Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 04:06 AM EDT

PDB ID	:	1X9Y
Title	:	The prostaphopain B structure
Authors	:	Filipek, R.; Szczepanowski, R.; Sabat, A.; Potempa, J.; Bochtler, M.
Deposited on	:	2004-08-24
Resolution	:	2.50 Å(reported)

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

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

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

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

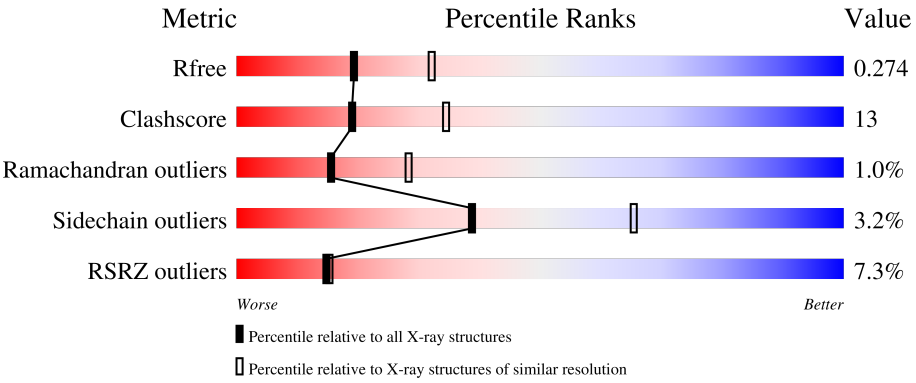
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	6% 71% 22% · 6%
1	B	367	5% 71% 21% · 6%
1	C	367	8% 72% 20% •• 6%
1	D	367	8% 72% 21% · 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11355 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 cysteine proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2778	1756	463	551	8			
1	B	346	Total	C	N	O	S	0	0	0
			2778	1756	463	551	8			
1	C	346	Total	C	N	O	S	0	0	0
			2778	1756	463	551	8			
1	D	346	Total	C	N	O	S	0	0	0
			2778	1756	463	551	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	cloning artifact	UNP Q70UQ8
A	36	SER	-	cloning artifact	UNP Q70UQ8
A	394	LEU	-	cloning artifact	UNP Q70UQ8
A	395	GLU	-	cloning artifact	UNP Q70UQ8
A	396	VAL	-	cloning artifact	UNP Q70UQ8
A	397	PRO	-	cloning artifact	UNP Q70UQ8
A	398	ILE	-	cloning artifact	UNP Q70UQ8
A	399	HIS	-	cloning artifact	UNP Q70UQ8
A	400	ARG	-	cloning artifact	UNP Q70UQ8
A	401	ASP	-	cloning artifact	UNP Q70UQ8
B	35	GLY	-	cloning artifact	UNP Q70UQ8
B	36	SER	-	cloning artifact	UNP Q70UQ8
B	394	LEU	-	cloning artifact	UNP Q70UQ8
B	395	GLU	-	cloning artifact	UNP Q70UQ8
B	396	VAL	-	cloning artifact	UNP Q70UQ8
B	397	PRO	-	cloning artifact	UNP Q70UQ8
B	398	ILE	-	cloning artifact	UNP Q70UQ8
B	399	HIS	-	cloning artifact	UNP Q70UQ8
B	400	ARG	-	cloning artifact	UNP Q70UQ8
B	401	ASP	-	cloning artifact	UNP Q70UQ8
C	35	GLY	-	cloning artifact	UNP Q70UQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	36	SER	-	cloning artifact	UNP Q70UQ8
C	394	LEU	-	cloning artifact	UNP Q70UQ8
C	395	GLU	-	cloning artifact	UNP Q70UQ8
C	396	VAL	-	cloning artifact	UNP Q70UQ8
C	397	PRO	-	cloning artifact	UNP Q70UQ8
C	398	ILE	-	cloning artifact	UNP Q70UQ8
C	399	HIS	-	cloning artifact	UNP Q70UQ8
C	400	ARG	-	cloning artifact	UNP Q70UQ8
C	401	ASP	-	cloning artifact	UNP Q70UQ8
D	35	GLY	-	cloning artifact	UNP Q70UQ8
D	36	SER	-	cloning artifact	UNP Q70UQ8
D	394	LEU	-	cloning artifact	UNP Q70UQ8
D	395	GLU	-	cloning artifact	UNP Q70UQ8
D	396	VAL	-	cloning artifact	UNP Q70UQ8
D	397	PRO	-	cloning artifact	UNP Q70UQ8
D	398	ILE	-	cloning artifact	UNP Q70UQ8
D	399	HIS	-	cloning artifact	UNP Q70UQ8
D	400	ARG	-	cloning artifact	UNP Q70UQ8
D	401	ASP	-	cloning artifact	UNP Q70UQ8

- Molecule 2 is water.

