



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 6FCV / pdb_00006fcv
Title : Structure of the human DDB1-CSA complex
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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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

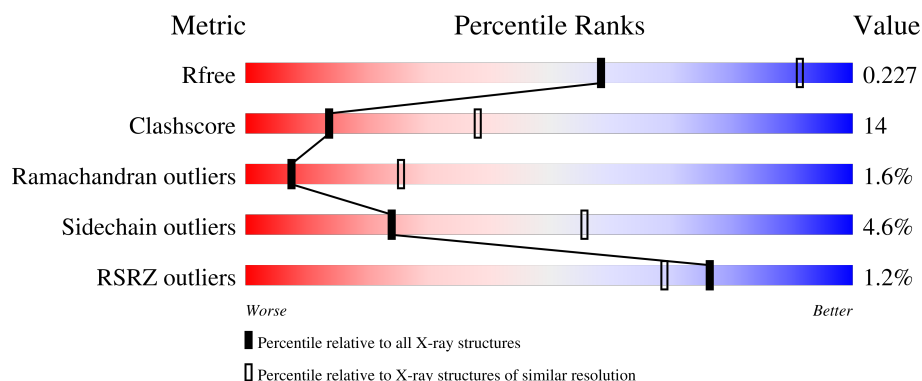
1 Overall quality at a glance

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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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 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 $\leq 5\%$. 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	
2	B	416	

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
			Total	C	N	O	S			
1	A	1091	8563	5439	1443	1634	47	0	0	0

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
			Total	C	N	O	S			
2	B	365	2849	1775	507	548	19	0	0	0

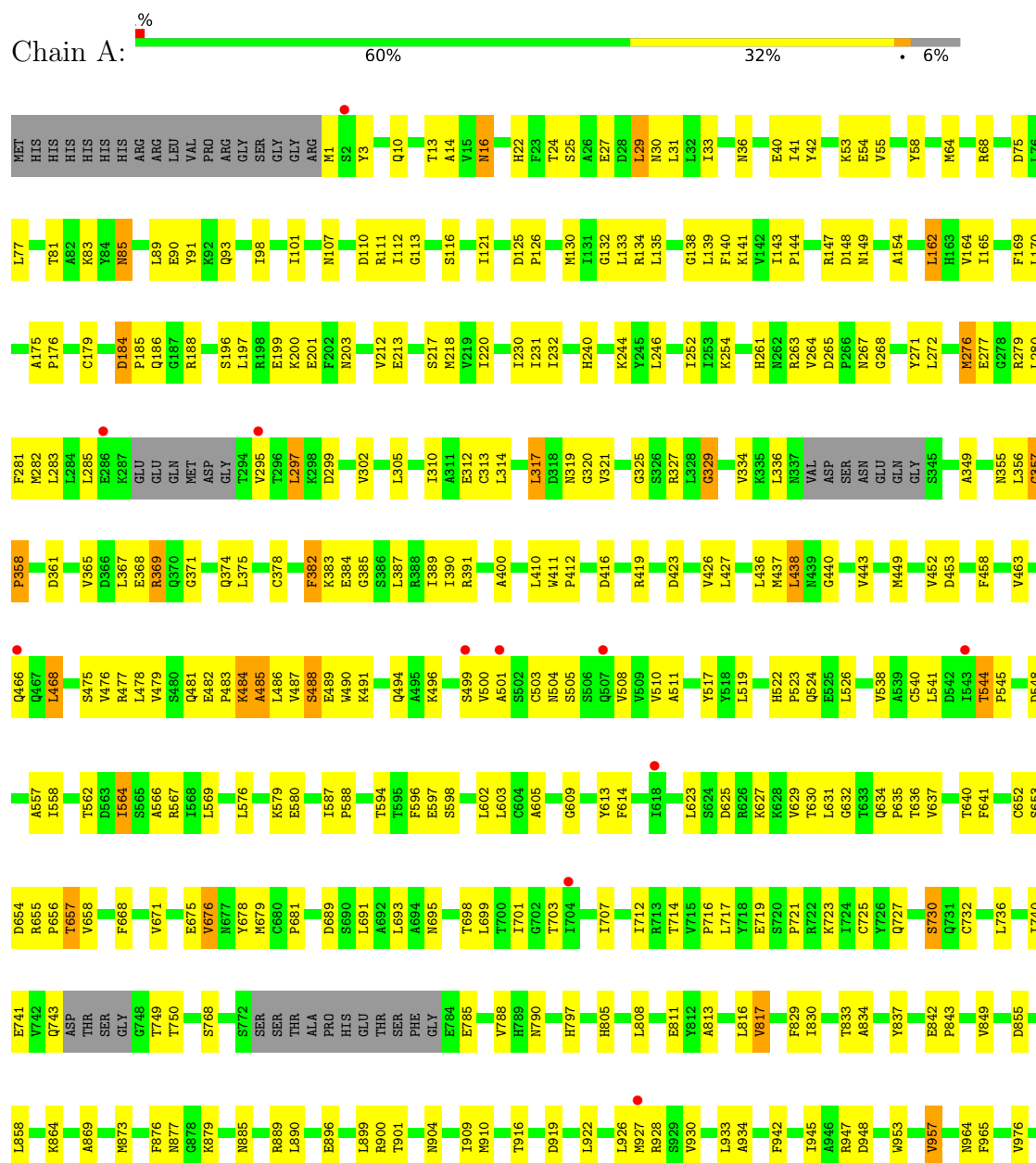
There are 20 discrepancies between the modelled and reference sequences:

