Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:45 PM EDT

PDB ID	:	1KUT
Title	:	Structural Genomics, Protein TM1243, (SAICAR synthetase)
Authors	:	Zhang, R.; Skarina, T.; Beasley, S.; Edwards, A.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2002-01-22
Resolution	:	2.20 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:

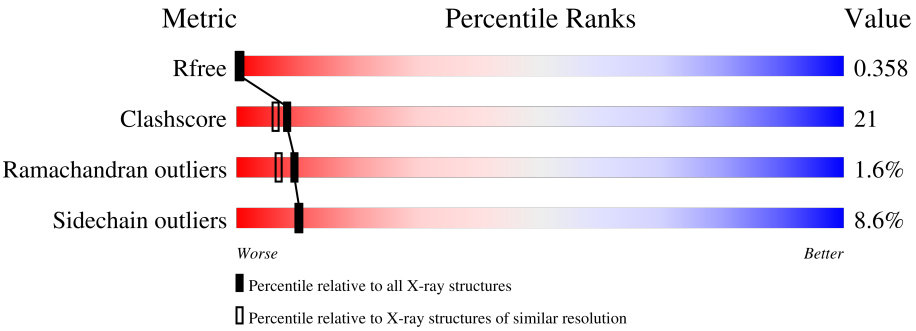
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	230	47% 41% · 7%
1	B	230	58% 32% 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3583 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 Phosphoribosylaminoimidazole-succinocarboxamide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	Se	0	0	0
			1718	1109	286	316	3	4			
1	B	222	Total	C	N	O	S	Se	0	0	0
			1784	1149	298	330	3	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
A	51	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
A	124	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
A	144	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
B	51	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
B	124	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0
B	144	MSE	MET	MODIFIED RESIDUE	UNP Q9X0X0

- Molecule 2 is water.

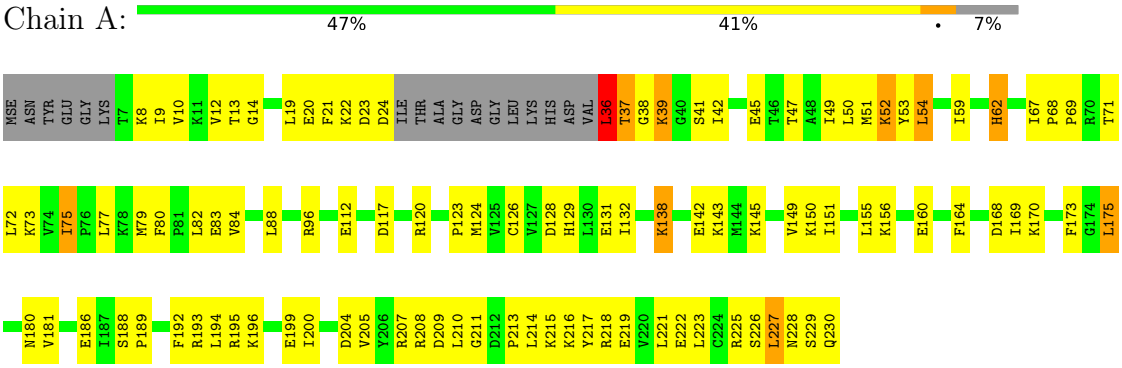
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	39	Total	O	0	0
			39	39		

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. 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. 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.

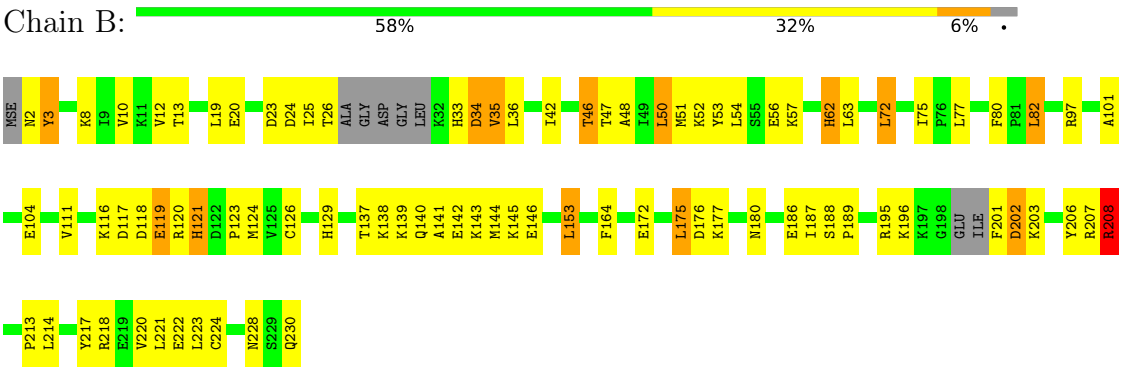
• Molecule 1: Phosphoribosylaminoimidazole-succinocarboxamide synthase

