



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 04:19 AM EDT

PDB ID : 3KLI  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

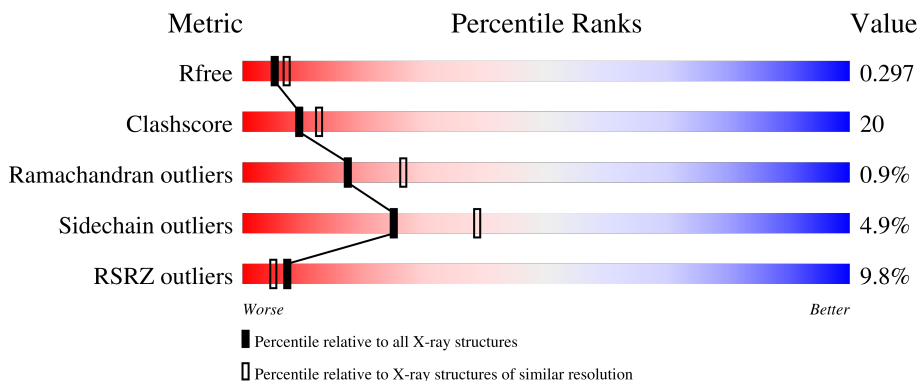
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	
2	B	437	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	551	4495	2911	749	828	7	0	0	0

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
			Total	C	N	O	S			
2	B	427	3529	2300	584	638	7	0	0	0

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

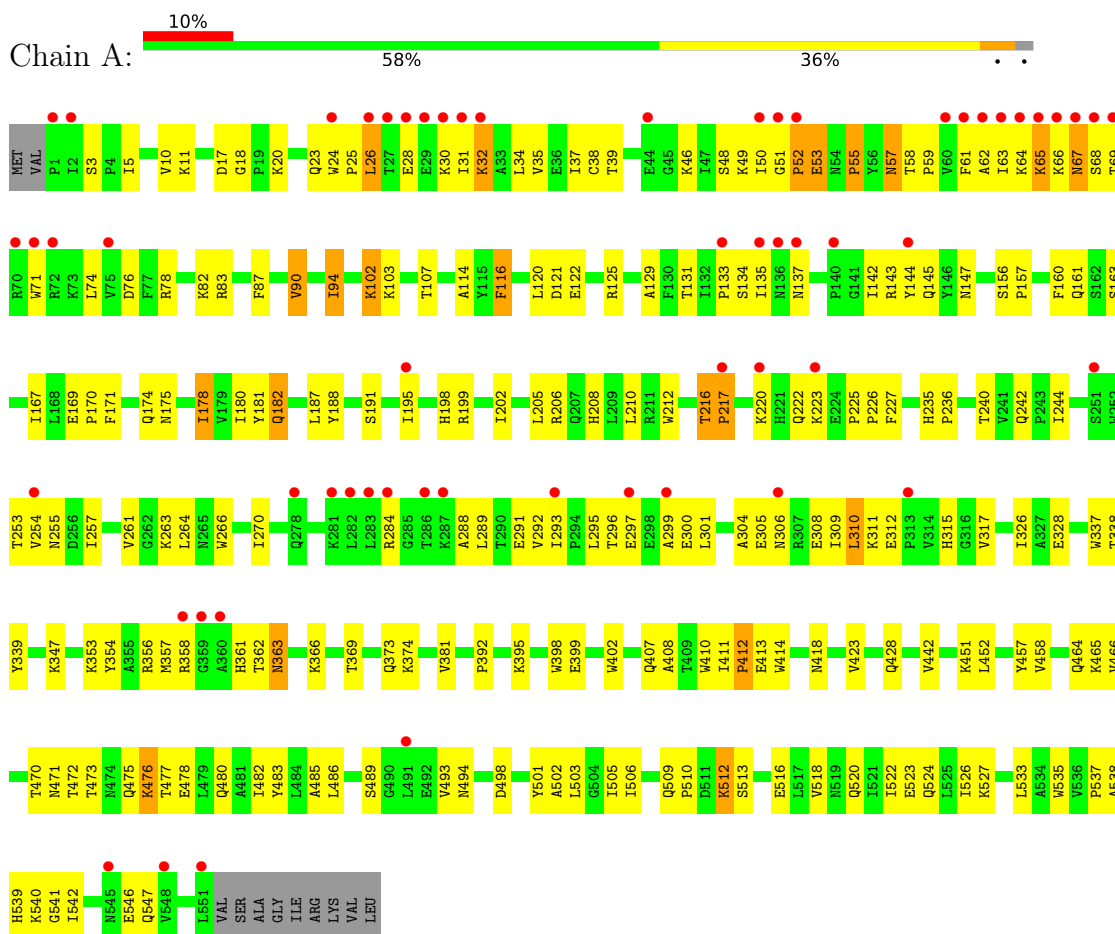
- Molecule 3 is water.

