Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 04:57 PM JST

PDB ID	:	8HAX
Title	:	Brucella melitensis 7alpha-Hydroxysteroid Dehydrogenase mutant-I258M/K262T
Authors	:	Liu, Z.Y.; Zhang, R.Z.
Deposited on	:	2022-10-27
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:

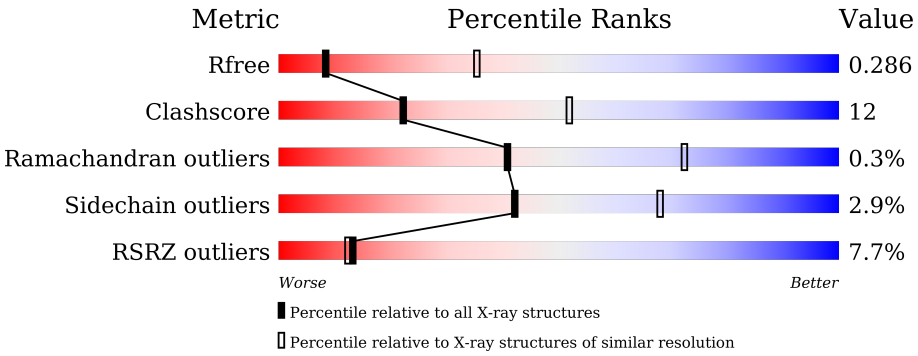
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	304	6% 60% 18% 21%
1	B	304	3% 62% 18% 20%
1	C	304	5% 62% 16% 21%
1	D	304	10% 59% 18% 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6908 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	A	239	Total	C	N	O	S	0	0	0
			1718	1079	309	320	10			
1	B	242	Total	C	N	O	S	0	0	0
			1742	1095	312	325	10			
1	C	239	Total	C	N	O	S	0	0	0
			1716	1079	308	319	10			
1	D	241	Total	C	N	O	S	0	0	0
			1732	1088	311	323	10			

There are 4 discrepancies between the modelled and reference sequences:

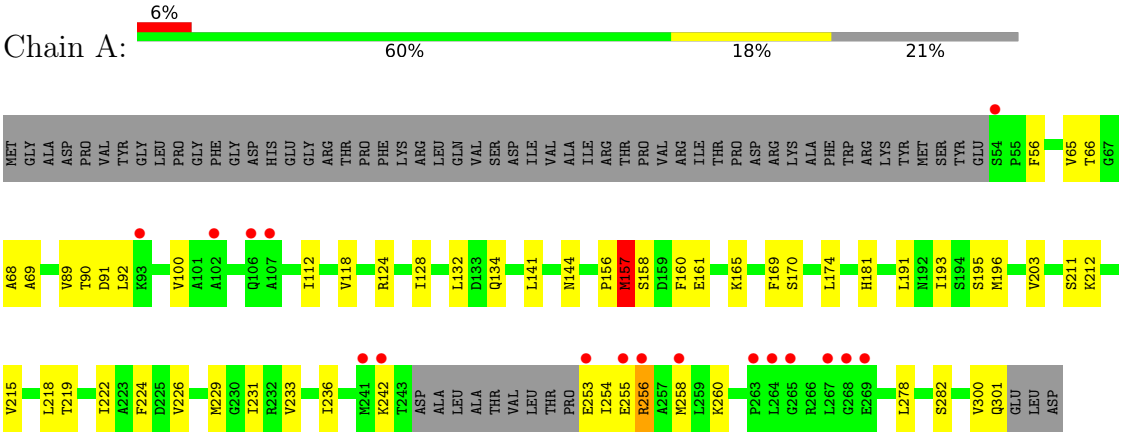
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	ILE	conflict	UNP Q8YIN7
B	241	MET	ILE	conflict	UNP Q8YIN7
C	241	MET	ILE	conflict	UNP Q8YIN7
D	241	MET	ILE	conflict	UNP Q8YIN7

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.

