Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 12:11 AM JST

PDB ID	:	5YIK
Title	:	Structure of a Legionella effector with its substrate
Authors	:	Feng, Y.; Dong, Y.; Liu, Z.
Deposited on	:	2017-10-05
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

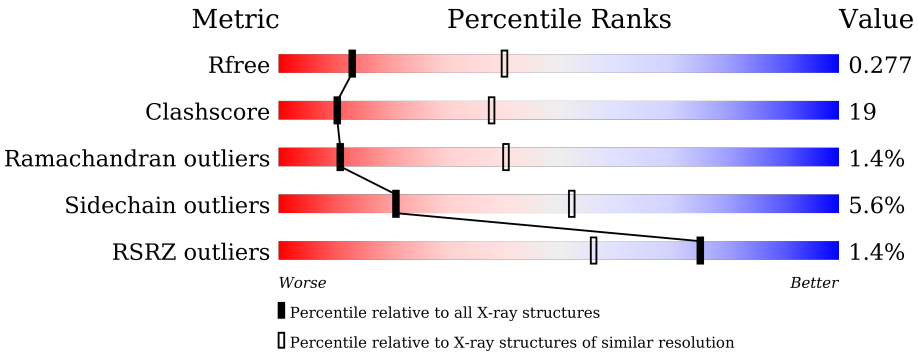
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	968	69% 28%
2	C	78	12% 31% 37% 23% 9%
2	D	78	3% 69% 24%
2	F	78	3% 77% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9381 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 SdeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	0	0
			7601	4767	1330	1477	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1191	LEU	-	expression tag	UNP Q6RCR0
A	1192	GLU	-	expression tag	UNP Q6RCR0
A	1193	HIS	-	expression tag	UNP Q6RCR0
A	1194	HIS	-	expression tag	UNP Q6RCR0
A	1195	HIS	-	expression tag	UNP Q6RCR0
A	1196	HIS	-	expression tag	UNP Q6RCR0
A	1197	HIS	-	expression tag	UNP Q6RCR0
A	1198	HIS	-	expression tag	UNP Q6RCR0

- Molecule 2 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	71	Total	C	N	O	S	0	0	0
			563	356	94	112	1			
2	D	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	F	78	Total	C	N	O	S	0	0	0
			616	387	109	119	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP P0CG47
C	0	HIS	-	expression tag	UNP P0CG47
D	-1	SER	-	expression tag	UNP P0CG47
D	0	HIS	-	expression tag	UNP P0CG47

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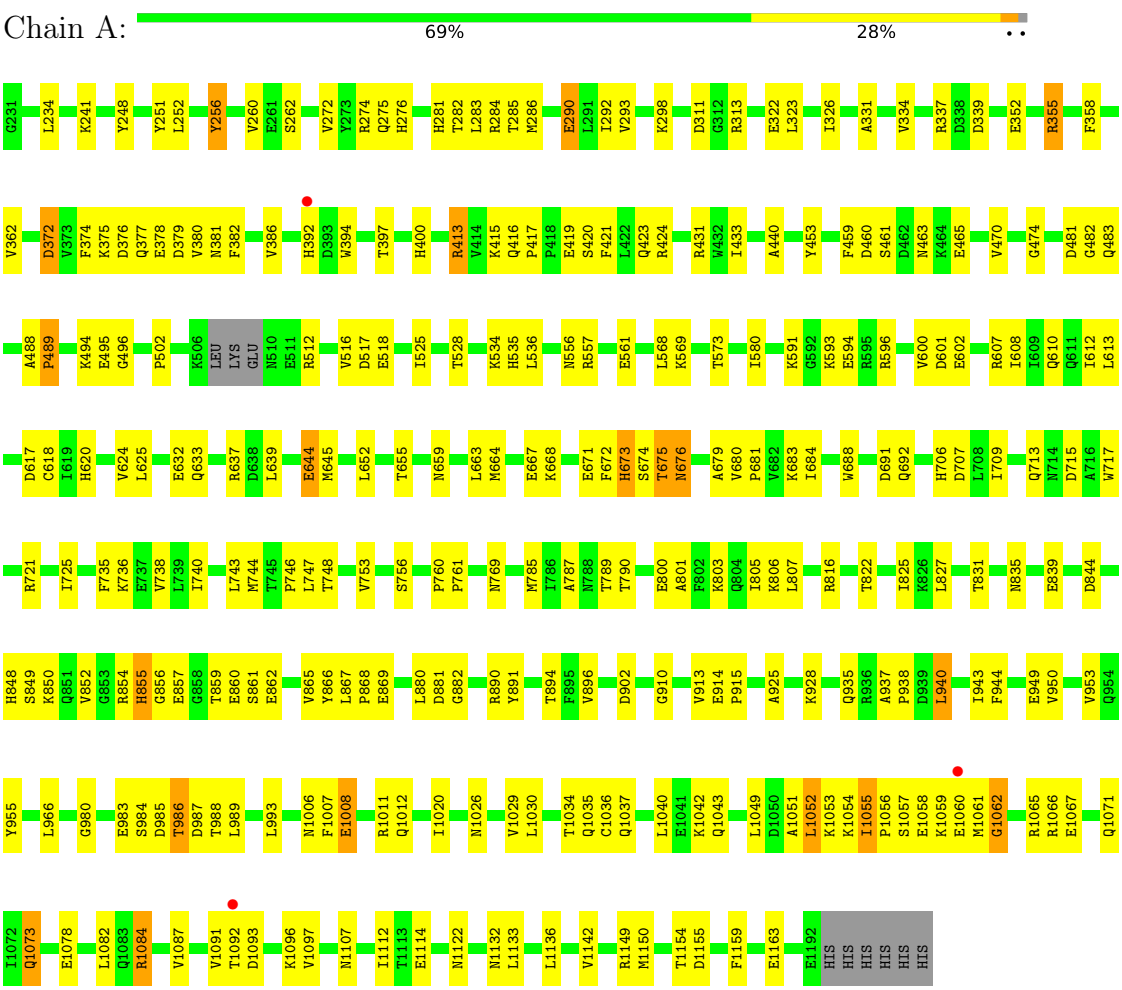
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	SER	-	expression tag	UNP P0CG47
F	0	HIS	-	expression tag	UNP P0CG47