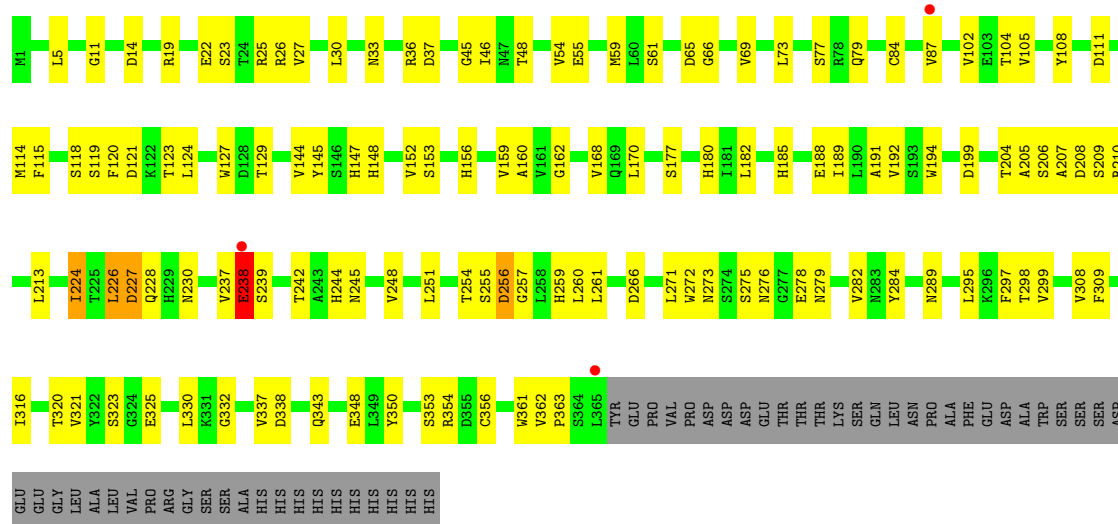
Chain	Residue	Modelled	Actual	Comment	Reference
B	397	LEU	-	expression tag	UNP Q13216
B	398	ALA	-	expression tag	UNP Q13216
B	399	LEU	-	expression tag	UNP Q13216
B	400	VAL	-	expression tag	UNP Q13216
B	401	PRO	-	expression tag	UNP Q13216
B	402	ARG	-	expression tag	UNP Q13216
B	403	GLY	-	expression tag	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, 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: DNA damage-binding protein 1





