Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:45 PM GMT

PDB ID	:	4G1T
Title	:	Crystal structure of interferon-stimulated gene 54
Authors	:	Yang, Z.; Liang, H.; Zhou, Q.; Li, Y.; Chen, H.; Ye, W.; Chen, D.; Fleming, J.; Shu, H.; Liu, Y.
Deposited on	:	2012-07-11
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	Percentile Ranks	Value
Rfree		0.305
Clashscore		28
Ramachandran outliers		0.2%
Sidechain outliers		7.6%
RSRZ outliers		2.9%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
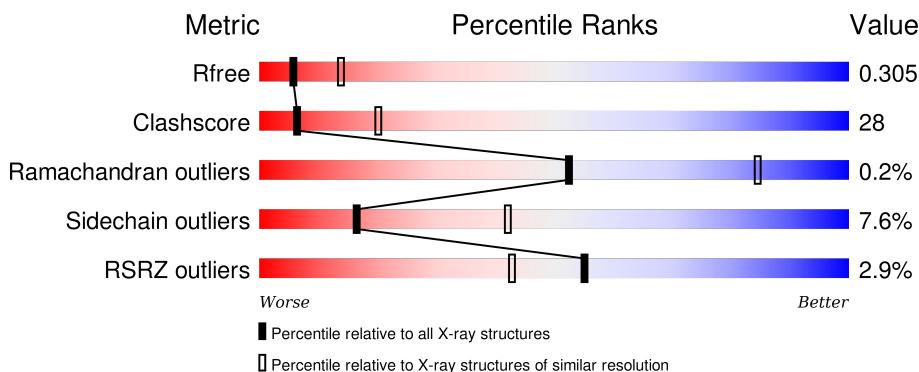
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	472	3% / 54% 33% • 10%
1	B	472	3% / 52% 36% • 9%
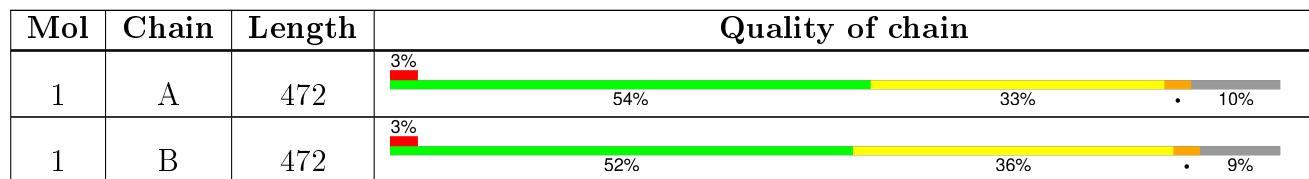
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6870 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 Interferon-induced protein with tetratricopeptide repeats 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3425	2176	602	627	20			
1	B	429	Total	C	N	O	S	0	0	0
			3422	2170	603	629	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLU	ASP	SEE REMARK 999	UNP P09913
B	352	GLU	ASP	SEE REMARK 999	UNP P09913

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	5	Total	O	0	0
			5	5		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Interferon-induced protein with tetratricopeptide repeats 2
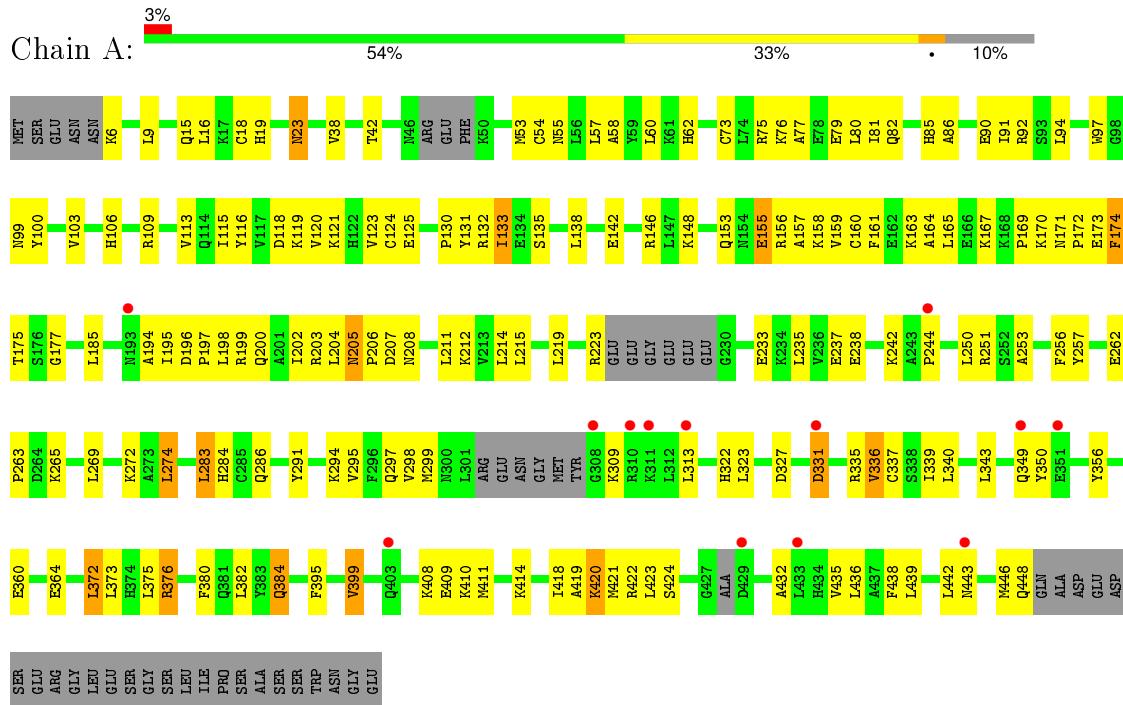
- Molecule 1: Interferon-induced protein with tetratricopeptide repeats 2
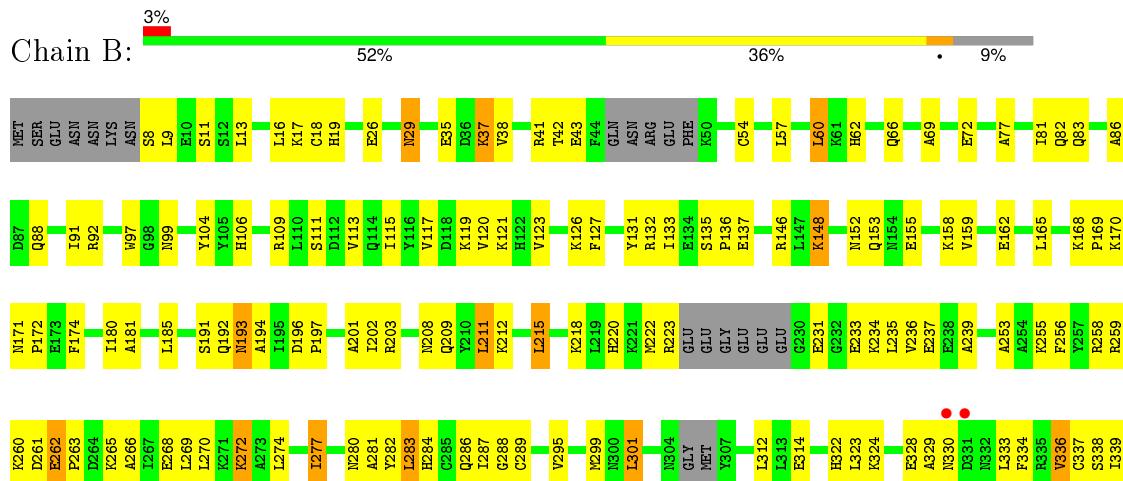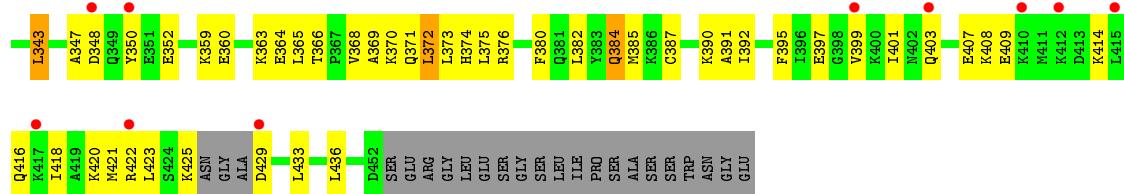
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.02Å　　95.21Å　　155.90Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	39.57　–　2.80 48.17　–　2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.57-2.80) 98.5 (48.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.234　,　0.287 0.266　,　0.305	Depositor DCC
R_{free} test set	1505 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 29702 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/3488	0.60	2/4685 (0.0%)
1	B	0.46	0/3484	0.57	0/4683
All	All	0.47	0/6972	0.59	2/9368 (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	349	GLN	N-CA-C	-5.29	96.72	111.00
1	A	331	ASP	CB-CG-OD2	5.19	122.97	118.30

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	3425	0	3394	177	0
1	B	3422	0	3358	226	0
2	A	18	0	0	1	0
2	B	5	0	0	0	0
All	All	6870	0	6752	377	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 28.

All (377) 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:330:ASN:ND2	1:B:333:LEU:HD12	1.63	1.13
1:B:350:TYR:CE1	1:B:384:GLN:HB2	1.84	1.11
1:B:359:LYS:HE2	1:B:363:LYS:HZ3	1.09	1.10
1:B:359:LYS:HG2	1:B:363:LYS:HE3	1.27	1.09