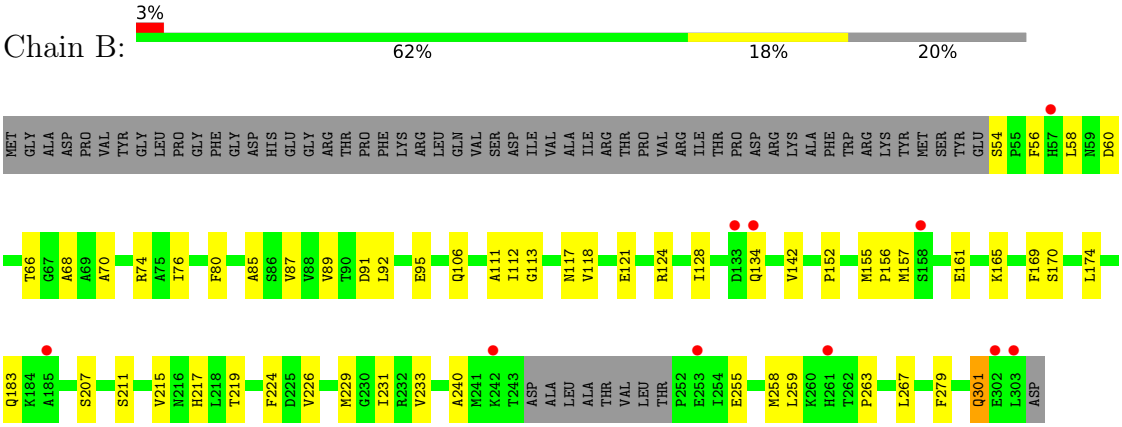
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain A:



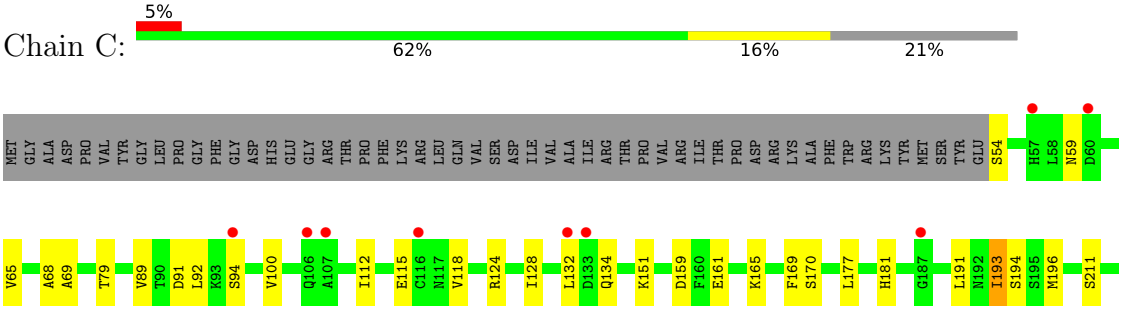
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

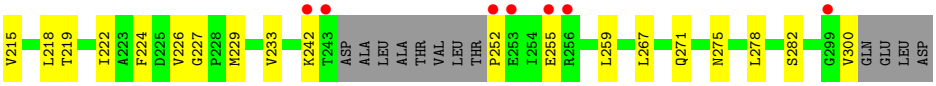
Chain B:



• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

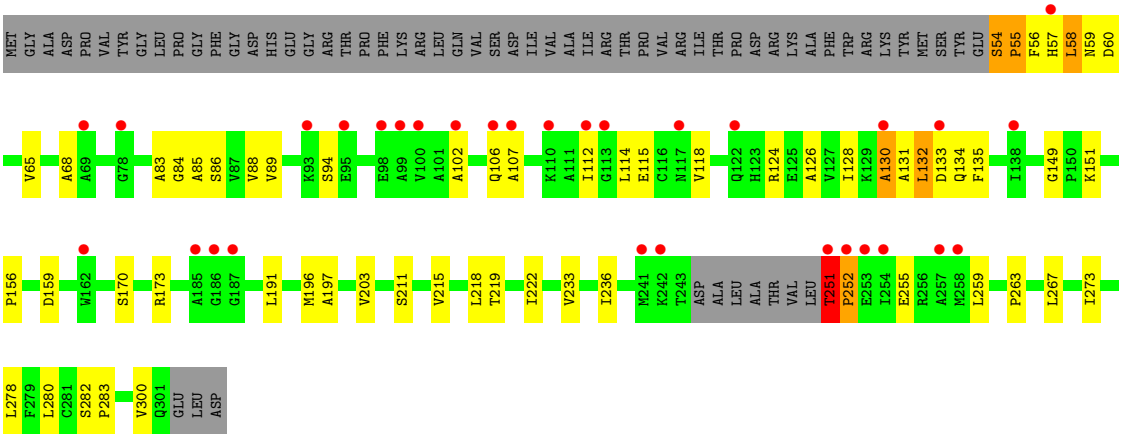
Chain C:





• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain D:



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}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.23Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.239 , 0.285 0.240 , 0.286	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 , 49.4	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	6908	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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	0.31	1/1745 (0.1%)	0.49	0/2359
1	B	0.29	0/1770	0.49	0/2393
1	C	0.31	0/1744	0.49	0/2358
1	D	0.37	1/1760 (0.1%)	0.56	0/2381
All	All	0.32	2/7019 (0.0%)	0.51	0/9491

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	251	THR	C-N	8.56	1.50	1.34
1	A	157	MET	C-O	6.09	1.34	1.23

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	1718	0	1735	45	0
1	B	1742	0	1760	39	0
1	C	1716	0	1735	33	1
1	D	1732	0	1749	62	1
All	All	6908	0	6979	163	1

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 12.

