Full wwPDB X-ray Structure Validation Report ⓘ

Dec 26, 2023 – 08:10 PM JST

PDB ID	:	8HS6
Title	:	Brucella melitensis 7-alpha-Hydroxysteroid Dehydrogenase mutant:1-53 truncation
Authors	:	Liu, Z.Y.; Zhang, R.Z.
Deposited on	:	2022-12-17
Resolution	:	2.35 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:

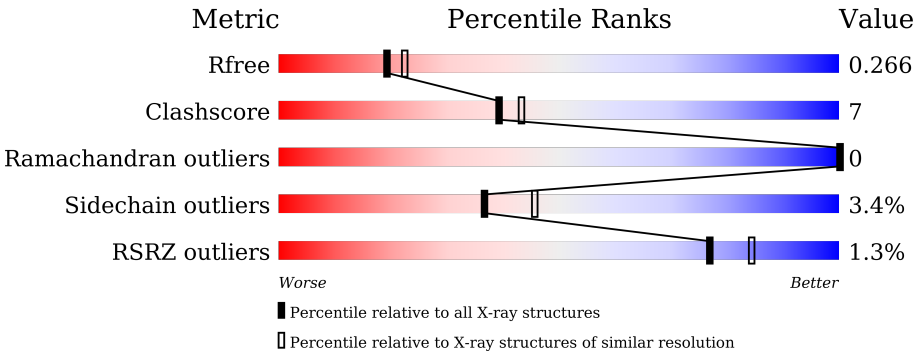
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	249	2% 78% 14% • 7%
1	B	249	83% 14% ••
1	C	249	% 80% 12% 8%
1	D	249	90% 9% •
1	E	249	% 85% 14% •
1	F	249	% 81% 10% 9%

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Mol	Chain	Length	Quality of chain
1	G	249	2% 78% 13% 9%
1	H	249	% 83% 17%
1	I	249	2% 66% 24% 9%
1	J	249	% 68% 21% 11%
1	K	249	% 69% 29%
1	L	249	3% 68% 27%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20848 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	232	Total	C	N	O	S	0	0	0
			1656	1041	297	310	8			
1	B	245	Total	C	N	O	S	0	0	0
			1766	1112	316	330	8			
1	C	229	Total	C	N	O	S	0	0	0
			1633	1027	292	306	8			
1	D	247	Total	C	N	O	S	0	0	0
			1773	1118	317	330	8			
1	E	248	Total	C	N	O	S	0	0	0
			1782	1123	319	332	8			
1	F	227	Total	C	N	O	S	0	0	0
			1629	1026	293	302	8			
1	G	227	Total	C	N	O	S	0	0	0
			1623	1023	291	301	8			
1	H	249	Total	C	N	O	S	0	0	0
			1791	1128	320	335	8			
1	I	226	Total	C	N	O	S	0	0	0
			1612	1013	290	301	8			
1	J	221	Total	C	N	O	S	0	0	0
			1577	993	281	295	8			
1	K	246	Total	C	N	O	S	0	0	0
			1766	1113	316	329	8			
1	L	239	Total	C	N	O	S	0	0	0
			1718	1083	309	318	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ILE	MET	engineered mutation	UNP Q8YIN7
A	262	LYS	THR	engineered mutation	UNP Q8YIN7
B	258	ILE	MET	engineered mutation	UNP Q8YIN7
B	262	LYS	THR	engineered mutation	UNP Q8YIN7
C	258	ILE	MET	engineered mutation	UNP Q8YIN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	262	LYS	THR	engineered mutation	UNP Q8YIN7
D	258	ILE	MET	engineered mutation	UNP Q8YIN7
D	262	LYS	THR	engineered mutation	UNP Q8YIN7
E	258	ILE	MET	engineered mutation	UNP Q8YIN7
E	262	LYS	THR	engineered mutation	UNP Q8YIN7
F	258	ILE	MET	engineered mutation	UNP Q8YIN7
F	262	LYS	THR	engineered mutation	UNP Q8YIN7
G	258	ILE	MET	engineered mutation	UNP Q8YIN7
G	262	LYS	THR	engineered mutation	UNP Q8YIN7
H	258	ILE	MET	engineered mutation	UNP Q8YIN7
H	262	LYS	THR	engineered mutation	UNP Q8YIN7
I	258	ILE	MET	engineered mutation	UNP Q8YIN7
I	262	LYS	THR	engineered mutation	UNP Q8YIN7
J	258	ILE	MET	engineered mutation	UNP Q8YIN7
J	262	LYS	THR	engineered mutation	UNP Q8YIN7
K	258	ILE	MET	engineered mutation	UNP Q8YIN7
K	262	LYS	THR	engineered mutation	UNP Q8YIN7
L	258	ILE	MET	engineered mutation	UNP Q8YIN7
L	262	LYS	THR	engineered mutation	UNP Q8YIN7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	59	Total O 59 59	0	0
2	C	65	Total O 65 65	0	0
2	D	53	Total O 53 53	0	0
2	E	48	Total O 48 48	0	0
2	F	49	Total O 49 49	0	0
2	G	52	Total O 52 52	0	0
2	H	63	Total O 63 63	0	0
2	I	17	Total O 17 17	0	0
2	J	16	Total O 16 16	0	0

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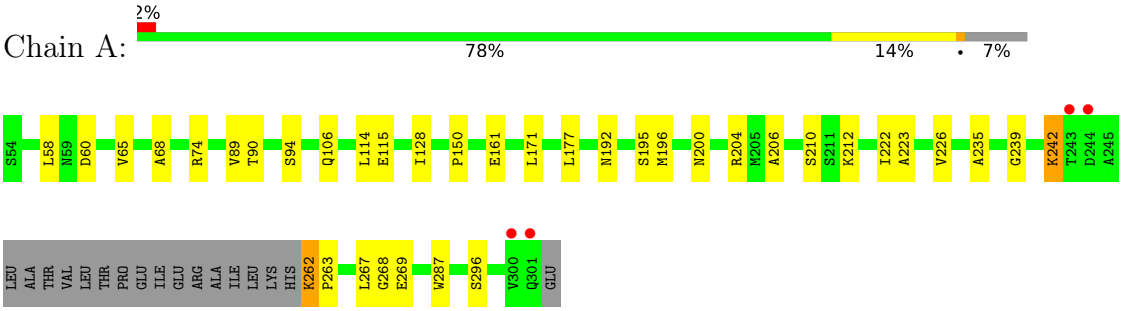
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	13	Total O 13 13	0	0
2	L	11	Total O 11 11	0	0

3 Residue-property plots

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.