Chain A:



• Molecule 1: Phosphoribosylaminoimidazole-succinocarboxamide synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.51Å 43.07Å 80.22Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 40.08 – 2.01	Depositor EDS
% Data completeness (in resolution range)	82.0 (10.00-2.20) 92.2 (40.08-2.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.281 0.363 , 0.358	Depositor DCC
R_{free} test set	1359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	3583	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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	0.44	0/1744	0.72	3/2334 (0.1%)
1	B	0.46	0/1811	1.37	10/2425 (0.4%)
All	All	0.45	0/3555	1.10	13/4759 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ARG	NE-CZ-NH1	-34.03	103.29	120.30
1	B	208	ARG	NE-CZ-NH2	28.74	134.67	120.30
1	B	207	ARG	NE-CZ-NH2	-25.71	107.44	120.30
1	B	207	ARG	NE-CZ-NH1	24.04	132.32	120.30
1	A	36	LEU	CB-CG-CD2	9.85	127.75	111.00
1	A	36	LEU	CB-CG-CD1	-9.23	95.31	111.00
1	B	207	ARG	CD-NE-CZ	7.87	134.62	123.60
1	B	208	ARG	CA-CB-CG	6.53	127.76	113.40
1	B	207	ARG	CG-CD-NE	6.42	125.27	111.80
1	B	208	ARG	CG-CD-NE	6.31	125.05	111.80
1	B	207	ARG	CA-CB-CG	6.19	127.01	113.40
1	B	208	ARG	CB-CG-CD	-6.05	95.86	111.60
1	A	36	LEU	CA-CB-CG	5.78	128.59	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ARG	Sidechain

5.2 Too-close contacts (i)

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	1775	81	0
1	B	1784	0	1823	72	0
2	A	42	0	0	1	0
2	B	39	0	0	3	0
All	All	3583	0	3598	149	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 21.