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.

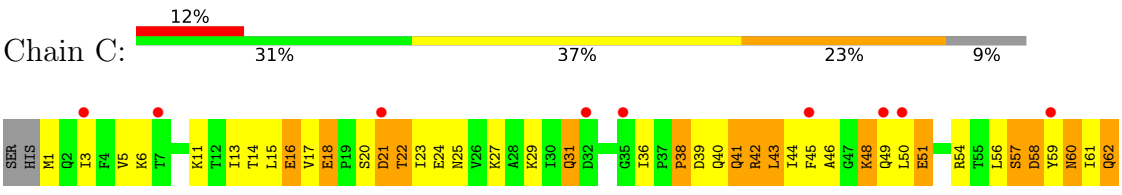
• Molecule 1: SdeA

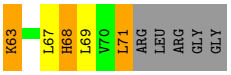
Chain A:



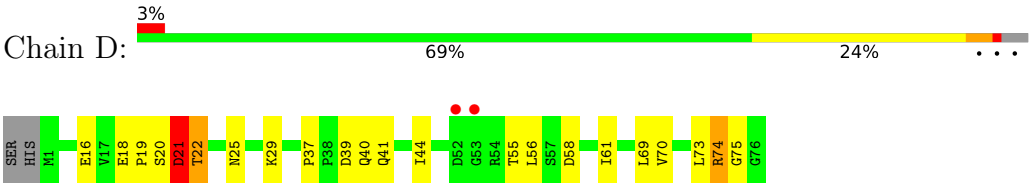
• Molecule 2: ubiquitin

Chain C:

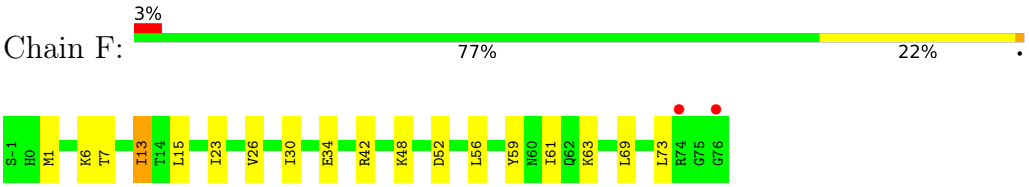




• Molecule 2: ubiquitin



• Molecule 2: ubiquitin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.85Å 145.89Å 104.09Å 90.00° 104.46° 90.00°	Depositor
Resolution (Å)	42.54 – 3.10 47.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.54-3.10) 88.5 (47.85-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.279 0.234 , 0.277	Depositor DCC
R_{free} test set	1290 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9381	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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	0/7734	0.50	2/10439 (0.0%)
2	C	0.48	0/569	0.71	0/767
2	D	0.39	0/607	0.56	0/816
2	F	0.27	0/623	0.53	0/838
All	All	0.43	0/9533	0.52	2/12860 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	676	ASN	C-N-CD	5.78	140.53	128.40
1	A	938	PRO	N-CA-CB	5.33	109.69	103.30

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	7601	0	7518	255	0
2	C	563	0	586	74	0
2	D	601	0	629	21	0
2	F	616	0	638	11	0
All	All	9381	0	9371	349	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 19.