1:B:366:THR:HG23	1:B:369:ALA:H	1.17	1.07
1:B:359:LYS:HG2	1:B:363:LYS:CE	1.84	1.06
1:B:301:LEU:HD13	1:B:301:LEU:H	1.20	1.05
1:B:261:ASP:O	1:B:263:PRO:HD3	1.60	1.02
1:B:88:GLN:HG3	1:B:92:ARG:HH21	1.23	1.02
1:A:204:LEU:C	1:A:205:ASN:HD22	1.62	1.01
1:A:205:ASN:HD21	1:B:172:PRO:HB3	1.19	1.01
1:A:309:LYS:O	1:A:313:LEU:HG	1.60	0.99
1:A:262:GLU:OE1	1:A:265:LYS:HD2	1.63	0.98
1:A:194:ALA:O	1:A:197:PRO:HD2	1.64	0.98
1:A:55:ASN:HD22	1:A:99:ASN:HD22	1.10	0.96
1:B:359:LYS:HE2	1:B:363:LYS:NZ	1.80	0.96
1:B:330:ASN:HD22	1:B:333:LEU:HD12	1.21	0.95
1:B:301:LEU:N	1:B:301:LEU:CD1	2.30	0.94
1:A:146:ARG:HB3	1:A:153:GLN:HG3	1.50	0.94
1:B:350:TYR:CE1	1:B:384:GLN:CB	2.50	0.94
1:A:38:VAL:O	1:A:42:THR:HG23	1.68	0.92
1:A:284:HIS:HD2	1:A:322:HIS:HD2	1.19	0.91
1:B:301:LEU:HD13	1:B:301:LEU:N	1.88	0.89
1:B:18:CYS:HB2	1:B:99:ASN:ND2	1.88	0.88
1:A:380:PHE:CD1	1:A:384:GLN:HG3	2.10	0.86
1:A:446:MET:HA	1:A:448:GLN:C	1.96	0.85
1:B:350:TYR:HE1	1:B:384:GLN:CB	1.86	0.85
1:B:117:VAL:CG1	1:B:121:LYS:HE3	2.06	0.85
1:A:251:ARG:HG3	1:A:286:GLN:HE22	1.40	0.85
1:B:301:LEU:H	1:B:301:LEU:CD1	1.89	0.85
1:A:159:VAL:HG21	1:B:159:VAL:HG21	1.59	0.84
1:A:132:ARG:HH21	1:B:17:LYS:HE2	1.41	0.84
1:B:66:GLN:O	1:B:69:ALA:HB3	1.78	0.83
1:B:359:LYS:CG	1:B:363:LYS:HE3	2.09	0.82
1:B:350:TYR:HE1	1:B:384:GLN:HB2	1.44	0.81
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.47	0.80
1:B:9:LEU:HD11	1:B:13:LEU:HD11	1.63	0.80
1:B:280:ASN:HD22	1:B:283:LEU:H	1.29	0.80
1:A:284:HIS:CD2	1:A:322:HIS:HD2	1.99	0.80
1:A:309:LYS:O	1:A:313:LEU:CG	2.30	0.79
1:B:359:LYS:HG2	1:B:363:LYS:NZ	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:THR:HG22	1:B:369:ALA:CB	2.13	0.79
1:A:284:HIS:HD2	1:A:322:HIS:CD2	2.00	0.79
1:A:55:ASN:HD22	1:A:99:ASN:ND2	1.81	0.79
1:A:205:ASN:ND2	1:B:172:PRO:HB3	1.96	0.78
1:B:117:VAL:HG12	1:B:121:LYS:HE3	1.63	0.78
1:B:218:LYS:O	1:B:222:MET:HG2	1.84	0.78
1:B:260:LYS:O	1:B:261:ASP:HB2	1.83	0.78
1:B:9:LEU:HD13	1:B:9:LEU:O	1.83	0.77
1:B:19:HIS:H	1:B:19:HIS:CD2	2.01	0.76
1:B:280:ASN:HD21	1:B:282:TYR:HB2	1.50	0.76
1:B:9:LEU:HD13	1:B:9:LEU:C	2.06	0.75
1:B:366:THR:HG23	1:B:369:ALA:N	1.99	0.75
1:A:85:HIS:HB3	1:A:92:ARG:CD	2.17	0.74
1:B:284:HIS:HD2	1:B:322:HIS:HD2	1.35	0.74
1:B:366:THR:CG2	1:B:369:ALA:CB	2.66	0.74
1:B:171:ASN:OD1	1:B:172:PRO:HD2	1.87	0.73
1:B:347:ALA:O	1:B:348:ASP:HB2	1.89	0.73
1:A:438:PHE:O	1:A:442:LEU:HD13	1.89	0.72
1:A:410:LYS:HE3	1:A:414:LYS:HE3	1.70	0.72
1:A:198:LEU:O	1:A:202:ILE:HG13	1.88	0.72
1:B:366:THR:CG2	1:B:369:ALA:HB2	2.20	0.72
1:B:391:ALA:HB1	1:B:395:PHE:CE2	2.25	0.72
1:A:205:ASN:HD22	1:A:205:ASN:N	1.83	0.72
1:B:155:GLU:HA	1:B:185:LEU:HD11	1.71	0.71
