



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 09:06 AM EDT

PDB ID : 3KLI / pdb_00003kli
Title : Crystal structure of unliganded AZT-resistant HIV-1 Reverse Transcriptase
Authors : Tu, X.; Sarafianos, S.G.; Arnold, E.
Deposited on : 2009-11-08
Resolution : 2.65 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

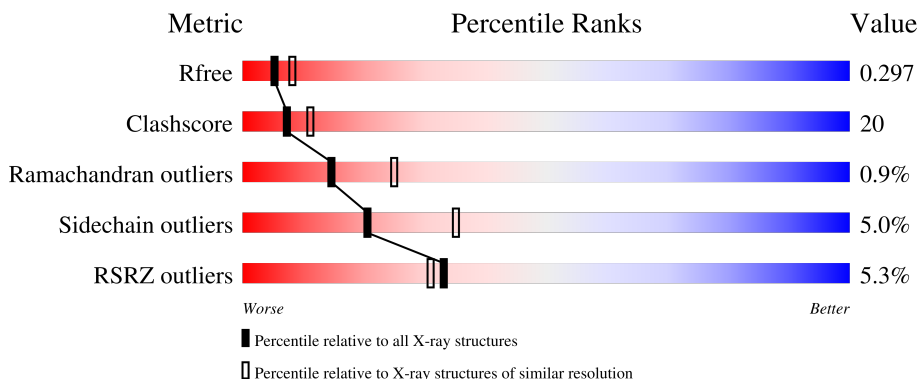
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	562	<div> <div>6%</div> <div>56%</div> <div>37%</div> <div>.</div> <div>.</div> </div>
2	B	437	<div> <div>5%</div> <div>58%</div> <div>35%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8062 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4495	2911	749	828	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	41	LEU	MET	engineered mutation	UNP P03366
A	67	ASN	ASP	engineered mutation	UNP P03366
A	70	ARG	LYS	engineered mutation	UNP P03366
A	215	TYR	THR	engineered mutation	UNP P03366
A	219	GLN	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	559	VAL	ILE	SEE REMARK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3529	2300	584	638	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	429	GLY	-	expression tag	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	HIS	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

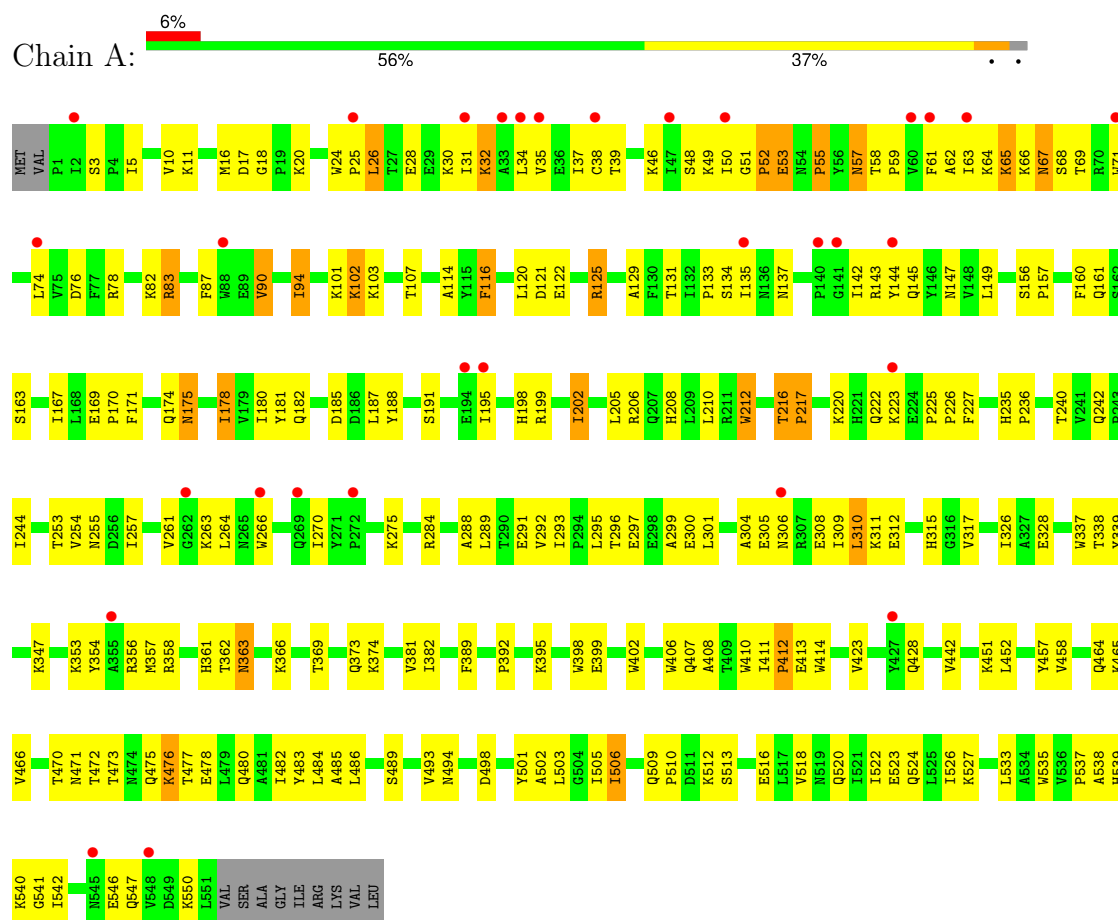
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	19	Total	O	0	0
			19	19		

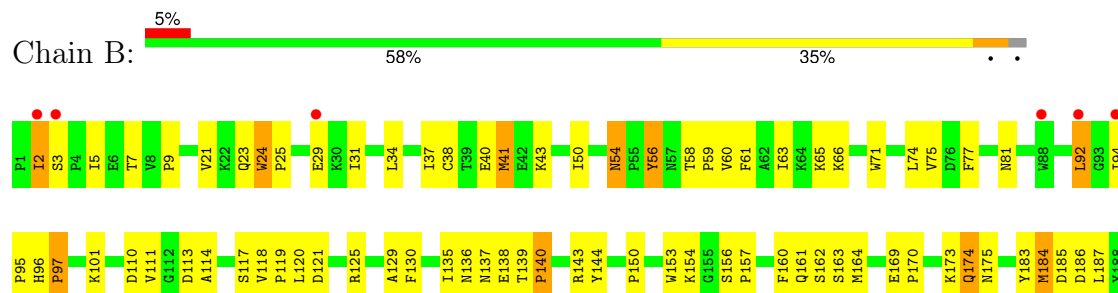
3 Residue-property plots

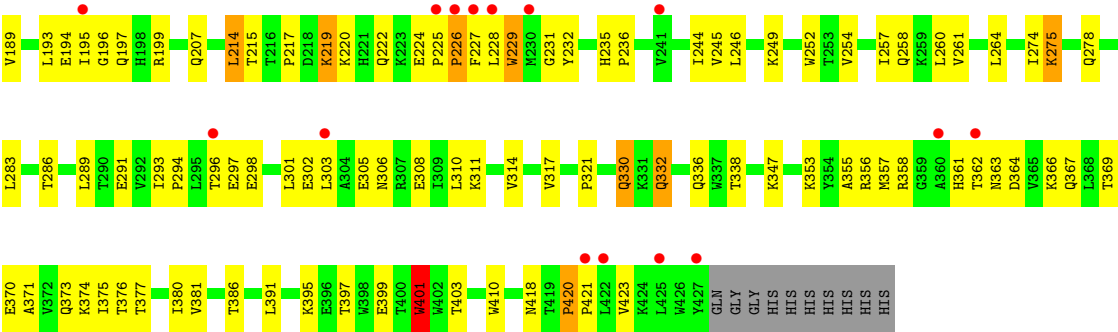
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.07Å 71.22Å 94.63Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.65 28.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (28.64-2.65) 94.3 (28.64-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.260 , 0.294 0.260 , 0.297	Depositor DCC
R_{free} test set	1293 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8062	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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 ⓘ