All (349) 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:A:822:THR:HG21	1:A:827:LEU:CD2	1.33	1.57
2:C:42:ARG:HG2	2:C:49:GLN:NE2	1.54	1.20
1:A:419:GLU:HG3	1:A:516:VAL:HG11	1.21	1.12
1:A:822:THR:CG2	1:A:827:LEU:CD2	2.29	1.10
1:A:822:THR:CG2	1:A:827:LEU:HD23	1.80	1.10
2:C:48:LYS:NZ	2:C:49:GLN:O	1.88	1.06
1:A:822:THR:HG21	1:A:827:LEU:HD23	1.03	1.01
2:C:20:SER:O	2:C:56:LEU:HD22	1.59	1.01
2:C:1:MET:HB3	2:C:17:VAL:O	1.61	1.00
1:A:822:THR:HG21	1:A:827:LEU:HD22	1.43	1.00
1:A:1058:GLU:HG2	1:A:1059:LYS:HD3	1.45	0.98
1:A:940:LEU:HD12	1:A:940:LEU:H	1.29	0.97
1:A:375:LYS:HB3	1:A:379:ASP:OD2	1.65	0.97
1:A:709:ILE:CG2	1:A:852:VAL:HG23	1.95	0.96
1:A:1154:THR:O	1:A:1155:ASP:OD1	1.82	0.96
1:A:993:LEU:HD21	1:A:1060:GLU:HB3	1.45	0.94
1:A:415:LYS:HD3	1:A:421:PHE:CE2	2.02	0.94
2:C:42:ARG:HG2	2:C:49:GLN:HE22	1.22	0.93
1:A:1055:ILE:HG12	1:A:1071:GLN:OE1	1.69	0.92
2:C:21:ASP:O	2:C:22:THR:OG1	1.89	0.90
1:A:993:LEU:CD2	1:A:1060:GLU:HB3	2.01	0.90
2:C:42:ARG:CG	2:C:49:GLN:NE2	2.35	0.89
1:A:1093:ASP:HB3	1:A:1096:LYS:HB3	1.54	0.89
1:A:928:LYS:HE2	1:A:1034:THR:HG22	1.55	0.89
1:A:415:LYS:CD	1:A:421:PHE:CE2	2.56	0.88
2:C:58:ASP:O	2:C:59:TYR:CD2	2.27	0.88
1:A:1058:GLU:N	1:A:1058:GLU:OE2	2.07	0.87
1:A:709:ILE:HG22	1:A:852:VAL:HG23	1.57	0.86
1:A:940:LEU:O	1:A:944:PHE:HD1	1.57	0.86
2:C:20:SER:O	2:C:56:LEU:CD2	2.23	0.86
2:C:17:VAL:HG22	2:C:18:GLU:H	1.39	0.86
1:A:397:THR:HG1	1:A:400:HIS:HD1	1.24	0.85
2:C:51:GLU:OE2	2:C:51:GLU:N	2.09	0.85
1:A:1056:PRO:O	1:A:1057:SER:OG	1.91	0.85
2:C:20:SER:O	2:C:56:LEU:HD13	1.76	0.84
1:A:706:HIS:CD2	2:D:75:GLY:HA3	2.13	0.83
2:C:43:LEU:C	2:C:44:ILE:HD12	1.98	0.83
1:A:855:HIS:HA	1:A:859:THR:HG21	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:GLN:HG2	2:D:73:LEU:HD13	1.58	0.82
2:D:41:GLN:HB2	2:D:69:LEU:HD11	1.60	0.81
1:A:1035:GLN:OE1	1:A:1054:LYS:NZ	2.14	0.81
2:C:24:GLU:HG3	2:C:25:ASN:N	1.96	0.80
2:C:42:ARG:CG	2:C:49:GLN:HE22	1.93	0.80
1:A:985:ASP:O	1:A:986:THR:OG1	1.98	0.79
2:C:56:LEU:HB3	2:C:61:ILE:HD13	1.65	0.78
2:C:56:LEU:HB3	2:C:61:ILE:CD1	2.14	0.78
1:A:744:MET:O	1:A:748:THR:HG23	1.85	0.77
1:A:1036:CYS:SG	1:A:1052:LEU:CD2	2.73	0.77
1:A:803:LYS:O	1:A:807:LEU:HG	1.86	0.76
2:C:44:ILE:HA	2:C:48:LYS:O	1.84	0.76
1:A:928:LYS:CE	1:A:1034:THR:HG22	2.16	0.75
2:C:20:SER:O	2:C:56:LEU:CD1	2.35	0.75
2:C:43:LEU:HD22	2:C:43:LEU:H	1.51	0.75
1:A:986:THR:OG1	1:A:988:THR:HG22	1.87	0.74
2:C:43:LEU:HB2	2:C:50:LEU:HD12	1.66	0.74
1:A:1036:CYS:SG	1:A:1052:LEU:HD23	2.29	0.73
1:A:859:THR:HG23	1:A:861:SER:H	1.53	0.73
2:C:17:VAL:HG22	2:C:18:GLU:N	2.03	0.73
1:A:419:GLU:HG3	1:A:516:VAL:CG1	2.10	0.72
2:C:43:LEU:HD22	2:C:43:LEU:N	2.04	0.72
1:A:940:LEU:HD12	1:A:940:LEU:N	2.03	0.72
1:A:633:GLN:OE1	1:A:637:ARG:NH1	2.22	0.72
2:C:58:ASP:O	2:C:59:TYR:HD2	1.70	0.71
1:A:854:ARG:O	1:A:855:HIS:HB2	1.89	0.71
1:A:822:THR:HG21	1:A:827:LEU:HD21	1.62	0.71
1:A:481:ASP:O	1:A:483:GLN:N	2.23	0.71
1:A:415:LYS:HD2	1:A:421:PHE:CE2	2.24	0.71
2:C:62:GLN:N	2:C:62:GLN:OE1	2.24	0.70
1:A:1026:ASN:HD22	1:A:1061:MET:CE	2.05	0.69
1:A:674:SER:HA	1:A:721:ARG:NH2	2.08	0.69
1:A:1091:VAL:O	1:A:1093:ASP:N	2.26	0.69
1:A:415:LYS:CD	1:A:421:PHE:HE2	2.07	0.68
1:A:831:THR:CG2	2:D:44:ILE:HD12	2.23	0.68
1:A:663:LEU:O	1:A:667:GLU:HG2	1.93	0.68
1:A:707:ASP:OD1	2:D:74:ARG:HD3	1.94	0.68
1:A:910:GLY:HA2	1:A:913:VAL:HG12	1.74	0.67
1:A:1051:ALA:O	1:A:1054:LYS:HB2	1.94	0.67
1:A:1055:ILE:CG1	1:A:1071:GLN:OE1	2.43	0.67
2:C:22:THR:OG1	2:C:25:ASN:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:LYS:O	1:A:1061:MET:N	2.27	0.67
2:C:1:MET:HG3	2:C:63:LYS:HB3	1.77	0.66
1:A:857:GLU:O	1:A:857:GLU:HG2	1.95	0.66
2:C:45:PHE:HD2	2:C:67:LEU:CD2	2.09	0.66
2:C:44:ILE:HG23	2:C:48:LYS:N	2.12	0.65
2:C:43:LEU:HA	2:C:69:LEU:HD22	1.79	0.65
1:A:953:VAL:HG21	1:A:966:LEU:HD12	1.79	0.64
2:C:45:PHE:HD2	2:C:67:LEU:HD23	1.62	0.64
1:A:985:ASP:HA	1:A:989:LEU:HD13	1.80	0.64
1:A:593:LYS:HE3	1:A:844:ASP:O	1.98	0.64
1:A:1036:CYS:SG	1:A:1052:LEU:HD21	2.38	0.63