All (163) 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:D:251:THR:N	1:D:252:PRO:HD3	1.44	1.24
1:A:56:PHE:CD2	1:D:56:PHE:CE2	2.26	1.22
1:A:56:PHE:CD2	1:D:56:PHE:CD2	2.33	1.17
1:D:124:ARG:HH21	1:D:173:ARG:HG2	1.03	1.16
1:D:88:VAL:HG21	1:D:131:ALA:HB2	1.35	1.07
1:D:128:ILE:O	1:D:132:LEU:HB2	1.62	1.00
1:D:88:VAL:HG21	1:D:131:ALA:CB	1.93	0.98
1:D:251:THR:N	1:D:252:PRO:CD	2.25	0.98
1:A:56:PHE:CD2	1:D:56:PHE:HE2	1.89	0.89
1:D:58:LEU:HB2	1:D:83:ALA:CB	2.01	0.89
1:D:124:ARG:NH2	1:D:173:ARG:HG2	1.88	0.89
1:D:55:PRO:HB3	1:D:283:PRO:HB2	1.54	0.88
1:D:124:ARG:HH21	1:D:173:ARG:CG	1.86	0.88
1:A:56:PHE:HD2	1:D:56:PHE:CE2	1.93	0.86
1:B:112:ILE:HD13	1:B:134:GLN:HG3	1.59	0.85
1:C:271:GLN:O	1:C:275:ASN:ND2	2.13	0.81
1:A:157:MET:O	1:A:160:PHE:N	2.14	0.80
1:A:56:PHE:CG	1:D:56:PHE:CD2	2.70	0.79
1:A:56:PHE:CE2	1:D:56:PHE:CD2	2.71	0.78
1:B:91:ASP:OD1	1:B:92:LEU:N	2.17	0.75
1:D:58:LEU:HB2	1:D:83:ALA:HB1	1.67	0.75
1:A:56:PHE:CE2	1:D:56:PHE:CE2	2.76	0.73
1:B:219:THR:HG23	1:B:233:VAL:HG12	1.74	0.69
1:B:224:PHE:HB3	1:D:203:VAL:HG22	1.75	0.68
1:C:91:ASP:OD1	1:C:92:LEU:N	2.26	0.68
1:A:56:PHE:CD2	1:D:56:PHE:HD2	2.03	0.67
1:A:196:MET:HE1	1:A:300:VAL:HA	1.79	0.65
1:A:56:PHE:CE2	1:D:56:PHE:HD2	2.11	0.64
1:D:58:LEU:HB2	1:D:83:ALA:HB3	1.79	0.64
1:A:219:THR:HG23	1:A:233:VAL:HG12	1.79	0.64
1:C:219:THR:HG23	1:C:233:VAL:HG12	1.78	0.64
1:C:118:VAL:O	1:C:124:ARG:NH1	2.29	0.63
1:A:118:VAL:O	1:A:124:ARG:NH1	2.31	0.62
1:D:68:ALA:HB3	1:D:89:VAL:HG13	1.81	0.62
1:D:54:SER:O	1:D:54:SER:OG	2.10	0.61
1:C:118:VAL:HB	1:C:170:SER:HB2	1.83	0.60
1:A:191:LEU:HD11	1:A:236:ILE:HG12	1.83	0.60
1:C:271:GLN:HG3	1:C:275:ASN:HD21	1.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HG22	1:C:193:ILE:O	2.01	0.59
1:D:124:ARG:HE	1:D:173:ARG:HG3	1.67	0.59
1:D:58:LEU:O	1:D:84:GLY:C	2.42	0.58
1:D:58:LEU:N	1:D:83:ALA:O	2.36	0.58
1:D:124:ARG:HE	1:D:173:ARG:CG	2.17	0.57
1:A:112:ILE:HG21	1:A:134:GLN:HG3	1.86	0.57
1:D:211:SER:O	1:D:215:VAL:HG23	2.04	0.57
1:B:124:ARG:O	1:B:128:ILE:HG12	2.05	0.57
1:D:251:THR:O	1:D:251:THR:HG23	2.04	0.56
1:C:94:SER:HB2	1:C:115:GLU:HB2	1.87	0.56
1:C:132:LEU:HD11	1:C:181:HIS:CD2	2.41	0.56
1:B:121:GLU:HA	1:B:124:ARG:HB2	1.88	0.56
1:A:218:LEU:O	1:A:222:ILE:HG12	2.06	0.56
1:A:211:SER:O	1:A:215:VAL:HG23	2.06	0.56
1:B:157:MET:O	1:B:161:GLU:HB2	2.06	0.55
1:D:118:VAL:HB	1:D:170:SER:HB2	1.88	0.55
1:D:88:VAL:HG21	1:D:131:ALA:HB1	1.86	0.54
1:B:70:ALA:HA	1:B:74:ARG:HD3	1.89	0.54
1:C:222:ILE:HG13	1:C:233:VAL:HG21	1.90	0.54
1:B:92:LEU:HD11	1:B:117:ASN:HD22	1.73	0.53
1:B:229:MET:HB2	1:B:231:ILE:HG13	1.90	0.53
1:D:219:THR:HG23	1:D:233:VAL:HG12	1.91	0.53
1:C:65:VAL:HG12	1:C:68:ALA:HB2	1.91	0.53
1:D:65:VAL:HG12	1:D:68:ALA:HB2	1.90	0.53
1:D:112:ILE:HG21	1:D:134:GLN:OE1	2.09	0.53
1:A:195:SER:HB3	1:A:212:LYS:HG3	1.90	0.53
1:B:89:VAL:O	1:B:113:GLY:HA2	2.08	0.53
1:D:196:MET:HE1	1:D:300:VAL:HA	1.91	0.52
1:A:224:PHE:HA	1:D:263:PRO:HB3	1.90	0.52
1:A:158:SER:HA	1:A:161:GLU:OE1	2.10	0.52
1:B:76:ILE:HG23	1:B:80:PHE:CD2	2.44	0.52
1:C:226:VAL:HA	1:C:229:MET:HG3	1.90	0.52
1:A:65:VAL:HG12	1:A:68:ALA:HB2	1.91	0.52
1:B:58:LEU:HB3	1:B:85:ALA:HB2	1.93	0.51
1:C:211:SER:O	1:C:215:VAL:HG23	2.09	0.51
1:A:229:MET:HB2	1:A:231:ILE:HG13	1.93	0.51
1:B:76:ILE:HG23	1:B:80:PHE:HD2	1.76	0.51
1:B:240:ALA:HB2	1:B:301:GLN:HG3	1.92	0.51
1:A:203:VAL:HG22	1:C:224:PHE:HB3	1.93	0.50
1:D:58:LEU:HD13	1:D:85:ALA:HB2	1.92	0.50
1:D:58:LEU:CD1	1:D:85:ALA:HB2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:O	1:A:260:LYS:HG2	2.11	0.50
1:B:240:ALA:CB	1:B:301:GLN:HG3	2.42	0.50
1:C:165:LYS:HA	1:C:169:PHE:HB2	1.94	0.49
1:B:76:ILE:HG21	1:B:142:VAL:HG11	1.94	0.49
