Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:41 pm BST

PDB ID	:	6FCV
Title	:	Structure of the human DDB1-CSA complex
Authors	:	Meulenbroek, E.M.; Pannu, N.S.
Deposited on	:	2017-12-21
Resolution	:	2.92 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 following versions of software and data (see references ①) were used in the production of this report:

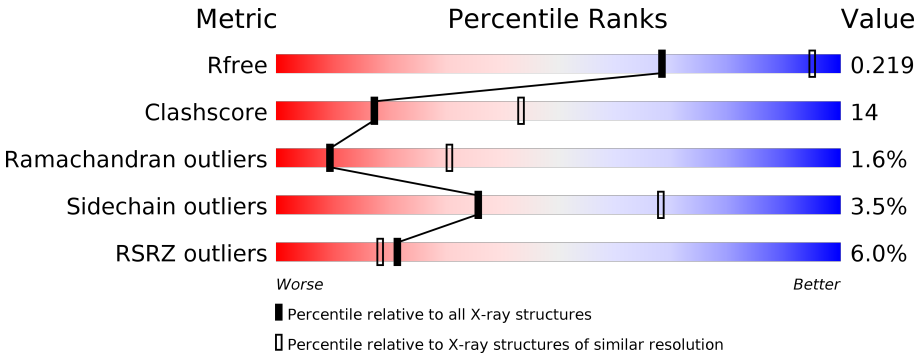
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	1158	8%, 62%, 31%, 6%
2	B	416	60%, 27%, 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11412 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1091	Total	C	N	O	S	0	0	0
			8563	5439	1443	1634	47			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	S	0	0	0
			2849	1775	507	548	19			

There are 20 discrepancies between the modelled and reference sequences:

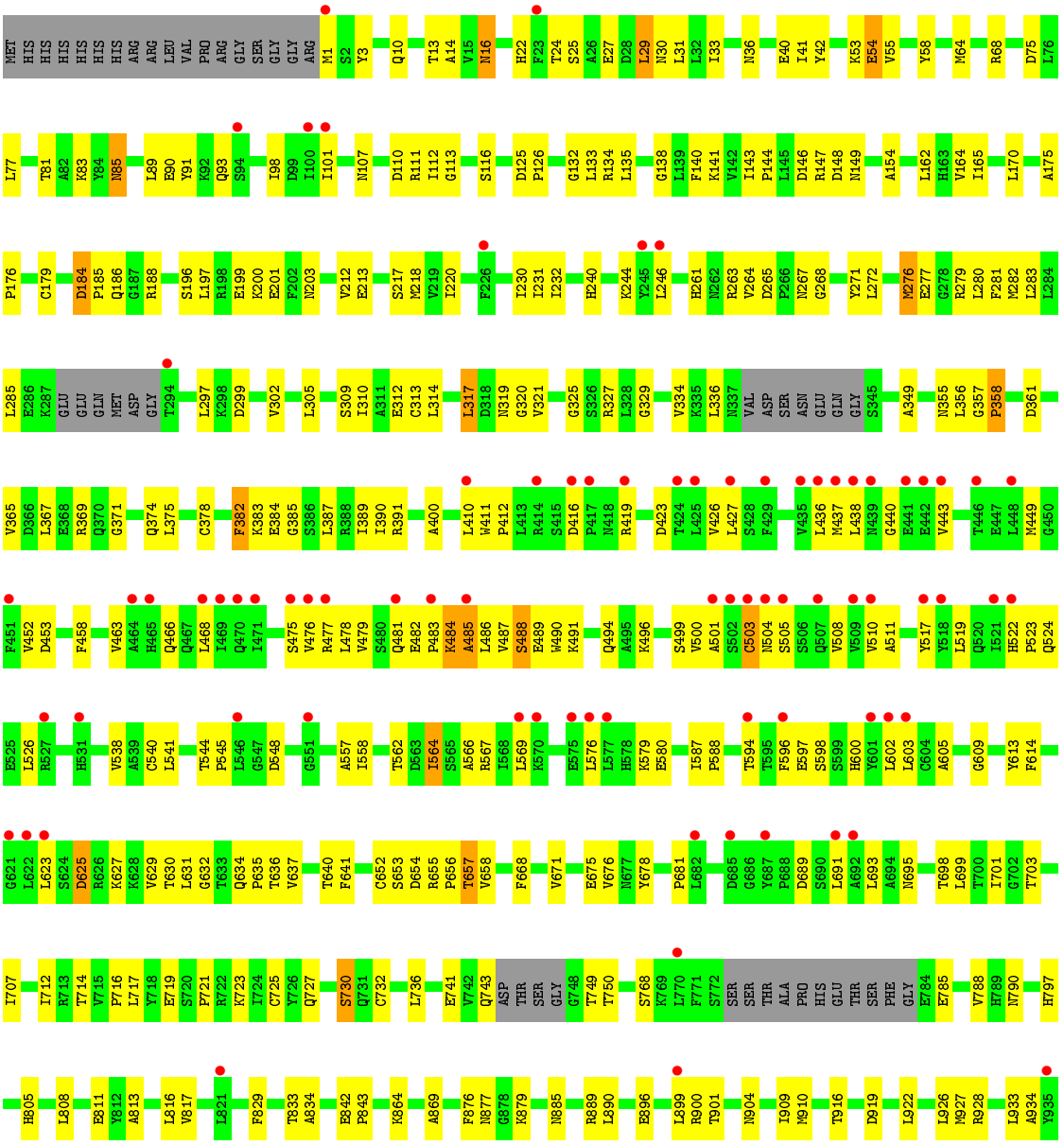
Chain	Residue	Modelled	Actual	Comment	Reference
B	397	LEU	-	expression tag	UNP Q13216
B	398	ALA	-	expression tag	UNP Q13216
B	399	LEU	-	expression tag	UNP Q13216
B	400	VAL	-	expression tag	UNP Q13216
B	401	PRO	-	expression tag	UNP Q13216
B	402	ARG	-	expression tag	UNP Q13216
B	403	GLY	-	expression tag	UNP Q13216
B	404	SER	-	expression tag	UNP Q13216
B	405	SER	-	expression tag	UNP Q13216
B	406	ALA	-	expression tag	UNP Q13216