2:C:21:ASP:C	2:C:22:THR:HG1	1.99	0.63
1:A:940:LEU:O	1:A:944:PHE:CD1	2.48	0.63
1:A:1059:LYS:HD2	1:A:1059:LYS:N	2.12	0.63
1:A:707:ASP:OD1	2:D:74:ARG:NE	2.30	0.63
1:A:902:ASP:HA	1:A:1149:ARG:HH22	1.63	0.63
2:C:22:THR:OG1	2:C:25:ASN:CB	2.48	0.62
1:A:417:PRO:HG2	1:A:420:SER:HB2	1.82	0.62
1:A:880:LEU:HD13	1:A:891:TYR:CE1	2.35	0.62
1:A:1029:VAL:HG22	1:A:1056:PRO:HD2	1.82	0.62
1:A:1049:LEU:O	1:A:1053:LYS:HG3	2.00	0.61
1:A:709:ILE:HG22	1:A:852:VAL:CG2	2.29	0.61
2:C:56:LEU:O	2:C:61:ILE:HG23	2.00	0.61
1:A:512:ARG:NH2	1:A:518:GLU:OE2	2.34	0.60
1:A:709:ILE:HG21	1:A:852:VAL:HG23	1.80	0.60
1:A:607:ARG:NH1	1:A:610:GLN:OE1	2.34	0.60
1:A:1058:GLU:HG2	1:A:1059:LYS:CD	2.26	0.60
1:A:596:ARG:NH1	1:A:869:GLU:OE2	2.35	0.59
1:A:620:HIS:O	1:A:736:LYS:NZ	2.35	0.59
1:A:692:GLN:NE2	1:A:707:ASP:OD2	2.36	0.59
1:A:707:ASP:OD1	2:D:74:ARG:CD	2.50	0.59
1:A:983:GLU:O	1:A:984:SER:OG	2.11	0.59
1:A:1159:PHE:O	1:A:1163:GLU:HG2	2.03	0.59
2:C:60:ASN:O	2:C:62:GLN:NE2	2.35	0.59
1:A:282:THR:CG2	1:A:334:VAL:HG12	2.33	0.58
1:A:362:VAL:HG11	1:A:380:VAL:HG11	1.85	0.58
2:D:16:GLU:O	2:D:29:LYS:NZ	2.33	0.58
2:D:20:SER:O	2:D:21:ASP:HB2	2.02	0.58
1:A:377:GLN:O	1:A:381:ASN:ND2	2.35	0.58
2:F:13:ILE:HD13	2:F:34:GLU:HG3	1.85	0.58
1:A:415:LYS:HD3	1:A:421:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:VAL:CG2	2:C:18:GLU:H	2.13	0.58
2:C:58:ASP:O	2:C:59:TYR:CB	2.52	0.58
1:A:806:LYS:NZ	1:A:902:ASP:O	2.36	0.58
2:D:56:LEU:HB3	2:D:61:ILE:HB	1.85	0.57
1:A:596:ARG:NH2	1:A:602:GLU:OE1	2.37	0.57
2:C:44:ILE:HD12	2:C:44:ILE:N	2.18	0.57
1:A:256:TYR:HB3	1:A:262:SER:HB3	1.87	0.57
1:A:676:ASN:O	1:A:679:ALA:HB3	2.05	0.57
1:A:377:GLN:HG3	1:A:381:ASN:ND2	2.19	0.57
1:A:248:TYR:HA	1:A:252:LEU:HB2	1.87	0.57
2:C:45:PHE:O	2:C:46:ALA:HB3	2.05	0.57
1:A:260:VAL:N	1:A:339:ASP:OD2	2.37	0.56
1:A:241:LYS:HD3	1:A:568:LEU:HD12	1.86	0.56
1:A:474:GLY:HA2	1:A:502:PRO:HD3	1.87	0.56
1:A:593:LYS:CE	1:A:844:ASP:O	2.54	0.56
1:A:1112:ILE:HG12	1:A:1136:LEU:HD13	1.87	0.56
1:A:925:ALA:HB2	1:A:1037:GLN:HE22	1.70	0.56
2:C:31:GLN:HB2	2:C:38:PRO:HG3	1.89	0.55
2:C:1:MET:HE2	2:C:17:VAL:O	2.07	0.55
1:A:673:HIS:HB3	1:A:675:THR:O	2.07	0.55
1:A:715:ASP:HB3	1:A:717:TRP:NE1	2.22	0.55
1:A:849:SER:HB3	1:A:865:VAL:HG22	1.89	0.55
2:C:56:LEU:N	2:C:56:LEU:HD12	2.22	0.55
1:A:517:ASP:N	1:A:517:ASP:OD1	2.39	0.54
1:A:613:LEU:HD11	1:A:747:LEU:HD11	1.88	0.54
2:F:1:MET:HB2	2:F:63:LYS:HG2	1.89	0.54
1:A:928:LYS:NZ	1:A:1034:THR:CG2	2.70	0.54
1:A:311:ASP:OD1	1:A:311:ASP:N	2.36	0.54
1:A:1007:PHE:CZ	1:A:1011:ARG:HD3	2.43	0.54
2:C:20:SER:H	2:C:56:LEU:HD22	1.73	0.54
1:A:600:VAL:HG23	1:A:601:ASP:N	2.22	0.54
1:A:416:GLN:HA	1:A:417:PRO:C	2.28	0.53
1:A:935:GLN:OE1	1:A:1026:ASN:ND2	2.41	0.53
1:A:706:HIS:HD2	2:D:75:GLY:HA3	1.70	0.53
1:A:655:THR:O	1:A:659:ASN:ND2	2.31	0.53
2:C:56:LEU:HB3	2:C:61:ILE:HD11	1.89	0.53
1:A:859:THR:OG1	1:A:860:GLU:N	2.41	0.53
1:A:949:GLU:OE2	2:F:6:LYS:NZ	2.37	0.53
1:A:1058:GLU:O	1:A:1059:LYS:HG2	2.09	0.53
1:A:372:ASP:OD1	1:A:372:ASP:N	2.41	0.53
2:C:56:LEU:CD1	2:C:56:LEU:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:LEU:CD1	2:C:56:LEU:N	2.72	0.52
1:A:955:TYR:HB3	2:F:42:ARG:NH1	2.24	0.52
1:A:859:THR:HG23	1:A:861:SER:N	2.24	0.52
1:A:789:THR:HG22	1:A:801:ALA:HB1	1.91	0.52
2:C:44:ILE:N	2:C:44:ILE:CD1	2.73	0.52
1:A:753:VAL:HA	1:A:850:LYS:HE3	1.92	0.52
1:A:1059:LYS:N	1:A:1061:MET:O	2.43	0.52
1:A:1065:ARG:O	1:A:1067:GLU:N	2.40	0.52
1:A:854:ARG:O	1:A:855:HIS:CB	2.53	0.52
2:F:23:ILE:HB	2:F:52:ASP:HA	1.91	0.52
1:A:985:ASP:CB	1:A:989:LEU:HD22	2.40	0.52
2:C:17:VAL:HG22	2:C:18:GLU:O	2.10	0.52
1:A:674:SER:OG	1:A:675:THR:N	2.43	0.51
1:A:691:ASP:OD1	2:D:74:ARG:NH2	2.43	0.51
2:C:60:ASN:O	2:C:62:GLN:CD	2.48	0.51
1:A:985:ASP:CA	1:A:989:LEU:HD13	2.39	0.51
1:A:460:ASP:HB3	1:A:463:ASN:HB2	1.92	0.51
1:A:1059:LYS:N	1:A:1059:LYS:CD	2.73	0.50
1:A:283:LEU:HD22	1:A:568:LEU:HD21	1.94	0.50
2:C:58:ASP:O	2:C:59:TYR:CG	2.63	0.50
1:A:375:LYS:CB	1:A:379:ASP:OD2	2.50	0.50