1:D:218:LEU:O	1:D:222:ILE:HG12	2.12	0.49
1:C:112:ILE:HG21	1:C:134:GLN:HG3	1.95	0.49
1:A:258:MET:HG3	1:A:301:GLN:HB3	1.94	0.49
1:D:236:ILE:HG21	1:D:273:ILE:HG23	1.96	0.48
1:B:183:GLN:HG3	1:B:229:MET:HB3	1.95	0.48
1:B:259:LEU:HD11	1:B:267:LEU:HG	1.94	0.48
1:A:68:ALA:HB3	1:A:89:VAL:HG13	1.95	0.48
1:A:169:PHE:CE2	1:C:161:GLU:HG3	2.48	0.48
1:C:252:PRO:HB2	1:C:255:GLU:HB3	1.94	0.48
1:A:132:LEU:HD11	1:A:181:HIS:NE2	2.29	0.47
1:B:66:THR:HG21	1:B:174:LEU:HD11	1.96	0.47
1:D:278:LEU:O	1:D:282:SER:HB3	2.13	0.47
1:B:56:PHE:HE1	1:B:279:PHE:HD1	1.61	0.47
1:D:54:SER:N	1:D:55:PRO:HD3	2.29	0.47
1:B:255:GLU:O	1:B:258:MET:HG2	2.15	0.47
1:B:118:VAL:O	1:B:124:ARG:NH1	2.41	0.46
1:B:226:VAL:HA	1:B:229:MET:HG3	1.97	0.46
1:B:87:VAL:O	1:B:111:ALA:HA	2.15	0.46
1:A:91:ASP:OD1	1:A:92:LEU:N	2.46	0.46
1:A:165:LYS:HA	1:A:169:PHE:HB2	1.98	0.46
1:B:217:HIS:NE2	1:D:197:ALA:O	2.44	0.46
1:C:68:ALA:HB3	1:C:89:VAL:HG13	1.98	0.46
1:D:102:ALA:O	1:D:106:GLN:HG3	2.16	0.45
1:D:86:SER:HB3	1:D:135:PHE:CD1	2.51	0.45
1:B:58:LEU:HD12	1:B:80:PHE:CD1	2.51	0.45
1:C:193:ILE:N	1:C:193:ILE:CD1	2.78	0.45
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.83	0.45
1:A:222:ILE:O	1:A:226:VAL:HG22	2.16	0.45
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.74	0.44
1:A:278:LEU:O	1:A:282:SER:HB3	2.17	0.44
1:C:278:LEU:O	1:C:282:SER:HB3	2.18	0.44
1:A:144:ASN:HA	1:A:193:ILE:HB	1.98	0.44
1:A:156:PRO:O	1:A:157:MET:C	2.52	0.44
1:A:253:GLU:HA	1:A:256:ARG:HB2	1.99	0.44
1:B:165:LYS:HG2	1:B:169:PHE:CD2	2.53	0.44
1:A:69:ALA:HA	1:A:100:VAL:HG21	1.99	0.44
1:C:259:LEU:HD11	1:C:267:LEU:HG	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:MET:HE1	1:C:300:VAL:HA	1.98	0.43
1:B:112:ILE:CD1	1:B:134:GLN:HG3	2.39	0.43
1:B:152:PRO:O	1:B:155:MET:HB3	2.19	0.43
1:D:58:LEU:HB2	1:D:83:ALA:C	2.39	0.43
1:D:124:ARG:NH2	1:D:173:ARG:CG	2.64	0.43
1:A:212:LYS:HD3	1:A:212:LYS:HA	1.82	0.43
1:B:58:LEU:HD12	1:B:80:PHE:HD1	1.83	0.43
1:B:155:MET:HG3	1:B:156:PRO:O	2.18	0.43
1:A:124:ARG:O	1:A:128:ILE:HG12	2.18	0.43
1:B:118:VAL:CG1	1:B:170:SER:HB2	2.49	0.43
1:C:69:ALA:HA	1:C:100:VAL:HG21	1.99	0.43
1:C:79:THR:HG22	1:C:278:LEU:HD22	2.01	0.43
1:A:56:PHE:CE2	1:D:56:PHE:HE2	2.24	0.42
1:D:94:SER:HB2	1:D:115:GLU:HB2	2.00	0.42
1:C:222:ILE:O	1:C:226:VAL:HG22	2.19	0.42
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.88	0.42
1:C:191:LEU:CD2	1:C:193:ILE:HD11	2.49	0.42
1:D:126:ALA:O	1:D:130:ALA:HB2	2.20	0.42
1:A:132:LEU:HD11	1:A:181:HIS:CD2	2.54	0.42
1:C:128:ILE:HG13	1:C:177:LEU:HB3	2.01	0.42
1:A:141:LEU:HD21	1:A:174:LEU:HB3	2.01	0.42
1:D:259:LEU:HD11	1:D:267:LEU:HG	2.02	0.42
1:C:151:LYS:HD3	1:C:159:ASP:HB3	2.00	0.42
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.69	0.42
1:D:149:GLY:O	1:D:151:LYS:HG3	2.20	0.42
1:B:68:ALA:HB3	1:B:89:VAL:HG13	2.01	0.41
1:C:218:LEU:O	1:C:222:ILE:HG12	2.20	0.41
1:D:114:LEU:HD11	1:D:130:ALA:HB1	2.01	0.41
1:B:95:GLU:H	1:B:95:GLU:HG2	1.61	0.41
1:D:191:LEU:HD11	1:D:236:ILE:HG12	2.03	0.41
1:B:211:SER:O	1:B:215:VAL:HG23	2.21	0.41
1:B:263:PRO:HB2	1:C:227:GLY:HA3	2.03	0.41
1:C:267:LEU:HD23	1:C:267:LEU:HA	1.82	0.41
1:A:118:VAL:HB	1:A:170:SER:HB2	2.03	0.41
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.82	0.41
1:C:191:LEU:HD23	1:C:193:ILE:HD11	2.01	0.40
1:D:86:SER:HB3	1:D:135:PHE:CE1	2.56	0.40
1:A:66:THR:HA	1:A:90:THR:OG1	2.20	0.40
1:A:242:LYS:HD3	1:A:242:LYS:HA	1.83	0.40
1:D:252:PRO:HB2	1:D:255:GLU:HB3	2.03	0.40
1:D:55:PRO:O	1:D:283:PRO:HD2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PRO:O	1:D:159:ASP:HB2	2.22	0.40
1:D:251:THR:O	1:D:251:THR:CG2	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:ND2	1:D:107:ALA:O[1_654]	1.99	0.21