B	407	HIS	-	expression tag	UNP Q13216
B	408	HIS	-	expression tag	UNP Q13216
B	409	HIS	-	expression tag	UNP Q13216
B	410	HIS	-	expression tag	UNP Q13216
B	411	HIS	-	expression tag	UNP Q13216
B	412	HIS	-	expression tag	UNP Q13216
B	413	HIS	-	expression tag	UNP Q13216
B	414	HIS	-	expression tag	UNP Q13216
B	415	HIS	-	expression tag	UNP Q13216
B	416	HIS	-	expression tag	UNP Q13216

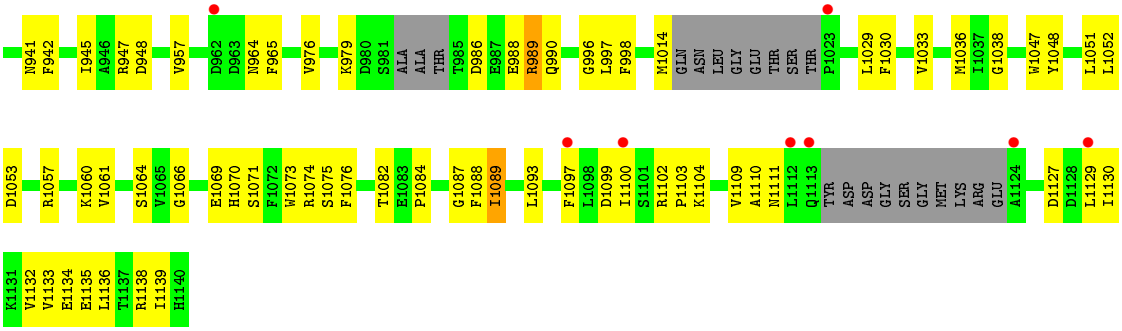
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: DNA damage-binding protein 1

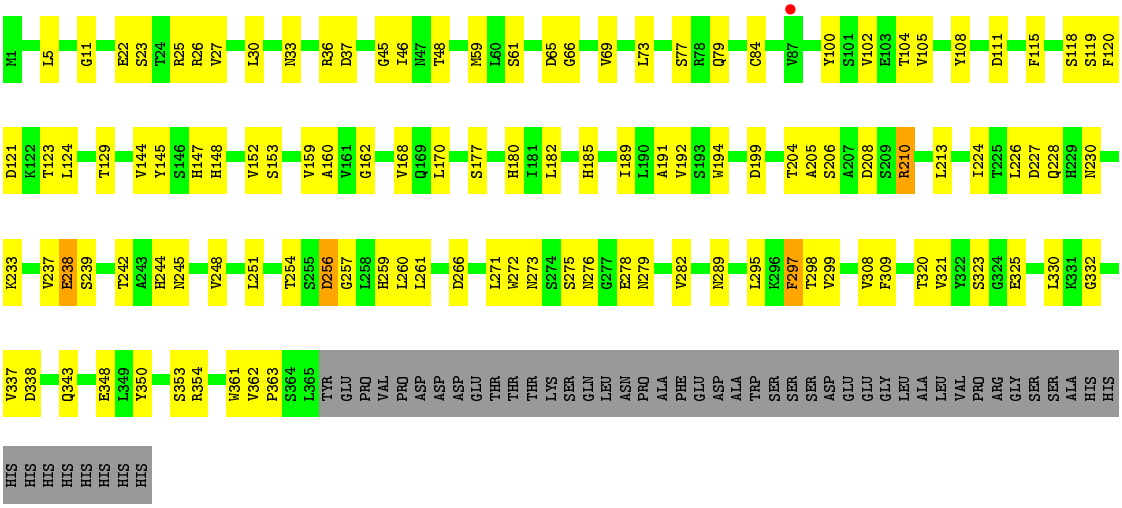
Chain A:





- Molecule 2: DNA excision repair protein ERCC-8

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.79Å 140.79Å 249.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.67 – 2.92 68.67 – 2.92	Depositor EDS
% Data completeness (in resolution range)	88.7 (68.67-2.92) 90.6 (68.67-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.193 , 0.245 0.181 , 0.219	Depositor DCC
R_{free} test set	2923 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	0.61	0/8717	0.57	0/11800
2	B	0.73	0/2908	0.59	0/3939
All	All	0.65	0/11625	0.57	0/15739

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	8563	0	8574	235	0
2	B	2849	0	2778	82	0
All	All	11412	0	11352	314	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 14.