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	0.54	0/4614	0.92	16/6270 (0.3%)
2	B	0.63	1/3634 (0.0%)	1.03	22/4940 (0.4%)
All	All	0.58	1/8248 (0.0%)	0.97	38/11210 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	MET	SD-CE	5.39	1.93	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	SER	N-CA-C	7.97	120.98	111.33
1	A	149	LEU	CA-C-N	7.95	127.71	119.76
1	A	149	LEU	C-N-CA	7.95	127.71	119.76
2	B	139	THR	CA-C-N	-7.54	112.97	120.21
2	B	139	THR	C-N-CA	-7.54	112.97	120.21
2	B	391	LEU	N-CA-C	7.22	118.75	109.72
2	B	125	ARG	N-CA-C	6.91	119.69	111.33
2	B	214	LEU	N-CA-C	6.67	119.97	109.96
2	B	401	TRP	N-CA-C	6.51	124.17	113.89
2	B	162	SER	CB-CA-C	-6.43	99.74	110.68
1	A	212	TRP	CB-CA-C	-6.40	101.17	111.28
2	B	220	LYS	N-CA-C	6.38	117.92	110.97
2	B	184	MET	CB-CA-C	-6.19	109.42	116.54
1	A	382	ILE	N-CA-C	6.00	116.64	110.82
1	A	101	LYS	N-CA-C	-6.00	101.12	110.42
2	B	92	LEU	N-CA-C	-5.75	105.52	112.54
1	A	406	TRP	N-CA-C	5.67	119.94	113.19
1	A	57	ASN	CB-CA-C	5.62	121.06	110.95
1	A	275	LYS	N-CA-C	-5.50	99.93	108.90
1	A	202	ILE	CB-CA-C	-5.47	104.97	111.81
1	A	175	ASN	CA-C-N	5.41	126.60	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	C-N-CA	5.41	126.60	119.84
2	B	186	ASP	N-CA-C	5.40	118.29	109.59
2	B	140	PRO	N-CA-C	-5.40	103.66	111.22
2	B	54	ASN	CA-C-N	5.36	125.05	119.64
2	B	54	ASN	C-N-CA	5.36	125.05	119.64
1	A	389	PHE	N-CA-C	5.34	118.19	109.59
1	A	58	THR	N-CA-CB	5.32	120.22	111.17
2	B	235	HIS	CA-C-N	5.31	126.47	119.84
2	B	235	HIS	C-N-CA	5.31	126.47	119.84
1	A	125	ARG	N-CA-C	5.30	117.05	111.28
1	A	185	ASP	N-CA-C	5.29	117.95	111.82
2	B	164	MET	N-CA-C	-5.19	105.07	111.40
2	B	189	VAL	N-CA-C	5.19	115.24	107.51
2	B	163	SER	N-CA-C	-5.18	106.65	113.17
1	A	550	LYS	N-CA-C	-5.16	107.05	113.55
2	B	38	CYS	N-CA-C	5.03	117.66	111.82
2	B	56	TYR	N-CA-C	5.03	117.34	110.55

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	4495	0	4549	211	0
2	B	3529	0	3568	135	0
3	A	19	0	0	0	0
3	B	19	0	0	3	0
All	All	8062	0	8117	327	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 20.