1:B:38:VAL:O	1:B:42:THR:HG23	1.90	0.71
1:B:77:ALA:O	1:B:81:ILE:HG13	1.90	0.71
1:A:121:LYS:HE3	1:B:131:TYR:HE1	1.54	0.71
1:A:446:MET:CA	1:A:448:GLN:C	2.59	0.71
1:B:366:THR:HG22	1:B:369:ALA:HB2	1.73	0.71
1:B:323:LEU:HD22	1:B:336:VAL:HG21	1.72	0.71
1:A:197:PRO:HA	1:A:200:GLN:HE21	1.57	0.70
1:B:324:LYS:O	1:B:328:GLU:HG3	1.92	0.69
1:A:263:PRO:HG2	1:A:297:GLN:OE1	1.92	0.69
1:B:397:GLU:O	1:B:401:ILE:HG13	1.93	0.69
1:A:132:ARG:NH2	1:B:17:LYS:HG2	2.07	0.69
1:B:88:GLN:HB2	1:B:92:ARG:HE	1.56	0.69
1:B:208:ASN:ND2	1:B:211:LEU:HD22	2.07	0.68
1:B:88:GLN:CB	1:B:92:ARG:HE	2.06	0.68
1:B:158:LYS:HE3	1:B:162:GLU:OE2	1.93	0.68
1:B:109:ARG:O	1:B:113:VAL:HG23	1.93	0.68
1:A:175:THR:HG22	1:B:201:ALA:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLU:HG3	1:B:373:LEU:HD22	1.76	0.67
1:B:359:LYS:HG2	1:B:363:LYS:HZ1	1.57	0.67
1:A:130:PRO:O	1:B:121:LYS:HA	1.95	0.67
1:B:359:LYS:CG	1:B:363:LYS:CE	2.68	0.67
1:A:121:LYS:HE3	1:B:131:TYR:CE1	2.30	0.67
1:A:171:ASN:OD1	1:A:172:PRO:HD2	1.95	0.67
1:A:205:ASN:HD21	1:B:172:PRO:CB	2.02	0.66
1:A:131:TYR:CE1	1:B:121:LYS:HE2	2.30	0.66
1:B:347:ALA:O	1:B:348:ASP:CB	2.42	0.65
1:A:253:ALA:O	1:A:256:PHE:HB3	1.96	0.65
1:B:364:GLU:O	1:B:365:LEU:HD23	1.97	0.65
1:B:337:CYS:SG	1:B:359:LYS:HD3	2.38	0.64
1:B:301:LEU:HD12	1:B:301:LEU:N	2.12	0.64
1:A:196:ASP:HB2	1:A:197:PRO:HD3	1.80	0.64
1:B:391:ALA:HB1	1:B:395:PHE:HE2	1.61	0.64
1:B:366:THR:HG22	1:B:369:ALA:HB3	1.79	0.64
1:B:375:LEU:HD12	1:B:407:GLU:HB3	1.78	0.64
1:A:291:TYR:O	1:A:295:VAL:HG23	1.98	0.64
1:A:262:GLU:OE1	1:A:265:LYS:CD	2.41	0.63
1:A:323:LEU:HD22	1:A:336:VAL:HG21	1.81	0.63
1:A:58:ALA:HB2	1:A:73:CYS:HB2	1.79	0.63
1:B:171:ASN:OD1	1:B:172:PRO:CD	2.46	0.63
1:A:132:ARG:NH2	1:B:17:LYS:HE2	2.12	0.63
1:B:268:GLU:O	1:B:272:LYS:HD2	1.98	0.63
1:A:53:MET:HE3	1:A:53:MET:HA	1.80	0.62
1:B:233:GLU:O	1:B:237:GLU:HG3	1.98	0.62
1:B:265:LYS:O	1:B:269:LEU:HD12	1.99	0.62
1:A:294:LYS:O	1:A:298:VAL:HG23	2.00	0.62
1:A:423:LEU:HD11	1:A:436:LEU:HD22	1.82	0.62
1:B:88:GLN:HG3	1:B:92:ARG:NH2	2.05	0.62
1:B:9:LEU:CD1	1:B:13:LEU:HD11	2.29	0.62
1:B:169:PRO:O	1:B:170:LYS:HB3	2.00	0.62
1:B:255:LYS:O	1:B:259:ARG:HG2	2.00	0.61
1:A:295:VAL:O	1:A:299:MET:HG3	2.00	0.61
1:A:75:ARG:O	1:A:79:GLU:HG3	2.01	0.61
1:B:284:HIS:HD2	1:B:322:HIS:CD2	2.18	0.61
1:A:169:PRO:O	1:A:170:LYS:HB2	2.00	0.60
1:A:153:GLN:NE2	1:A:156:ARG:NH1	2.49	0.60
1:B:284:HIS:CD2	1:B:322:HIS:HD2	2.18	0.60
1:A:16:LEU:HD23	1:B:131:TYR:HB3	1.84	0.60
1:B:371:GLN:NE2	1:B:403:GLN:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:HB2	1:A:420:LYS:NZ	2.17	0.59
1:A:23:ASN:ND2	2:A:515:HOH:O	2.35	0.59
1:B:35:GLU:HB2	1:B:60:LEU:HD11	1.84	0.59
1:B:359:LYS:CE	1:B:363:LYS:NZ	2.62	0.59
