Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:23 am BST

PDB ID	:	1JAL
Title	:	YCHF PROTEIN (HI0393)
Authors	:	Teplyakov, A.; Gilliland, G.L.; Structure 2 Function Project (S2F)
Deposited on	:	2001-05-30
Resolution	:	2.40 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:

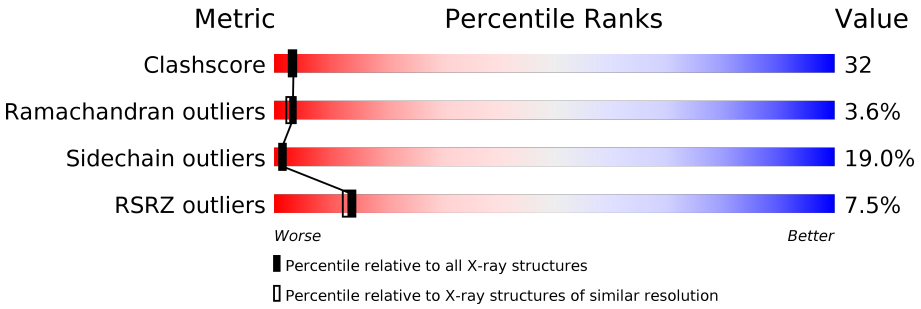
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	363	6% 58% 30% 6%
1	B	363	8% 38% 38% 15% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5727 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 YchF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2659	1686	450	512	11			
1	B	335	Total	C	N	O	S	0	0	0
			2584	1641	436	496	11			

- Molecule 2 is water.

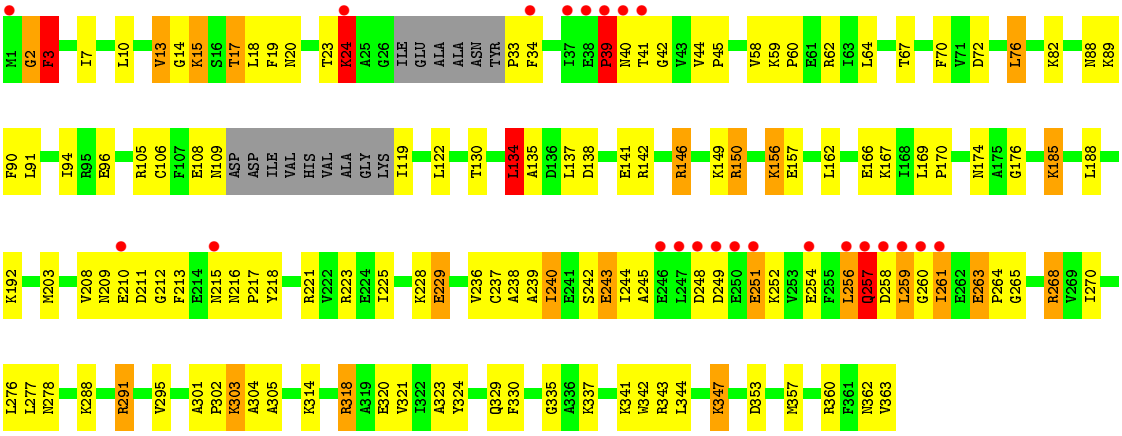
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	314	Total	O	0	0
			314	314		
2	B	170	Total	O	0	0
			170	170		

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.

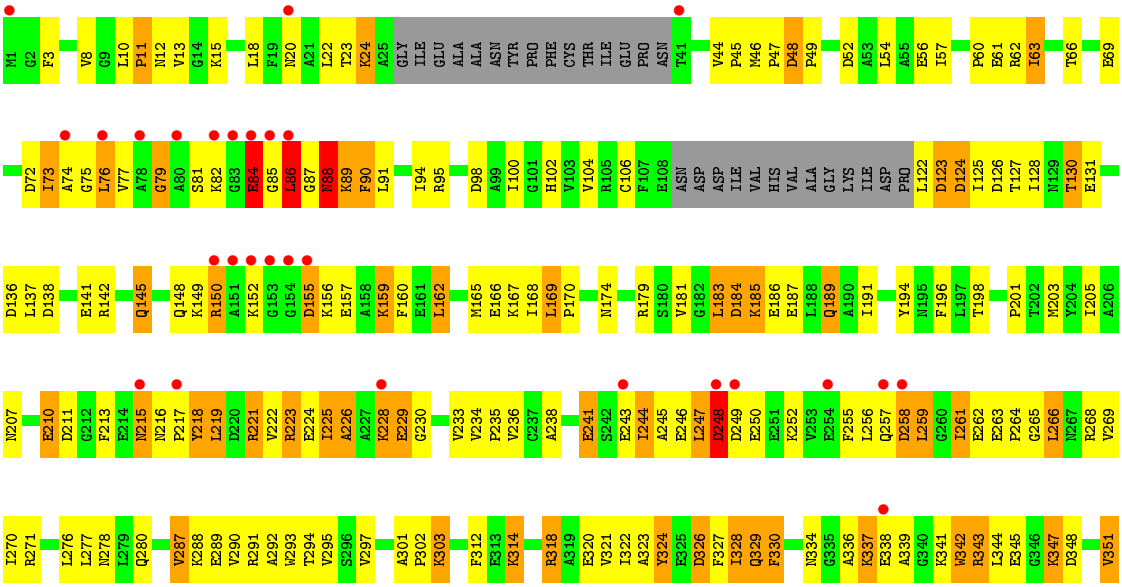
- Molecule 1: YchF protein

Chain A:



- Molecule 1: YchF protein

Chain B:




Q352
D353
M357
H358
F359
R360
F361
N362
V363

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.00Å 93.60Å 85.20Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-2.40) 95.4 (10.00-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.204 , 0.247 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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	0.80	0/2699	0.94	4/3648 (0.1%)
1	B	0.64	1/2623 (0.0%)	0.84	12/3542 (0.3%)
All	All	0.73	1/5322 (0.0%)	0.89	16/7190 (0.2%)

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	A	0	2
1	B	0	8
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	VAL	CB-CG2	-5.53	1.41	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	LEU	CA-CB-CG	7.91	133.49	115.30
1	B	48	ASP	CB-CG-OD2	7.08	124.68	118.30
1	B	353	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	353	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	33	PRO	N-CA-CB	6.24	110.79	103.30
1	A	39	PRO	N-CA-CB	6.21	110.75	103.30
1	B	348	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	249	ASP	CB-CG-OD2	6.12	123.80	118.30
1	B	72	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	184	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	138	ASP	CB-CG-OD2	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	326	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	155	ASP	CB-CG-OD2	5.49	123.25	118.30
1	B	248	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	123	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	258	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	PHE	Peptide
1	A	39	PRO	Peptide
1	B	12	ASN	Peptide
1	B	211	ASP	Peptide
1	B	215	ASN	Peptide
1	B	248	ASP	Peptide
1	B	314	LYS	Peptide
1	B	81	SER	Peptide
1	B	84	GLU	Peptide
1	B	86	LEU	Peptide

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	2659	0	2642	127	0
1	B	2584	0	2596	214	0
2	A	314	0	0	14	0
2	B	170	0	0	18	0
All	All	5727	0	5238	338	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 32.