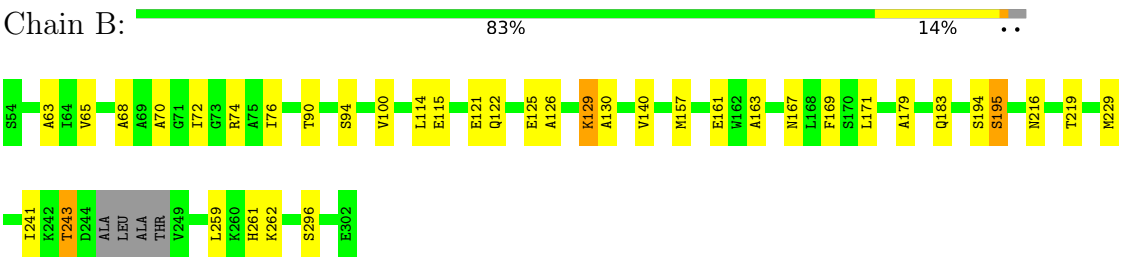
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain A:



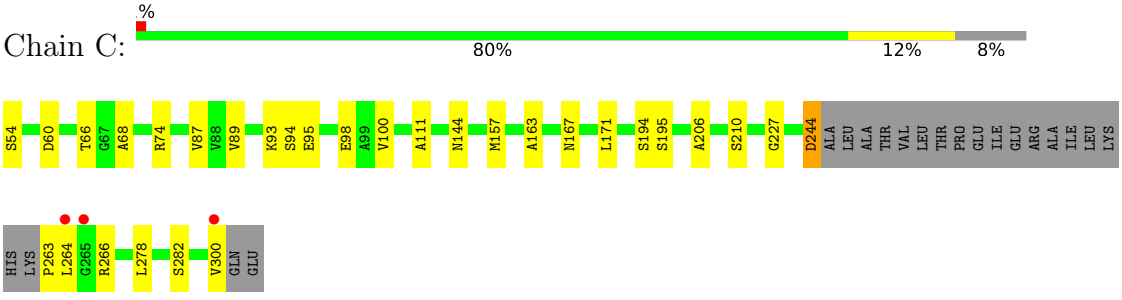
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain B:



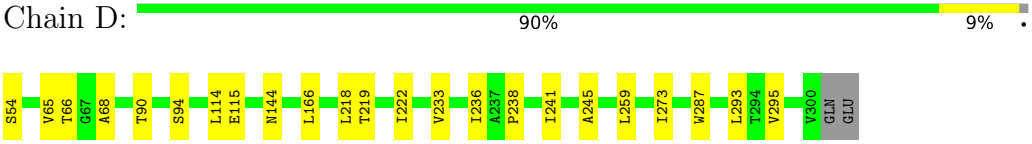
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain C:



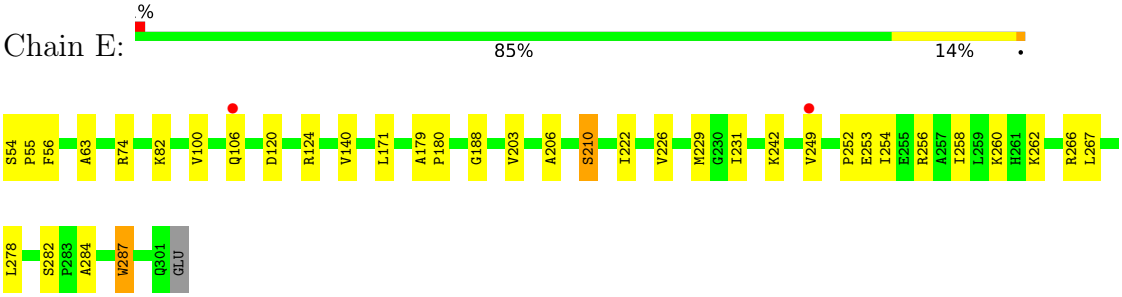
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain D:



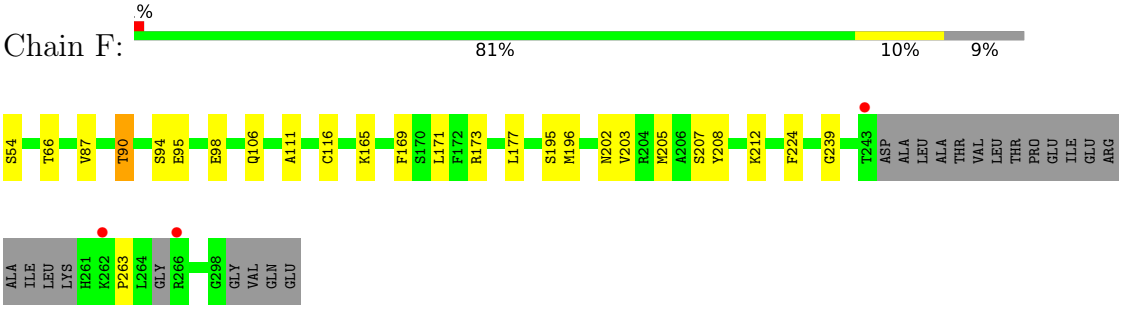
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain E:



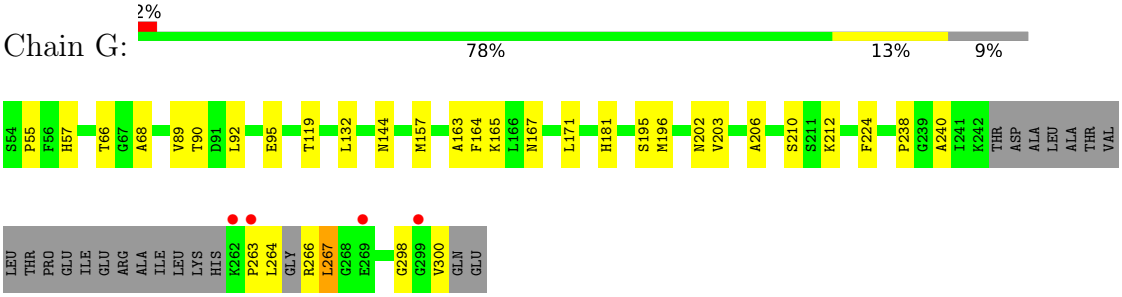
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain F:



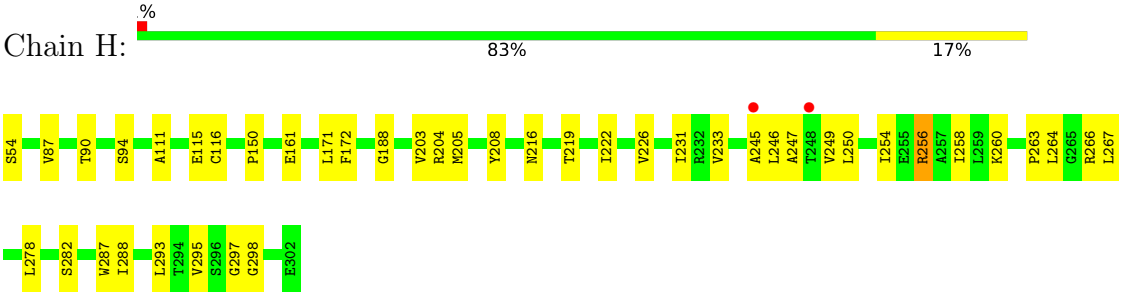
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain G:



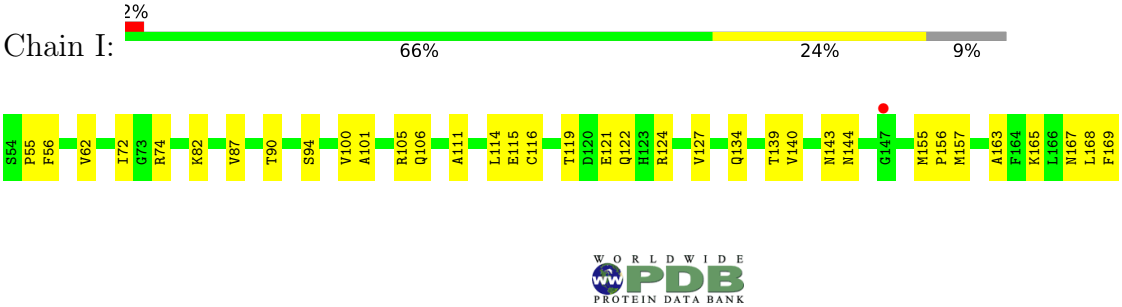
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

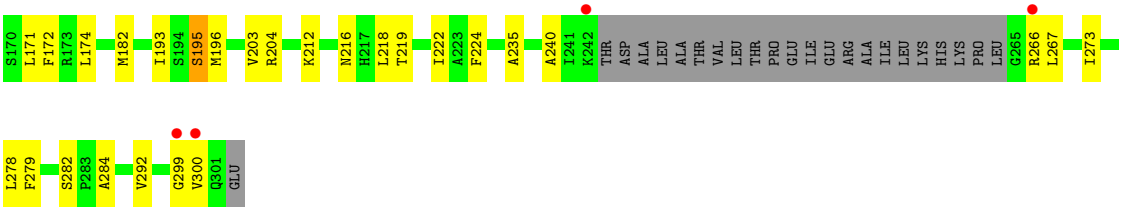
Chain H:



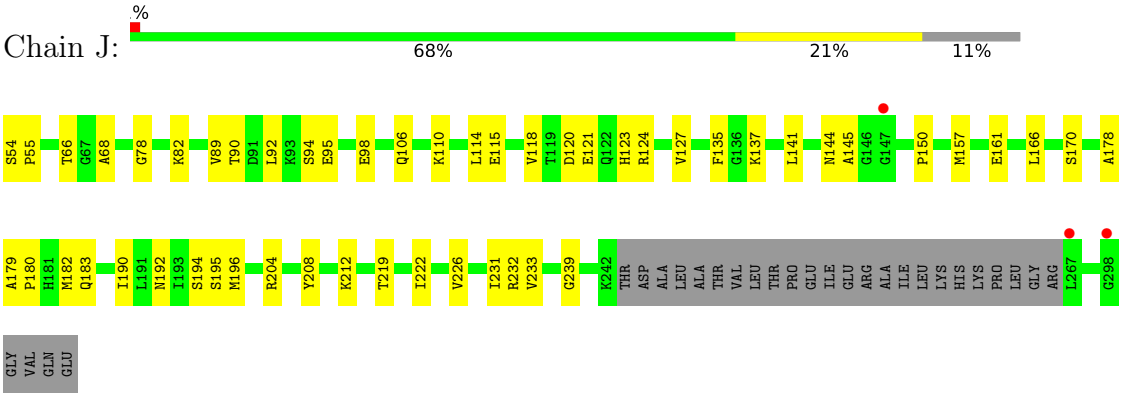
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain I:

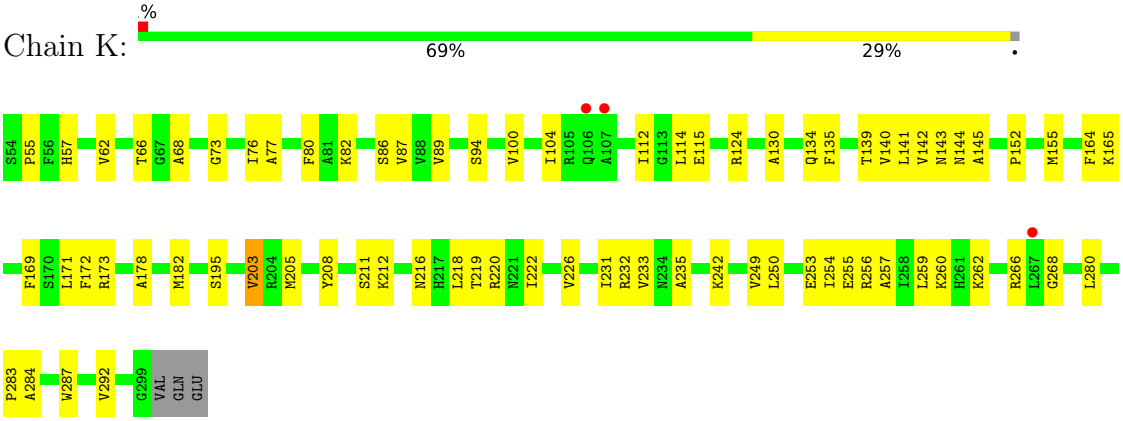




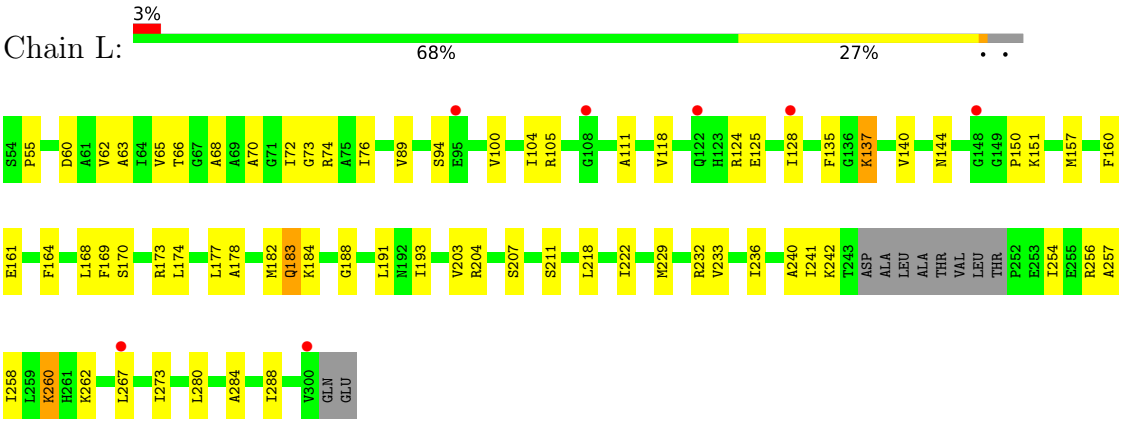
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.08Å 99.91Å 103.42Å 87.43° 78.84° 78.37°	Depositor
Resolution (Å)	23.75 – 2.35 23.75 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.4 (23.75-2.35) 93.4 (23.75-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.36Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.217 , 0.266 0.219 , 0.266	Depositor DCC
R_{free} test set	6448 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.157 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20848	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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	0.47	0/1682	0.63	0/2276
1	B	0.45	0/1794	0.63	0/2428
1	C	0.48	0/1659	0.64	0/2245
1	D	0.46	0/1802	0.65	0/2442
1	E	0.45	0/1811	0.63	0/2454
1	F	0.45	0/1655	0.63	0/2238
1	G	0.48	0/1648	0.67	0/2228
1	H	0.48	0/1820	0.64	0/2466
1	I	0.37	0/1637	0.57	0/2214
1	J	0.35	0/1602	0.56	0/2168
1	K	0.33	0/1795	0.55	0/2432
1	L	0.37	0/1746	0.55	0/2361
All	All	0.43	0/20651	0.61	0/27952

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	1656	0	1671	24	0
1	B	1766	0	1789	23	0
1	C	1633	0	1646	20	0
1	D	1773	0	1804	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1782	0	1812	22	0
1	F	1629	0	1645	18	0
1	G	1623	0	1643	27	0
1	H	1791	0	1818	28	0
1	I	1612	0	1624	35	0
1	J	1577	0	1588	27	0
1	K	1766	0	1795	47	0
1	L	1718	0	1745	42	0
2	A	76	0	0	3	0
2	B	59	0	0	0	0
2	C	65	0	0	1	0
2	D	53	0	0	0	0
2	E	48	0	0	1	0
2	F	49	0	0	1	0
2	G	52	0	0	0	0
2	H	63	0	0	0	0
2	I	17	0	0	0	0
2	J	16	0	0	0	0
2	K	13	0	0	1	0
2	L	11	0	0	1	0
All	All	20848	0	20580	301	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 7.