All (327) 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:494:ASN:HD22	2:B:289:LEU:HD12	1.19	1.06
1:A:51:GLY:N	1:A:52:PRO:HD3	1.76	0.95
1:A:222:GLN:O	1:A:222:GLN:HG3	1.67	0.93
1:A:63:ILE:HG12	1:A:64:LYS:H	1.34	0.90
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.54	0.89
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.56	0.86
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.57	0.86
1:A:51:GLY:H	1:A:52:PRO:HD3	1.40	0.84
1:A:369:THR:HG23	1:A:411:ILE:HD11	1.57	0.84
1:A:522:ILE:O	1:A:526:ILE:HD13	1.82	0.80
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.62	0.79
1:A:63:ILE:CG1	1:A:64:LYS:H	1.95	0.78
2:B:363:ASN:O	2:B:367:GLN:HG3	1.83	0.78
1:A:398:TRP:CH2	1:A:411:ILE:HD13	2.18	0.77
2:B:420:PRO:HB2	2:B:421:PRO:HD2	1.65	0.77
1:A:541:GLY:HA2	1:A:546:GLU:HB3	1.68	0.76
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.51	0.75
2:B:66:LYS:HZ1	2:B:232:TYR:H	1.35	0.75
2:B:355:ALA:O	2:B:358:ARG:HB3	1.85	0.74
2:B:2:ILE:HD13	2:B:2:ILE:O	1.87	0.74
2:B:246:LEU:HD21	2:B:264:LEU:HD21	1.70	0.73
1:A:63:ILE:HG12	1:A:64:LYS:N	2.04	0.72
2:B:2:ILE:HG12	2:B:117:SER:HA	1.71	0.72
1:A:288:ALA:HB3	1:A:291:GLU:HG2	1.70	0.72
1:A:198:HIS:O	1:A:202:ILE:HG12	1.89	0.72
1:A:410:TRP:O	1:A:411:ILE:HD12	1.91	0.71
1:A:131:THR:OG1	1:A:143:ARG:HG2	1.91	0.70
2:B:224:GLU:HG2	2:B:228:LEU:HB2	1.72	0.70
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.57	0.70
2:B:214:LEU:H	2:B:214:LEU:HD23	1.56	0.69
1:A:50:ILE:HD12	1:A:145:GLN:HG2	1.75	0.68
2:B:366:LYS:O	2:B:370:GLU:HG3	1.94	0.67
2:B:317:VAL:HG22	2:B:347:LYS:HB3	1.74	0.67
1:A:257:ILE:O	1:A:261:VAL:HG23	1.96	0.65
1:A:402:TRP:CZ2	2:B:361:HIS:O	2.49	0.65
2:B:195:ILE:O	2:B:199:ARG:HG3	1.97	0.65
1:A:102:LYS:HD3	1:A:103:LYS:N	2.11	0.65
1:A:288:ALA:HB3	1:A:291:GLU:CG	2.27	0.65
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.33	0.64
2:B:9:PRO:HA	2:B:121:ASP:OD2	1.97	0.64
2:B:174:GLN:HG3	2:B:175:ASN:ND2	2.13	0.63
1:A:102:LYS:HD3	1:A:103:LYS:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:HE22	2:B:60:VAL:HG12	1.64	0.63
1:A:206:ARG:HG2	1:A:216:THR:HG23	1.80	0.63
1:A:222:GLN:O	1:A:227:PHE:CE1	2.51	0.63
1:A:407:GLN:NE2	2:B:418:ASN:HA	2.14	0.63
1:A:32:LYS:HE3	1:A:32:LYS:HA	1.82	0.62
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.29	0.62
1:A:305:GLU:O	1:A:309:ILE:HG13	1.99	0.62
1:A:338:THR:HG22	1:A:353:LYS:HG2	1.79	0.62
1:A:37:ILE:HD11	1:A:71:TRP:O	1.99	0.62
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.00	0.62
2:B:296:THR:HG23	2:B:297:GLU:HG2	1.81	0.62
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.34	0.62
1:A:410:TRP:C	1:A:411:ILE:HD12	2.25	0.62
1:A:510:PRO:O	1:A:522:ILE:HD12	1.99	0.62
1:A:63:ILE:CG1	1:A:64:LYS:N	2.61	0.61
2:B:332:GLN:HB3	2:B:336:GLN:HB3	1.82	0.61
1:A:402:TRP:CH2	2:B:361:HIS:O	2.54	0.61
1:A:53:GLU:O	1:A:55:PRO:HD3	2.01	0.61
1:A:369:THR:HG23	1:A:411:ILE:CD1	2.28	0.61
1:A:17:ASP:OD2	1:A:18:GLY:N	2.33	0.61
1:A:191:SER:OG	1:A:198:HIS:HD2	1.84	0.61
1:A:506:ILE:HD12	1:A:506:ILE:H	1.67	0.60