All (338) 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:287:VAL:HG23	1:B:288:LYS:N	1.62	1.12
1:A:318:ARG:HD2	1:A:360:ARG:HG3	1.12	1.11
1:B:287:VAL:CG2	1:B:288:LYS:H	1.61	1.11
1:A:13:VAL:HG23	1:A:105:ARG:HB2	1.19	1.09
1:A:185:LYS:H	1:A:185:LYS:HD2	1.17	1.06
1:B:343:ARG:HH11	1:B:343:ARG:HG3	1.22	1.04
1:B:287:VAL:HA	2:B:500:HOH:O	1.59	1.01
1:B:287:VAL:HG23	1:B:288:LYS:H	0.84	1.00
1:B:241:GLU:OE1	1:B:241:GLU:HA	1.58	0.98
1:A:13:VAL:CG2	1:A:105:ARG:HB2	1.95	0.95
1:A:17:THR:HG22	1:A:242:SER:HB2	1.48	0.94
1:A:185:LYS:CD	1:A:185:LYS:H	1.81	0.94
1:A:210:GLU:CB	1:A:240:ILE:HD12	1.98	0.94
1:B:60:PRO:HD2	2:B:441:HOH:O	1.71	0.91
1:A:258:ASP:O	1:A:259:LEU:HD23	1.69	0.90
1:B:85:GLY:HA3	1:B:88:ASN:HB2	1.54	0.90
1:B:246:GLU:O	1:B:247:LEU:HD23	1.73	0.89
1:B:10:LEU:HD23	1:B:77:VAL:CG1	2.03	0.88
1:B:85:GLY:HA3	1:B:88:ASN:CA	2.03	0.87
1:A:192:LYS:HE2	2:A:598:HOH:O	1.74	0.87
1:B:85:GLY:HA3	1:B:88:ASN:CB	2.03	0.87
1:B:343:ARG:HG3	1:B:343:ARG:NH1	1.88	0.87
1:A:318:ARG:HD2	1:A:360:ARG:CG	2.01	0.85
1:B:126:ASP:O	1:B:130:THR:HG23	1.76	0.85
1:B:73:ILE:HG22	1:B:73:ILE:O	1.74	0.84
1:B:57:ILE:HD11	1:B:328:ILE:HD13	1.58	0.84
1:A:248:ASP:HB3	1:A:251:GLU:HB2	1.58	0.84
1:B:318:ARG:HE	1:B:344:LEU:HD22	1.45	0.82
1:B:76:LEU:HB2	1:B:87:GLY:HA3	1.59	0.82
1:B:86:LEU:H	1:B:86:LEU:HD23	1.43	0.82
1:A:318:ARG:CD	1:A:360:ARG:HG3	2.06	0.81
1:B:218:TYR:H	1:B:218:TYR:HD1	1.29	0.81
1:B:203:MET:HG2	1:B:276:LEU:HD22	1.63	0.81
1:A:185:LYS:HD2	1:A:185:LYS:N	1.96	0.80
1:A:3:PHE:CE1	1:A:67:THR:O	2.35	0.80
1:B:73:ILE:CG2	1:B:73:ILE:O	2.30	0.80
1:A:17:THR:HG22	1:A:242:SER:CB	2.12	0.80
1:B:241:GLU:OE2	1:B:265:GLY:N	2.15	0.80
1:B:318:ARG:HH11	1:B:360:ARG:HG3	1.47	0.79
1:B:330:PHE:N	1:B:330:PHE:CD1	2.47	0.78
1:A:210:GLU:CA	1:A:240:ILE:HD12	2.14	0.77
1:B:318:ARG:NE	1:B:344:LEU:HD22	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:HIS:CE1	1:B:128:ILE:HG21	2.20	0.76
1:B:91:LEU:O	1:B:95:ARG:HB2	1.85	0.76
1:B:330:PHE:CE2	1:B:341:LYS:HG3	2.21	0.76
1:A:210:GLU:HA	1:A:240:ILE:HD12	1.66	0.75
1:A:210:GLU:CB	1:A:240:ILE:CD1	2.64	0.75
1:B:320:GLU:OE1	1:B:342:TRP:HZ2	1.69	0.75
1:B:86:LEU:HG	1:B:91:LEU:HD11	1.67	0.75
1:A:248:ASP:HB2	2:A:436:HOH:O	1.87	0.74
1:A:237:CYS:SG	1:A:240:ILE:HB	2.26	0.74
1:B:330:PHE:HE2	1:B:341:LYS:CG	2.00	0.74
1:B:169:LEU:HB3	1:B:170:PRO:HD3	1.70	0.74
1:B:166:GLU:HG3	2:B:523:HOH:O	1.88	0.73
1:A:277:LEU:HA	2:A:494:HOH:O	1.87	0.73
1:B:10:LEU:HD23	1:B:77:VAL:HG11	1.70	0.73
1:A:243:GLU:O	1:A:245:ALA:N	2.22	0.73
1:B:86:LEU:H	1:B:86:LEU:CD2	2.01	0.73
1:A:64:LEU:HB2	1:A:291:ARG:CG	2.18	0.73
1:B:90:PHE:CD1	1:B:91:LEU:HD23	2.23	0.73
1:A:210:GLU:HB2	1:A:240:ILE:CD1	2.19	0.73
1:B:126:ASP:O	1:B:130:THR:CG2	2.37	0.72
1:A:320:GLU:OE2	1:A:360:ARG:HD3	1.90	0.72
1:A:268:ARG:HH11	1:A:268:ARG:HG3	1.55	0.71
1:B:330:PHE:HE2	1:B:341:LYS:HG3	1.55	0.71
1:A:329:GLN:OE1	1:A:330:PHE:CZ	2.44	0.71
1:B:347:LYS:HD2	2:B:468:HOH:O	1.91	0.71