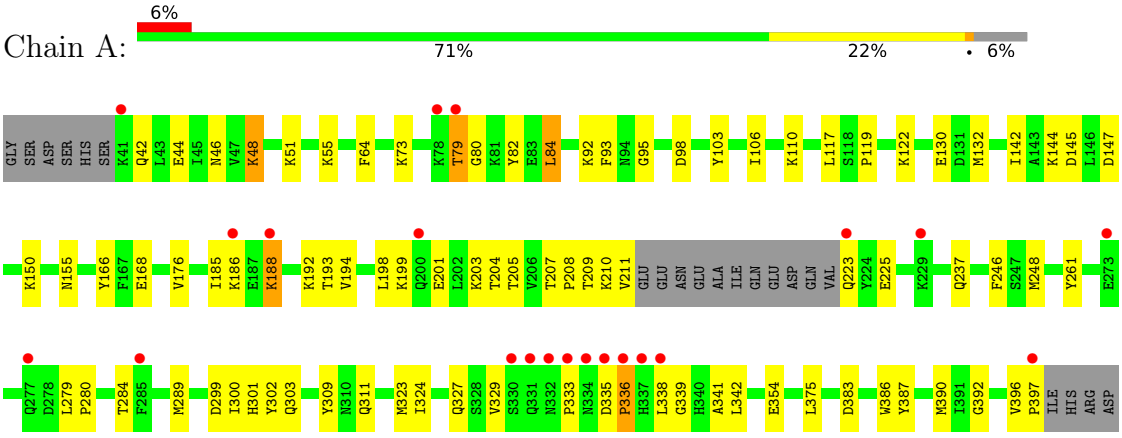
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	68	Total O 68 68	0	0
2	B	58	Total O 58 58	0	0
2	C	49	Total O 49 49	0	0
2	D	68	Total O 68 68	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

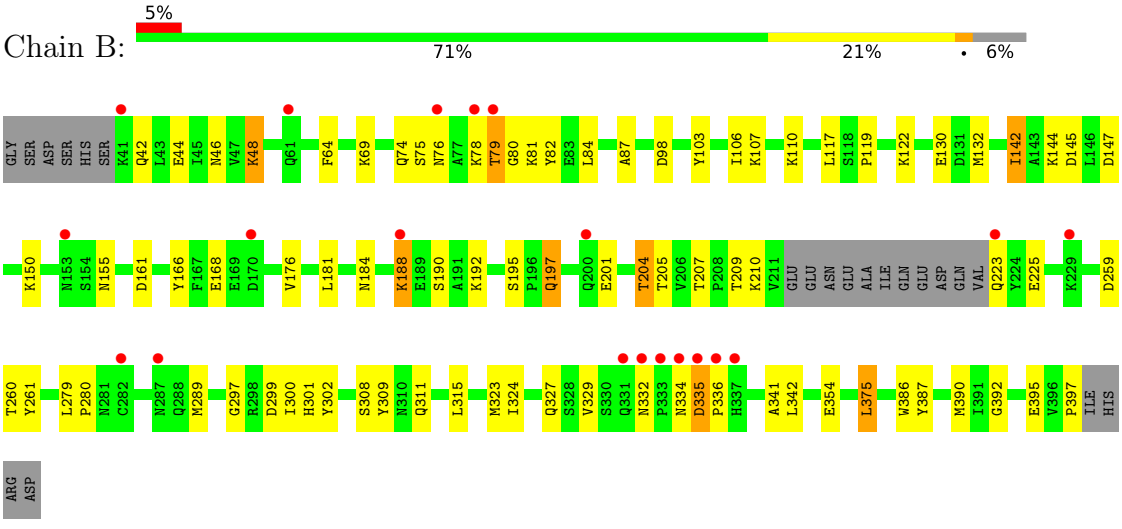
• Molecule 1: cysteine proteinase

Chain A:



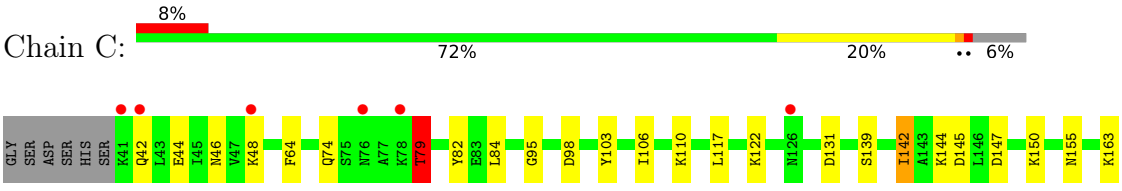
• Molecule 1: cysteine proteinase

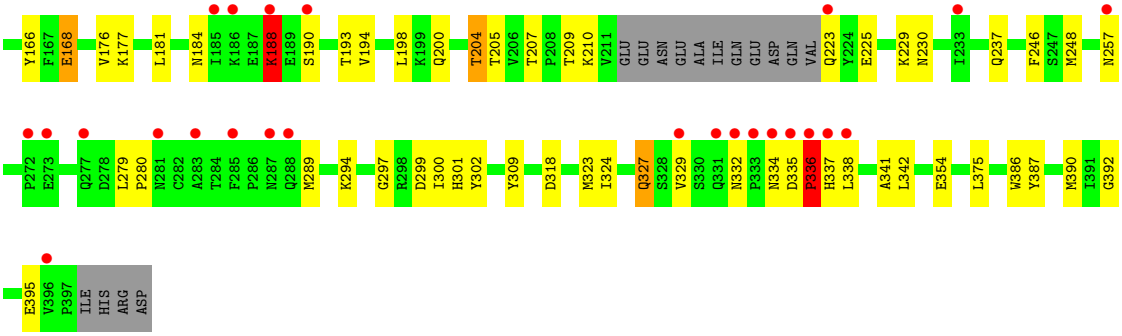
Chain B:



• Molecule 1: cysteine proteinase

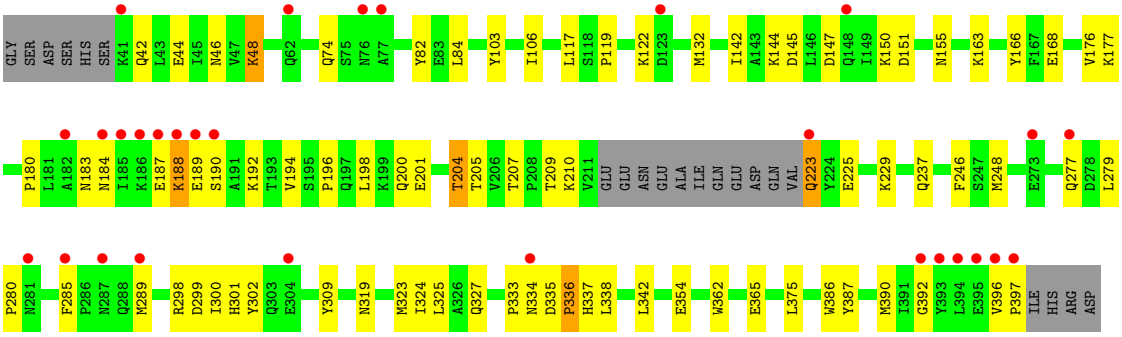
Chain C:





• Molecule 1: cysteine proteinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.62Å 104.92Å 173.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.86-2.50) 99.2 (19.86-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.276 0.242 , 0.274	Depositor DCC
R_{free} test set	2730 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11355	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.07% 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	0.39	0/2833	0.60	0/3831
1	B	0.39	0/2833	0.61	0/3831
1	C	0.38	0/2833	0.60	0/3831
1	D	0.39	0/2833	0.61	0/3831
All	All	0.39	0/11332	0.61	0/15324

There are no bond length outliers.

There are no bond angle outliers.