All (149) 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:B:51:MSE:HE3	1:B:63:LEU:HB2	1.53	0.91
1:A:37:THR:HG22	1:A:214:LEU:HD13	1.58	0.85
1:B:46:THR:HG22	1:B:221:LEU:HD13	1.58	0.84
1:B:121:HIS:O	1:B:123:PRO:HD3	1.77	0.83
1:B:126:CYS:H	1:B:129:HIS:HD2	1.24	0.82
1:B:36:LEU:HD11	1:B:213:PRO:HB2	1.61	0.82
1:B:42:ILE:O	1:B:46:THR:HG23	1.80	0.82
1:A:37:THR:CG2	1:A:214:LEU:HD13	2.10	0.81
1:B:47:THR:HG22	1:B:51:MSE:HE2	1.62	0.81
1:A:156:LYS:O	1:A:160:GLU:HG3	1.79	0.81
1:B:42:ILE:HD12	1:B:214:LEU:HD11	1.63	0.80
1:A:168:ASP:OD1	1:A:193:ARG:HG3	1.82	0.80
1:A:189:PRO:HB3	1:A:216:LYS:HE2	1.61	0.79
1:A:54:LEU:HD21	1:A:151:ILE:HG23	1.68	0.76
1:B:42:ILE:HG21	1:B:217:TYR:HB3	1.67	0.76
1:A:218:ARG:O	1:A:222:GLU:HG3	1.86	0.76
1:B:52:LYS:O	1:B:56:GLU:HG2	1.87	0.74
1:B:51:MSE:CE	1:B:63:LEU:HB2	2.17	0.74
1:A:227:LEU:C	1:A:229:SER:H	1.90	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:CYS:H	1:B:129:HIS:CD2	2.05	0.73
1:A:84:VAL:HG11	1:A:173:PHE:HE1	1.54	0.72
1:A:225:ARG:O	1:A:230:GLN:HB2	1.91	0.71
1:A:209:ASP:OD1	1:A:215:LYS:HD3	1.91	0.71
1:A:10:VAL:HG22	1:A:19:LEU:HD13	1.73	0.70
1:B:142:GLU:O	1:B:146:GLU:HG3	1.92	0.68
1:A:225:ARG:C	1:A:230:GLN:HB2	2.15	0.68
1:A:42:ILE:HG23	1:A:221:LEU:HD22	1.77	0.67
1:B:218:ARG:O	1:B:222:GLU:HG3	1.95	0.66
1:A:83:GLU:HG2	1:A:170:LYS:HE2	1.77	0.65
1:A:128:ASP:O	1:A:132:ILE:HD13	1.97	0.65
1:B:189:PRO:HG3	1:B:220:VAL:HG21	1.79	0.64
1:A:138:LYS:O	1:A:142:GLU:HB2	1.99	0.63
1:A:145:LYS:O	1:A:149:VAL:HG23	2.00	0.62
1:A:39:LYS:HB3	1:A:214:LEU:HD11	1.82	0.62
1:A:169:ILE:HG13	1:A:192:PHE:HB3	1.82	0.62
1:A:96:ARG:O	1:B:120:ARG:HD3	1.99	0.62
1:B:3:TYR:HB3	1:B:10:VAL:HG12	1.81	0.61
1:A:208:ARG:HG3	1:A:209:ASP:N	2.15	0.61
1:A:84:VAL:HG11	1:A:173:PHE:CE1	2.36	0.61
1:B:34:ASP:CG	1:B:35:VAL:H	2.03	0.61
1:A:131:GLU:CD	1:A:138:LYS:HD3	2.20	0.61
1:B:23:ASP:HB3	1:B:36:LEU:O	2.00	0.59
1:B:25:ILE:HG22	1:B:26:THR:N	2.17	0.59
1:B:137:THR:OG1	1:B:140:GLN:HG3	2.02	0.59
1:A:8:LYS:HB2	1:A:20:GLU:O	2.04	0.58
1:B:62:HIS:HB3	1:B:77:LEU:HD11	1.86	0.58
1:A:200:ILE:O	1:A:200:ILE:HG13	2.04	0.57
1:A:52:LYS:O	1:A:52:LYS:HD3	2.04	0.57
1:A:205:VAL:O	1:A:209:ASP:HB3	2.05	0.56
1:B:2:ASN:O	1:B:3:TYR:HB2	2.05	0.56
1:A:227:LEU:C	1:A:229:SER:N	2.56	0.56
1:A:9:ILE:HG23	1:A:22:LYS:NZ	2.21	0.55
1:A:194:LEU:C	1:A:195:ARG:HD3	2.28	0.55
1:B:177:LYS:HG3	2:B:315:HOH:O	2.08	0.54
1:B:33:HIS:ND1	1:B:34:ASP:N	2.55	0.54
1:B:119:GLU:C	1:B:121:HIS:H	2.11	0.54
1:B:139:LYS:HE3	1:B:143:LYS:NZ	2.23	0.54
1:A:8:LYS:HB3	1:A:21:PHE:HA	1.89	0.54
1:A:41:SER:HA	1:A:69:PRO:O	2.07	0.54
