.86	0.57
1:C:211:SER:O	1:C:215:VAL:HG23	2.04	0.57
1:A:124:ARG:O	1:A:128:ILE:HG12	2.05	0.57
1:A:241:ILE:CG2	1:A:268:GLY:C	2.73	0.56
1:B:94:SER:HB2	1:B:115:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD11	1:B:181:HIS:CD2	2.41	0.56
1:A:121:GLU:HA	1:A:124:ARG:HB2	1.88	0.56
1:E:218:LEU:O	1:E:222:ILE:HG12	2.06	0.56
1:E:211:SER:O	1:E:215:VAL:HG23	2.06	0.56
1:A:157:MET:O	1:A:161:GLU:HB2	2.06	0.55
1:B:259:LEU:HD11	1:B:267:LEU:HG	1.89	0.54
1:A:70:ALA:HA	1:A:74:ARG:HD3	1.89	0.54
1:B:222:ILE:HG13	1:B:233:VAL:HG21	1.90	0.54
1:C:105:ARG:HA	1:C:105:ARG:HE	1.73	0.53
1:C:124:ARG:O	1:C:125:GLU:C	2.47	0.53
1:A:92:LEU:HD11	1:A:117:ASN:HD22	1.73	0.53
1:A:229:MET:HB2	1:A:231:ILE:HG13	1.90	0.53
1:C:219:THR:HG23	1:C:233:VAL:HG12	1.91	0.53
1:B:65:VAL:HG12	1:B:68:ALA:HB2	1.91	0.53
1:C:65:VAL:HG12	1:C:68:ALA:HB2	1.90	0.53
1:E:195:SER:HB3	1:E:212:LYS:HG3	1.90	0.53
1:A:89:VAL:O	1:A:113:GLY:HA2	2.08	0.53
1:C:128:ILE:CD1	1:C:128:ILE:N	2.72	0.53
1:C:196:MET:HE1	1:C:300:VAL:HA	1.91	0.52
1:E:224:PHE:HA	1:C:263:PRO:HB3	1.90	0.52
1:C:60:ASP:O	1:C:137:LYS:NZ	2.29	0.52
1:C:120:ASP:HB3	1:C:123:HIS:HB2	1.91	0.52
1:E:163:ALA:O	1:E:167:ASN:HB2	2.09	0.52
1:A:76:ILE:HG23	1:A:80:PHE:CD2	2.44	0.52
1:B:226:VAL:HA	1:B:229:MET:HG3	1.90	0.52
1:E:65:VAL:HG12	1:E:68:ALA:HB2	1.91	0.52
1:C:64:ILE:HG13	1:C:140:VAL:O	2.08	0.52
1:B:61:ALA:HB1	1:B:139:THR:OG1	2.10	0.51
1:A:58:LEU:HB3	1:A:85:ALA:HB2	1.93	0.51
1:B:211:SER:O	1:B:215:VAL:HG23	2.09	0.51
1:E:229:MET:HB2	1:E:231:ILE:HG13	1.93	0.51
1:B:54:SER:C	1:B:56:PHE:N	2.63	0.51
1:E:160:PHE:CE1	1:E:207:SER:HA	2.45	0.51
1:C:128:ILE:N	1:C:128:ILE:HD12	2.26	0.51
1:A:76:ILE:HG23	1:A:80:PHE:HD2	1.76	0.51
1:A:240:ALA:HB2	1:A:301:GLN:HG3	1.92	0.51
1:E:203:VAL:HG22	1:B:224:PHE:HB3	1.93	0.50
1:E:256:ARG:O	1:E:260:LYS:HG2	2.11	0.50
1:A:240:ALA:CB	1:A:301:GLN:HG3	2.42	0.50
1:A:275:ASN:HD21	1:B:55:PRO:HD2	1.78	0.49
1:B:165:LYS:HA	1:B:169:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG21	1:A:142:VAL:HG11	1.94	0.49
1:C:218:LEU:O	1:C:222:ILE:HG12	2.12	0.49
1:B:112:ILE:HG21	1:B:134:GLN:HG3	1.95	0.49
1:E:258:MET:HG3	1:E:301:GLN:HB3	1.94	0.49
1:C:236:ILE:HG21	1:C:273:ILE:HG23	1.96	0.48
1:A:275:ASN:ND2	1:B:55:PRO:HD2	2.27	0.48
1:A:183:GLN:HG3	1:A:229:MET:HB3	1.95	0.48
1:A:259:LEU:HD11	1:A:267:LEU:HG	1.94	0.48
1:C:184:LYS:O	1:C:185:ALA:C	2.50	0.48
1:E:68:ALA:HB3	1:E:89:VAL:HG13	1.95	0.48
1:B:252:PRO:HB2	1:B:255:GLU:HB3	1.94	0.48
1:C:124:ARG:O	1:C:126:ALA:N	2.47	0.48
1:E:132:LEU:HD11	1:E:181:HIS:NE2	2.29	0.47
1:A:66:THR:HG21	1:A:174:LEU:HD11	1.96	0.47
1:C:278:LEU:O	1:C:282:SER:HB3	2.13	0.47
1:A:56:PHE:HE1	1:A:279:PHE:HD1	1.61	0.47
1:B:58:LEU:CD1	1:B:85:ALA:HB2	2.44	0.47
1:E:157:MET:CE	1:E:157:MET:CA	2.85	0.47
1:A:255:GLU:O	1:A:258:MET:HG2	2.15	0.47
1:B:57:HIS:HB2	1:B:59:ASN:ND2	2.30	0.47