4 Data and refinement statistics

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) 90.1 (68.67-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.193 , 0.245 (Not available) , 0.227	Depositor DCC
R_{free} test set	2923 reflections (4.66%)	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)	0.32 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.81	3/8717 (0.0%)	0.75	5/11800 (0.0%)
2	B	0.95	2/2908 (0.1%)	0.75	2/3939 (0.1%)
All	All	0.85	5/11625 (0.0%)	0.75	7/15739 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLY	C-O	-6.58	1.18	1.24
2	B	226	LEU	C-O	-5.71	1.17	1.24
2	B	284	TYR	N-CA	5.31	1.53	1.46
1	A	999	HIS	CA-C	-5.21	1.46	1.52
1	A	139	LEU	C-O	5.08	1.29	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	THR	CA-C-N	5.59	126.83	119.84
1	A	544	THR	C-N-CA	5.59	126.83	119.84
2	B	14	ASP	CA-C-N	5.39	124.58	118.97
2	B	14	ASP	C-N-CA	5.39	124.58	118.97
1	A	837	TYR	CA-C-N	5.10	126.21	119.84
1	A	837	TYR	C-N-CA	5.10	126.21	119.84
1	A	930	VAL	N-CA-C	5.03	115.51	108.17

There are no chirality outliers.

There are no planarity outliers.