1:A:860:GLU:HG2	2:D:70:VAL:HG11	1.93	0.50
1:A:675:THR:HB	1:A:676:ASN:HD22	1.75	0.50
1:A:985:ASP:CG	1:A:986:THR:H	2.13	0.50
1:A:668:LYS:HG2	1:A:683:LYS:HD2	1.93	0.50
1:A:1154:THR:O	1:A:1155:ASP:CG	2.48	0.50
1:A:985:ASP:HB2	1:A:989:LEU:HD22	1.93	0.49
2:C:71:LEU:H	2:C:71:LEU:HD22	1.77	0.49
2:D:25:ASN:O	2:D:29:LYS:HG3	2.11	0.49
1:A:419:GLU:OE1	1:A:460:ASP:O	2.30	0.49
2:C:43:LEU:CB	2:C:50:LEU:HD12	2.41	0.49
1:A:852:VAL:HG12	1:A:862:GLU:O	2.11	0.49
1:A:988:THR:HG23	1:A:989:LEU:HD12	1.94	0.49
1:A:928:LYS:CE	1:A:1034:THR:CG2	2.90	0.49
1:A:358:PHE:O	1:A:362:VAL:HG23	2.12	0.49
1:A:453:TYR:OH	1:A:556:ASN:ND2	2.36	0.49
1:A:580:ILE:HG12	1:A:896:VAL:HG11	1.94	0.49
1:A:608:ILE:O	1:A:612:ILE:HG12	2.13	0.49
1:A:313:ARG:NH2	1:A:322:GLU:OE1	2.45	0.49
1:A:985:ASP:HA	1:A:989:LEU:CD1	2.41	0.49
1:A:993:LEU:HD21	1:A:1060:GLU:CB	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:TYR:HB3	2:F:42:ARG:HH11	1.78	0.49
1:A:292:ILE:HG23	1:A:433:ILE:HD12	1.94	0.49
1:A:1008:GLU:O	1:A:1011:ARG:NH2	2.45	0.49
2:C:16:GLU:H	2:C:16:GLU:CD	2.16	0.48
2:C:24:GLU:O	2:C:27:LYS:HB2	2.13	0.48
2:C:20:SER:O	2:C:56:LEU:CG	2.61	0.48
1:A:323:LEU:HA	1:A:326:ILE:HD12	1.94	0.48
1:A:557:ARG:NH2	1:A:561:GLU:OE2	2.47	0.48
1:A:902:ASP:HA	1:A:1149:ARG:NH2	2.29	0.48
1:A:624:VAL:HG23	1:A:735:PHE:HZ	1.79	0.48
1:A:785:MET:HG2	1:A:805:ILE:HG12	1.96	0.48
1:A:1026:ASN:HD22	1:A:1061:MET:HE3	1.78	0.48
1:A:1030:LEU:O	1:A:1034:THR:HG23	2.14	0.48
1:A:334:VAL:HG22	1:A:337:ARG:HG3	1.96	0.47
1:A:800:GLU:OE1	1:A:803:LYS:NZ	2.39	0.47
2:C:45:PHE:CD2	2:C:67:LEU:CD2	2.94	0.47
1:A:807:LEU:HD21	1:A:1142:VAL:CG2	2.44	0.47
1:A:852:VAL:O	1:A:852:VAL:HG13	2.13	0.47
1:A:459:PHE:HB3	1:A:536:LEU:HB2	1.96	0.47
1:A:785:MET:O	1:A:789:THR:HG23	2.15	0.47
1:A:1026:ASN:HD22	1:A:1061:MET:HE1	1.79	0.47
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.73	0.47
2:C:6:LYS:O	2:C:68:HIS:HA	2.15	0.47
2:C:43:LEU:O	2:C:44:ILE:HD12	2.14	0.47
2:C:58:ASP:O	2:C:59:TYR:HB2	2.13	0.47
1:A:256:TYR:HD2	1:A:262:SER:HA	1.80	0.47
1:A:950:VAL:HG22	1:A:966:LEU:HB3	1.97	0.47
1:A:1084:ARG:NE	1:A:1084:ARG:O	2.48	0.47
2:C:22:THR:HB	2:C:24:GLU:HG2	1.96	0.47
1:A:807:LEU:HD21	1:A:1142:VAL:HG21	1.97	0.46
1:A:1026:ASN:HA	1:A:1061:MET:HE1	1.97	0.46
1:A:382:PHE:O	1:A:386:VAL:HG23	2.16	0.46
2:C:45:PHE:CD1	2:C:46:ALA:N	2.84	0.46
2:F:7:THR:HG22	2:F:69:LEU:HD23	1.98	0.46
1:A:854:ARG:HH12	1:A:856:GLY:HA3	1.81	0.46
1:A:1042:LYS:O	1:A:1043:GLN:HB2	2.16	0.46
2:C:6:LYS:N	2:C:67:LEU:O	2.38	0.46
1:A:1061:MET:HG3	1:A:1062:GLY:N	2.31	0.46
1:A:596:ARG:HD2	1:A:1087:VAL:HG21	1.98	0.46
1:A:831:THR:HG22	2:D:44:ILE:HD12	1.95	0.46
1:A:671:GLU:HG3	1:A:684:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLU:OE2	1:A:1107:ASN:ND2	2.49	0.45
1:A:839:GLU:HB3	1:A:894:THR:HA	1.98	0.45
1:A:286:MET:HE2	1:A:331:ALA:HA	1.97	0.45
1:A:463:ASN:OD1	1:A:465:GLU:HG2	2.16	0.45
1:A:1011:ARG:HG3	1:A:1012:GLN:N	2.32	0.45
2:C:56:LEU:O	2:C:61:ILE:CG2	2.64	0.45
2:D:41:GLN:HB2	2:D:69:LEU:CD1	2.41	0.45
1:A:397:THR:OG1	1:A:400:HIS:ND1	2.25	0.45
1:A:461:SER:HB3	1:A:535:HIS:CE1	2.52	0.45
1:A:352:GLU:O	1:A:355:ARG:HG3	2.16	0.45
1:A:419:GLU:OE1	1:A:460:ASP:N	2.44	0.45
1:A:1040:LEU:HA	1:A:1040:LEU:HD23	1.76	0.45
2:F:26:VAL:O	2:F:30:ILE:HG13	2.17	0.45
1:A:725:ILE:HG21	1:A:738:VAL:HA	1.99	0.45
1:A:358:PHE:CE2	1:A:380:VAL:HG13	2.52	0.45
1:A:822:THR:CB	1:A:827:LEU:HD23	2.46	0.45
1:A:1122:ASN:OD1	1:A:1122:ASN:N	2.49	0.45
2:C:22:THR:OG1	2:C:25:ASN:HB3	2.17	0.45
2:C:60:ASN:O	2:C:62:GLN:HG3	2.17	0.45
1:A:251:TYR:O	1:A:274:ARG:NH2	2.49	0.44
1:A:293:VAL:HG21	1:A:323:LEU:HD13	1.99	0.44
1:A:980:GLY:HA3	1:A:989:LEU:CD1	2.47	0.44
2:D:22:THR:OG1	2:D:25:ASN:HB2	2.16	0.44
1:A:612:ILE:HD12	1:A:624:VAL:HG11	1.99	0.44
1:A:807:LEU:CD2	1:A:1142:VAL:HG21	2.48	0.44
1:A:983:GLU:C	1:A:984:SER:HG	2.11	0.44
2:D:18:GLU:C	2:D:20:SER:H	2.21	0.44
1:A:1097:VAL:HG12	1:A:1150:MET:HE3	2.00	0.44
1:A:481:ASP:N	1:A:481:ASP:OD1	2.49	0.44
1:A:645:MET:SD	1:A:746:PRO:HG3	2.58	0.44