1:A:118:VAL:O	1:A:124:ARG:NH1	2.41	0.46
1:A:226:VAL:HA	1:A:229:MET:HG3	1.97	0.46
1:A:241:ILE:HA	1:A:268:GLY:O	2.15	0.46
1:A:87:VAL:O	1:A:111:ALA:HA	2.15	0.46
1:E:91:ASP:OD1	1:E:92:LEU:N	2.46	0.46
1:E:165:LYS:HA	1:E:169:PHE:HB2	1.98	0.46
1:A:217:HIS:NE2	1:C:197:ALA:O	2.44	0.46
1:B:68:ALA:HB3	1:B:89:VAL:HG13	1.98	0.46
1:A:58:LEU:HD12	1:A:80:PHE:CD1	2.51	0.45
1:B:193:ILE:N	1:B:193:ILE:CD1	2.78	0.45
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.83	0.45
1:E:222:ILE:O	1:E:226:VAL:HG22	2.16	0.45
1:B:59:ASN:OD1	1:B:84:GLY:HA3	2.16	0.45
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.69	0.45
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.74	0.44
1:B:258:MET:HE3	1:B:258:MET:HB3	1.80	0.44
1:E:278:LEU:O	1:E:282:SER:HB3	2.17	0.44
1:B:278:LEU:O	1:B:282:SER:HB3	2.18	0.44
1:E:144:ASN:HA	1:E:193:ILE:HB	1.98	0.44
1:E:253:GLU:HA	1:E:256:ARG:HB2	1.99	0.44
1:A:165:LYS:HG2	1:A:169:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ALA:HA	1:E:100:VAL:HG21	1.99	0.44
1:A:204:ARG:HA	1:A:204:ARG:HD2	1.62	0.44
1:B:196:MET:HE1	1:B:300:VAL:HA	1.98	0.43
1:C:128:ILE:HG23	1:C:138:ILE:HD11	1.99	0.43
1:A:112:ILE:CD1	1:A:134:GLN:HG3	2.39	0.43
1:A:152:PRO:O	1:A:155:MET:HB3	2.19	0.43
1:C:121:GLU:O	1:C:125:GLU:N	2.43	0.43
1:C:122:GLN:O	1:C:123:HIS:C	2.57	0.43
1:E:212:LYS:HD3	1:E:212:LYS:HA	1.82	0.43
1:A:58:LEU:HD12	1:A:80:PHE:HD1	1.83	0.43
1:A:155:MET:HG3	1:A:156:PRO:O	2.18	0.43
1:C:181:HIS:HA	1:C:184:LYS:HB3	2.01	0.43
1:E:124:ARG:O	1:E:128:ILE:HG12	2.18	0.43
1:A:118:VAL:CG1	1:A:170:SER:HB2	2.49	0.43
1:B:69:ALA:HA	1:B:100:VAL:HG21	1.99	0.43
1:B:79:THR:HG22	1:B:278:LEU:HD22	2.01	0.43
1:E:241:ILE:HD12	1:E:241:ILE:C	2.39	0.43
1:A:205:MET:HE3	1:A:205:MET:HA	2.01	0.42
1:B:222:ILE:O	1:B:226:VAL:HG22	2.19	0.42
1:E:254:ILE:HD13	1:E:254:ILE:HA	1.88	0.42
1:C:124:ARG:HD2	1:C:174:LEU:HG	2.00	0.42
1:B:191:LEU:CD2	1:B:193:ILE:HD11	2.49	0.42
1:E:132:LEU:HD11	1:E:181:HIS:CD2	2.54	0.42
1:B:128:ILE:HG13	1:B:177:LEU:HB3	2.01	0.42
1:E:141:LEU:HD21	1:E:174:LEU:HB3	2.01	0.42
1:C:259:LEU:HD11	1:C:267:LEU:HG	2.02	0.42
1:C:104:ILE:O	1:C:105:ARG:C	2.58	0.42
1:C:149:GLY:O	1:C:151:LYS:HG3	2.20	0.42
1:A:68:ALA:HB3	1:A:89:VAL:HG13	2.01	0.41
1:C:132:LEU:HD11	1:C:181:HIS:NE2	2.35	0.41
1:B:58:LEU:O	1:B:58:LEU:CD1	2.62	0.41
1:E:157:MET:O	1:E:157:MET:HG3	2.18	0.41
1:B:218:LEU:O	1:B:222:ILE:HG12	2.20	0.41
1:C:64:ILE:HB	1:C:141:LEU:HD12	2.03	0.41
1:A:95:GLU:H	1:A:95:GLU:HG2	1.61	0.41
1:C:102:ALA:O	1:C:105:ARG:HB2	2.20	0.41
1:C:191:LEU:HD11	1:C:236:ILE:HG12	2.03	0.41
1:A:211:SER:O	1:A:215:VAL:HG23	2.21	0.41
1:A:263:PRO:HB2	1:B:227:GLY:HA3	2.03	0.41
1:C:120:ASP:C	1:C:122:GLN:N	2.73	0.41
1:E:118:VAL:HB	1:E:170:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.82	0.41
1:C:64:ILE:HD11	1:C:138:ILE:HG21	1.99	0.41