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	235/304 (77%)	226 (96%)	9 (4%)	0	100 100
1	B	238/304 (78%)	224 (94%)	14 (6%)	0	100 100
1	C	235/304 (77%)	227 (97%)	8 (3%)	0	100 100
1	D	237/304 (78%)	227 (96%)	7 (3%)	3 (1%)	12 41
All	All	945/1216 (78%)	904 (96%)	38 (4%)	3 (0%)	41 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	130	ALA
1	D	252	PRO
1	D	55	PRO

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	169/224 (75%)	166 (98%)	3 (2%)	59	77
1	B	172/224 (77%)	167 (97%)	5 (3%)	42	68
1	C	169/224 (75%)	165 (98%)	4 (2%)	49	72
1	D	171/224 (76%)	163 (95%)	8 (5%)	26	57
All	All	681/896 (76%)	661 (97%)	20 (3%)	42	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	MET
1	A	255	GLU
1	A	256	ARG
1	B	54	SER
1	B	60	ASP
1	B	106	GLN
1	B	207	SER
1	B	301	GLN
1	C	54	SER
1	C	193	ILE
1	C	194	SER
1	C	242	LYS
1	D	54	SER
1	D	57	HIS
1	D	58	LEU
1	D	59	ASN
1	D	60	ASP
1	D	132	LEU
1	D	133	ASP
1	D	251	THR