1:A:410:LYS:HE3	1:A:414:LYS:CE	2.33	0.59
1:B:196:ASP:HB2	1:B:197:PRO:HD3	1.83	0.59
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.03	0.59
1:B:170:LYS:O	1:B:170:LYS:HG2	2.03	0.58
1:B:280:ASN:ND2	1:B:282:TYR:HB2	2.18	0.58
1:B:104:TYR:HE1	1:B:109:ARG:NH1	2.01	0.58
1:B:260:LYS:O	1:B:261:ASP:CB	2.50	0.58
1:A:19:HIS:CD2	1:A:99:ASN:HD21	2.21	0.58
1:A:85:HIS:HB3	1:A:92:ARG:NE	2.18	0.58
1:B:281:ALA:HB1	1:B:334:PHE:CE2	2.38	0.58
1:B:395:PHE:O	1:B:399:VAL:HG23	2.04	0.58
1:A:131:TYR:HE1	1:B:121:LYS:HE2	1.68	0.58
1:B:263:PRO:O	1:B:266:ALA:HB3	2.03	0.57
1:A:55:ASN:ND2	1:A:99:ASN:HD22	1.91	0.57
1:A:331:ASP:O	1:A:331:ASP:OD1	2.22	0.57
1:B:202:ILE:HD11	1:B:212:LYS:HA	1.85	0.57
1:A:238:GLU:OE2	1:A:242:LYS:HE2	2.03	0.57
1:A:54:CYS:HB2	1:A:77:ALA:HB2	1.86	0.57
1:B:171:ASN:OD1	1:B:172:PRO:N	2.37	0.57
1:A:53:MET:HE3	1:A:53:MET:CA	2.34	0.57
1:B:236:VAL:HG21	1:B:256:PHE:CD1	2.40	0.57
1:B:368:VAL:HG22	1:B:403:GLN:HG2	1.86	0.57
1:A:174:PHE:N	1:A:174:PHE:CD2	2.70	0.57
1:A:339:ILE:O	1:A:343:LEU:HB2	2.04	0.57
1:B:126:LYS:HD2	1:B:127:PHE:CE2	2.39	0.57
1:B:16:LEU:HD22	1:B:120:VAL:HG11	1.87	0.56
1:B:9:LEU:CD1	1:B:13:LEU:CD1	2.83	0.56
1:B:350:TYR:OH	1:B:384:GLN:HB3	2.06	0.56
1:A:82:GLN:O	1:A:86:ALA:HB2	2.06	0.56
1:B:433:LEU:HA	1:B:436:LEU:HD12	1.87	0.56
1:B:350:TYR:HD1	1:B:380:PHE:CZ	2.24	0.56
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.20	0.55
1:A:339:ILE:N	1:A:339:ILE:CD1	2.69	0.55
1:A:171:ASN:OD1	1:A:172:PRO:CD	2.53	0.55
1:B:193:ASN:HD21	1:B:196:ASP:H	1.55	0.55
1:B:37:LYS:O	1:B:41:ARG:HG3	2.05	0.55
1:A:340:LEU:HD13	1:A:356:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLU:O	1:B:365:LEU:HD11	2.06	0.55
1:B:368:VAL:CG2	1:B:403:GLN:NE2	2.70	0.55
1:A:335:ARG:NH2	1:A:364:GLU:OE2	2.40	0.55
1:A:418:ILE:HA	1:A:421:MET:HE3	1.88	0.55
1:B:9:LEU:CD1	1:B:9:LEU:C	2.75	0.54
1:B:19:HIS:HD2	1:B:19:HIS:H	1.55	0.54
1:A:23:ASN:C	1:A:23:ASN:HD22	2.10	0.54
1:A:97:TRP:HZ3	1:A:119:LYS:O	1.90	0.54
1:A:337:CYS:HB2	1:A:360:GLU:HG2	1.88	0.54
1:A:116:TYR:HA	1:A:119:LYS:HG3	1.88	0.54
1:A:414:LYS:O	1:A:418:ILE:HG13	2.08	0.53
1:A:195:ILE:O	1:A:199:ARG:HG3	2.09	0.53
1:B:115:ILE:O	1:B:119:LYS:HG3	2.08	0.53
1:B:359:LYS:O	1:B:363:LYS:HG3	2.08	0.53
1:A:153:GLN:HE22	1:A:156:ARG:NH1	2.06	0.53
1:B:29:ASN:HD22	1:B:29:ASN:H	1.55	0.53
1:B:35:GLU:HG2	1:B:35:GLU:O	2.09	0.53
1:B:352:GLU:OE1	1:B:352:GLU:N	2.42	0.53
1:B:220:HIS:HA	1:B:223:ARG:HG3	1.89	0.53
1:B:323:LEU:HD22	1:B:336:VAL:CG2	2.39	0.53
1:B:368:VAL:HG22	1:B:403:GLN:HE21	1.73	0.53
1:B:35:GLU:CB	1:B:60:LEU:HD11	2.39	0.53
1:B:392:ILE:HD11	1:B:422:ARG:HH21	1.74	0.53
1:B:368:VAL:HG22	1:B:403:GLN:NE2	2.24	0.52
1:B:202:ILE:HD13	1:B:212:LYS:HG2	1.91	0.52