All (301) 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:I:139:THR:HG22	1:I:140:VAL:HG23	1.60	0.82
1:I:203:VAL:HG13	1:I:204:ARG:HG3	1.64	0.80
1:K:257:ALA:HA	1:K:260:LYS:HE3	1.64	0.80
1:C:264:LEU:HD11	1:C:266:ARG:HE	1.51	0.75
1:K:195:SER:HB3	1:K:212:LYS:HG3	1.68	0.75
1:K:219:THR:HG23	1:K:233:VAL:HG22	1.68	0.75
1:E:203:VAL:HG12	1:G:224:PHE:HB3	1.69	0.73
1:J:114:LEU:HD11	1:J:127:VAL:HG22	1.71	0.72
1:F:195:SER:HB3	1:F:212:LYS:HG3	1.71	0.70
1:A:287:TRP:CZ3	1:G:266:ARG:HB3	2.25	0.70
1:L:151:LYS:HE3	2:L:409:HOH:O	1.91	0.69
1:I:121:GLU:HA	1:I:124:ARG:HE	1.58	0.68
1:C:157:MET:H	1:I:134:GLN:HE22	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:ALA:HB1	1:I:267:LEU:HD12	1.75	0.67
1:K:205:MET:HE3	1:K:208:TYR:HB3	1.77	0.67
1:I:114:LEU:HD11	1:I:127:VAL:HG22	1.76	0.66
1:L:72:ILE:HD11	1:L:241:ILE:HG21	1.76	0.66
1:F:165:LYS:HD2	1:F:169:PHE:HD2	1.61	0.65
1:I:224:PHE:HB3	1:L:203:VAL:HG22	1.76	0.65
1:L:105:ARG:NH1	1:L:111:ALA:O	2.29	0.65
1:B:94:SER:HB3	1:B:115:GLU:HB2	1.79	0.64
1:K:124:ARG:HE	1:K:173:ARG:HG2	1.62	0.64
1:I:195:SER:HB3	1:I:212:LYS:HG3	1.78	0.64
1:J:94:SER:HB3	1:J:115:GLU:HB2	1.79	0.64
1:I:121:GLU:HA	1:I:124:ARG:NE	2.13	0.64
1:E:63:ALA:HA	1:E:140:VAL:HG13	1.79	0.64
1:D:94:SER:HB3	1:D:115:GLU:HB2	1.79	0.64
1:G:195:SER:HB3	1:G:212:LYS:HG3	1.82	0.62
1:K:232:ARG:NH2	1:K:280:LEU:O	2.27	0.62
1:L:128:ILE:HD12	1:L:177:LEU:HB3	1.81	0.62
1:F:205:MET:HE3	1:F:208:TYR:HB3	1.81	0.61
1:K:165:LYS:HA	1:K:169:PHE:HB2	1.83	0.61
1:K:254:ILE:HD12	1:K:255:GLU:N	2.15	0.61
1:L:240:ALA:HB1	1:L:267:LEU:HD23	1.82	0.61
1:D:219:THR:HG23	1:D:233:VAL:HG12	1.81	0.60
1:B:74:ARG:HD3	1:B:100:VAL:HG22	1.82	0.60
1:A:206:ALA:O	1:A:210:SER:OG	2.20	0.60
1:L:68:ALA:HA	1:L:73:GLY:HA3	1.84	0.59
1:F:165:LYS:HE3	2:F:425:HOH:O	2.02	0.59
1:K:235:ALA:HB3	1:K:292:VAL:HG22	1.83	0.59
1:K:139:THR:HG22	1:K:140:VAL:HG23	1.83	0.59
1:L:70:ALA:HA	1:L:74:ARG:HE	1.68	0.59
1:G:164:PHE:HZ	1:G:210:SER:HG	1.49	0.59
1:G:264:LEU:HB3	1:G:266:ARG:NH1	2.17	0.59
1:C:94:SER:O	1:C:98:GLU:HG3	2.03	0.58
1:K:112:ILE:HG21	1:K:134:GLN:HG2	1.86	0.58
1:C:206:ALA:O	1:C:210:SER:OG	2.20	0.58
1:C:264:LEU:HD21	1:C:266:ARG:HH21	1.69	0.58
1:E:206:ALA:O	1:E:210:SER:HB3	2.04	0.57
1:I:94:SER:OG	1:I:115:GLU:HB2	2.04	0.57
1:G:206:ALA:O	1:G:210:SER:HB3	2.03	0.57
1:G:264:LEU:HB3	1:G:266:ARG:HH11	1.69	0.57
1:E:258:ILE:HG23	1:H:254:ILE:HD12	1.87	0.57
1:K:259:LEU:HD11	1:K:266:ARG:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:MET:HE1	1:F:208:TYR:HD2	1.68	0.56
1:K:62:VAL:H	1:K:139:THR:HB	1.69	0.56
1:E:203:VAL:CG1	1:G:224:PHE:HB3	2.35	0.56
1:G:266:ARG:HB2	1:G:266:ARG:CZ	2.35	0.56
1:I:62:VAL:H	1:I:139:THR:HB	1.71	0.55
1:H:245:ALA:C	1:H:247:ALA:H	2.09	0.55
1:H:256:ARG:O	1:H:260:LYS:HG2	2.07	0.55
1:J:208:TYR:O	1:J:212:LYS:HG2	2.07	0.55
1:I:196:MET:HE1	1:I:300:VAL:HA	1.89	0.54
1:K:114:LEU:HD11	1:K:130:ALA:HB3	1.89	0.54
1:G:119:THR:HB	1:G:165:LYS:HE3	1.89	0.53
1:I:74:ARG:HD3	1:I:100:VAL:HG22	1.89	0.53
1:A:287:TRP:HZ3	1:G:266:ARG:HB3	1.69	0.53
1:E:179:ALA:HB1	1:E:229:MET:HE1	1.90	0.53
1:A:65:VAL:HG12	1:A:68:ALA:HB2	1.90	0.52
1:F:90:THR:HG23	1:F:116:CYS:HB3	1.92	0.52
1:E:55:PRO:HG2	1:E:284:ALA:HB2	1.91	0.52
1:K:66:THR:HB	1:K:145:ALA:HB2	1.92	0.52
1:K:171:LEU:HD12	1:K:172:PHE:N	2.24	0.52
1:G:240:ALA:O	1:G:267:LEU:O	2.27	0.52
1:L:118:VAL:CG1	1:L:170:SER:HB3	2.39	0.52
1:A:161:GLU:HG2	1:B:169:PHE:CE2	2.45	0.51
1:G:196:MET:CE	1:G:300:VAL:HA	2.40	0.51
1:G:66:THR:O	1:G:144:ASN:HB3	2.10	0.51
1:J:196:MET:HE2	1:J:239:GLY:HA3	1.93	0.51
1:B:296:SER:HA	1:E:287:TRP:CZ3	2.45	0.51
1:F:95:GLU:CD	1:F:95:GLU:H	2.14	0.51
1:E:254:ILE:O	1:E:258:ILE:HG13	2.11	0.51
1:I:143:ASN:OD1	1:I:174:LEU:HD23	2.10	0.51
1:K:55:PRO:HG2	1:K:284:ALA:HB2	1.92	0.51
1:D:293:LEU:HD13	1:H:293:LEU:HD13	1.92	0.51
1:L:100:VAL:O	1:L:104:ILE:HG13	2.10	0.51
1:A:195:SER:HB3	1:A:212:LYS:HG3	1.92	0.51
1:L:222:ILE:HD11	1:L:233:VAL:HG11	1.92	0.51
1:B:70:ALA:HA	1:B:74:ARG:HE	1.76	0.51
1:C:244:ASP:OD1	1:C:244:ASP:N	2.44	0.51
1:H:278:LEU:O	1:H:282:SER:HB3	2.09	0.51
1:K:55:PRO:HA	1:K:57:HIS:CE1	2.46	0.51
1:D:65:VAL:HG12	1:D:68:ALA:HB2	1.92	0.51
1:L:157:MET:O	1:L:161:GLU:HG3	2.11	0.51
1:G:55:PRO:HA	1:G:57:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:SER:HB3	1:H:115:GLU:HB2	1.93	0.50
1:H:266:ARG:HG3	1:H:267:LEU:O	2.11	0.50
1:A:94:SER:HB3	1:A:115:GLU:HB2	1.93	0.50
1:B:259:LEU:HD23	1:B:262:LYS:HG3	1.93	0.50
1:K:94:SER:HB3	1:K:115:GLU:HB3	1.93	0.50
1:B:216:ASN:O	1:B:219:THR:HB	2.10	0.50
1:K:203:VAL:O	1:K:205:MET:HG2	2.11	0.50
1:I:90:THR:HB	1:I:116:CYS:HB3	1.94	0.50
1:K:68:ALA:HA	1:K:73:GLY:HA3	1.94	0.50
1:L:89:VAL:HG11	1:L:100:VAL:HG11	1.92	0.50
1:L:218:LEU:O	1:L:222:ILE:HG12	2.11	0.50
1:B:122:GLN:OE1	1:J:137:LYS:HD3	2.11	0.50
1:E:222:ILE:O	1:E:226:VAL:HG22	2.11	0.50
1:J:94:SER:O	1:J:98:GLU:HG3	2.12	0.50
1:J:157:MET:O	1:J:161:GLU:HG3	2.12	0.50
1:B:163:ALA:O	1:B:167:ASN:HB2	2.12	0.50
1:F:196:MET:SD	1:F:239:GLY:HA3	2.52	0.50
1:G:196:MET:HE1	1:G:300:VAL:HA	1.94	0.50
1:L:257:ALA:O	1:L:260:LYS:HG2	2.11	0.49
1:J:78:GLY:O	1:J:82:LYS:HG3	2.12	0.49
1:J:196:MET:CE	1:J:239:GLY:HA3	2.42	0.49
1:F:224:PHE:HB3	1:H:203:VAL:CG1	2.42	0.49
1:K:76:ILE:HG21	1:K:142:VAL:HG11	1.94	0.49
1:G:164:PHE:HZ	1:G:210:SER:OG	1.96	0.49
1:B:126:ALA:HA	1:B:129:LYS:HE3	1.93	0.49
1:D:295:VAL:HG13	1:H:288:ILE:HG12	1.95	0.49
1:K:164:PHE:CE1	1:K:211:SER:HA	2.47	0.49
1:K:262:LYS:NZ	2:K:401:HOH:O	2.45	0.49
1:L:178:ALA:O	1:L:182:MET:HG3	2.12	0.49
1:A:287:TRP:CZ2	1:G:267:LEU:O	2.66	0.48
1:C:87:VAL:O	1:C:111:ALA:HA	2.13	0.48
1:I:216:ASN:O	1:I:219:THR:HB	2.14	0.48
1:B:157:MET:O	1:B:161:GLU:HG3	2.14	0.48
1:B:241:ILE:HD12	1:B:241:ILE:O	2.13	0.48
1:B:129:LYS:HD2	1:B:130:ALA:N	2.28	0.48
1:F:165:LYS:HD2	1:F:169:PHE:CD2	2.46	0.48
1:C:278:LEU:O	1:C:282:SER:HB3	2.14	0.48
1:K:212:LYS:HA	1:K:212:LYS:HD3	1.69	0.48
1:B:63:ALA:HA	1:B:140:VAL:O	2.13	0.48
1:B:183:GLN:HB2	1:B:229:MET:HB3	1.96	0.48
1:A:58:LEU:HA	2:A:405:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:MET:HE1	1:H:208:TYR:HD2	1.79	0.47
1:D:66:THR:O	1:D:144:ASN:HB3	2.14	0.47
1:L:118:VAL:HG12	1:L:170:SER:HB3	1.95	0.47
1:L:182:MET:HE3	1:L:188:GLY:HA3	1.96	0.47
1:L:183:GLN:HG3	1:L:184:LYS:N	2.30	0.47
1:J:66:THR:HA	1:J:90:THR:OG1	2.15	0.47
1:A:128:ILE:HG13	1:A:177:LEU:HB3	1.95	0.47
1:J:194:SER:OG	1:J:195:SER:N	2.46	0.47
1:L:236:ILE:HG21	1:L:273:ILE:HG23	1.97	0.47
1:I:157:MET:HG3	1:L:173:ARG:HD3	1.97	0.47
1:K:205:MET:HE1	1:K:208:TYR:HD2	1.80	0.47
1:A:242:LYS:HB2	1:A:268:GLY:O	2.15	0.46
1:C:74:ARG:HG3	1:C:100:VAL:HG22	1.97	0.46
1:C:93:LYS:HA	1:C:93:LYS:HD3	1.44	0.46
1:L:89:VAL:HG11	1:L:100:VAL:CG1	2.45	0.46
1:L:168:LEU:HD23	1:L:169:PHE:CE1	2.49	0.46
1:J:179:ALA:N	1:J:180:PRO:HD2	2.29	0.46
1:H:222:ILE:O	1:H:226:VAL:HG22	2.15	0.46
1:F:169:PHE:CE2	1:H:161:GLU:HG2	2.50	0.46
1:E:74:ARG:HD3	1:E:100:VAL:HG22	1.96	0.46
1:J:166:LEU:O	1:J:170:SER:OG	2.25	0.46
1:K:242:LYS:N	1:K:268:GLY:O	2.37	0.46
1:I:74:ARG:HD3	1:I:100:VAL:CG2	2.46	0.46
1:E:179:ALA:HB1	1:E:229:MET:CE	2.46	0.45
1:G:263:PRO:HG2	1:G:298:GLY:HA3	1.98	0.45
1:K:222:ILE:O	1:K:226:VAL:HG22	2.16	0.45
1:B:121:GLU:HG2	1:J:135:PHE:HA	1.97	0.45
1:E:82:LYS:HE2	2:E:448:HOH:O	2.16	0.45
1:H:203:VAL:O	1:H:205:MET:HG2	2.16	0.45