1:A:652:LEU:HD11	1:A:746:PRO:HB2	2.00	0.44
1:A:807:LEU:CD2	1:A:1142:VAL:CG2	2.96	0.44
1:A:392:HIS:CG	1:A:392:HIS:O	2.70	0.44
1:A:760:PRO:HA	1:A:761:PRO:HD2	1.83	0.44
1:A:1082:LEU:HD23	1:A:1082:LEU:HA	1.90	0.44
1:A:618:CYS:HB2	1:A:625:LEU:O	2.18	0.44
2:C:3:ILE:HD13	2:C:17:VAL:HG12	2.00	0.44
2:C:24:GLU:HG3	2:C:25:ASN:H	1.80	0.44
1:A:275:GLN:HG3	1:A:276:HIS:ND1	2.33	0.44
1:A:453:TYR:CE1	1:A:556:ASN:HB3	2.53	0.44
2:F:56:LEU:HD22	2:F:61:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:PRO:HD3	1:A:495:GLU:HB2	2.00	0.43
1:A:569:LYS:O	1:A:573:THR:HG23	2.18	0.43
1:A:645:MET:HB2	1:A:866:TYR:CZ	2.53	0.43
1:A:488:ALA:HA	1:A:489:PRO:HD3	1.84	0.43
1:A:1006:ASN:HB3	1:A:1007:PHE:H	1.41	0.43
1:A:675:THR:HB	1:A:676:ASN:ND2	2.34	0.43
1:A:1071:GLN:HE21	1:A:1071:GLN:HB2	1.57	0.43
1:A:234:LEU:HB2	1:A:290:GLU:HG3	2.00	0.43
1:A:272:VAL:HG11	1:A:561:GLU:HB2	1.99	0.43
1:A:377:GLN:HG3	1:A:381:ASN:HD21	1.83	0.43
1:A:672:PHE:CD1	1:A:681:PRO:HB3	2.54	0.43
1:A:914:GLU:HB2	1:A:915:PRO:HD3	2.01	0.43
1:A:1059:LYS:C	1:A:1061:MET:N	2.72	0.43
1:A:461:SER:HB2	1:A:534:LYS:O	2.18	0.43
1:A:664:MET:HG3	1:A:688:TRP:CD1	2.52	0.43
1:A:282:THR:O	1:A:286:MET:HG3	2.18	0.43
1:A:525:ILE:HA	1:A:528:THR:HG22	2.00	0.43
2:C:43:LEU:HB2	2:C:50:LEU:CD1	2.45	0.43
2:D:55:THR:OG1	2:D:58:ASP:OD2	2.23	0.42
1:A:1040:LEU:HD21	1:A:1078:GLU:OE2	2.19	0.42
1:A:284:ARG:HH22	1:A:413:ARG:NH2	2.17	0.42
1:A:1061:MET:HG3	1:A:1062:GLY:H	1.84	0.42
2:F:48:LYS:HE2	2:F:59:TYR:HE1	1.84	0.42
1:A:298:LYS:HG2	1:A:787:ALA:HA	2.00	0.42
1:A:376:ASP:OD1	1:A:378:GLU:HB3	2.20	0.42
2:D:18:GLU:HB3	2:D:19:PRO:HD2	2.01	0.42
2:D:37:PRO:HB2	2:D:39:ASP:OD1	2.20	0.42
2:F:15:LEU:HD21	2:F:30:ILE:HG12	2.01	0.42
1:A:1029:VAL:CG2	1:A:1056:PRO:HD2	2.49	0.42
2:C:21:ASP:HA	2:C:56:LEU:HD13	2.00	0.42
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.91	0.42
1:A:943:ILE:HD13	1:A:1020:ILE:HG12	2.00	0.42
1:A:1026:ASN:ND2	1:A:1061:MET:CE	2.78	0.42
1:A:1058:GLU:C	1:A:1059:LYS:CG	2.88	0.42
1:A:1073:GLN:HE21	1:A:1073:GLN:HB3	1.61	0.41
2:C:57:SER:O	2:C:58:ASP:C	2.58	0.41
1:A:676:ASN:HB3	1:A:679:ALA:HB2	2.02	0.41
1:A:867:LEU:HD12	1:A:868:PRO:HD2	2.01	0.41
1:A:392:HIS:CE1	1:A:394:TRP:CZ2	3.09	0.41
1:A:852:VAL:HG11	1:A:862:GLU:HG2	2.01	0.41
1:A:1059:LYS:C	1:A:1060:GLU:HG3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:O	1:A:285:THR:HG23	2.20	0.41
1:A:322:GLU:O	1:A:326:ILE:HG13	2.20	0.41
1:A:980:GLY:HA3	1:A:989:LEU:HD12	2.02	0.41
1:A:374:PHE:CD2	1:A:380:VAL:HG22	2.56	0.41
1:A:612:ILE:HG21	1:A:743:LEU:HD21	2.01	0.41
1:A:756:SER:HB3	1:A:850:LYS:HD2	2.02	0.41
1:A:769:ASN:HA	1:A:835:ASN:OD1	2.21	0.41
2:C:14:THR:O	2:C:15:LEU:HD23	2.21	0.41
1:A:881:ASP:O	1:A:890:ARG:HB3	2.21	0.41
1:A:984:SER:OG	1:A:985:ASP:N	2.51	0.41
2:C:27:LYS:HG2	2:C:41:GLN:CD	2.41	0.41
1:A:362:VAL:HG11	1:A:380:VAL:HG21	2.03	0.41
1:A:470:VAL:O	1:A:470:VAL:HG12	2.20	0.41
2:C:23:ILE:HG22	2:C:27:LYS:HD2	2.03	0.41
1:A:925:ALA:HB2	1:A:1037:GLN:NE2	2.34	0.41
1:A:988:THR:HG23	1:A:989:LEU:N	2.35	0.41
2:C:43:LEU:O	2:C:49:GLN:HA	2.21	0.41
1:A:1056:PRO:HB2	1:A:1061:MET:HB3	2.03	0.40
1:A:282:THR:CG2	1:A:334:VAL:CG1	2.99	0.40
1:A:440:ALA:HB2	1:A:790:THR:HB	2.04	0.40
1:A:740:ILE:O	1:A:744:MET:HG2	2.22	0.40
1:A:949:GLU:O	1:A:953:VAL:HG13	2.21	0.40
1:A:825:ILE:H	1:A:825:ILE:HG13	1.66	0.40
1:A:1058:GLU:O	1:A:1059:LYS:CB	2.70	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	955/968 (99%)	891 (93%)	51 (5%)	13 (1%)	11 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	69/78 (88%)	64 (93%)	3 (4%)	2 (3%)	4 24
2	D	74/78 (95%)	71 (96%)	2 (3%)	1 (1%)	11 40
2	F	76/78 (97%)	75 (99%)	1 (1%)	0	100 100
All	All	1174/1202 (98%)	1101 (94%)	57 (5%)	16 (1%)	11 40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	PRO
1	A	1092	THR
2	C	38	PRO
1	A	482	GLY
1	A	496	GLY
1	A	848	HIS
1	A	882	GLY
1	A	1008	GLU
1	A	644	GLU
1	A	1066	ARG
2	C	22	THR
1	A	632	GLU
1	A	986	THR
2	D	21	ASP
1	A	937	ALA
1	A	1062	GLY