2:B:135:ILE:HG12	3:B:449:HOH:O	2.01	0.60
2:B:278:GLN:HB3	2:B:302:GLU:CD	2.26	0.60
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.84	0.60
1:A:361:HIS:CD2	1:A:505:ILE:HD12	2.37	0.60
2:B:225:PRO:HB2	2:B:226:PRO:HD3	1.84	0.59
1:A:270:ILE:N	1:A:270:ILE:HD12	2.17	0.59
1:A:208:HIS:O	1:A:212:TRP:HD1	1.85	0.59
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.85	0.59
1:A:64:LYS:HB3	1:A:71:TRP:CE3	2.38	0.59
1:A:518:VAL:O	1:A:522:ILE:HG12	2.03	0.59
1:A:392:PRO:O	1:A:423:VAL:HG22	2.03	0.59
1:A:181:TYR:CZ	2:B:138:GLU:HG2	2.38	0.58
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.85	0.58
1:A:296:THR:HG23	1:A:299:ALA:H	1.68	0.58
1:A:90:VAL:CG1	2:B:143:ARG:HD2	2.34	0.58
1:A:202:ILE:HG21	1:A:220:LYS:HB2	1.86	0.57
1:A:134:SER:OG	1:A:137:ASN:HA	2.05	0.57
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.39	0.57
1:A:51:GLY:N	1:A:52:PRO:CD	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.53	0.56
1:A:64:LYS:HD3	1:A:71:TRP:CH2	2.39	0.56
1:A:90:VAL:HG11	2:B:143:ARG:HD2	1.87	0.56
1:A:244:ILE:HG23	1:A:263:LYS:HE2	1.87	0.56
2:B:66:LYS:HZ1	2:B:232:TYR:N	2.00	0.56
1:A:26:LEU:HD12	1:A:30:LYS:HD2	1.86	0.56
1:A:506:ILE:HD12	1:A:506:ILE:N	2.20	0.56
2:B:66:LYS:NZ	2:B:232:TYR:H	2.04	0.56
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.31	0.56
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.88	0.55
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.88	0.55
2:B:303:LEU:HD23	2:B:303:LEU:O	2.05	0.55
1:A:50:ILE:HD12	1:A:145:GLN:CG	2.37	0.55
1:A:522:ILE:O	1:A:526:ILE:CD1	2.54	0.55
2:B:293:ILE:O	2:B:293:ILE:HG23	2.06	0.55
1:A:244:ILE:HB	1:A:310:LEU:HD22	1.89	0.55
2:B:50:ILE:HD12	2:B:54:ASN:ND2	2.22	0.55
2:B:156:SER:N	2:B:157:PRO:HD2	2.21	0.55
2:B:3:SER:O	2:B:5:ILE:N	2.39	0.54
1:A:395:LYS:O	1:A:399:GLU:HG2	2.08	0.54
2:B:246:LEU:HD12	2:B:246:LEU:N	2.23	0.54
1:A:57:ASN:HD21	1:A:131:THR:N	2.06	0.54
1:A:142:ILE:CG2	1:A:144:TYR:CE2	2.91	0.54
2:B:23:GLN:HE22	2:B:60:VAL:H	1.54	0.54
1:A:50:ILE:O	1:A:143:ARG:HB2	2.08	0.53
1:A:216:THR:O	1:A:217:PRO:C	2.51	0.53
2:B:246:LEU:HD11	2:B:310:LEU:HD12	1.89	0.53
2:B:219:LYS:HG3	2:B:229:TRP:HZ2	1.73	0.53
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.89	0.53
1:A:142:ILE:HG21	1:A:144:TYR:CE2	2.43	0.53
2:B:135:ILE:O	2:B:138:GLU:HG3	2.08	0.53
1:A:163:SER:O	1:A:167:ILE:HG12	2.08	0.53
2:B:92:LEU:HD23	2:B:92:LEU:H	1.72	0.53
1:A:357:MET:HG2	1:A:358:ARG:N	2.23	0.53
1:A:398:TRP:CZ2	1:A:411:ILE:HD13	2.43	0.52
1:A:20:LYS:HD3	1:A:55:PRO:O	2.09	0.52
1:A:57:ASN:HA	1:A:129:ALA:O	2.10	0.52
1:A:512:LYS:HD2	1:A:513:SER:N	2.25	0.52
2:B:66:LYS:HD2	2:B:231:GLY:HA3	1.91	0.52
1:A:122:GLU:O	1:A:125:ARG:HB2	2.10	0.52
2:B:23:GLN:NE2	2:B:60:VAL:HG12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLN:N	1:A:510:PRO:HD3	2.25	0.51
2:B:275:LYS:HB2	2:B:275:LYS:NZ	2.25	0.51
1:A:129:ALA:HA	1:A:144:TYR:O	2.10	0.51
1:A:50:ILE:O	1:A:143:ARG:CB	2.58	0.51
1:A:107:THR:OG1	1:A:198:HIS:HE1	1.93	0.51
2:B:2:ILE:HG12	2:B:117:SER:CA	2.40	0.51
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.45	0.51