1:A:265:LYS:O	1:A:269:LEU:HG	2.09	0.52
1:B:260:LYS:HE2	1:B:262:GLU:OE2	2.09	0.52
1:A:274:LEU:HD11	1:A:283:LEU:HB3	1.90	0.52
1:B:359:LYS:O	1:B:363:LYS:HE3	2.09	0.52
1:A:115:ILE:O	1:A:118:ASP:HB2	2.09	0.52
1:A:16:LEU:HD22	1:A:120:VAL:HG11	1.92	0.52
1:B:422:ARG:HB3	1:B:429:ASP:N	2.24	0.52
1:A:205:ASN:N	1:A:205:ASN:ND2	2.52	0.52
1:A:97:TRP:CZ3	1:A:119:LYS:O	2.63	0.52
1:A:155:GLU:HG2	1:A:156:ARG:N	2.25	0.51
1:A:42:THR:CG2	1:A:53:MET:HE1	2.39	0.51
1:B:54:CYS:HB2	1:B:77:ALA:HB2	1.92	0.51
1:B:104:TYR:HD1	1:B:109:ARG:HD3	1.74	0.51
1:A:171:ASN:OD1	1:A:172:PRO:N	2.44	0.51
1:A:323:LEU:HD22	1:A:336:VAL:CG2	2.39	0.51
1:A:194:ALA:C	1:A:197:PRO:HD2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:GLN:O	1:B:372:LEU:C	2.49	0.51
1:B:392:ILE:CD1	1:B:422:ARG:HH21	2.23	0.51
1:B:330:ASN:ND2	1:B:333:LEU:CD1	2.55	0.51
1:B:88:GLN:O	1:B:92:ARG:HG2	2.11	0.51
1:B:421:MET:SD	1:B:425:LYS:HD3	2.50	0.51
1:A:395:PHE:CD1	1:A:411:MET:HG2	2.46	0.50
1:B:350:TYR:CE1	1:B:384:GLN:HB3	2.45	0.50
1:A:53:MET:O	1:A:57:LEU:HG	2.11	0.50
1:B:123:VAL:O	1:B:127:PHE:HD2	1.93	0.50
1:A:75:ARG:HH11	1:A:75:ARG:CG	2.23	0.50
1:A:133:ILE:HD11	1:B:91:ILE:HD11	1.93	0.50
1:B:387:CYS:HB3	1:B:390:LYS:HG3	1.92	0.50
1:A:199:ARG:O	1:A:203:ARG:HG3	2.11	0.50
1:B:19:HIS:CD2	1:B:19:HIS:N	2.76	0.50
1:B:364:GLU:OE2	1:B:364:GLU:HA	2.12	0.50
1:B:97:TRP:CZ3	1:B:123:VAL:HG21	2.47	0.49
1:A:16:LEU:CD2	1:A:120:VAL:HG11	2.42	0.49
1:A:423:LEU:CD1	1:A:436:LEU:HD22	2.42	0.49
1:A:185:LEU:HD23	1:B:192:GLN:NE2	2.27	0.49
1:A:85:HIS:HB3	1:A:92:ARG:HD3	1.93	0.49
1:A:195:ILE:HD11	1:A:219:LEU:HD23	1.95	0.49
1:A:340:LEU:HD13	1:A:356:TYR:CE1	2.47	0.49
1:A:419:ALA:HB1	1:A:432:ALA:HB1	1.94	0.49
1:A:443:ASN:O	1:A:446:MET:O	2.30	0.49
1:B:368:VAL:CG2	1:B:403:GLN:HE21	2.26	0.49
1:A:274:LEU:CD1	1:A:283:LEU:HB3	2.43	0.49
1:B:9:LEU:HD13	1:B:13:LEU:HG	1.95	0.49
1:B:104:TYR:HE1	1:B:109:ARG:CZ	2.26	0.49
1:B:350:TYR:CZ	1:B:384:GLN:CB	2.96	0.49
1:B:350:TYR:HE1	1:B:384:GLN:CG	2.26	0.49
1:B:215:LEU:O	1:B:215:LEU:HD22	2.13	0.49
1:A:380:PHE:HD1	1:A:384:GLN:HG3	1.68	0.48
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.46	0.48
1:B:54:CYS:CB	1:B:77:ALA:HB2	2.44	0.48
1:B:348:ASP:O	1:B:350:TYR:CD2	2.66	0.48
1:A:153:GLN:NE2	1:A:153:GLN:HA	2.29	0.48
1:A:53:MET:CE	1:A:53:MET:HA	2.26	0.48
1:A:15:GLN:OE1	1:B:131:TYR:HD2	1.96	0.48
1:B:295:VAL:O	1:B:299:MET:HG3	2.13	0.48
1:A:284:HIS:CD2	1:A:322:HIS:CD2	2.87	0.48
1:A:446:MET:HA	1:A:448:GLN:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:N	1:A:174:PHE:HD2	2.11	0.48
1:A:327:ASP:HB2	1:A:336:VAL:HG12	1.95	0.48
1:B:350:TYR:CZ	1:B:384:GLN:HB2	2.44	0.48
1:A:169:PRO:O	1:A:170:LYS:CB	2.62	0.48