1:B:301:ALA:N	1:B:302:PRO:HD2	2.06	0.71
1:B:221:ARG:O	1:B:225:ILE:HG13	1.91	0.70
1:B:297:VAL:HG22	2:B:502:HOH:O	1.92	0.70
1:B:90:PHE:C	1:B:90:PHE:CD1	2.65	0.70
1:B:10:LEU:HB2	1:B:13:VAL:HG21	1.74	0.69
1:B:57:ILE:CD1	1:B:328:ILE:HD13	2.23	0.69
1:B:216:ASN:HB3	1:B:219:LEU:HB3	1.73	0.69
1:A:363:VAL:HG22	2:A:635:HOH:O	1.92	0.68
1:B:301:ALA:H	1:B:302:PRO:HD2	1.58	0.68
1:A:44:VAL:HG21	1:A:270:ILE:HD13	1.76	0.68
1:B:287:VAL:CG2	1:B:288:LYS:N	2.33	0.68
1:B:318:ARG:HH21	1:B:344:LEU:HD21	1.59	0.68
1:B:85:GLY:HA3	1:B:88:ASN:HA	1.75	0.67
1:B:221:ARG:O	1:B:224:GLU:HB3	1.94	0.67
1:B:330:PHE:HD1	1:B:330:PHE:N	1.91	0.67
1:B:76:LEU:CD1	1:B:87:GLY:HA2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:O	1:A:258:ASP:N	2.28	0.67
1:B:236:VAL:HG11	1:B:269:VAL:CG2	2.26	0.66
1:A:254:GLU:HA	1:A:257:GLN:NE2	2.10	0.66
1:B:162:LEU:HB3	2:B:399:HOH:O	1.96	0.66
1:A:248:ASP:OD1	1:A:249:ASP:N	2.27	0.66
1:A:64:LEU:HB2	1:A:291:ARG:HG3	1.78	0.66
1:B:222:VAL:HA	1:B:225:ILE:HD12	1.77	0.65
1:A:142:ARG:HD2	2:A:608:HOH:O	1.94	0.65
1:B:347:LYS:HG2	2:B:459:HOH:O	1.97	0.65
1:A:254:GLU:O	1:A:257:GLN:OE1	2.14	0.65
1:A:167:LYS:HD3	2:B:417:HOH:O	1.98	0.64
1:B:321:VAL:HG22	1:B:357:MET:HG2	1.80	0.64
1:B:10:LEU:HB3	1:B:11:PRO:HD2	1.78	0.64
1:A:209:ASN:C	1:A:211:ASP:H	2.01	0.64
1:B:76:LEU:HD13	1:B:87:GLY:HA2	1.80	0.64
1:A:3:PHE:HE1	1:A:67:THR:O	1.81	0.64
1:B:244:ILE:CG2	1:B:252:LYS:HE2	2.28	0.63
1:B:301:ALA:HB3	1:B:302:PRO:CD	2.28	0.63
1:A:257:GLN:OE1	1:A:258:ASP:OD1	2.17	0.63
1:A:301:ALA:HB3	1:A:302:PRO:HD3	1.82	0.62
1:A:3:PHE:CZ	1:A:67:THR:O	2.52	0.62
1:A:64:LEU:HB2	1:A:291:ARG:HG2	1.80	0.62
1:B:330:PHE:HD2	1:B:336:ALA:HA	1.63	0.62
1:B:201:PRO:HA	2:B:431:HOH:O	1.99	0.62
1:B:90:PHE:C	1:B:90:PHE:HD1	2.02	0.62
1:B:87:GLY:O	1:B:90:PHE:N	2.33	0.61
1:A:295:VAL:HG11	1:A:304:ALA:HA	1.82	0.61
1:B:203:MET:HG2	1:B:276:LEU:CD2	2.30	0.61
1:A:146:ARG:HG2	2:A:453:HOH:O	2.00	0.60
1:B:184:ASP:O	1:B:187:GLU:HB2	2.01	0.60
1:B:257:GLN:C	1:B:259:LEU:H	2.05	0.60
1:B:330:PHE:CD2	1:B:339:ALA:HB3	2.37	0.60
1:B:85:GLY:O	1:B:88:ASN:N	2.35	0.60
1:A:156:LYS:HG3	1:A:157:GLU:N	2.17	0.59
1:B:181:VAL:HG12	1:B:183:LEU:HD13	1.84	0.59
1:A:318:ARG:NH1	1:A:320:GLU:OE2	2.36	0.59
1:A:146:ARG:HD3	2:A:480:HOH:O	2.02	0.59
1:B:255:PHE:O	1:B:259:LEU:HB2	2.03	0.59
1:B:320:GLU:OE1	1:B:342:TRP:CZ2	2.54	0.58
1:A:243:GLU:C	1:A:245:ALA:H	2.06	0.58
1:B:186:GLU:H	1:B:186:GLU:CD	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLY:CA	1:B:88:ASN:HA	2.33	0.58
1:A:318:ARG:NE	1:A:344:LEU:HD22	2.19	0.58
1:A:88:ASN:OD1	1:A:89:LYS:N	2.37	0.58
1:B:223:ARG:HA	1:B:226:ALA:HB3	1.86	0.58
1:B:257:GLN:O	1:B:259:LEU:N	2.32	0.58
1:B:301:ALA:HB3	1:B:302:PRO:HD3	1.85	0.57
1:A:44:VAL:HB	1:A:45:PRO:HD2	1.85	0.57
1:B:218:TYR:N	1:B:218:TYR:HD1	2.01	0.57
1:A:301:ALA:N	1:A:302:PRO:CD	2.68	0.57
1:B:219:LEU:HD11	1:B:223:ARG:HE	1.66	0.57
1:A:237:CYS:SG	1:A:240:ILE:N	2.63	0.57
1:B:106:CYS:HB2	1:B:207:ASN:O	2.04	0.56