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	827/844 (98%)	798 (96%)	29 (4%)	36 68
2	C	65/70 (93%)	41 (63%)	24 (37%)	0 0
2	D	68/70 (97%)	65 (96%)	3 (4%)	28 61
2	F	69/70 (99%)	67 (97%)	2 (3%)	42 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1029/1054 (98%)	971 (94%)	58 (6%)	21 52

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	TYR
1	A	290	GLU
1	A	355	ARG
1	A	372	ASP
1	A	413	ARG
1	A	423	GLN
1	A	424	ARG
1	A	431	ARG
1	A	494	LYS
1	A	591	LYS
1	A	594	GLU
1	A	617	ASP
1	A	639	LEU
1	A	644	GLU
1	A	673	HIS
1	A	675	THR
1	A	680	VAL
1	A	713	GLN
1	A	816	ARG
1	A	855	HIS
1	A	940	LEU
1	A	987	ASP
1	A	1052	LEU
1	A	1055	ILE
1	A	1073	GLN
1	A	1084	ARG
1	A	1114	GLU
1	A	1132	ASN
1	A	1133	LEU
2	C	5	VAL
2	C	11	LYS
2	C	13	ILE
2	C	16	GLU
2	C	18	GLU
2	C	21	ASP
2	C	29	LYS
2	C	31	GLN