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	8563	0	8574	244	0
2	B	2849	0	2778	89	0
All	All	11412	0	11352	329	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 (329) 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
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
2:B:148:HIS:HD1	2:B:194:TRP:CD1	2.05	0.74
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:830:ILE:HG22	1:A:873:MET:HE1	1.72	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:41:ILE:HD12	1:A:53:LYS:HB3	1.80	0.64
1:A:1109:VAL:O	1:A:1111:ASN:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PHE:HB3	1:A:501:ALA:HB3	1.80	0.64
1:A:483:PRO:O	1:A:484:LYS:HB2	1.98	0.63
1:A:218:MET:HB3	1:A:232:ILE:HB	1.80	0.63
1:A:138:GLY:CA	1:A:162:LEU:HD23	2.29	0.63
1:A:1057:ARG:HA	1:A:1060:LYS:HD3	1.80	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
1:A:641:PHE:HB3	1:A:679:MET:HE1	1.83	0.61
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:45:GLY:HA3	2:B:354:ARG:HA	1.84	0.60
2:B:337:VAL:HA	2:B:353:SER:HB2	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:24:THR:HG22	1:A:91:TYR:CE1	2.37	0.59
1:A:476:VAL:HB	1:A:490:TRP:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:426:VAL:C	1:A:427:LEU:HD12	2.34	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
2:B:237:VAL:C	2:B:239:SER:H	2.16	0.52
1:A:112:ILE:HG13	1:A:113:GLY:H	1.73	0.52
1:A:89:LEU:HD21	1:A:1066:GLY:HA2	1.93	0.51
1:A:196:SER:HB2	1:A:203:ASN:HD21	1.75	0.51
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:MET:HE2	1:A:169:PHE:CZ	2.45	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: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:1127:ASP:HA	1:A:1130:ILE:HD12	1.94	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
1:A:134:ARG:HE	1:A:164:VAL:HB	1.78	0.49
2:B:320:THR:O	2:B:321:VAL:C	2.55	0.49
1:A:64:MET:HG3	1:A:77:LEU:HD11	1.95	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:387:LEU:HG	1:A:717:LEU:HD11	1.95	0.49
1:A:1048:TYR:CD2	1:A:1089:ILE:HD12	2.47	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:130:MET:HE2	1:A:169:PHE:HZ	1.78	0.49
1:A:246:LEU:HD21	1:A:299:ASP:HA	1.93	0.49
1:A:437:MET:O	1:A:438:LEU:HG	2.13	0.49
1:A:1075:SER:OG	1:A:1084:PRO:HA	2.12	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:896:GLU:O	1:A:896:GLU:HG2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:GLU:HA	2:B:22:GLU:OE1	2.14	0.48
2:B:168:VAL:HB	2:B:182:LEU:HB2	1.96	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:227:ASP:C	2:B:227:ASP:OD1	2.55	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:O	1:A:785:GLU:HG3	2.14	0.47
1:A:463:VAL:HG12	1:A:505:SER:HA	1.96	0.47
1:A:479:VAL:HG13	1:A:485:ALA:O	2.14	0.47
1:A:1033:VAL:HG11	2:B:11:GLY:HA3	1.96	0.47
2:B:48:THR:HG23	2:B:105:VAL:HG12	1.97	0.47
1:A:53:LYS:HG3	1:A:55:VAL:HG13	1.97	0.47
1:A:1047:TRP:O	1:A:1051:LEU:HG	2.15	0.47
2:B:330:LEU:HB3	2:B:361:TRP:CZ3	2.49	0.47
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
2:B:77:SER:C	2:B:79:GLN:H	2.21	0.47
1:A:768:SER:HB3	1:A:808:LEU:HD11	1.97	0.47
2:B:33:ASN:C	2:B:33:ASN:OD1	2.58	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:30:LEU:HD21	2:B:361:TRP:CB	2.44	0.46
2:B:237:VAL:HG12	2:B:238:GLU:N	2.30	0.46
1:A:953:TRP:CD1	2:B:19:ARG:HE	2.33	0.46
2:B:210:ARG:HG2	2:B:242:THR:HG22	1.98	0.46
1:A:175:ALA:O	1:A:176:PRO:C	2.58	0.46
1:A:277:GLU:CD	1:A:279:ARG:HH11	2.24	0.46
2:B:185:HIS:CE1	2:B:206:SER:HB3	2.51	0.46
1:A:58:TYR:HD1	1:A:1073:TRP:CD1	2.33	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.43	0.46
1:A:110:ASP:O	1:A:111:ARG:C	2.57	0.46
1:A:361:ASP:OD2	1:A:723:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:85:ASN:OD1	1:A:85:ASN:N	2.49	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:279:ARG:HB3	1:A:281:PHE:HE1	1.82	0.45
2:B:354:ARG:C	2:B:356:CYS:H	2.24	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
1:A:357:GLY:O	1:A:358:PRO:C	2.58	0.45
1:A:629:VAL:HG21	1:A:668:PHE:CE2	2.51	0.45
1:A:1071:SER:O	1:A:1075:SER:OG	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:O	1:A:579:LYS:HG3	2.17	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
1:A:1070:HIS:CE1	1:A:1074:ARG:HG3	2.51	0.44
2:B:273:ASN:HB3	2:B:278:GLU:H	1.82	0.44
1:A:138:GLY:HA3	1:A:162:LEU:HD23	2.00	0.44
1:A:282:MET:HE2	1:A:305:LEU:HD11	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
1:A:1061:VAL:HG11	1:A:1104:LYS:HB3	2.00	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
1:A:3:TYR:CD1	1:A:1087:GLY:HA2	2.53	0.43
1:A:641:PHE:CB	1:A:679:MET:HE1	2.46	0.43
1:A:965:PHE:O	1:A:976:VAL:HA	2.18	0.43
1:A:1136:LEU:O	1:A:1139:ILE:HG12	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:605:ALA:HB3	1:A:636:THR:O	2.18	0.43
1:A:609:GLY:HA2	1:A:636:THR:OG1	2.19	0.43
2:B:104:THR:OG1	2:B:147:HIS:ND1	2.40	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
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:24:THR:HA	1:A:91:TYR:HD1	1.84	0.42
1:A:368:GLU:O	1:A:369:ARG:C	2.62	0.42
1:A:817:VAL:O	1:A:829:PHE:HA	2.19	0.42
1:A:116:SER:HB3	1:A:134:ARG:NH2	2.34	0.42
2:B:33:ASN:CG	2:B:36:ARG:HB2	2.44	0.42
2:B:254:THR:CG2	2:B:259:HIS:HB2	2.49	0.42
1:A:68:ARG:NE	1:A:75:ASP:OD1	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:TRP:CE2	1:A:519:LEU:HD11	2.54	0.42
1:A:1053:ASP:O	1:A:1057:ARG:HG3	2.19	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: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
1:A:1129:LEU:O	1:A:1133:VAL:HG23	2.20	0.41
2:B:185:HIS:ND1	2:B:206:SER:CB	2.83	0.41
2:B:254:THR:O	2:B:255:SER:C	2.62	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:30:ASN:HA	1:A:42:TYR:O	2.20	0.41
1:A:147:ARG:O	1:A:149:ASN:N	2.52	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: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:358:PRO:HA	1:A:1033:VAL:O	2.20	0.41
2:B:207:ALA:C	2:B:209:SER:H	2.28	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:OD1	2:B:65:ASP:N	2.54	0.41
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:OE1	1:A:27:GLU:HA	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:HD13	1:A:945:ILE:HA	1.93	0.41
1:A:947:ARG:HG2	1:A:948:ASP:N	2.36	0.41
1:A:58:TYR:CE2	1:A:1064:SER:HB2	2.56	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
2:B:121:ASP:O	2:B:123:THR:HG23	2.21	0.41
2:B:156:HIS:ND1	2:B:156:HIS:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD13	1:A:283:LEU:HD21	2.01	0.41
1:A:271:TYR:HB2	1:A:283:LEU:HD23	2.02	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
2:B:114:MET:HE2	2:B:127:TRP:O	2.21	0.40
1:A:83:LYS:O	1:A:107:ASN:ND2	2.47	0.40
1:A:475:SER:HB3	1:A:491:LYS:HD2	2.03	0.40
1:A:707:ILE:O	1:A:707:ILE:HG13	2.21	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%)	6	22
2	B	363/416 (87%)	326 (90%)	34 (9%)	3 (1%)	16	43
All	All	1438/1574 (91%)	1267 (88%)	148 (10%)	23 (2%)	7	25