1:B:218:TYR:N	1:B:218:TYR:CD1	2.69	0.56
1:B:244:ILE:HG21	1:B:264:PRO:HB3	1.88	0.56
1:A:210:GLU:HB2	1:A:240:ILE:HD11	1.87	0.56
1:B:150:ARG:NH1	1:B:155:ASP:OD2	2.39	0.56
1:B:85:GLY:CA	1:B:88:ASN:CA	2.82	0.56
1:B:235:PRO:O	1:B:268:ARG:NH1	2.30	0.56
1:A:261:ILE:O	1:A:261:ILE:CG2	2.53	0.56
1:A:210:GLU:HB3	1:A:240:ILE:HD12	1.87	0.56
1:B:102:HIS:CE1	1:B:128:ILE:CG2	2.89	0.56
1:B:318:ARG:NH1	1:B:360:ARG:HG3	2.20	0.56
1:B:343:ARG:CG	1:B:343:ARG:NH1	2.63	0.55
1:B:174:ASN:ND2	2:B:496:HOH:O	2.40	0.55
1:B:76:LEU:HB2	1:B:87:GLY:CA	2.34	0.55
1:A:176:GLY:HA2	1:B:174:ASN:ND2	2.23	0.54
1:B:337:LYS:NZ	1:B:337:LYS:HB2	2.23	0.54
1:B:352:GLN:O	1:B:353:ASP:C	2.46	0.54
1:A:40:ASN:C	1:A:42:GLY:H	2.11	0.54
1:B:79:GLY:HA2	2:B:376:HOH:O	2.06	0.53
1:A:170:PRO:O	1:A:174:ASN:ND2	2.41	0.53
1:B:291:ARG:HD3	1:B:293:TRP:CZ2	2.44	0.53
1:A:208:VAL:HB	1:A:212:GLY:HA3	1.90	0.53
1:A:347:LYS:HE3	2:A:609:HOH:O	2.08	0.53
1:B:219:LEU:O	1:B:223:ARG:HG3	2.08	0.53
1:B:84:GLU:OE1	1:B:84:GLU:O	2.26	0.53
1:B:10:LEU:CB	1:B:11:PRO:HD2	2.37	0.53
1:B:280:GLN:HG3	1:B:295:VAL:CG1	2.37	0.53
1:B:136:ASP:OD2	1:B:198:THR:HG23	2.08	0.53
1:B:77:VAL:CG2	1:B:90:PHE:HE2	2.22	0.53
1:B:90:PHE:O	1:B:90:PHE:CD1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HD11	1:A:263:GLU:HA	1.91	0.53
1:B:213:PHE:CE2	1:B:235:PRO:HB2	2.44	0.53
1:A:209:ASN:C	1:A:211:ASP:N	2.61	0.53
1:B:94:ILE:HD11	1:B:100:ILE:CD1	2.39	0.53
1:B:62:ARG:O	1:B:289:GLU:HA	2.08	0.52
1:B:330:PHE:HE2	1:B:341:LYS:HG2	1.74	0.52
1:B:48:ASP:C	1:B:48:ASP:OD1	2.45	0.52
1:B:160:PHE:HE2	1:B:186:GLU:O	1.93	0.52
1:A:2:GLY:O	1:A:3:PHE:CB	2.57	0.52
1:B:102:HIS:HE1	1:B:128:ILE:CG2	2.22	0.52
1:B:85:GLY:O	1:B:86:LEU:C	2.47	0.52
1:B:312:PHE:CZ	1:B:359:PHE:HB2	2.44	0.52
1:A:257:GLN:O	1:A:259:LEU:N	2.43	0.52
1:A:237:CYS:SG	1:A:239:ALA:HB3	2.50	0.52
1:A:90:PHE:CZ	1:A:94:ILE:HD11	2.45	0.52
1:B:77:VAL:HG22	1:B:90:PHE:HE2	1.74	0.52
1:B:94:ILE:HD11	1:B:100:ILE:HD11	1.91	0.52
1:A:185:LYS:CD	1:A:185:LYS:N	2.61	0.51
1:A:19:PHE:CD2	1:A:72:ASP:HB2	2.46	0.51
1:B:74:ALA:HB1	2:B:393:HOH:O	2.11	0.51
1:B:87:GLY:O	1:B:89:LYS:N	2.44	0.51
1:B:241:GLU:OE1	1:B:244:ILE:HD12	2.10	0.51
1:A:303:LYS:HG3	2:A:422:HOH:O	2.11	0.51
1:B:75:GLY:O	1:B:77:VAL:N	2.43	0.51
1:B:86:LEU:CG	1:B:91:LEU:HD11	2.39	0.50
1:A:150:ARG:HD3	2:A:524:HOH:O	2.12	0.50
1:B:343:ARG:NH1	1:B:345:GLU:OE2	2.44	0.50
1:B:79:GLY:CA	2:B:376:HOH:O	2.60	0.50
1:A:122:LEU:HD13	1:A:225:ILE:HG12	1.93	0.50
1:B:122:LEU:HD13	1:B:225:ILE:HD13	1.93	0.50
1:A:330:PHE:O	1:A:335:GLY:HA3	2.12	0.50
1:B:183:LEU:HD23	1:B:191:ILE:HD11	1.94	0.50
1:B:244:ILE:HG23	1:B:252:LYS:HE2	1.94	0.50
1:A:268:ARG:NH1	1:A:268:ARG:HG3	2.26	0.50
1:A:176:GLY:HA2	1:B:174:ASN:HD21	1.77	0.49
1:A:254:GLU:HG2	1:A:257:GLN:HE22	1.76	0.49
1:B:76:LEU:HD12	1:B:87:GLY:HA2	1.94	0.49
1:B:301:ALA:N	1:B:302:PRO:CD	2.74	0.49
1:B:10:LEU:HA	1:B:77:VAL:HG11	1.93	0.49
1:A:7:ILE:HD11	1:A:70:PHE:CD1	2.47	0.49