1:A:337:TRP:O	1:A:353:LYS:HA	2.10	0.51
1:A:458:VAL:HG13	1:A:464:GLN:HE21	1.76	0.51
1:A:59:PRO:HB2	1:A:76:ASP:HB3	1.93	0.50
1:A:222:GLN:O	1:A:227:PHE:CD1	2.64	0.50
2:B:56:TYR:O	2:B:143:ARG:NH2	2.43	0.50
1:A:412:PRO:HG3	2:B:401:TRP:CH2	2.47	0.50
1:A:442:VAL:HG21	1:A:482:ILE:HD13	1.94	0.50
2:B:113:ASP:OD1	2:B:215:THR:HG22	2.10	0.50
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.37	0.50
1:A:31:ILE:O	1:A:35:VAL:HG23	2.12	0.50
1:A:473:THR:O	1:A:477:THR:HG23	2.11	0.50
1:A:135:ILE:H	1:A:135:ILE:HD12	1.76	0.50
2:B:245:VAL:C	2:B:246:LEU:HD12	2.37	0.50
1:A:16:MET:HE2	1:A:83:ARG:HB3	1.95	0.49
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.47	0.49
2:B:308:GLU:HA	2:B:311:LYS:HD3	1.93	0.49
2:B:94:ILE:N	2:B:95:PRO:HD3	2.27	0.49
2:B:257:ILE:O	2:B:261:VAL:HG23	2.12	0.49
2:B:293:ILE:CG1	2:B:294:PRO:HD2	2.43	0.49
1:A:326:ILE:HD12	1:A:326:ILE:N	2.26	0.49
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.48	0.49
1:A:308:GLU:O	1:A:311:LYS:HG2	2.12	0.49
1:A:540:LYS:HA	1:A:540:LYS:HE2	1.94	0.49
2:B:361:HIS:ND1	2:B:362:THR:N	2.61	0.49
1:A:254:VAL:HB	1:A:289:LEU:O	2.13	0.48
1:A:478:GLU:O	1:A:482:ILE:HG12	2.12	0.48
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.48	0.48
1:A:225:PRO:HA	1:A:226:PRO:C	2.38	0.48
1:A:114:ALA:HB3	1:A:160:PHE:CE1	2.48	0.48
2:B:65:LYS:HE3	2:B:232:TYR:HE1	1.77	0.48
2:B:293:ILE:O	2:B:294:PRO:C	2.57	0.48
2:B:303:LEU:HD23	2:B:303:LEU:C	2.38	0.48
1:A:30:LYS:O	1:A:34:LEU:HD23	2.13	0.48
2:B:2:ILE:CG1	2:B:117:SER:HA	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.48	0.48
1:A:328:GLU:O	1:A:339:TYR:HA	2.14	0.48
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.39	0.48
2:B:356:ARG:O	2:B:357:MET:HB2	2.12	0.48
1:A:65:LYS:C	1:A:67:ASN:H	2.22	0.48
1:A:506:ILE:H	1:A:506:ILE:CD1	2.27	0.48
2:B:154:LYS:HA	2:B:184:MET:HE1	1.96	0.48
2:B:293:ILE:HG13	2:B:294:PRO:HD2	1.96	0.48
1:A:181:TYR:CE1	2:B:138:GLU:HA	2.49	0.47
2:B:29:GLU:OE2	2:B:71:TRP:HZ2	1.96	0.47
2:B:302:GLU:HA	2:B:305:GLU:HB3	1.96	0.47
1:A:46:LYS:HD2	1:A:116:PHE:HD2	1.79	0.47
1:A:61:PHE:HB2	1:A:74:LEU:O	2.14	0.47
1:A:476:LYS:HE3	1:A:476:LYS:HA	1.95	0.47
2:B:25:PRO:HA	3:B:457:HOH:O	2.14	0.47
1:A:57:ASN:HD22	1:A:143:ARG:NH1	2.12	0.47
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.95	0.47
2:B:376:THR:HG23	2:B:386:THR:HG22	1.96	0.47
1:A:270:ILE:HD12	1:A:270:ILE:H	1.79	0.47
1:A:452:LEU:HD23	1:A:470:THR:HA	1.97	0.47
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.96	0.47
2:B:214:LEU:H	2:B:214:LEU:CD2	2.26	0.47
1:A:175:ASN:HB2	1:A:178:ILE:HD12	1.96	0.47
1:A:242:GLN:O	1:A:242:GLN:HG3	2.14	0.47
2:B:54:ASN:HD21	2:B:129:ALA:CB	2.28	0.47
1:A:49:LYS:C	1:A:50:ILE:HG13	2.40	0.46
1:A:457:TYR:CZ	1:A:465:LYS:HB3	2.51	0.46
1:A:485:ALA:O	1:A:489:SER:HB3	2.16	0.46
1:A:537:PRO:HB3	3:B:455:HOH:O	2.15	0.46
1:A:57:ASN:HD21	1:A:131:THR:CB	2.28	0.46
1:A:161:GLN:HG3	1:A:182:GLN:HE22	1.80	0.46
1:A:357:MET:HG2	1:A:358:ARG:H	1.79	0.46
1:A:46:LYS:O	1:A:147:ASN:HB2	2.15	0.46