All (314) 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)
2:B:30:LEU:HA	2:B:363:PRO:HA	1.42	1.01
2:B:152:VAL:HG11	2:B:199:ASP:HA	1.45	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:HIS:HD1	2:B:194:TRP:HD1	1.23	0.85
1:A:199:GLU:HG2	1:A:201:GLU:HB3	1.65	0.77
1:A:564:ILE:HG23	1:A:588:PRO:HD3	1.65	0.77
2:B:189:ILE:HG13	2:B:206:SER:HB2	1.67	0.75
1:A:218:MET:SD	1:A:261:HIS:HD2	2.10	0.75
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.68	0.74
1:A:468:LEU:HD13	1:A:481:GLN:HB3	1.70	0.73
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.68	0.73
1:A:1:MET:HA	1:A:964:ASN:ND2	2.05	0.71
1:A:813:ALA:HA	1:A:833:THR:HG22	1.73	0.71
1:A:93:GLN:HG3	1:A:98:ILE:HA	1.74	0.69
1:A:743:GLN:HA	1:A:749:THR:HG22	1.74	0.69
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.28	0.69
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.74	0.68
1:A:641:PHE:HB2	1:A:681:PRO:HB3	1.76	0.68
2:B:115:PHE:HD2	2:B:129:THR:HG22	1.57	0.68
1:A:790:ASN:HA	1:A:805:HIS:O	1.94	0.68
1:A:282:MET:HB2	1:A:305:LEU:HD21	1.77	0.66
2:B:191:ALA:HB3	2:B:205:ALA:HB3	1.77	0.65
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.78	0.65
1:A:40:GLU:HG3	1:A:54:GLU:HG2	1.78	0.64
1:A:1109:VAL:O	1:A:1111:ASN:N	2.31	0.64
1:A:41:ILE:HD12	1:A:53:LYS:HB3	1.80	0.64
1:A:385:GLY:HA3	1:A:719:GLU:O	1.97	0.64
2:B:189:ILE:HA	2:B:206:SER:HA	1.80	0.64
1:A:483:PRO:O	1:A:484:LYS:HB2	1.98	0.64
1:A:458:PHE:HB3	1:A:501:ALA:HB3	1.80	0.64
2:B:104:THR:HG1	2:B:147:HIS:HD1	1.46	0.63
1:A:218:MET:HB3	1:A:232:ILE:HB	1.80	0.63
1:A:1057:ARG:HA	1:A:1060:LYS:HD3	1.80	0.63
1:A:138:GLY:CA	1:A:162:LEU:HD23	2.29	0.63
2:B:185:HIS:ND1	2:B:206:SER:HB3	2.14	0.63
1:A:276:MET:HA	1:A:310:ILE:HG23	1.81	0.62
1:A:277:GLU:HB3	1:A:279:ARG:HD3	1.80	0.62
1:A:282:MET:O	1:A:302:VAL:HA	2.00	0.62
1:A:500:VAL:HG11	1:A:540:CYS:HA	1.82	0.61
2:B:271:LEU:HD23	2:B:282:VAL:HG21	1.81	0.61
1:A:714:THR:HG22	1:A:716:PRO:HD3	1.83	0.61
1:A:13:THR:HB	1:A:355:ASN:HA	1.82	0.61
2:B:206:SER:HB3	2:B:208:ASP:OD1	2.00	0.61
1:A:478:LEU:HG	1:A:487:VAL:HG23	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PHE:HB3	1:A:501:ALA:CB	2.31	0.60
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.82	0.60
2:B:337:VAL:HA	2:B:353:SER:HB2	1.84	0.60
2:B:45:GLY:HA3	2:B:354:ARG:HA	1.84	0.60
1:A:910:MET:HB3	1:A:926:LEU:HB2	1.84	0.60
1:A:14:ALA:HB1	1:A:327:ARG:HA	1.84	0.59
2:B:33:ASN:HB2	2:B:362:VAL:HG22	1.84	0.59
1:A:476:VAL:HB	1:A:490:TRP:HB3	1.84	0.59
1:A:24:THR:HG22	1:A:91:TYR:CE1	2.37	0.59
1:A:265:ASP:HB3	1:A:267:ASN:OD1	2.02	0.59
2:B:115:PHE:CD2	2:B:129:THR:HG22	2.36	0.59
1:A:486:LEU:HD21	1:A:489:GLU:HB2	1.83	0.59
1:A:614:PHE:CD2	1:A:623:LEU:HB3	2.38	0.59
1:A:477:ARG:HB3	1:A:486:LEU:HD11	1.84	0.58
1:A:81:THR:HG22	1:A:83:LYS:H	1.68	0.58
1:A:212:VAL:HG22	1:A:213:GLU:H	1.68	0.58
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.37	0.58
1:A:1134:GLU:HB3	1:A:1138:ARG:HH12	1.69	0.57
2:B:119:SER:OG	2:B:120:PHE:N	2.36	0.57