1:B:169:LEU:HB3	1:B:170:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PRO:HG2	1:B:218:TYR:HD1	1.78	0.49
1:A:91:LEU:HD13	1:A:135:ALA:HB2	1.93	0.49
1:B:324:TYR:O	1:B:327:PHE:N	2.46	0.49
1:A:13:VAL:CG2	1:A:105:ARG:CB	2.82	0.49
1:B:257:GLN:C	1:B:259:LEU:N	2.66	0.49
1:B:10:LEU:CD2	1:B:77:VAL:CG1	2.84	0.49
1:B:10:LEU:HD12	1:B:124:ASP:HB3	1.95	0.48
1:B:233:VAL:O	1:B:235:PRO:HD2	2.12	0.48
1:A:2:GLY:O	1:A:3:PHE:HB2	2.12	0.48
1:B:24:LYS:HA	1:B:24:LYS:HE2	1.95	0.48
1:A:248:ASP:O	1:A:249:ASP:C	2.53	0.47
1:B:261:ILE:HG21	2:B:499:HOH:O	2.12	0.47
1:A:362:ASN:O	1:A:363:VAL:C	2.53	0.47
1:B:150:ARG:O	1:B:155:ASP:HB3	2.15	0.47
1:A:261:ILE:HG12	1:A:263:GLU:O	2.15	0.47
1:B:303:LYS:HA	2:B:425:HOH:O	2.14	0.47
1:A:19:PHE:CE2	1:A:72:ASP:HB2	2.50	0.47
1:A:318:ARG:NH1	1:A:360:ARG:NH1	2.63	0.47
1:B:90:PHE:HD1	1:B:91:LEU:HD23	1.73	0.47
1:B:219:LEU:CD1	1:B:223:ARG:HE	2.29	0.46
1:B:217:PRO:HG2	1:B:218:TYR:CD1	2.49	0.46
1:B:244:ILE:HG22	1:B:252:LYS:HE2	1.97	0.46
1:B:362:ASN:O	1:B:363:VAL:C	2.53	0.46
1:A:210:GLU:HB3	1:A:240:ILE:CD1	2.44	0.46
1:A:337:LYS:HE3	1:A:342:TRP:CE2	2.51	0.46
1:A:256:LEU:CD2	1:A:261:ILE:HG23	2.45	0.46
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.58	0.46
1:B:277:LEU:O	1:B:278:ASN:CB	2.64	0.46
1:B:8:VAL:HG22	1:B:73:ILE:CG2	2.45	0.46
1:A:221:ARG:O	1:A:225:ILE:HD12	2.15	0.46
1:B:145:GLN:HB2	1:B:145:GLN:HE21	1.51	0.46
1:B:196:PHE:HB2	2:B:366:HOH:O	2.14	0.46
1:B:318:ARG:HH21	1:B:344:LEU:CD2	2.27	0.46
1:A:137:LEU:O	1:A:141:GLU:HG3	2.15	0.46
1:B:122:LEU:HD12	1:B:122:LEU:O	2.16	0.46
1:B:57:ILE:HD11	2:B:490:HOH:O	2.15	0.46
1:B:165:MET:CE	1:B:194:TYR:CE2	2.99	0.46
1:B:8:VAL:HG22	1:B:73:ILE:HG21	1.98	0.46
1:B:185:LYS:O	1:B:189:GLN:HB2	2.16	0.46
1:B:22:LEU:O	1:B:44:VAL:HG11	2.15	0.46
1:B:47:PRO:HD2	1:B:270:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:HA	1:B:49:PRO:HD3	1.81	0.46
1:A:256:LEU:HD22	1:A:261:ILE:O	2.16	0.45
1:B:326:ASP:O	1:B:329:GLN:N	2.49	0.45
1:B:323:ALA:O	1:B:324:TYR:C	2.53	0.45
1:B:122:LEU:HB2	1:B:225:ILE:HD11	1.97	0.45
1:B:137:LEU:O	1:B:141:GLU:HG3	2.16	0.45
1:B:18:LEU:HD21	1:B:236:VAL:HG21	1.98	0.45
1:A:88:ASN:OD1	1:A:88:ASN:C	2.55	0.45
1:B:244:ILE:O	1:B:252:LYS:HE3	2.16	0.45
1:B:337:LYS:HB2	1:B:337:LYS:HZ2	1.82	0.45
1:B:85:GLY:C	1:B:88:ASN:N	2.70	0.45
1:B:226:ALA:O	1:B:229:GLU:HB3	2.17	0.45
1:B:54:LEU:HD23	1:B:327:PHE:CD1	2.52	0.45
1:A:14:GLY:O	1:A:15:LYS:C	2.53	0.45
1:A:188:LEU:HA	1:A:188:LEU:HD23	1.73	0.45
1:A:254:GLU:CG	1:A:257:GLN:HE22	2.30	0.45
1:B:156:LYS:O	1:B:159:LYS:N	2.49	0.45
1:B:162:LEU:O	1:B:166:GLU:HG2	2.17	0.45
1:B:225:ILE:O	1:B:226:ALA:C	2.56	0.45
1:B:263:GLU:CD	1:B:271:ARG:HH22	2.21	0.45
1:B:330:PHE:CE2	1:B:339:ALA:HB3	2.52	0.45
1:B:207:ASN:HD21	1:B:238:ALA:HB2	1.81	0.44
1:B:241:GLU:CA	1:B:241:GLU:OE1	2.42	0.44
1:A:108:GLU:HG3	1:A:218:TYR:OH	2.18	0.44
1:B:236:VAL:HG11	1:B:269:VAL:HG22	2.00	0.44
1:A:138:ASP:CG	1:A:142:ARG:HE	2.20	0.44
1:A:248:ASP:CB	1:A:251:GLU:HB2	2.39	0.44