1:A:195:ILE:CD1	1:A:199:ARG:HH12	2.29	0.46
1:A:526:ILE:N	1:A:526:ILE:HD12	2.30	0.46
1:A:369:THR:CG2	1:A:411:ILE:HD11	2.38	0.46
2:B:40:GLU:OE2	2:B:43:LYS:HD3	2.16	0.46
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.51	0.46
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.97	0.46
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.31	0.46
1:A:222:GLN:O	1:A:227:PHE:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.98	0.46
2:B:224:GLU:OE2	2:B:226:PRO:HD2	2.16	0.46
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.98	0.45
2:B:380:ILE:HD11	2:B:386:THR:HG23	1.98	0.45
1:A:35:VAL:O	1:A:39:THR:HG23	2.17	0.45
1:A:63:ILE:O	1:A:71:TRP:HA	2.17	0.45
1:A:362:THR:O	1:A:510:PRO:HA	2.16	0.45
2:B:81:ASN:HD21	2:B:153:TRP:HA	1.82	0.45
1:A:412:PRO:O	1:A:414:TRP:HD1	1.98	0.45
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.45
1:A:131:THR:HG23	1:A:142:ILE:C	2.41	0.45
1:A:195:ILE:CD1	1:A:223:LYS:HG2	2.47	0.45
2:B:94:ILE:HG22	2:B:94:ILE:O	2.16	0.45
1:A:354:TYR:HE1	1:A:374:LYS:HE2	1.81	0.45
2:B:101:LYS:O	2:B:236:PRO:HB2	2.16	0.45
1:A:120:LEU:HD23	1:A:121:ASP:N	2.32	0.45
1:A:222:GLN:HG3	1:A:227:PHE:HD1	1.81	0.45
1:A:284:ARG:HD2	1:A:284:ARG:O	2.16	0.45
1:A:125:ARG:NE	1:A:147:ASN:HA	2.33	0.44
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.47	0.44
2:B:156:SER:N	2:B:157:PRO:CD	2.80	0.44
1:A:301:LEU:O	1:A:305:GLU:HG2	2.17	0.44
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.52	0.44
2:B:376:THR:O	2:B:380:ILE:HG12	2.17	0.44
2:B:160:PHE:O	2:B:161:GLN:C	2.60	0.44
1:A:49:LYS:O	1:A:50:ILE:HG13	2.18	0.44
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.99	0.44
2:B:244:ILE:N	2:B:244:ILE:HD12	2.32	0.44
1:A:412:PRO:CG	2:B:401:TRP:CH2	3.00	0.44
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.00	0.44
2:B:37:ILE:O	2:B:41:MET:HG2	2.18	0.44
2:B:330:GLN:NE2	2:B:338:THR:OG1	2.49	0.44
1:A:263:LYS:O	1:A:266:TRP:HB3	2.18	0.43
2:B:225:PRO:CB	2:B:226:PRO:HD3	2.48	0.43
2:B:252:TRP:HZ3	2:B:260:LEU:HD22	1.82	0.43
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.83	0.43
2:B:278:GLN:NE2	2:B:301:LEU:HD23	2.32	0.43
2:B:296:THR:HG23	2:B:297:GLU:N	2.33	0.43
1:A:65:LYS:HE2	1:A:65:LYS:HB3	1.63	0.43
1:A:131:THR:HG23	1:A:142:ILE:O	2.18	0.43
1:A:546:GLU:HG3	1:A:547:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:HD2	1:A:513:SER:H	1.82	0.43
2:B:169:GLU:HG3	2:B:173:LYS:HE2	2.00	0.43
2:B:376:THR:HB	2:B:410:TRP:CH2	2.54	0.43
1:A:48:SER:HB2	1:A:145:GLN:HE21	1.83	0.43
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.99	0.43
2:B:254:VAL:HG23	2:B:291:GLU:O	2.19	0.43
1:A:181:TYR:CE1	2:B:138:GLU:HG2	2.53	0.43
2:B:24:TRP:CD1	2:B:24:TRP:N	2.85	0.43
1:A:78:ARG:O	1:A:82:LYS:HG3	2.18	0.43
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.54	0.43
1:A:120:LEU:O	1:A:121:ASP:C	2.62	0.43
1:A:373:GLN:NE2	2:B:397:THR:HA	2.34	0.43
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.49	0.43
1:A:244:ILE:HD12	1:A:244:ILE:N	2.33	0.43
1:A:493:VAL:HG22	1:A:494:ASN:N	2.33	0.43
2:B:2:ILE:HA	2:B:117:SER:O	2.18	0.43