1:A:365:VAL:HG23	1:A:374:GLN:HB3	1.85	0.57
2:B:343:GLN:HB3	2:B:348:GLU:HB2	1.85	0.57
1:A:741:GLU:OE1	1:A:788:VAL:HG21	2.05	0.57
2:B:30:LEU:HD21	2:B:361:TRP:HB3	1.87	0.57
1:A:631:LEU:HD22	1:A:657:THR:HG21	1.87	0.57
1:A:695:ASN:HD21	1:A:698:THR:CG2	2.17	0.57
2:B:61:SER:OG	2:B:69:VAL:HB	2.05	0.56
1:A:478:LEU:HD23	1:A:488:SER:HB2	1.87	0.56
2:B:254:THR:O	2:B:257:GLY:N	2.37	0.56
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.70	0.56
2:B:26:ARG:O	2:B:363:PRO:HB3	2.06	0.56
2:B:254:THR:HG21	2:B:259:HIS:HB2	1.87	0.56
1:A:165:ILE:HG21	1:A:217:SER:HA	1.88	0.56
1:A:540:CYS:O	1:A:558:ILE:HA	2.06	0.56
2:B:152:VAL:HG13	2:B:153:SER:N	2.21	0.56
1:A:423:ASP:HA	1:A:438:LEU:HD11	1.88	0.56
2:B:226:LEU:HD23	2:B:272:TRP:CD2	2.40	0.56
1:A:133:LEU:HB3	1:A:135:LEU:HD21	1.89	0.55
1:A:389:ILE:O	1:A:712:ILE:HA	2.07	0.55
1:A:693:LEU:O	1:A:699:LEU:HD22	2.07	0.55
1:A:3:TYR:HD1	1:A:1087:GLY:HA2	1.72	0.55
2:B:213:LEU:HD22	2:B:224:ILE:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLY:HA2	2:B:102:VAL:HG23	1.88	0.55
1:A:16:ASN:HA	1:A:312:GLU:HG2	1.88	0.55
1:A:654:ASP:O	1:A:656:PRO:HD3	2.08	0.54
1:A:334:VAL:HA	1:A:349:ALA:HA	1.89	0.54
1:A:197:LEU:O	1:A:200:LYS:HG2	2.07	0.54
1:A:313:CYS:SG	1:A:325:GLY:HA3	2.47	0.54
1:A:374:GLN:HG3	1:A:391:ARG:HB3	1.90	0.54
1:A:329:GLY:HA3	1:A:384:GLU:HB3	1.90	0.53
1:A:630:THR:HB	1:A:797:HIS:NE2	2.23	0.53
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.89	0.53
1:A:449:MET:HG2	1:A:485:ALA:H	1.73	0.53
1:A:1132:VAL:HA	1:A:1135:GLU:HB3	1.90	0.53
2:B:124:LEU:HD21	2:B:159:VAL:HG11	1.90	0.53
1:A:736:LEU:HD13	1:A:813:ALA:HB1	1.90	0.53
1:A:879:LYS:HD3	1:A:890:LEU:HD21	1.89	0.53
1:A:400:ALA:HB3	1:A:701:ILE:HD12	1.90	0.52
1:A:1:MET:HA	1:A:964:ASN:HD21	1.73	0.52
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.92	0.52
1:A:864:LYS:HE2	1:A:899:LEU:O	2.09	0.52
1:A:112:ILE:HG13	1:A:113:GLY:H	1.73	0.52
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.09	0.51
1:A:196:SER:HB2	1:A:203:ASN:HD21	1.75	0.51
1:A:89:LEU:HD21	1:A:1066:GLY:HA2	1.93	0.51
1:A:691:LEU:HD23	1:A:693:LEU:HD21	1.92	0.51
1:A:466:GLN:HA	1:A:481:GLN:HE21	1.76	0.51
1:A:695:ASN:HD21	1:A:698:THR:HG23	1.75	0.51
1:A:33:ILE:HD12	1:A:42:TYR:CE2	2.46	0.51
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.92	0.50
2:B:276:ASN:HD21	2:B:278:GLU:HB2	1.76	0.50
1:A:138:GLY:HA2	1:A:162:LEU:HD23	1.92	0.50
1:A:519:LEU:HD23	1:A:526:LEU:HD22	1.93	0.50
1:A:909:ILE:HD12	1:A:928:ARG:CG	2.41	0.50
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.94	0.50
1:A:13:THR:O	1:A:355:ASN:HB2	2.11	0.50
1:A:630:THR:HB	1:A:797:HIS:CD2	2.46	0.50
1:A:896:GLU:HG2	1:A:896:GLU:O	2.12	0.50
1:A:113:GLY:HA2	2:B:256:ASP:HB3	1.92	0.50
2:B:33:ASN:ND2	2:B:36:ARG:HB2	2.27	0.50
1:A:676:VAL:HG11	1:A:693:LEU:HD22	1.94	0.50
1:A:1102:ARG:HB2	1:A:1103:PRO:HD3	1.93	0.50
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HE	1:A:164:VAL:HB	1.78	0.49
1:A:261:HIS:HA	1:A:272:LEU:O	2.13	0.49