1:C:60:ASP:HA	2:C:450:HOH:O	2.15	0.45
1:J:120:ASP:HB3	1:J:123:HIS:HB2	1.97	0.45
1:K:77:ALA:HB1	1:K:87:VAL:HG11	1.99	0.45
1:K:114:LEU:HD11	1:K:130:ALA:CB	2.47	0.45
1:I:72:ILE:HD13	1:I:273:ILE:HG21	1.98	0.45
1:I:165:LYS:HA	1:I:169:PHE:HB2	1.99	0.45
1:J:150:PRO:HA	1:J:204:ARG:O	2.17	0.45
1:B:229:MET:HE2	1:B:229:MET:HB2	1.86	0.45
1:I:171:LEU:HD12	1:I:172:PHE:N	2.31	0.45
1:C:157:MET:H	1:I:134:GLN:NE2	2.11	0.45
1:J:226:VAL:HG23	1:J:231:ILE:O	2.17	0.45
1:L:55:PRO:HG2	1:L:284:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:ARG:NH2	1:L:173:ARG:HG2	2.32	0.45
1:H:219:THR:HG23	1:H:233:VAL:HG12	1.99	0.44
1:J:95:GLU:OE1	1:J:95:GLU:N	2.39	0.44
1:K:66:THR:O	1:K:144:ASN:HB3	2.16	0.44
1:G:132:LEU:HD11	1:G:181:HIS:NE2	2.32	0.44
1:K:218:LEU:O	1:K:222:ILE:HG12	2.17	0.44
1:K:178:ALA:O	1:K:182:MET:HG3	2.17	0.44
1:L:125:GLU:O	1:L:128:ILE:HG22	2.18	0.44
1:B:65:VAL:HG12	1:B:68:ALA:HB2	2.00	0.44
1:B:179:ALA:HB1	1:B:229:MET:HE1	2.00	0.44
1:J:121:GLU:OE1	1:J:124:ARG:NH2	2.47	0.44
1:A:106:GLN:NE2	2:A:402:HOH:O	2.51	0.44
1:I:144:ASN:HB2	1:I:193:ILE:HG13	2.00	0.44
1:A:60:ASP:HA	2:A:456:HOH:O	2.17	0.44
1:A:150:PRO:HA	1:A:204:ARG:O	2.18	0.44
1:A:262:LYS:N	1:A:263:PRO:HD3	2.32	0.44
1:E:55:PRO:HD2	1:E:56:PHE:CD1	2.53	0.44
1:L:183:GLN:HB3	1:L:229:MET:HB3	1.99	0.44
1:C:95:GLU:H	1:C:95:GLU:CD	2.20	0.44
1:J:141:LEU:HD23	1:J:190:ILE:HG23	1.99	0.44
1:G:68:ALA:HB3	1:G:89:VAL:HG13	1.99	0.43
1:K:124:ARG:NE	1:K:173:ARG:HG2	2.29	0.43
1:H:264:LEU:HD12	1:H:297:GLY:HA2	2.00	0.43
1:I:122:GLN:OE1	1:I:122:GLN:N	2.51	0.43
1:K:141:LEU:HD11	1:K:143:ASN:ND2	2.33	0.43
1:L:66:THR:O	1:L:144:ASN:HB3	2.18	0.43
1:D:218:LEU:O	1:D:222:ILE:HG12	2.17	0.43
1:H:150:PRO:HA	1:H:204:ARG:O	2.19	0.43
1:J:178:ALA:O	1:J:182:MET:HG3	2.17	0.43
1:E:252:PRO:HG2	1:H:208:TYR:CD2	2.54	0.43
1:E:278:LEU:O	1:E:282:SER:HB3	2.19	0.43
1:I:155:MET:HG3	1:I:156:PRO:O	2.19	0.43
1:D:90:THR:HA	1:D:114:LEU:O	2.19	0.43
1:E:256:ARG:O	1:E:260:LYS:HD3	2.18	0.43
1:H:254:ILE:O	1:H:258:ILE:HD12	2.17	0.43
1:C:66:THR:O	1:C:144:ASN:HB3	2.19	0.43
1:C:194:SER:OG	1:C:195:SER:N	2.50	0.43
1:I:168:LEU:HD12	1:I:171:LEU:HD11	1.99	0.43
1:K:256:ARG:O	1:K:260:LYS:HG3	2.18	0.43
1:A:222:ILE:O	1:A:226:VAL:HG22	2.17	0.43
1:C:227:GLY:HA3	1:F:263:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:SER:O	1:F:98:GLU:HB2	2.19	0.43
1:G:95:GLU:CD	1:G:95:GLU:H	2.21	0.43
1:L:63:ALA:HA	1:L:140:VAL:O	2.18	0.43
1:L:164:PHE:CE1	1:L:211:SER:HA	2.54	0.43
1:A:196:MET:HB3	1:A:200:ASN:ND2	2.33	0.43
1:F:87:VAL:O	1:F:111:ALA:HA	2.19	0.43
1:F:173:ARG:NH2	1:F:177:LEU:HD21	2.34	0.43
1:J:68:ALA:HB3	1:J:89:VAL:HG13	1.99	0.43
1:K:82:LYS:HA	1:K:82:LYS:HD3	1.76	0.43
1:K:242:LYS:HD2	1:K:250:LEU:HD22	2.00	0.43
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.69	0.42
1:B:72:ILE:O	1:B:76:ILE:HG13	2.18	0.42
1:F:66:THR:HA	1:F:90:THR:HG22	2.00	0.42
1:I:163:ALA:O	1:I:167:ASN:HB2	2.19	0.42
1:C:263:PRO:HB2	1:C:264:LEU:H	1.65	0.42
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.01	0.42
1:J:219:THR:HG23	1:J:233:VAL:HG22	2.01	0.42
1:L:191:LEU:HD21	1:L:236:ILE:HD12	2.01	0.42
1:A:223:ALA:O	1:G:263:PRO:HB3	2.20	0.42
1:C:68:ALA:HB3	1:C:89:VAL:HG13	2.02	0.42
1:E:262:LYS:HD2	1:E:262:LYS:HA	1.78	0.42
1:L:174:LEU:HD23	1:L:174:LEU:HA	1.86	0.42
1:G:66:THR:HA	1:G:90:THR:OG1	2.19	0.42
1:I:55:PRO:HG2	1:I:284:ALA:HB2	2.02	0.42
1:L:254:ILE:O	1:L:258:ILE:HG13	2.19	0.42
1:A:192:ASN:O	1:A:235:ALA:HA	2.20	0.42
1:I:87:VAL:O	1:I:111:ALA:HA	2.20	0.42
1:K:216:ASN:O	1:K:220:ARG:HG3	2.20	0.42
1:C:163:ALA:O	1:C:167:ASN:HB2	2.19	0.42
1:I:196:MET:HE1	1:I:299:GLY:O	2.20	0.42
1:L:62:VAL:HG11	1:L:135:PHE:HB3	2.02	0.42
1:B:194:SER:OG	1:B:195:SER:N	2.51	0.41
1:H:87:VAL:O	1:H:111:ALA:HA	2.20	0.41
1:I:101:ALA:O	1:I:105:ARG:HG3	2.19	0.41
1:L:150:PRO:HA	1:L:204:ARG:O	2.20	0.41
1:J:222:ILE:HG13	1:J:233:VAL:HG11	2.01	0.41
1:I:218:LEU:HG	1:I:222:ILE:HD13	2.03	0.41
1:K:222:ILE:HG13	1:K:233:VAL:HG11	2.02	0.41
1:L:60:ASP:O	1:L:137:LYS:NZ	2.52	0.41
1:B:241:ILE:HD13	1:B:243:THR:HG23	2.02	0.41
1:I:56:PHE:HE1	1:I:279:PHE:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:232:ARG:HD2	1:L:288:ILE:O	2.20	0.41
1:J:66:THR:O	1:J:144:ASN:HB3	2.20	0.41
1:K:80:PHE:HE2	1:K:140:VAL:HG11	1.86	0.41
1:K:152:PRO:O	1:K:155:MET:HB3	2.20	0.41
1:L:65:VAL:HG12	1:L:68:ALA:HB2	2.02	0.41
1:L:160:PHE:CD1	1:L:207:SER:HB3	2.55	0.41
1:A:242:LYS:HG3	1:A:267:LEU:HD12	2.03	0.41
1:F:224:PHE:HB3	1:H:203:VAL:HG13	2.03	0.41
1:G:163:ALA:O	1:G:167:ASN:HB2	2.20	0.41
1:H:188:GLY:O	1:H:231:ILE:HA	2.20	0.41
1:K:100:VAL:O	1:K:104:ILE:HG13	2.20	0.41
1:H:245:ALA:C	1:H:247:ALA:N	2.73	0.41
1:A:242:LYS:HE3	1:A:269:GLU:HG3	2.03	0.41
1:E:120:ASP:O	1:E:124:ARG:HG3	2.21	0.41
1:F:224:PHE:HB3	1:H:203:VAL:HG12	2.02	0.41
1:H:263:PRO:HG2	1:H:298:GLY:HA3	2.03	0.41
1:K:86:SER:HB3	1:K:135:PHE:CE1	2.56	0.41
1:L:76:ILE:HD11	1:L:193:ILE:HD11	2.03	0.41
1:L:124:ARG:CZ	1:L:173:ARG:HG2	2.50	0.41
1:A:68:ALA:HB3	1:A:89:VAL:HG13	2.02	0.41
1:C:74:ARG:HG3	1:C:100:VAL:CG2	2.51	0.41
1:E:188:GLY:O	1:E:231:ILE:HA	2.20	0.41
1:J:118:VAL:HG11	1:J:145:ALA:HB3	2.03	0.41
1:D:236:ILE:O	1:D:238:PRO:HD3	2.21	0.41
1:D:241:ILE:HD11	1:D:273:ILE:HD11	2.02	0.41
1:G:157:MET:CE	1:G:157:MET:HA	2.51	0.41
1:K:226:VAL:HB	1:K:231:ILE:HB	2.02	0.41
1:L:236:ILE:HD11	1:L:280:LEU:HD12	2.02	0.41
1:H:90:THR:HB	1:H:116:CYS:HB3	2.03	0.40
1:D:245:ALA:HB1	1:K:249:VAL:HG11	2.03	0.40
1:D:287:TRP:HD1	1:H:295:VAL:HG12	1.87	0.40
1:H:216:ASN:O	1:H:219:THR:HB	2.22	0.40
1:I:235:ALA:HB3	1:I:292:VAL:HG22	2.02	0.40
1:I:278:LEU:O	1:I:282:SER:HB3	2.21	0.40
1:A:90:THR:HA	1:A:114:LEU:O	2.22	0.40
1:B:90:THR:HA	1:B:114:LEU:O	2.21	0.40
1:J:54:SER:HA	1:J:55:PRO:HD3	1.90	0.40
1:A:239:GLY:HA3	1:A:296:SER:HB3	2.02	0.40
1:D:245:ALA:HB3	1:K:249:VAL:HG21	2.02	0.40
1:E:253:GLU:HA	1:E:256:ARG:NH1	2.36	0.40
1:G:132:LEU:HD11	1:G:181:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:LEU:HD12	1:H:172:PHE:N	2.37	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	228/249 (92%)	219 (96%)	9 (4%)	0	100	100
1	B	241/249 (97%)	235 (98%)	6 (2%)	0	100	100
1	C	225/249 (90%)	219 (97%)	6 (3%)	0	100	100
1	D	245/249 (98%)	239 (98%)	6 (2%)	0	100	100
1	E	246/249 (99%)	239 (97%)	7 (3%)	0	100	100
1	F	221/249 (89%)	212 (96%)	9 (4%)	0	100	100
1	G	221/249 (89%)	214 (97%)	7 (3%)	0	100	100
1	H	247/249 (99%)	239 (97%)	8 (3%)	0	100	100
1	I	222/249 (89%)	216 (97%)	6 (3%)	0	100	100
1	J	217/249 (87%)	209 (96%)	8 (4%)	0	100	100
1	K	244/249 (98%)	239 (98%)	5 (2%)	0	100	100
1	L	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
All	All	2792/2988 (93%)	2707 (97%)	85 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	162/177 (92%)	158 (98%)	4 (2%)	47	58
1	B	175/177 (99%)	169 (97%)	6 (3%)	37	46
1	C	160/177 (90%)	156 (98%)	4 (2%)	47	58
1	D	175/177 (99%)	173 (99%)	2 (1%)	73	84
1	E	176/177 (99%)	167 (95%)	9 (5%)	24	27
1	F	160/177 (90%)	153 (96%)	7 (4%)	28	34
1	G	159/177 (90%)	153 (96%)	6 (4%)	33	41
1	H	177/177 (100%)	171 (97%)	6 (3%)	37	46
1	I	157/177 (89%)	151 (96%)	6 (4%)	33	41
1	J	154/177 (87%)	148 (96%)	6 (4%)	32	40
1	K	174/177 (98%)	169 (97%)	5 (3%)	42	52
1	L	169/177 (96%)	162 (96%)	7 (4%)	30	37
All	All	1998/2124 (94%)	1930 (97%)	68 (3%)	37	46