1:A:34:PHE:CB	1:A:62:ARG:CD	2.96	0.44
1:B:228:LYS:HB2	1:B:228:LYS:HE3	1.65	0.44
1:B:266:LEU:HA	1:B:266:LEU:HD12	1.75	0.44
1:B:62:ARG:NH2	2:B:486:HOH:O	2.46	0.44
1:B:219:LEU:HD11	1:B:223:ARG:NE	2.33	0.44
1:B:337:LYS:HG3	1:B:342:TRP:HB2	2.01	0.43
1:A:217:PRO:HD2	2:A:507:HOH:O	2.19	0.43
1:B:185:LYS:O	1:B:187:GLU:N	2.52	0.43
1:B:168:ILE:O	1:B:169:LEU:C	2.56	0.43
1:A:203:MET:HG2	1:A:276:LEU:HD22	2.01	0.43
1:A:321:VAL:HG22	1:A:357:MET:HG2	1.99	0.43
1:B:226:ALA:O	1:B:230:GLY:N	2.52	0.43
1:A:142:ARG:CD	2:A:608:HOH:O	2.57	0.43
1:B:243:GLU:C	1:B:245:ALA:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:HB	1:B:292:ALA:O	2.18	0.43
1:B:207:ASN:ND2	1:B:238:ALA:HB2	2.33	0.42
1:B:280:GLN:HG3	1:B:295:VAL:HG12	2.00	0.42
1:B:86:LEU:N	1:B:86:LEU:CD2	2.74	0.42
1:B:203:MET:CG	1:B:276:LEU:HD22	2.42	0.42
1:A:19:PHE:O	1:A:19:PHE:CD1	2.72	0.42
1:B:330:PHE:CD2	1:B:336:ALA:HA	2.49	0.42
1:B:44:VAL:HB	1:B:45:PRO:HD2	2.00	0.42
1:A:142:ARG:O	1:A:146:ARG:HG3	2.20	0.42
1:A:176:GLY:CA	1:B:174:ASN:ND2	2.82	0.42
1:B:243:GLU:O	1:B:244:ILE:C	2.58	0.42
1:B:341:LYS:HD3	1:B:341:LYS:HA	1.76	0.42
1:B:322:ILE:HG22	1:B:323:ALA:O	2.19	0.42
1:A:17:THR:HB	1:A:238:ALA:HB1	2.01	0.42
1:A:323:ALA:O	1:A:324:TYR:C	2.57	0.42
1:B:252:LYS:O	1:B:256:LEU:HG	2.20	0.42
1:A:89:LYS:O	1:A:90:PHE:C	2.58	0.42
1:A:216:ASN:HA	1:A:217:PRO:HD3	1.89	0.41
1:B:127:THR:O	1:B:131:GLU:HG2	2.19	0.41
1:B:329:GLN:HB3	1:B:330:PHE:CD1	2.54	0.41
1:A:259:LEU:HB3	1:A:260:GLY:H	1.72	0.41
1:A:58:VAL:O	1:A:59:LYS:HB2	2.21	0.41
1:A:59:LYS:N	1:A:60:PRO:HD3	2.35	0.41
1:B:20:ASN:HD22	1:B:20:ASN:HA	1.66	0.41
1:A:169:LEU:HB3	1:A:170:PRO:HD3	2.02	0.41
1:B:248:ASP:O	1:B:250:GLU:N	2.53	0.41
1:A:169:LEU:HB3	1:A:170:PRO:CD	2.50	0.41
1:A:17:THR:CG2	1:A:242:SER:HB2	2.33	0.41
1:A:301:ALA:O	1:A:305:ALA:N	2.53	0.41
1:A:162:LEU:O	1:A:166:GLU:HG3	2.21	0.41
1:B:102:HIS:NE2	1:B:128:ILE:HG13	2.35	0.41
1:A:62:ARG:NH2	2:A:562:HOH:O	2.46	0.41
1:B:44:VAL:HB	1:B:45:PRO:CD	2.50	0.41
1:B:167:LYS:HE2	1:B:187:GLU:OE2	2.20	0.41
1:B:54:LEU:HD23	1:B:327:PHE:CE1	2.56	0.41
1:A:209:ASN:O	1:A:211:ASP:N	2.54	0.41
1:A:76:LEU:HD12	2:A:375:HOH:O	2.20	0.41
1:A:23:THR:O	1:A:24:LYS:C	2.59	0.41
1:A:261:ILE:HG22	1:A:261:ILE:O	2.21	0.41
1:B:63:ILE:HA	1:B:290:VAL:O	2.21	0.41
1:B:181:VAL:CG1	1:B:183:LEU:HD13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:O	1:B:90:PHE:HD1	2.04	0.40
1:B:156:LYS:O	1:B:159:LYS:HB2	2.20	0.40
1:B:3:PHE:HB3	1:B:277:LEU:HD22	2.01	0.40
1:A:130:THR:HG22	1:A:134:LEU:HD22	2.03	0.40
1:B:10:LEU:HD22	1:B:11:PRO:HD2	2.03	0.40
1:B:210:GLU:H	1:B:210:GLU:HG2	1.61	0.40
1:A:108:GLU:O	1:A:109:ASN:HB3	2.21	0.40
1:A:229:GLU:HG3	1:A:229:GLU:H	1.77	0.40
1:A:10:LEU:HA	1:A:10:LEU:HD23	1.61	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	342/363 (94%)	304 (89%)	28 (8%)	10 (3%)	4	4
1	B	329/363 (91%)	280 (85%)	35 (11%)	14 (4%)	2	2
All	All	671/726 (92%)	584 (87%)	63 (9%)	24 (4%)	3	3