1:A:602:LEU:HB3	1:A:614:PHE:HB2	1.94	0.49
1:A:603:LEU:HD23	1:A:613:TYR:HB3	1.93	0.49
1:A:64:MET:HG3	1:A:77:LEU:HD11	1.95	0.49
1:A:1048:TYR:CD2	1:A:1089:ILE:HD12	2.47	0.49
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.95	0.49
2:B:230:ASN:HD21	2:B:279:ASN:HB3	1.77	0.49
1:A:730:SER:HB3	1:A:732:CYS:SG	2.52	0.49
2:B:244:HIS:HB2	2:B:248:VAL:HG22	1.93	0.49
1:A:272:LEU:HD22	1:A:280:LEU:HD11	1.95	0.49
1:A:246:LEU:HD21	1:A:299:ASP:HA	1.93	0.49
1:A:1075:SER:OG	1:A:1084:PRO:HA	2.12	0.49
1:A:437:MET:O	1:A:438:LEU:HG	2.13	0.49
1:A:1076:PHE:O	1:A:1082:THR:HA	2.13	0.48
2:B:108:TYR:CD1	2:B:111:ASP:HB3	2.48	0.48
1:A:268:GLY:O	1:A:285:LEU:HD12	2.13	0.48
2:B:298:THR:OG1	2:B:299:VAL:N	2.47	0.48
1:A:282:MET:CB	1:A:305:LEU:HD21	2.43	0.48
1:A:605:ALA:HB1	1:A:636:THR:HB	1.96	0.48
2:B:108:TYR:HB3	2:B:111:ASP:O	2.14	0.48
2:B:152:VAL:CG1	2:B:153:SER:N	2.75	0.48
2:B:245:ASN:O	2:B:266:ASP:HB3	2.14	0.48
1:A:81:THR:HG22	1:A:83:LYS:N	2.28	0.48
2:B:168:VAL:HB	2:B:182:LEU:HB2	1.96	0.48
2:B:22:GLU:OE1	2:B:22:GLU:HA	2.14	0.48
1:A:558:ILE:HG22	1:A:567:ARG:O	2.12	0.48
1:A:566:ALA:HB3	1:A:580:GLU:HB3	1.96	0.48
2:B:37:ASP:O	2:B:84:CYS:N	2.47	0.48
2:B:298:THR:HG23	2:B:309:PHE:HD2	1.79	0.48
1:A:375:LEU:HD11	1:A:1029:LEU:HD13	1.97	0.47
1:A:785:GLU:HG3	1:A:785:GLU:O	2.14	0.47
1:A:426:VAL:C	1:A:427:LEU:HD12	2.34	0.47
1:A:463:VAL:HG12	1:A:505:SER:HA	1.96	0.47
2:B:237:VAL:C	2:B:239:SER:H	2.16	0.47
1:A:1033:VAL:HG11	2:B:11:GLY:HA3	1.96	0.47
1:A:479:VAL:HG13	1:A:485:ALA:O	2.14	0.47
2:B:48:THR:HG23	2:B:105:VAL:HG12	1.97	0.47
1:A:1047:TRP:O	1:A:1051:LEU:HG	2.15	0.47
1:A:53:LYS:HG3	1:A:55:VAL:HG13	1.97	0.47
2:B:330:LEU:HB3	2:B:361:TRP:CZ3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.96	0.47
1:A:613:TYR:CE1	1:A:627:LYS:HD2	2.49	0.47
2:B:297:PHE:HB2	2:B:309:PHE:O	2.15	0.47
1:A:596:PHE:O	1:A:598:SER:N	2.48	0.47
1:A:768:SER:HB3	1:A:808:LEU:HD11	1.97	0.47
1:A:90:GLU:HB3	1:A:101:ILE:HG13	1.96	0.47
1:A:636:THR:HA	1:A:652:CYS:O	2.14	0.46
1:A:327:ARG:O	1:A:358:PRO:HD3	2.15	0.46
2:B:237:VAL:HG12	2:B:238:GLU:N	2.30	0.46
2:B:30:LEU:HD21	2:B:361:TRP:CB	2.44	0.46
2:B:210:ARG:HG2	2:B:242:THR:HG22	1.98	0.46
2:B:185:HIS:CE1	2:B:206:SER:HB3	2.51	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.43	0.46
1:A:58:TYR:HD1	1:A:1073:TRP:CD1	2.33	0.46
1:A:361:ASP:OD2	1:A:723:LYS:HA	2.15	0.46
1:A:889:ARG:NE	1:A:904:ASN:OD1	2.41	0.46
2:B:118:SER:HB2	2:B:144:VAL:HG11	1.96	0.46
2:B:237:VAL:O	2:B:239:SER:N	2.49	0.46
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.16	0.46
2:B:205:ALA:HB2	2:B:251:LEU:HG	1.98	0.46
1:A:602:LEU:O	1:A:613:TYR:HA	2.16	0.46
2:B:46:ILE:O	2:B:338:ASP:HB2	2.16	0.46
1:A:933:LEU:HD11	1:A:942:PHE:HB3	1.98	0.46
2:B:348:GLU:HG2	2:B:362:VAL:HG12	1.98	0.46
1:A:133:LEU:HB2	1:A:141:LYS:HB3	1.97	0.45
1:A:605:ALA:CB	1:A:636:THR:O	2.64	0.45
2:B:104:THR:OG1	2:B:147:HIS:ND1	2.40	0.45
2:B:148:HIS:ND1	2:B:194:TRP:HD1	2.02	0.45