1:B:191:LEU:HD23	1:B:193:ILE:HD11	2.01	0.40
1:E:66:THR:HA	1:E:90:THR:OG1	2.20	0.40
1:A:150:PRO:HB3	1:A:204:ARG:HB3	2.04	0.40
1:C:156:PRO:O	1:C:159:ASP:HB2	2.22	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	238/251 (95%)	225 (94%)	13 (6%)	0	100 100
1	B	235/251 (94%)	226 (96%)	9 (4%)	0	100 100
1	C	209/251 (83%)	194 (93%)	14 (7%)	1 (0%)	29 62
1	E	235/251 (94%)	227 (97%)	8 (3%)	0	100 100
All	All	917/1004 (91%)	872 (95%)	44 (5%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	172/179 (96%)	162 (94%)	10 (6%)	20 50
1	B	169/179 (94%)	162 (96%)	7 (4%)	30 60
1	C	155/179 (87%)	145 (94%)	10 (6%)	17 46
1	E	169/179 (94%)	164 (97%)	5 (3%)	41 67
All	All	665/716 (93%)	633 (95%)	32 (5%)	25 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	157	MET
1	E	161	GLU
1	E	194	SER
1	E	255	GLU
1	E	256	ARG
1	A	54	SER
1	A	60	ASP
1	A	106	GLN
1	A	194	SER
1	A	203	VAL
1	A	205	MET
1	A	208	TYR
1	A	241	ILE
1	A	287	TRP
1	A	301	GLN
1	B	54	SER
1	B	157	MET
1	B	193	ILE
1	B	194	SER
1	B	242	LYS
1	B	243	THR
1	B	258	MET
1	C	64	ILE
1	C	90	THR
1	C	105	ARG
1	C	121	GLU
1	C	125	GLU
1	C	128	ILE
1	C	129	LYS
1	C	184	LYS
1	C	255	GLU

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Mol	Chain	Res	Type
1	C	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	200	ASN
1	B	200	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	242/251 (96%)	0.17	9 (3%) 41 38	25, 54, 87, 113	0
1	B	239/251 (95%)	0.27	13 (5%) 25 24	23, 57, 90, 116	0
1	C	219/251 (87%)	0.61	24 (10%) 5 5	29, 69, 97, 110	0
1	E	239/251 (95%)	0.16	12 (5%) 28 26	23, 49, 92, 117	0
All	All	939/1004 (93%)	0.30	58 (6%) 20 19	23, 57, 92, 117	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	256	ARG	4.1
1	B	252	PRO	3.9
1	C	57	HIS	3.8
1	A	253	GLU	3.8
1	B	255	GLU	3.6
1	B	106	GLN	3.5
1	E	255	GLU	3.4
1	E	102	ALA	3.1
1	C	98	GLU	3.1
1	E	258	MET	3.1
1	A	158	SER	3.0
1	E	264	LEU	3.0
1	C	241	ILE	3.0
1	E	253	GLU	3.0
1	C	138	ILE	2.9
1	A	302	GLU	2.9
1	B	256	ARG	2.8
1	A	242	LYS	2.8
1	B	132	LEU	2.8
1	A	303	LEU	2.7
1	C	69	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	93	LYS	2.7
1	C	96	GLY	2.7
1	C	258	MET	2.7
1	B	133	ASP	2.6
1	B	253	GLU	2.6
1	C	102	ALA	2.6
1	C	93	LYS	2.6
1	C	162	TRP	2.6
1	C	60	ASP	2.6
1	C	100	VAL	2.5
1	C	130	ALA	2.5
1	E	267	LEU	2.5
1	C	144	ASN	2.5
1	C	103	ALA	2.5
1	E	107	ALA	2.4
1	A	185	ALA	2.4
1	C	78	GLY	2.4
1	C	99	ALA	2.4
1	C	126	ALA	2.3
1	E	54	SER	2.3
1	C	54	SER	2.3
1	E	265	GLY	2.3
1	A	261	HIS	2.3
1	C	257	ALA	2.3
1	B	187	GLY	2.3
1	E	263	PRO	2.2
1	B	107	ALA	2.2
1	B	94	SER	2.2
1	C	240	ALA	2.2
1	A	186	GLY	2.2
1	B	60	ASP	2.2
1	C	86	SER	2.1
1	A	133	ASP	2.1
1	B	299	GLY	2.1
1	C	97	ALA	2.1
1	C	184	LYS	2.1
1	B	122	GLN	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 monosaccharides 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.