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

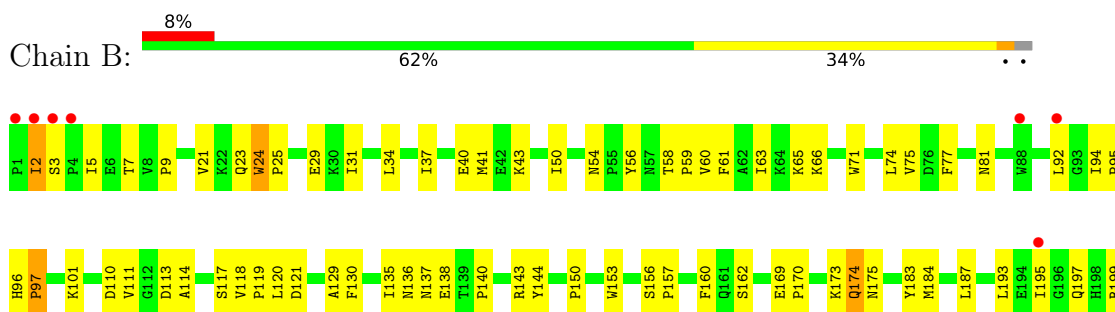
### 3 Residue-property plots

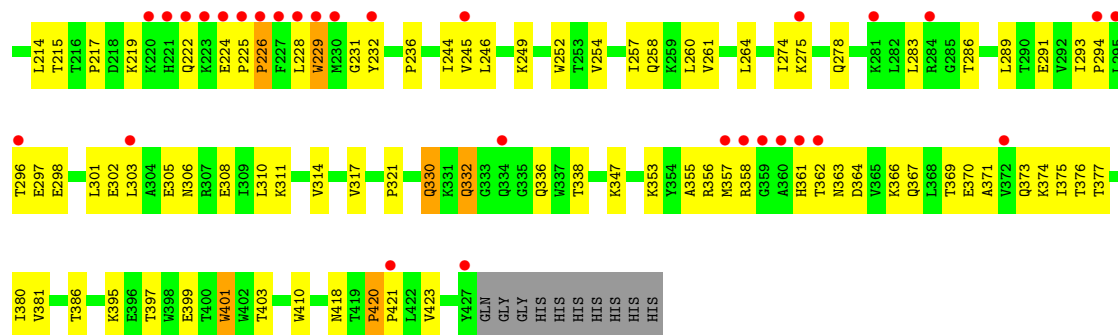
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	237.07Å 71.22Å 94.63Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.65 28.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (28.64-2.65) 92.5 (28.64-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.260 , 0.294 0.260 , 0.297	Depositor DCC
$R_{free}$ test set	1334 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/4614	0.61	2/6270 (0.0%)
2	B	0.50	0/3634	0.67	1/4940 (0.0%)
All	All	0.46	0/8248	0.64	3/11210 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	SER	CB-CA-C	-5.45	99.74	110.10
1	A	57	ASN	CB-CA-C	5.33	121.06	110.40
1	A	58	THR	N-CA-CB	5.22	120.22	110.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4495	0	4549	208	0
2	B	3529	0	3568	130	0
3	A	19	0	0	0	0
3	B	19	0	0	3	0
All	All	8062	0	8117	319	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 (319) 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:66:LYS:HZ1	2:B:232:TYR:H	1.34	0.76
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
2:B:66:LYS:HZ1	2:B:232:TYR:N	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:N	1:A:52:PRO:CD	2.60	0.57
1:A:410:TRP:C	1:A:411:ILE:HD12	2.25	0.57
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
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:278:GLN:HB3	2:B:302:GLU:CD	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:NE2	2:B:60:VAL:HG12	2.25	0.52
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
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:216:THR:O	1:A:217:PRO:C	2.51	0.48
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: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
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
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:356:ARG:O	2:B:357:MET:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:H	1:A:506:ILE:CD1	2.27	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: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
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	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
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
2:B:94:ILE:HG22	2:B:94:ILE:O	2.16	0.45
1:A:35:VAL:O	1:A:39:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:245:VAL:C	2:B:246:LEU:HD12	2.37	0.45
1:A:195:ILE:CD1	1:A:223:LYS:HG2	2.47	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
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:225:PRO:HA	1:A:226:PRO:C	2.38	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
2:B:293:ILE:O	2:B:294:PRO:C	2.57	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
1:A:512:LYS:HD2	1:A:513:SER:H	1.82	0.43
1:A:65:LYS:C	1:A:67:ASN:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG23	2:B:291:GLU:O	2.19	0.43
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.39	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
2:B:303:LEU:HD23	2:B:303:LEU:C	2.38	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: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:CG	1:A:402:TRP:O	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
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: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:49:LYS:C	1:A:50:ILE:HG13	2.40	0.42
1:A:486:LEU:HB3	1:A:524:GLN:HG2	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:LYS:HB2	2:B:219:LYS:NZ	2.34	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
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
2:B:66:LYS:HZ2	2:B:231:GLY:CA	2.34	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:131:THR:HG23	1:A:142:ILE:C	2.41	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%)	17	26
2	B	425/437 (97%)	381 (90%)	40 (9%)	4 (1%)	17	26
All	All	974/999 (98%)	872 (90%)	93 (10%)	9 (1%)	17	26