1:A:725:CYS:SG	1:A:816:LEU:HG	2.56	0.45
1:A:541:LEU:HA	1:A:557:ALA:O	2.16	0.45
1:A:900:ARG:NH1	1:A:901:THR:OG1	2.50	0.45
1:A:727:GLN:HE21	1:A:730:SER:HB2	1.81	0.45
2:B:147:HIS:HA	2:B:160:ALA:O	2.15	0.45
1:A:184:ASP:CB	1:A:185:PRO:HD2	2.45	0.45
1:A:382:PHE:HB2	1:A:383:LYS:H	1.67	0.45
1:A:629:VAL:O	1:A:631:LEU:HG	2.17	0.45
1:A:85:ASN:N	1:A:85:ASN:OD1	2.49	0.45
2:B:320:THR:O	2:B:321:VAL:C	2.55	0.45
1:A:279:ARG:HB3	1:A:281:PHE:HE1	1.82	0.45
1:A:1070:HIS:CE1	1:A:1093:LEU:HD22	2.52	0.45
2:B:170:LEU:HD12	2:B:180:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:SER:O	1:A:1075:SER:OG	2.24	0.45
1:A:629:VAL:HG21	1:A:668:PHE:CE2	2.51	0.45
1:A:569:LEU:HD23	1:A:576:LEU:HA	1.98	0.45
1:A:653:SER:O	1:A:675:GLU:HG3	2.16	0.45
1:A:979:LYS:NZ	1:A:989:ARG:HB3	2.32	0.45
2:B:145:TYR:HB2	2:B:162:GLY:O	2.17	0.45
1:A:280:LEU:HG	1:A:305:LEU:HD12	1.98	0.44
1:A:416:ASP:HB2	1:A:419:ARG:CZ	2.47	0.44
2:B:227:ASP:C	2:B:227:ASP:OD1	2.55	0.44
1:A:438:LEU:HA	1:A:443:VAL:HA	1.98	0.44
2:B:192:VAL:HG12	2:B:204:THR:HG22	2.00	0.44
1:A:934:ALA:HB3	1:A:945:ILE:HG12	1.99	0.44
1:A:244:LYS:NZ	1:A:297:LEU:O	2.37	0.44
2:B:23:SER:O	2:B:27:VAL:HG23	2.17	0.44
1:A:22:HIS:CE1	1:A:29:LEU:HD12	2.53	0.44
2:B:228:GLN:HA	2:B:272:TRP:CH2	2.52	0.44
1:A:579:LYS:O	1:A:579:LYS:HG3	2.17	0.44
1:A:1070:HIS:CE1	1:A:1074:ARG:HG3	2.51	0.44
1:A:410:LEU:HD23	1:A:427:LEU:HG	2.00	0.44
1:A:508:VAL:HB	1:A:519:LEU:HB2	1.98	0.44
1:A:988:GLU:O	1:A:990:GLN:N	2.51	0.44
2:B:273:ASN:HB3	2:B:278:GLU:H	1.82	0.44
1:A:1061:VAL:HG11	1:A:1104:LYS:HB3	2.00	0.44
1:A:138:GLY:HA3	1:A:162:LEU:HD23	2.00	0.44
1:A:523:PRO:O	1:A:524:GLN:HG2	2.18	0.44
1:A:864:LYS:HD3	1:A:899:LEU:HB2	1.99	0.44
2:B:237:VAL:O	2:B:238:GLU:HG2	2.18	0.43
1:A:31:LEU:HD13	1:A:317:LEU:HD21	2.00	0.43
2:B:77:SER:C	2:B:79:GLN:H	2.21	0.43
1:A:3:TYR:CD1	1:A:1087:GLY:HA2	2.53	0.43
1:A:110:ASP:O	1:A:111:ARG:C	2.57	0.43
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.18	0.43
1:A:965:PHE:O	1:A:976:VAL:HA	2.18	0.43
1:A:319:ASN:O	1:A:321:VAL:HG23	2.18	0.43
1:A:876:PHE:HD1	1:A:916:THR:HG21	1.82	0.43
2:B:289:ASN:ND2	2:B:295:LEU:HD22	2.34	0.43
1:A:170:LEU:HD11	1:A:179:CYS:HB2	2.01	0.43
1:A:609:GLY:HA2	1:A:636:THR:OG1	2.19	0.43
1:A:605:ALA:HB3	1:A:636:THR:O	2.18	0.43
1:A:165:ILE:HG13	1:A:188:ARG:HD3	2.01	0.42
2:B:59:MET:HB2	2:B:73:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HD22	2:B:350:TYR:CZ	2.54	0.42
1:A:877:ASN:ND2	1:A:919:ASP:OD1	2.52	0.42
1:A:817:VAL:O	1:A:829:PHE:HA	2.19	0.42
1:A:24:THR:HA	1:A:91:TYR:HD1	1.84	0.42
1:A:116:SER:HB3	1:A:134:ARG:NH2	2.34	0.42
2:B:254:THR:CG2	2:B:259:HIS:HB2	2.49	0.42
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.54	0.42
1:A:490:TRP:CH2	1:A:517:TYR:HB3	2.54	0.42
1:A:494:GLN:HB2	1:A:496:LYS:HE3	2.01	0.42
1:A:632:GLY:HA2	1:A:655:ARG:HB2	2.00	0.42
1:A:68:ARG:NE	1:A:75:ASP:OD1	2.52	0.42
1:A:10:GLN:O	1:A:1036:MET:HG2	2.18	0.42
1:A:483:PRO:O	1:A:484:LYS:CB	2.67	0.42