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

Mol	Chain	Res	Type
1	A	200	ASN
1	C	200	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 monosaccharides 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^{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	239/304 (78%)	0.20	17 (7%)	16	15	23, 49, 92, 117	0
1	B	242/304 (79%)	0.21	10 (4%)	37	34	25, 54, 87, 113	0
1	C	239/304 (78%)	0.31	16 (6%)	17	17	23, 57, 90, 116	0
1	D	241/304 (79%)	0.73	31 (12%)	3	3	29, 71, 98, 129	0
All	All	961/1216 (79%)	0.36	74 (7%)	13	12	23, 57, 93, 129	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	THR	6.1
1	D	254	ILE	5.3
1	D	133	ASP	5.0
1	A	256	ARG	4.4
1	D	57	HIS	4.2
1	D	186	GLY	4.1
1	D	253	GLU	3.9
1	C	252	PRO	3.8
1	C	106	GLN	3.8
1	A	255	GLU	3.6
1	B	253	GLU	3.5
1	A	264	LEU	3.5
1	D	242	LYS	3.5
1	D	241	MET	3.4
1	D	106	GLN	3.3
1	C	255	GLU	3.2
1	A	258	MET	3.1
1	C	57	HIS	3.1
1	C	133	ASP	3.1
1	A	241	MET	3.1
1	D	162	TRP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	GLU	3.0
1	B	158	SER	2.9
1	A	54	SER	2.9
1	C	253	GLU	2.9
1	C	256	ARG	2.9
1	A	102	ALA	2.9
1	C	132	LEU	2.8
1	D	252	PRO	2.8
1	C	60	ASP	2.8
1	B	185	ALA	2.7
1	C	107	ALA	2.7
1	B	303	LEU	2.7
1	C	299	GLY	2.7
1	B	133	ASP	2.6
1	D	122	GLN	2.6
1	B	242	LYS	2.6
1	A	93	LYS	2.6
1	A	265	GLY	2.6
1	D	117	ASN	2.6
1	D	98	GLU	2.5
1	A	106	GLN	2.5
1	A	107	ALA	2.5
1	D	93	LYS	2.5
1	D	185	ALA	2.5
1	D	258	MET	2.4
1	D	112	ILE	2.4
1	C	94	SER	2.3
1	D	102	ALA	2.3
1	A	242	LYS	2.3
1	D	110	LYS	2.3
1	D	100	VAL	2.3
1	B	302	GLU	2.3
1	D	78	GLY	2.2
1	C	187	GLY	2.2
1	D	99	ALA	2.2
1	D	138	ILE	2.2
1	B	261	HIS	2.2
1	A	267	LEU	2.2
1	D	187	GLY	2.2
1	C	116	CYS	2.1
1	A	269	GLU	2.1
1	D	113	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	130	ALA	2.1
1	A	268	GLY	2.1
1	A	263	PRO	2.1
1	D	69	ALA	2.1
1	D	95	GLU	2.1
1	C	242	LYS	2.1
1	D	257	ALA	2.1
1	C	243	THR	2.0
1	D	107	ALA	2.0
1	B	134	GLN	2.0
1	B	57	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.