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	244	ILE
1	A	257	GLN
1	B	11	PRO
1	B	88	ASN
1	B	226	ALA
1	A	3	PHE
1	B	76	LEU
1	B	244	ILE

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Mol	Chain	Res	Type
1	B	258	ASP
1	B	287	VAL
1	A	41	THR
1	A	243	GLU
1	B	215	ASN
1	A	24	LYS
1	B	353	ASP
1	A	2	GLY
1	B	324	TYR
1	A	265	GLY
1	B	169	LEU
1	A	264	PRO
1	B	125	ILE
1	B	225	ILE
1	B	79	GLY

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	275/294 (94%)	234 (85%)	41 (15%)	3 3
1	B	271/294 (92%)	208 (77%)	63 (23%)	1 1
All	All	546/588 (93%)	442 (81%)	104 (19%)	1 1

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	13	VAL
1	A	15	LYS
1	A	17	THR
1	A	18	LEU
1	A	20	ASN
1	A	24	LYS
1	A	76	LEU

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	96	GLU
1	A	106	CYS
1	A	119	ILE
1	A	134	LEU
1	A	146	ARG
1	A	149	LYS
1	A	150	ARG
1	A	156	LYS
1	A	185	LYS
1	A	215	ASN
1	A	223	ARG
1	A	228	LYS
1	A	229	GLU
1	A	236	VAL
1	A	240	ILE
1	A	251	GLU
1	A	252	LYS
1	A	256	LEU
1	A	257	GLN
1	A	259	LEU
1	A	261	ILE
1	A	263	GLU
1	A	268	ARG
1	A	278	ASN
1	A	288	LYS
1	A	291	ARG
1	A	303	LYS
1	A	314	LYS
1	A	318	ARG
1	A	341	LYS
1	A	343	ARG
1	A	347	LYS
1	B	15	LYS
1	B	23	THR
1	B	24	LYS
1	B	46	MET
1	B	52	ASP
1	B	56	GLU
1	B	61	GLU
1	B	63	ILE
1	B	69	GLU

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Mol	Chain	Res	Type
1	B	73	ILE
1	B	82	LYS
1	B	84	GLU
1	B	86	LEU
1	B	88	ASN
1	B	89	LYS
1	B	90	PHE
1	B	98	ASP
1	B	104	VAL
1	B	123	ASP
1	B	124	ASP
1	B	130	THR
1	B	142	ARG
1	B	145	GLN
1	B	148	GLN
1	B	149	LYS
1	B	150	ARG
1	B	152	LYS
1	B	157	GLU
1	B	159	LYS
1	B	162	LEU
1	B	179	ARG
1	B	183	LEU
1	B	185	LYS
1	B	189	GLN
1	B	205	ILE
1	B	210	GLU
1	B	218	TYR
1	B	219	LEU
1	B	221	ARG
1	B	223	ARG
1	B	228	LYS
1	B	229	GLU
1	B	234	VAL
1	B	241	GLU
1	B	247	LEU
1	B	259	LEU
1	B	261	ILE
1	B	262	GLU
1	B	266	LEU
1	B	294	THR
1	B	303	LYS

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Mol	Chain	Res	Type
1	B	314	LYS
1	B	318	ARG
1	B	328	ILE
1	B	329	GLN
1	B	330	PHE
1	B	334	ASN
1	B	337	LYS
1	B	338	GLU
1	B	342	TRP
1	B	343	ARG
1	B	347	LYS
1	B	351	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	129	ASN
1	A	257	GLN
1	A	362	ASN
1	B	20	ASN
1	B	88	ASN
1	B	93	ASN
1	B	102	HIS
1	B	145	GLN
1	B	148	GLN
1	B	174	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	348/363 (95%)	-0.15	23 (6%)	18	17	26, 45, 107, 117	0
1	B	335/363 (92%)	0.13	28 (8%)	11	10	34, 63, 105, 116	0
All	All	683/726 (94%)	-0.01	51 (7%)	14	13	26, 54, 106, 117	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ASP	10.2
1	B	76	LEU	7.5
1	A	39	PRO	7.4
1	B	82	LYS	7.3
1	A	259	LEU	6.9
1	A	247	LEU	5.9
1	B	78	ALA	5.9
1	A	249	ASP	5.7
1	B	83	GLY	5.4
1	B	80	ALA	4.7
1	A	251	GLU	4.6
1	A	258	ASP	4.4
1	B	153	GLY	4.3
1	A	1	MET	4.1
1	A	250	GLU	4.1
1	A	246	GLU	3.8
1	A	257	GLN	3.8
1	B	215	ASN	3.6
1	B	1	MET	3.6
1	B	217	PRO	3.5
1	A	41	THR	3.5
1	A	256	LEU	3.5
1	A	34	PHE	3.4
1	A	261	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	210	GLU	3.4
1	B	41	THR	3.3
1	A	254	GLU	3.3
1	B	258	ASP	3.2
1	B	151	ALA	3.1
1	B	248	ASP	3.1
1	B	338	GLU	3.0
1	A	260	GLY	2.8
1	A	215	ASN	2.8
1	B	152	LYS	2.7
1	B	155	ASP	2.6
1	B	249	ASP	2.6
1	B	74	ALA	2.5
1	B	154	GLY	2.5
1	B	254	GLU	2.4
1	B	20	ASN	2.4
1	B	257	GLN	2.4
1	B	243	GLU	2.4
1	B	150	ARG	2.3
1	B	84	GLU	2.3
1	A	38	GLU	2.3
1	B	86	LEU	2.2
1	B	228	LYS	2.2
1	B	85	GLY	2.2
1	A	40	ASN	2.1
1	A	24	LYS	2.1
1	A	37	ILE	2.1

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 carbohydrates 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.