1:A:1053:ASP:O	1:A:1057:ARG:HG3	2.19	0.42
1:A:490:TRP:CE2	1:A:519:LEU:HD11	2.54	0.42
2:B:33:ASN:C	2:B:33:ASN:OD1	2.58	0.42
1:A:132:GLY:HA3	1:A:140:PHE:CZ	2.55	0.42
1:A:811:GLU:HG3	1:A:833:THR:HB	2.00	0.42
1:A:220:ILE:HG12	1:A:261:HIS:NE2	2.34	0.42
1:A:1129:LEU:O	1:A:1133:VAL:HG23	2.20	0.41
1:A:132:GLY:HA3	1:A:140:PHE:HZ	1.84	0.41
1:A:411:TRP:HA	1:A:412:PRO:HD3	1.91	0.41
1:A:641:PHE:CB	1:A:681:PRO:HB3	2.48	0.41
2:B:185:HIS:ND1	2:B:206:SER:CB	2.83	0.41
1:A:175:ALA:O	1:A:176:PRO:C	2.58	0.41
1:A:277:GLU:CD	1:A:279:ARG:HH11	2.24	0.41
1:A:329:GLY:O	1:A:355:ASN:ND2	2.48	0.41
2:B:33:ASN:OD1	2:B:36:ARG:N	2.53	0.41
1:A:147:ARG:O	1:A:149:ASN:N	2.52	0.41
1:A:30:ASN:HA	1:A:42:TYR:O	2.20	0.41
1:A:927:MET:SD	2:B:26:ARG:NH1	2.94	0.41
2:B:22:GLU:OE1	2:B:25:ARG:NE	2.48	0.41
1:A:358:PRO:HA	1:A:1033:VAL:O	2.20	0.41
1:A:125:ASP:HA	1:A:126:PRO:HD2	1.79	0.41
1:A:264:VAL:CG2	1:A:272:LEU:HG	2.50	0.41
1:A:707:ILE:O	1:A:707:ILE:HG13	2.21	0.41
2:B:320:THR:OG1	2:B:325:GLU:N	2.54	0.41
1:A:3:TYR:HB3	1:A:1048:TYR:CD2	2.55	0.41
1:A:371:GLY:O	1:A:1014:MET:HG3	2.21	0.41
1:A:453:ASP:OD1	1:A:453:ASP:N	2.52	0.41
2:B:65:ASP:N	2:B:65:ASP:OD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HB3	1:A:281:PHE:CE1	2.55	0.41
1:A:500:VAL:H	1:A:511:ALA:HB3	1.84	0.41
1:A:27:GLU:HA	1:A:27:GLU:OE1	2.21	0.41
1:A:383:LYS:HE3	1:A:384:GLU:OE2	2.21	0.41
1:A:482:GLU:HB3	1:A:483:PRO:HD3	2.02	0.41
1:A:945:ILE:HA	1:A:945:ILE:HD13	1.93	0.41
1:A:947:ARG:HG2	1:A:948:ASP:N	2.36	0.41
1:A:320:GLY:O	1:A:336:LEU:HG	2.20	0.41
1:A:637:VAL:HG11	1:A:678:TYR:CD2	2.55	0.41
1:A:658:VAL:HG23	1:A:671:VAL:CG2	2.51	0.41
1:A:996:GLY:O	1:A:997:LEU:HD23	2.21	0.41
1:A:998:PHE:HB2	1:A:1088:PHE:CD2	2.56	0.41
1:A:58:TYR:CE2	1:A:1064:SER:HB2	2.56	0.41
2:B:121:ASP:O	2:B:123:THR:HG23	2.21	0.41
1:A:271:TYR:HB2	1:A:283:LEU:HD23	2.02	0.41
1:A:230:ILE:HD13	1:A:283:LEU:HD21	2.01	0.41
1:A:329:GLY:HA3	1:A:384:GLU:CB	2.51	0.41
1:A:503:CYS:SG	1:A:504:ASN:N	2.93	0.41
1:A:811:GLU:HA	1:A:834:ALA:O	2.21	0.41
1:A:143:ILE:HA	1:A:144:PRO:HD3	1.93	0.40
1:A:276:MET:HA	1:A:310:ILE:CG2	2.49	0.40
1:A:475:SER:HB3	1:A:491:LYS:HD2	2.03	0.40
1:A:83:LYS:O	1:A:107:ASN:ND2	2.47	0.40
2:B:261:LEU:HD13	2:B:308:VAL:HG21	2.03	0.40
2:B:226:LEU:HD23	2:B:272:TRP:CG	2.57	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	1075/1158 (93%)	941 (88%)	114 (11%)	20 (2%)	8 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	363/416 (87%)	326 (90%)	34 (9%)	3 (1%)	19 49
All	All	1438/1574 (91%)	1267 (88%)	148 (10%)	23 (2%)	9 31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	ASP
1	A	1110	ALA
1	A	484	LYS
1	A	544	THR
1	A	545	PRO
1	A	548	ASP
1	A	689	ASP
1	A	989	ARG
1	A	36	ASN
1	A	148	ASP
1	A	317	LEU
1	A	499	SER
1	A	597	GLU
2	B	332	GLY
1	A	184	ASP
1	A	357	GLY
1	A	485	ALA
2	B	238	GLU
1	A	369	ARG
2	B	177	SER
1	A	358	PRO
1	A	440	GLY
1	A	564	ILE

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	960/1014 (95%)	924 (96%)	36 (4%)	33 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	320/365 (88%)	311 (97%)	9 (3%)	43 75