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	171	LEU
1	A	242	LYS
1	A	262	LYS
1	B	125	GLU
1	B	129	LYS
1	B	171	LEU
1	B	195	SER
1	B	243	THR
1	B	261	HIS
1	C	54	SER
1	C	171	LEU
1	C	244	ASP
1	C	300	VAL
1	D	54	SER
1	D	166	LEU
1	E	54	SER
1	E	106	GLN

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Mol	Chain	Res	Type
1	E	171	LEU
1	E	210	SER
1	E	242	LYS
1	E	249	VAL
1	E	266	ARG
1	E	267	LEU
1	E	287	TRP
1	F	54	SER
1	F	90	THR
1	F	106	GLN
1	F	171	LEU
1	F	202	ASN
1	F	203	VAL
1	F	207	SER
1	G	92	LEU
1	G	171	LEU
1	G	202	ASN
1	G	203	VAL
1	G	238	PRO
1	G	267	LEU
1	H	54	SER
1	H	246	LEU
1	H	249	VAL
1	H	250	LEU
1	H	256	ARG
1	H	287	TRP
1	I	82	LYS
1	I	106	GLN
1	I	119	THR
1	I	182	MET
1	I	195	SER
1	I	266	ARG
1	J	92	LEU
1	J	106	GLN
1	J	110	LYS
1	J	183	GLN
1	J	192	ASN
1	J	232	ARG
1	K	89	VAL
1	K	203	VAL
1	K	253	GLU
1	K	283	PRO