1:A:402:TRP:O	1:A:402:TRP:CG	2.72	0.42
1:A:87:PHE:CD1	1:A:87:PHE:N	2.87	0.42
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.54	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.84	0.42
2:B:194:GLU:CD	2:B:196:GLY:H	2.27	0.42
1:A:49:LYS:HB3	1:A:144:TYR:HE1	1.83	0.42
1:A:50:ILE:HG22	1:A:52:PRO:HD2	2.00	0.42
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.01	0.42
2:B:330:GLN:HB3	2:B:423:VAL:HG13	2.00	0.42
2:B:395:LYS:O	2:B:399:GLU:HG3	2.20	0.42
1:A:523:GLU:O	1:A:527:LYS:HD3	2.20	0.42
1:A:538:ALA:O	1:A:539:HIS:HB2	2.20	0.42
2:B:371:ALA:O	2:B:375:ILE:HG13	2.19	0.42
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.94	0.42
1:A:90:VAL:HG23	2:B:140:PRO:HB3	2.00	0.42
1:A:484:LEU:O	1:A:485:ALA:C	2.62	0.42
1:A:90:VAL:CG2	2:B:140:PRO:HB3	2.50	0.42
1:A:223:LYS:HD2	1:A:223:LYS:HA	1.90	0.42
1:A:254:VAL:HG22	1:A:293:ILE:HD12	2.00	0.42
1:A:502:ALA:O	1:A:506:ILE:HD13	2.19	0.42
1:A:195:ILE:CD1	1:A:199:ARG:NH1	2.83	0.42
1:A:296:THR:OG1	1:A:297:GLU:N	2.53	0.42
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.54	0.42
2:B:330:GLN:HE21	2:B:330:GLN:HB2	1.61	0.42
1:A:486:LEU:HB3	1:A:524:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.91	0.41
1:A:69:THR:O	1:A:69:THR:HG22	2.20	0.41
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.55	0.41
1:A:480:GLN:O	1:A:483:TYR:HB3	2.21	0.41
1:A:539:HIS:O	1:A:540:LYS:HE2	2.20	0.41
2:B:66:LYS:HZ2	2:B:231:GLY:CA	2.33	0.41
2:B:219:LYS:HB2	2:B:219:LYS:NZ	2.34	0.41
2:B:225:PRO:C	2:B:227:PHE:H	2.28	0.41
1:A:3:SER:OG	1:A:5:ILE:HG22	2.20	0.41
1:A:216:THR:O	1:A:217:PRO:O	2.39	0.41
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.36	0.41
1:A:156:SER:N	1:A:157:PRO:CD	2.84	0.41
1:A:413:GLU:O	1:A:413:GLU:HG3	2.20	0.41
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.41
1:A:178:ILE:O	1:A:178:ILE:HD13	2.20	0.41
1:A:465:LYS:HG3	1:A:466:VAL:N	2.35	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
1:A:25:PRO:HA	1:A:133:PRO:HG2	2.02	0.41
1:A:131:THR:HA	1:A:142:ILE:O	2.20	0.41
1:A:363:ASN:O	1:A:366:LYS:HB2	2.20	0.41
2:B:154:LYS:C	2:B:157:PRO:HD2	2.46	0.41
1:A:381:VAL:HG22	2:B:25:PRO:HB3	2.03	0.41
2:B:377:THR:O	2:B:381:VAL:HG23	2.21	0.41
1:A:31:ILE:O	1:A:31:ILE:HG22	2.21	0.40
1:A:264:LEU:HD22	1:A:306:ASN:HD22	1.86	0.40
2:B:314:VAL:HB	2:B:317:VAL:HG21	2.02	0.40
2:B:338:THR:HA	2:B:353:LYS:HA	2.02	0.40
1:A:94:ILE:HD13	1:A:94:ILE:H	1.86	0.40
1:A:49:LYS:HB3	1:A:144:TYR:CE1	2.56	0.40
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.40
2:B:136:ASN:O	2:B:137:ASN:HB2	2.22	0.40
1:A:102:LYS:HE2	1:A:236:PRO:O	2.21	0.40
1:A:253:THR:HA	1:A:292:VAL:HA	2.03	0.40
1:A:304:ALA:O	1:A:308:GLU:HG2	2.21	0.40
1:A:465:LYS:O	1:A:466:VAL:HG23	2.21	0.40
2:B:110:ASP:HB3	2:B:217:PRO:HG2	2.04	0.40
1:A:71:TRP:CD1	1:A:71:TRP:N	2.90	0.40
1:A:180:ILE:HA	1:A:188:TYR:O	2.22	0.40
2:B:31:ILE:HD12	2:B:135:ILE:CD1	2.51	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	549/562 (98%)	491 (89%)	53 (10%)	5 (1%)	14	25
2	B	425/437 (97%)	381 (90%)	40 (9%)	4 (1%)	14	25