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	914 (95%)	46 (5%)	23	54
2	B	320/365 (88%)	307 (96%)	13 (4%)	27	60
All	All	1280/1379 (93%)	1221 (95%)	59 (5%)	24	56

All (59) 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	85	ASN
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	162	LEU
1	A	186	GLN
1	A	252	ILE
1	A	254	LYS
1	A	276	MET
1	A	295	VAL
1	A	297	LEU
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	438	LEU
1	A	452	VAL
1	A	468	LEU
1	A	488	SER
1	A	510	VAL
1	A	562	THR
1	A	587	ILE
1	A	594	THR
1	A	640	THR
1	A	657	THR
1	A	676	VAL
1	A	703	THR
1	A	730	SER
1	A	740	ILE
1	A	750	THR
1	A	817	VAL
1	A	842	GLU
1	A	849	VAL
1	A	855	ASP
1	A	858	LEU
1	A	885	ASN
1	A	957	VAL
1	A	986	ASP
1	A	1050	LEU
1	A	1069	GLU
1	A	1078	THR
1	A	1089	ILE
1	A	1099	ASP
2	B	5	LEU

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Mol	Chain	Res	Type
2	B	54	VAL
2	B	55	GLU
2	B	87	VAL
2	B	188	GLU
2	B	224	ILE
2	B	227	ASP
2	B	238	GLU
2	B	256	ASP
2	B	260	LEU
2	B	275	SER
2	B	316	ILE
2	B	323	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	156	ASN
1	A	183	GLN
1	A	203	ASN
1	A	240	HIS
1	A	261	HIS
1	A	262	ASN
1	A	465	HIS
1	A	481	GLN
1	A	695	ASN
1	A	711	HIS
1	A	727	GLN
1	A	743	GLN
1	A	797	HIS
1	A	852	GLN
1	A	908	ASN
1	A	1070	HIS
2	B	9	GLN
2	B	110	HIS
2	B	133	GLN
2	B	180	HIS
2	B	187	GLN
2	B	249	ASN
2	B	289	ASN
2	B	326	GLN
2	B	343	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	0.10	14 (1%) 75 67	48, 92, 142, 175	0
2	B	365/416 (87%)	-0.17	3 (0%) 82 76	50, 74, 101, 145	0
All	All	1456/1574 (92%)	0.03	17 (1%) 76 69	48, 86, 138, 175	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	VAL	3.2
2	B	87	VAL	3.2
2	B	365	LEU	3.1
1	A	704	ILE	2.8
1	A	1008	CYS	2.7
1	A	1054	MET	2.7
1	A	1023	PRO	2.5
1	A	501	ALA	2.5
2	B	238	GLU	2.5
1	A	286	GLU	2.4
1	A	618	ILE	2.4
1	A	927	MET	2.3
1	A	543	ILE	2.3
1	A	2	SER	2.3
1	A	499	SER	2.3
1	A	466	GLN	2.2
1	A	507	GLN	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 oligosaccharides 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.