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Mol	Chain	Res	Type
1	K	287	TRP
1	L	94	SER
1	L	137	LYS
1	L	183	GLN
1	L	242	LYS
1	L	256	ARG
1	L	260	LYS
1	L	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	200	ASN
1	B	59	ASN
1	I	134	GLN
1	I	183	GLN
1	J	183	GLN
1	L	181	HIS

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	232/249 (93%)	-0.56	4 (1%) 70 78	9, 18, 45, 81	0
1	B	245/249 (98%)	-0.56	0 100 100	11, 19, 51, 80	0
1	C	229/249 (91%)	-0.60	3 (1%) 77 84	10, 17, 38, 93	0
1	D	247/249 (99%)	-0.55	0 100 100	11, 19, 54, 80	0
1	E	248/249 (99%)	-0.52	2 (0%) 86 91	12, 20, 50, 75	0
1	F	227/249 (91%)	-0.61	3 (1%) 77 84	10, 18, 41, 101	0
1	G	227/249 (91%)	-0.57	4 (1%) 68 77	11, 18, 40, 83	0
1	H	249/249 (100%)	-0.57	2 (0%) 86 91	10, 20, 45, 102	0
1	I	226/249 (90%)	-0.17	5 (2%) 62 72	26, 39, 59, 88	0
1	J	221/249 (88%)	-0.23	3 (1%) 75 83	25, 40, 56, 70	0
1	K	246/249 (98%)	0.17	3 (1%) 79 86	36, 53, 67, 82	0
1	L	239/249 (95%)	0.20	7 (2%) 51 62	36, 53, 71, 86	0
All	All	2836/2988 (94%)	-0.38	36 (1%) 77 84	9, 23, 62, 102	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	249	VAL	4.6
1	C	300	VAL	4.5
1	A	244	ASP	4.4
1	C	265	GLY	4.3
1	G	299	GLY	4.0
1	H	248	THR	3.8
1	L	267	LEU	3.4
1	I	266	ARG	3.1
1	F	266	ARG	3.0
1	F	262	LYS	3.0
1	L	95	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	300	VAL	2.9
1	K	107	ALA	2.8
1	A	300	VAL	2.7
1	I	242	LYS	2.7
1	H	245	ALA	2.6
1	K	106	GLN	2.4
1	L	108	GLY	2.4
1	G	262	LYS	2.4
1	C	264	LEU	2.4
1	L	148	GLY	2.4
1	G	269	GLU	2.4
1	J	267	LEU	2.2
1	E	106	GLN	2.2
1	J	147	GLY	2.2
1	J	298	GLY	2.2
1	A	301	GLN	2.2
1	F	243	THR	2.1
1	L	128	ILE	2.1
1	A	243	THR	2.1
1	L	300	VAL	2.1
1	I	299	GLY	2.1
1	L	122	GLN	2.1
1	K	267	LEU	2.0
1	I	147	GLY	2.0
1	G	263	PRO	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.