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%)	464 (94%)	29 (6%)	19	30
2	B	389/397 (98%)	375 (96%)	14 (4%)	35	51
All	All	882/899 (98%)	839 (95%)	43 (5%)	25	38

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
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	182	GLN
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	418	ASN
1	A	428	GLN
1	A	472	THR
1	A	476	LYS
1	A	512	LYS
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	222	GLN
2	B	229	TRP
2	B	249	LYS
2	B	330	GLN
2	B	332	GLN
2	B	374	LYS

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Mol	Chain	Res	Type
2	B	401	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	91	GLN
1	A	137	ASN
1	A	145	GLN
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	198	HIS
1	A	269	GLN
1	A	332	GLN
1	A	336	GLN
1	A	363	ASN
1	A	373	GLN
1	A	394	GLN
1	A	407	GLN
1	A	418	ASN
1	A	428	GLN
1	A	464	GLN
1	A	471	ASN
1	A	475	GLN
1	A	494	ASN
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	278	GLN
2	B	306	ASN
2	B	330	GLN
2	B	332	GLN
2	B	340	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/562 (98%)	0.63	59 (10%) <b>6</b> <b>4</b>	53, 97, 138, 148	0
2	B	427/437 (97%)	0.55	37 (8%) <b>10</b> <b>8</b>	43, 86, 138, 152	0
All	All	978/999 (97%)	0.60	96 (9%) <b>7</b> <b>5</b>	43, 94, 138, 152	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PRO	9.9
2	B	360	ALA	9.8
2	B	230	MET	8.8
2	B	359	GLY	8.4
2	B	227	PHE	8.2
1	A	71	TRP	7.6
1	A	135	ILE	7.1
2	B	229	TRP	6.5
2	B	220	LYS	6.3
1	A	27	THR	6.2
1	A	1	PRO	6.1
2	B	2	ILE	6.0
2	B	221	HIS	5.9
2	B	228	LEU	5.8
1	A	551	LEU	5.7
2	B	358	ARG	5.4
1	A	66	LYS	5.0
1	A	136	ASN	5.0
2	B	295	LEU	4.9
1	A	297	GLU	4.8
2	B	357	MET	4.8
2	B	225	PRO	4.7
1	A	70	ARG	4.5
2	B	3	SER	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	64	LYS	4.5
1	A	223	LYS	4.3
2	B	4	PRO	4.3
1	A	358	ARG	4.2
2	B	1	PRO	4.1
1	A	26	LEU	4.1
1	A	65	LYS	3.8
2	B	284	ARG	3.7
1	A	144	TYR	3.6
1	A	217	PRO	3.6
1	A	282	LEU	3.6
2	B	224	GLU	3.5
2	B	223	LYS	3.5
2	B	88	TRP	3.5
2	B	294	PRO	3.5
1	A	63	ILE	3.4
1	A	30	LYS	3.4
1	A	69	THR	3.4
1	A	220	LYS	3.4
1	A	491	LEU	3.3
1	A	251	SER	3.3
1	A	306	ASN	3.3
1	A	61	PHE	3.2
1	A	278	GLN	3.1
1	A	51	GLY	3.1
2	B	296	THR	3.0
1	A	67	ASN	3.0
1	A	29	GLU	2.9
1	A	283	LEU	2.8
1	A	2	ILE	2.8
1	A	68	SER	2.8
2	B	362	THR	2.7
2	B	421	PRO	2.7
1	A	137	ASN	2.6
2	B	427	TYR	2.6
1	A	50	ILE	2.6
2	B	232	TYR	2.6
1	A	60	VAL	2.6
1	A	28	GLU	2.6
1	A	133	PRO	2.6
1	A	299	ALA	2.6
1	A	281	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	281	LYS	2.5
2	B	222	GLN	2.5
2	B	92	LEU	2.5
1	A	72	ARG	2.5
1	A	313	PRO	2.5
1	A	286	THR	2.5
1	A	31	ILE	2.5
2	B	195	ILE	2.5
1	A	293	ILE	2.4
1	A	545	ASN	2.4
1	A	284	ARG	2.4
1	A	287	LYS	2.4
2	B	334	GLN	2.4
1	A	62	ALA	2.4
1	A	254	VAL	2.4
2	B	361	HIS	2.3
1	A	359	GLY	2.3
1	A	360	ALA	2.3
2	B	275	LYS	2.3
1	A	52	PRO	2.2
2	B	245	VAL	2.2
1	A	24	TRP	2.2
1	A	32	LYS	2.2
1	A	75	VAL	2.2
2	B	303	LEU	2.2
1	A	140	PRO	2.1
1	A	195	ILE	2.1
2	B	372	VAL	2.0
1	A	44	GLU	2.0
1	A	548	VAL	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.