1:A:399:VAL:HG22	1:A:408:LYS:HG3	1.96	0.47
1:B:82:GLN:O	1:B:86:ALA:HB2	2.14	0.47
1:B:414:LYS:O	1:B:418:ILE:HG13	2.14	0.47
1:A:251:ARG:HG3	1:A:286:GLN:NE2	2.18	0.47
1:B:146:ARG:HB3	1:B:153:GLN:HB3	1.95	0.47
1:A:23:ASN:C	1:A:23:ASN:ND2	2.68	0.47
1:A:395:PHE:HD1	1:A:411:MET:HG2	1.79	0.47
1:B:69:ALA:O	1:B:72:GLU:HB2	2.14	0.47
1:B:43:GLU:OE1	1:B:280:ASN:HB2	2.14	0.47
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.68	0.47
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.15	0.47
1:B:83:GLN:OE1	1:B:83:GLN:N	2.48	0.47
1:A:131:TYR:HB3	1:B:16:LEU:HD23	1.95	0.47
1:A:42:THR:HB	1:A:53:MET:HE2	1.96	0.47
1:A:85:HIS:CB	1:A:92:ARG:CD	2.92	0.47
1:B:360:GLU:CG	1:B:373:LEU:HD22	2.44	0.46
1:B:255:LYS:HB2	1:B:255:LYS:HE3	1.73	0.46
1:B:168:LYS:HB3	1:B:174:PHE:HE1	1.79	0.46
1:B:329:ALA:O	1:B:330:ASN:OD1	2.33	0.46
1:B:360:GLU:HG3	1:B:373:LEU:CD2	2.44	0.46
1:B:350:TYR:HB3	1:B:385:MET:CE	2.46	0.46
1:B:359:LYS:CG	1:B:363:LYS:NZ	2.74	0.46
1:A:350:TYR:CE1	1:A:384:GLN:HB3	2.51	0.46
1:A:133:ILE:HD11	1:B:91:ILE:CD1	2.46	0.46
1:B:359:LYS:CG	1:B:363:LYS:HZ1	2.24	0.46
1:A:167:LYS:HZ1	1:B:132:ARG:CZ	2.29	0.46
1:B:253:ALA:O	1:B:256:PHE:HB3	2.16	0.46
1:A:207:ASP:OD2	1:A:208:ASN:N	2.48	0.46
1:A:135:SER:HB3	1:A:138:LEU:HB2	1.98	0.46
1:A:194:ALA:O	1:A:197:PRO:CD	2.51	0.45
1:A:233:GLU:O	1:A:237:GLU:CD	2.55	0.45
1:A:42:THR:HG22	1:A:53:MET:HE1	1.97	0.45
1:A:339:ILE:N	1:A:339:ILE:HD12	2.30	0.45
1:A:62:HIS:CE1	1:A:106:HIS:CD2	3.04	0.45
1:B:337:CYS:SG	1:B:363:LYS:NZ	2.88	0.45
1:A:196:ASP:O	1:A:199:ARG:HB2	2.17	0.45
1:A:81:ILE:HD13	1:A:92:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:HG3	1:B:60:LEU:HD12	1.99	0.45
1:A:208:ASN:C	1:A:208:ASN:OD1	2.54	0.45
1:B:277:ILE:HD11	1:B:283:LEU:CD2	2.47	0.45
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.72	0.45
1:A:335:ARG:NH2	1:A:364:GLU:HG2	2.32	0.45
1:A:197:PRO:CA	1:A:200:GLN:HE21	2.28	0.45
1:A:373:LEU:O	1:A:373:LEU:HD12	2.17	0.45
1:B:170:LYS:O	1:B:170:LYS:CG	2.65	0.45
1:B:152:ASN:ND2	1:B:152:ASN:H	2.15	0.44
1:A:164:ALA:HB1	1:A:174:PHE:CD1	2.51	0.44
1:B:416:GLN:HA	1:B:416:GLN:OE1	2.18	0.44
1:B:119:LYS:O	1:B:123:VAL:HG23	2.16	0.44
1:A:206:PRO:O	1:A:212:LYS:NZ	2.50	0.44
1:A:53:MET:SD	1:B:148:LYS:NZ	2.91	0.44
1:A:167:LYS:NZ	1:B:132:ARG:CZ	2.80	0.44
1:B:287:ILE:CG2	1:B:288:GLY:N	2.80	0.44
1:A:85:HIS:CB	1:A:92:ARG:HD3	2.46	0.44
1:A:119:LYS:HE2	1:A:119:LYS:HB3	1.51	0.44
1:A:76:LYS:O	1:A:80:LEU:HG	2.17	0.44
1:A:161:PHE:CE1	1:A:177:GLY:HA3	2.53	0.44
1:A:146:ARG:HB2	1:A:157:ALA:HB2	2.00	0.43
1:A:159:VAL:HG21	1:B:159:VAL:CG2	2.41	0.43
1:A:138:LEU:HA	1:A:138:LEU:HD23	1.84	0.43
1:A:124:CYS:SG	1:B:133:ILE:HG23	2.58	0.43