All	All	1280/1379 (93%)	1235 (96%)	45 (4%)	36 68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	25	SER
1	A	29	LEU
1	A	54	GLU
1	A	85	ASN
1	A	146	ASP
1	A	186	GLN
1	A	276	MET
1	A	309	SER
1	A	314	LEU
1	A	356	LEU
1	A	367	LEU
1	A	382	PHE
1	A	390	ILE
1	A	436	LEU
1	A	452	VAL
1	A	488	SER
1	A	503	CYS
1	A	510	VAL
1	A	562	THR
1	A	587	ILE
1	A	594	THR
1	A	600	HIS
1	A	625	ASP
1	A	640	THR
1	A	657	THR
1	A	703	THR
1	A	730	SER
1	A	750	THR
1	A	842	GLU
1	A	885	ASN
1	A	941	ASN
1	A	986	ASP
1	A	1069	GLU
1	A	1089	ILE
1	A	1099	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	5	LEU
2	B	100	TYR
2	B	210	ARG
2	B	233	LYS
2	B	256	ASP
2	B	260	LEU
2	B	275	SER
2	B	297	PHE
2	B	323	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	203	ASN
1	A	261	HIS
1	A	481	GLN
1	A	497	ASN
1	A	695	ASN
1	A	711	HIS
1	A	727	GLN
1	A	743	GLN
1	A	964	ASN
1	A	1070	HIS
2	B	79	GLN
2	B	133	GLN
2	B	180	HIS
2	B	187	GLN
2	B	249	ASN
2	B	289	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 carbohydrates 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	1091/1158 (94%)	0.36	87 (7%) 12 10	48, 92, 142, 175	0
2	B	365/416 (87%)	-0.12	1 (0%) 94 94	50, 74, 101, 145	0
All	All	1456/1574 (92%)	0.24	88 (6%) 21 18	48, 86, 138, 175	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	LEU	5.6
1	A	417	PRO	5.1
1	A	546	LEU	5.0
1	A	1113	GLN	4.9
1	A	485	ALA	4.7
1	A	622	LEU	4.5
1	A	521	ILE	4.4
1	A	481	GLN	4.1
1	A	1023	PRO	3.9
1	A	1112	LEU	3.9
1	A	1124	ALA	3.9
1	A	438	LEU	3.8
1	A	435	VAL	3.8
1	A	443	VAL	3.7
1	A	575	GLU	3.7
1	A	100	ILE	3.6
1	A	601	TYR	3.5
1	A	442	GLU	3.5
1	A	682	LEU	3.5
1	A	245	TYR	3.4
1	A	770	LEU	3.4
1	A	1	MET	3.3
1	A	507	GLN	3.3
1	A	451	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	502	SER	3.3
1	A	471	ILE	3.3
1	A	425	LEU	3.3
1	A	503	CYS	3.3
1	A	594	THR	3.2
1	A	531	HIS	3.2
1	A	504	ASN	3.2
1	A	419	ARG	3.1
1	A	437	MET	3.0
1	A	517	TYR	3.0
1	A	468	LEU	3.0
1	A	505	SER	3.0
1	A	603	LEU	3.0
1	A	294	THR	3.0
1	A	685	ASP	3.0
1	A	1129	LEU	2.9
1	A	1097	PHE	2.9
1	A	821	LEU	2.9
1	A	429	PHE	2.8
1	A	691	LEU	2.8
1	A	596	PHE	2.8
1	A	246	LEU	2.7
1	A	469	ILE	2.7
1	A	501	ALA	2.7
1	A	441	GLU	2.7
1	A	436	LEU	2.6
1	A	935	TYR	2.6
1	A	623	LEU	2.6
1	A	424	THR	2.6
1	A	569	LEU	2.6
1	A	1100	ILE	2.5
1	A	621	GLY	2.5
1	A	410	LEU	2.5
1	A	416	ASP	2.5
1	A	518	TYR	2.5
1	A	476	VAL	2.5
1	A	226	PHE	2.5
1	A	551	GLY	2.4
1	A	509	VAL	2.4
1	A	962	ASP	2.4
1	A	94	SER	2.4
1	A	414	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	2.3
1	A	527	ARG	2.3
1	A	427	LEU	2.3
1	A	23	PHE	2.3
1	A	470	GLN	2.3
1	A	475	SER	2.3
1	A	510	VAL	2.3
1	A	477	ARG	2.3
1	A	522	HIS	2.3
1	A	439	ASN	2.2
2	B	87	VAL	2.2
1	A	464	ALA	2.2
1	A	577	LEU	2.2
1	A	446	THR	2.2
1	A	483	PRO	2.2
1	A	448	LEU	2.2
1	A	465	HIS	2.1
1	A	602	LEU	2.1
1	A	899	LEU	2.1
1	A	687	TYR	2.1
1	A	570	LYS	2.1
1	A	692	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.