1:A:188:SER:HB2	1:A:189:PRO:HD2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:OE1	1:A:138:LYS:HD3	2.07	0.54
1:B:82:LEU:O	1:B:172:GLU:HG2	2.08	0.54
1:A:67:ILE:HD11	1:A:73:LYS:HB2	1.89	0.54
1:A:143:LYS:HB3	1:A:181:VAL:HG21	1.89	0.54
1:B:3:TYR:HB3	1:B:10:VAL:CG1	2.37	0.54
1:A:188:SER:HB2	1:A:189:PRO:CD	2.37	0.54
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.70	0.54
1:A:45:GLU:O	1:A:49:ILE:HG13	2.08	0.54
1:B:8:LYS:HD2	1:B:19:LEU:HD11	1.90	0.53
1:A:123:PRO:HG3	1:B:97:ARG:O	2.09	0.53
1:A:126:CYS:H	1:A:129:HIS:CD2	2.26	0.53
1:A:112:GLU:OE2	1:B:129:HIS:HE1	1.91	0.53
1:A:156:LYS:HE2	1:A:160:GLU:OE2	2.09	0.53
1:B:75:ILE:O	1:B:75:ILE:HG13	2.09	0.53
1:A:42:ILE:HG23	1:A:221:LEU:CD2	2.38	0.52
1:A:62:HIS:HA	1:A:75:ILE:HG23	1.91	0.52
1:A:12:VAL:HG12	1:A:14:GLY:H	1.75	0.52
1:A:47:THR:O	1:A:51:MSE:HB2	2.10	0.51
1:B:63:LEU:HD13	1:B:72:LEU:HG	1.93	0.51
1:A:189:PRO:HB2	1:A:217:TYR:CE2	2.46	0.50
1:B:2:ASN:HB2	1:B:10:VAL:O	2.12	0.50
1:A:62:HIS:HB3	1:A:77:LEU:HD11	1.94	0.50
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.76	0.50
1:A:214:LEU:HA	1:A:217:TYR:HD1	1.76	0.50
1:B:53:TYR:O	1:B:57:LYS:HG3	2.12	0.49
1:A:169:ILE:CG1	1:A:192:PHE:HB3	2.42	0.49
1:B:175:LEU:HA	1:B:180:ASN:O	2.12	0.49
1:B:117:ASP:O	1:B:121:HIS:O	2.31	0.49
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.27	0.49
1:B:118:ASP:OD2	1:B:118:ASP:N	2.46	0.48
1:B:201:PHE:O	1:B:202:ASP:C	2.50	0.48
1:A:207:ARG:O	1:A:210:LEU:HB3	2.14	0.48
1:B:24:ASP:O	1:B:25:ILE:HD13	2.13	0.48
1:B:223:LEU:C	1:B:223:LEU:HD23	2.34	0.48
1:B:46:THR:HG22	1:B:221:LEU:CD1	2.40	0.47
1:B:46:THR:HG21	2:B:310:HOH:O	2.13	0.47
1:A:226:SER:HA	1:A:230:GLN:HB3	1.96	0.47
1:B:195:ARG:CZ	1:B:195:ARG:HB2	2.44	0.47
1:A:117:ASP:OD2	1:A:120:ARG:HD2	2.14	0.47
1:B:13:THR:HG23	1:B:13:THR:O	2.15	0.46
1:B:111:VAL:HG11	1:B:145:LYS:HG2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:O	1:A:210:LEU:CB	2.63	0.46
1:B:188:SER:HB2	1:B:189:PRO:HD2	1.97	0.46
1:B:224:CYS:O	1:B:228:ASN:HB2	2.16	0.46
1:A:80:PHE:CE2	1:A:175:LEU:HD13	2.51	0.45
1:A:227:LEU:O	1:A:229:SER:N	2.48	0.45
1:A:164:PHE:HB3	1:A:194:LEU:HD11	1.98	0.45
1:A:8:LYS:NZ	1:A:186:GLU:OE1	2.47	0.45
1:B:141:ALA:HA	1:B:144:MSE:HE3	1.97	0.45
1:A:59:ILE:HD11	1:A:150:LYS:HE2	1.98	0.45
1:A:37:THR:HG21	1:A:214:LEU:HD13	1.96	0.45
1:A:42:ILE:HG23	1:A:221:LEU:HB2	1.98	0.45
1:B:80:PHE:HE1	1:B:175:LEU:HD13	1.82	0.45
1:B:164:PHE:CD1	1:B:223:LEU:HD11	2.52	0.45
1:B:188:SER:HB2	1:B:189:PRO:CD	2.46	0.44
1:B:164:PHE:CE2	1:B:196:LYS:HD2	2.53	0.44
1:A:204:ASP:O	1:A:208:ARG:HG2	2.18	0.44