1:A:18:CYS:HB2	1:A:99:ASN:OD1	2.18	0.43
1:B:336:VAL:HG13	1:B:336:VAL:O	2.18	0.43
1:A:82:GLN:O	1:A:86:ALA:CB	2.66	0.43
1:B:136:PRO:HG2	1:B:137:GLU:OE2	2.19	0.43
1:A:263:PRO:CG	1:A:297:GLN:OE1	2.66	0.43
1:B:104:TYR:CE1	1:B:109:ARG:CZ	3.01	0.43
1:B:169:PRO:O	1:B:170:LYS:CB	2.66	0.43
1:B:62:HIS:CE1	1:B:106:HIS:CD2	3.07	0.43
1:B:420:LYS:NZ	1:B:420:LYS:HB2	2.33	0.43
1:B:280:ASN:HB3	1:B:283:LEU:HB2	2.01	0.43
1:B:180:ILE:O	1:B:181:ALA:C	2.56	0.43
1:B:366:THR:CG2	1:B:369:ALA:HB3	2.40	0.43
1:B:272:LYS:HA	1:B:272:LYS:HE3	2.00	0.43
1:B:193:ASN:ND2	1:B:196:ASP:H	2.16	0.43
1:A:158:LYS:NZ	1:B:192:GLN:HE22	2.17	0.43
1:A:109:ARG:O	1:A:113:VAL:HG23	2.19	0.43
1:B:196:ASP:N	1:B:197:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:HIS:ND1	1:B:220:HIS:C	2.72	0.43
1:B:209:GLN:HB3	1:B:239:ALA:HB1	2.00	0.43
1:B:384:GLN:HG2	1:B:384:GLN:H	1.36	0.42
1:B:372:LEU:HD23	1:B:373:LEU:N	2.33	0.42
1:B:165:LEU:O	1:B:169:PRO:N	2.52	0.42
1:A:148:LYS:HD3	1:A:148:LYS:HA	1.87	0.42
1:B:231:GLU:O	1:B:234:LYS:HB2	2.18	0.42
1:B:18:CYS:HB2	1:B:99:ASN:HD21	1.77	0.42
1:A:372:LEU:HD23	1:A:373:LEU:N	2.34	0.42
1:B:194:ALA:C	1:B:197:PRO:HD2	2.40	0.42
1:A:435:VAL:O	1:A:439:LEU:HG	2.19	0.42
1:A:97:TRP:O	1:A:100:TYR:HB2	2.18	0.42
1:B:280:ASN:ND2	1:B:283:LEU:H	2.07	0.42
1:B:220:HIS:O	1:B:220:HIS:ND1	2.52	0.42
1:B:215:LEU:HD13	1:B:235:LEU:CD1	2.49	0.42
1:A:94:LEU:HA	1:A:94:LEU:HD23	1.73	0.42
1:A:91:ILE:HG12	1:A:91:ILE:O	2.20	0.42
1:B:104:TYR:HB2	1:B:113:VAL:HG22	2.02	0.42
1:A:99:ASN:O	1:A:103:VAL:HG23	2.20	0.41
1:A:157:ALA:O	1:A:160:CYS:HB2	2.19	0.41
1:A:90:GLU:O	1:A:123:VAL:HG11	2.20	0.41
1:A:167:LYS:NZ	1:B:132:ARG:NH1	2.67	0.41
1:B:370:LYS:O	1:B:374:HIS:CD2	2.73	0.41
1:A:38:VAL:HG11	1:A:60:LEU:HD11	2.01	0.41
1:A:257:TYR:HB3	1:A:262:GLU:HB2	2.02	0.41
1:A:262:GLU:OE1	1:A:265:LYS:NZ	2.52	0.41
1:B:403:GLN:O	1:B:408:LYS:HD2	2.20	0.41
1:B:366:THR:HG23	1:B:369:ALA:CB	2.48	0.41
1:A:159:VAL:CG1	1:A:163:LYS:HE3	2.51	0.41
1:B:57:LEU:HA	1:B:57:LEU:HD23	1.80	0.41
1:B:360:GLU:OE1	1:B:360:GLU:HA	2.21	0.41
1:B:9:LEU:O	1:B:13:LEU:HG	2.21	0.41
1:B:277:ILE:HD11	1:B:283:LEU:HD22	2.03	0.41
1:A:171:ASN:ND2	1:A:174:PHE:CE2	2.89	0.41
1:A:372:LEU:C	1:A:372:LEU:HD23	2.41	0.41
1:B:343:LEU:HA	1:B:343:LEU:HD12	1.72	0.41
1:B:8:SER:O	1:B:11:SER:OG	2.28	0.41
1:A:446:MET:CB	1:A:448:GLN:C	2.89	0.41
1:B:423:LEU:C	1:B:423:LEU:HD13	2.41	0.41
1:A:198:LEU:HD21	1:A:214:LEU:HB2	2.02	0.40
1:B:208:ASN:ND2	1:B:211:LEU:CD2	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:O	1:A:250:LEU:HG	2.21	0.40
1:B:421:MET:C	1:B:421:MET:SD	3.00	0.40
1:B:270:LEU:HB2	1:B:287:ILE:HG13	2.04	0.40
1:A:376:ARG:HA	1:A:376:ARG:NE	2.37	0.40