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Mol	Chain	Res	Type
2	C	36	ILE
2	C	39	ASP
2	C	40	GLN
2	C	41	GLN
2	C	42	ARG
2	C	43	LEU
2	C	48	LYS
2	C	51	GLU
2	C	54	ARG
2	C	57	SER
2	C	58	ASP
2	C	60	ASN
2	C	62	GLN
2	C	63	LYS
2	C	68	HIS
2	C	71	LEU
2	D	21	ASP
2	D	22	THR
2	D	74	ARG
2	F	13	ILE
2	F	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	392	HIS
1	A	620	HIS
1	A	676	ASN
1	A	706	HIS
1	A	713	GLN
1	A	1016	GLN
1	A	1026	ASN
1	A	1037	GLN
1	A	1073	GLN
2	C	41	GLN
2	C	49	GLN

5.3.3 RNA

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	959/968 (99%)	-0.28	3 (0%) 94 88	13, 47, 78, 99	0
2	C	71/78 (91%)	0.79	9 (12%) 3 1	26, 118, 141, 152	0
2	D	76/78 (97%)	0.19	2 (2%) 56 33	54, 83, 103, 117	0
2	F	78/78 (100%)	0.12	2 (2%) 56 33	37, 63, 92, 104	0
All	All	1184/1202 (98%)	-0.16	16 (1%) 75 56	13, 51, 103, 152	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	76	GLY	5.5
2	C	32	ASP	4.2
2	C	21	ASP	4.2
2	C	35	GLY	4.1
2	D	53	GLY	2.8
1	A	1060	GLU	2.7
1	A	1092	THR	2.5
2	C	3	ILE	2.3
2	F	74	ARG	2.1
2	C	59	TYR	2.1
2	C	45	PHE	2.1
2	C	49	GLN	2.1
2	C	7	THR	2.1
2	C	50	LEU	2.1
1	A	392	HIS	2.1
2	D	52	ASP	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 (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.