1:B:50:LEU:HD23	1:B:187:ILE:HG22	2.00	0.44
1:A:164:PHE:CE2	1:A:196:LYS:HB3	2.53	0.44
1:A:124:MSE:O	1:B:124:MSE:HE1	2.18	0.43
1:B:101:ALA:HB3	1:B:104:GLU:HB2	1.99	0.43
1:B:177:LYS:HE3	1:B:177:LYS:HB2	1.76	0.43
1:B:25:ILE:HG22	1:B:26:THR:H	1.83	0.43
1:A:71:THR:HG22	1:A:72:LEU:N	2.34	0.43
1:A:22:LYS:HE2	1:A:24:ASP:OD2	2.19	0.43
1:A:216:LYS:HG3	1:A:217:TYR:N	2.34	0.42
1:B:203:LYS:H	1:B:203:LYS:HG2	1.61	0.42
1:A:68:PRO:HA	1:A:69:PRO:HA	1.74	0.42
1:B:20:GLU:HB2	2:B:372:HOH:O	2.20	0.42
1:B:47:THR:CG2	1:B:51:MSE:HE2	2.43	0.42
1:B:164:PHE:CE1	1:B:223:LEU:HD12	2.56	0.41
1:A:196:LYS:NZ	1:A:199:GLU:HG3	2.35	0.41
1:A:47:THR:OG1	1:A:186:GLU:HB2	2.19	0.41
1:B:34:ASP:CG	1:B:35:VAL:N	2.72	0.41
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.91	0.41
1:A:219:GLU:O	1:A:223:LEU:HB2	2.20	0.41
1:B:220:VAL:O	1:B:223:LEU:HB3	2.19	0.41
1:A:126:CYS:HB3	2:A:305:HOH:O	2.20	0.41
1:A:39:LYS:HB3	1:A:214:LEU:CD1	2.50	0.41
1:A:188:SER:CB	1:A:189:PRO:CD	2.97	0.41
1:B:33:HIS:ND1	1:B:33:HIS:C	2.74	0.41
1:B:176:ASP:OD2	1:B:180:ASN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:C	1:A:213:PRO:HD3	2.42	0.40
1:B:48:ALA:HA	1:B:63:LEU:HD22	2.03	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.87	0.40
1:A:23:ASP:O	1:A:36:LEU:HD23	2.22	0.40
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.87	0.40
1:B:25:ILE:CG2	1:B:26:THR:N	2.84	0.40
1:B:8:LYS:NZ	1:B:186:GLU:OE1	2.53	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	209/230 (91%)	202 (97%)	4 (2%)	3 (1%)	11 8
1	B	216/230 (94%)	201 (93%)	11 (5%)	4 (2%)	8 5
All	All	425/460 (92%)	403 (95%)	15 (4%)	7 (2%)	9 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	B	3	TYR
1	A	228	ASN
1	B	34	ASP
1	B	119	GLU
1	A	38	GLY
1	B	35	VAL

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	188/196 (96%)	171 (91%)	17 (9%)	9 9
1	B	194/196 (99%)	178 (92%)	16 (8%)	11 11
All	All	382/392 (97%)	349 (91%)	33 (9%)	10 10

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	36	LEU
1	A	39	LYS
1	A	50	LEU
1	A	52	LYS
1	A	53	TYR
1	A	54	LEU
1	A	62	HIS
1	A	75	ILE
1	A	79	MSE
1	A	82	LEU
1	A	88	LEU
1	A	138	LYS
1	A	155	LEU
1	A	175	LEU
1	A	180	ASN
1	A	227	LEU
1	B	12	VAL
1	B	46	THR
1	B	50	LEU
1	B	54	LEU
1	B	62	HIS
1	B	72	LEU
1	B	82	LEU
1	B	116	LYS
1	B	121	HIS
1	B	138	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	LEU
1	B	175	LEU
1	B	202	ASP
1	B	206	TYR
1	B	208	ARG
1	B	230	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	228	ASN
1	B	2	ASN
1	B	129	HIS
1	B	230	GLN

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.