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.89	0.40
1:B:258:ARG:O	1:B:261:ASP:N	2.54	0.40
1:B:148:LYS:HZ2	1:B:148:LYS:HG2	1.57	0.40
1:A:420:LYS:HB2	1:A:420:LYS:HZ3	1.86	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	416/472 (88%)	390 (94%)	25 (6%)	1 (0%)	52	84
1	B	419/472 (89%)	396 (94%)	22 (5%)	1 (0%)	52	84
All	All	835/944 (88%)	786 (94%)	47 (6%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	GLU
1	A	133	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	358/411 (87%)	333 (93%)	25 (7%)	19	47
1	B	352/411 (86%)	323 (92%)	29 (8%)	14	38
All	All	710/822 (86%)	656 (92%)	54 (8%)	16	42

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	9	LEU
1	A	23	ASN
1	A	125	GLU
1	A	155	GLU
1	A	173	GLU
1	A	174	PHE
1	A	205	ASN
1	A	211	LEU
1	A	215	LEU
1	A	223	ARG
1	A	272	LYS
1	A	274	LEU
1	A	283	LEU
1	A	336	VAL
1	A	372	LEU
1	A	375	LEU
1	A	376	ARG
1	A	382	LEU
1	A	384	GLN
1	A	399	VAL
1	A	409	GLU
1	A	420	LYS
1	A	422	ARG
1	A	424	SER
1	B	29	ASN
1	B	37	LYS
1	B	60	LEU
1	B	111	SER
1	B	135	SER
1	B	148	LYS
1	B	191	SER
1	B	193	ASN
1	B	203	ARG

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Mol	Chain	Res	Type
1	B	211	LEU
1	B	215	LEU
1	B	272	LYS
1	B	274	LEU
1	B	277	ILE
1	B	283	LEU
1	B	286	GLN
1	B	289	CYS
1	B	301	LEU
1	B	312	LEU
1	B	314	GLU
1	B	336	VAL
1	B	338	SER
1	B	339	ILE
1	B	343	LEU
1	B	372	LEU
1	B	376	ARG
1	B	382	LEU
1	B	384	GLN
1	B	409	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	23	ASN
1	A	46	ASN
1	A	55	ASN
1	A	62	HIS
1	A	82	GLN
1	A	106	HIS
1	A	192	GLN
1	A	200	GLN
1	A	205	ASN
1	A	280	ASN
1	A	284	HIS
1	A	286	GLN
1	A	322	HIS
1	B	19	HIS
1	B	23	ASN
1	B	29	ASN
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	66	GLN
1	B	99	ASN
1	B	106	HIS
1	B	152	ASN
1	B	154	ASN
1	B	192	GLN
1	B	193	ASN
1	B	280	ASN
1	B	284	HIS
1	B	297	GLN
1	B	322	HIS
1	B	330	ASN

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 carbohydrates 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	426/472 (90%)	0.20	13 (3%)	52	40	30, 65, 92, 118	0
1	B	429/472 (90%)	0.27	12 (2%)	56	44	45, 68, 127, 170	0
All	All	855/944 (90%)	0.24	25 (2%)	55	43	30, 66, 112, 170	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	PRO	4.4
1	B	415	LEU	4.3
1	B	429	ASP	4.0
1	B	422	ARG	4.0
1	B	412	LYS	3.9
1	B	330	ASN	3.6
1	A	351	GLU	3.3
1	A	193	ASN	3.2
1	A	429	ASP	3.0
1	A	310	ARG	3.0
1	B	331	ASP	2.9
1	A	313	LEU	2.9
1	B	350	TYR	2.9
1	B	403	GLN	2.5
1	A	331	ASP	2.4
1	B	410	LYS	2.4
1	A	349	GLN	2.3
1	A	308	GLY	2.3
1	B	399	VAL	2.2
1	A	443	ASN	2.2
1	A	403	GLN	2.2
1	A	311	LYS	2.2
1	B	417	LYS	2.1
1	B	348	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	433	LEU	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.