All	All	974/999 (98%)	872 (90%)	93 (10%)	9 (1%)	14	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	217	PRO
1	A	412	PRO
1	A	55	PRO
1	A	90	VAL
2	B	97	PRO
2	B	226	PRO
2	B	321	PRO
2	B	420	PRO

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	493/502 (98%)	467 (95%)	26 (5%)	19	33
2	B	389/397 (98%)	371 (95%)	18 (5%)	23	38
All	All	882/899 (98%)	838 (95%)	44 (5%)	20	35

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	26	LEU
1	A	32	LYS
1	A	53	GLU
1	A	65	LYS
1	A	66	LYS
1	A	67	ASN
1	A	68	SER
1	A	83	ARG
1	A	94	ILE
1	A	102	LYS
1	A	116	PHE
1	A	174	GLN
1	A	178	ILE
1	A	187	LEU
1	A	210	LEU
1	A	216	THR
1	A	310	LEU
1	A	312	GLU
1	A	356	ARG
1	A	363	ASN
1	A	428	GLN
1	A	472	THR
1	A	476	LYS
1	A	506	ILE
1	A	533	LEU
2	B	2	ILE
2	B	24	TRP
2	B	34	LEU
2	B	58	THR
2	B	63	ILE
2	B	120	LEU
2	B	174	GLN
2	B	185	ASP
2	B	207	GLN
2	B	219	LYS
2	B	222	GLN
2	B	229	TRP
2	B	249	LYS
2	B	275	LYS
2	B	330	GLN
2	B	332	GLN

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Mol	Chain	Res	Type
2	B	374	LYS
2	B	401	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	137	ASN
1	A	145	GLN
1	A	147	ASN
1	A	161	GLN
1	A	182	GLN
1	A	198	HIS
1	A	235	HIS
1	A	269	GLN
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	348	ASN
1	A	373	GLN
1	A	394	GLN
1	A	407	GLN
1	A	418	ASN
1	A	428	GLN
1	A	447	ASN
1	A	464	GLN
1	A	471	ASN
1	A	474	ASN
1	A	475	GLN
1	A	494	ASN
1	A	520	GLN
1	A	545	ASN
2	B	23	GLN
2	B	54	ASN
2	B	81	ASN
2	B	137	ASN
2	B	174	GLN
2	B	207	GLN
2	B	258	GLN
2	B	269	GLN
2	B	306	ASN

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Mol	Chain	Res	Type
2	B	330	GLN
2	B	332	GLN
2	B	334	GLN
2	B	340	GLN
2	B	407	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

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, 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	551/562 (98%)	0.41	31 (5%) 31 29	53, 97, 138, 148	0
2	B	427/437 (97%)	0.18	21 (4%) 36 33	43, 86, 138, 152	0
All	All	978/999 (97%)	0.31	52 (5%) 33 31	43, 94, 138, 152	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	5.7
1	A	144	TYR	4.3
2	B	228	LEU	4.1
1	A	50	ILE	4.0
2	B	422	LEU	3.7
2	B	421	PRO	3.5
2	B	427	TYR	3.2
1	A	88	TRP	3.2
2	B	226	PRO	3.2
1	A	272	PRO	3.2
2	B	94	ILE	3.2
1	A	33	ALA	3.0
1	A	60	VAL	3.0
1	A	223	LYS	2.9
1	A	355	ALA	2.9
2	B	3	SER	2.8
2	B	2	ILE	2.8
1	A	35	VAL	2.7
2	B	230	MET	2.7
1	A	63	ILE	2.7
1	A	38	CYS	2.7
2	B	88	TRP	2.7
1	A	269	GLN	2.7
1	A	71	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	2.6
1	A	74	LEU	2.5
1	A	34	LEU	2.5
2	B	225	PRO	2.4
2	B	362	THR	2.4
1	A	194	GLU	2.4
1	A	25	PRO	2.4
1	A	140	PRO	2.4
2	B	425	LEU	2.4
2	B	241	VAL	2.3
1	A	195	ILE	2.3
1	A	427	TYR	2.3
1	A	266	TRP	2.3
1	A	31	ILE	2.3
2	B	92	LEU	2.2
1	A	548	VAL	2.2
1	A	61	PHE	2.2
2	B	303	LEU	2.2
2	B	29	GLU	2.2
1	A	306	ASN	2.2
1	A	2	ILE	2.1
1	A	545	ASN	2.1
1	A	262	GLY	2.1
2	B	195	ILE	2.1
2	B	360	ALA	2.1
2	B	227	PHE	2.1
1	A	47	ILE	2.0
2	B	296	THR	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 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.