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	2778	0	2724	79	0
1	B	2778	0	2724	83	0
1	C	2778	0	2724	75	0
1	D	2778	0	2724	72	0
2	A	68	0	0	10	0
2	B	58	0	0	6	0
2	C	49	0	0	6	0
2	D	68	0	0	7	0
All	All	11355	0	10896	287	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 13.

All (287) 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:195:SER:HB3	1:B:197:GLN:HG3	1.31	1.09
1:C:122:LYS:HE2	1:C:329:VAL:HG13	1.46	0.96
1:B:308:SER:HB3	1:C:257:ASN:CG	1.86	0.95
1:A:204:THR:HG22	1:A:205:THR:H	1.33	0.94
1:B:332:ASN:HD22	1:B:335:ASP:HB3	1.34	0.92
1:B:79:THR:HG22	1:B:80:GLY:H	1.37	0.89
1:D:204:THR:HG22	1:D:205:THR:H	1.38	0.89
1:C:336:PRO:HB3	1:C:387:TYR:CE1	2.07	0.88
1:A:336:PRO:HD2	1:D:397:PRO:HB3	1.57	0.87
1:D:207:THR:OG1	1:D:210:LYS:HB2	1.76	0.86
1:B:204:THR:HG22	1:B:205:THR:H	1.39	0.85
1:C:294:LYS:HD3	2:C:435:HOH:O	1.75	0.85
1:B:207:THR:OG1	1:B:210:LYS:HB2	1.75	0.85
1:D:302:TYR:HA	1:D:390:MET:HE1	1.59	0.84
1:B:302:TYR:HA	1:B:390:MET:HE1	1.58	0.84
1:C:207:THR:OG1	1:C:210:LYS:HB2	1.77	0.84
1:C:302:TYR:HA	1:C:390:MET:HE1	1.60	0.83
1:A:302:TYR:HA	1:A:390:MET:HE1	1.60	0.83
1:A:207:THR:OG1	1:A:210:LYS:HB2	1.77	0.83
1:B:315:LEU:HD21	1:C:229:LYS:HE3	1.64	0.80
1:C:204:THR:HG22	1:C:205:THR:H	1.46	0.80
1:C:144:LYS:HE3	2:C:434:HOH:O	1.83	0.78
1:A:79:THR:HG22	1:A:80:GLY:N	1.99	0.77
1:A:188:LYS:N	1:A:188:LYS:HE3	2.02	0.75
1:D:48:LYS:HE3	1:D:201:GLU:O	1.86	0.75
1:B:46:ASN:HD21	1:B:155:ASN:ND2	1.85	0.75
1:B:308:SER:CB	1:C:257:ASN:OD1	2.34	0.75
1:C:131:ASP:HA	1:D:277:GLN:HE22	1.52	0.74
1:A:122:LYS:NZ	1:A:333:PRO:HB3	2.03	0.73
1:D:46:ASN:HD21	1:D:155:ASN:ND2	1.86	0.73
1:A:79:THR:HG22	1:A:80:GLY:H	1.54	0.73
1:C:46:ASN:HD21	1:C:155:ASN:ND2	1.86	0.72
1:D:188:LYS:HD2	1:D:188:LYS:N	2.03	0.72
1:B:79:THR:HG22	1:B:80:GLY:N	2.06	0.71
1:A:144:LYS:HE2	1:A:144:LYS:HA	1.72	0.71
1:D:144:LYS:HA	1:D:144:LYS:HE2	1.73	0.71
1:B:144:LYS:HA	1:B:144:LYS:HE2	1.72	0.70
1:D:196:PRO:O	1:D:200:GLN:HG2	1.91	0.70
1:B:375:LEU:HB3	2:B:423:HOH:O	1.91	0.70
1:D:177:LYS:HE2	2:D:412:HOH:O	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HG2	1:A:207:THR:HG22	1.73	0.69
1:C:144:LYS:HE2	1:C:144:LYS:HA	1.74	0.69
1:A:329:VAL:HG23	1:A:383:ASP:O	1.92	0.69
1:B:48:LYS:HB2	2:B:422:HOH:O	1.93	0.69
1:A:46:ASN:HD21	1:A:155:ASN:ND2	1.91	0.69
1:B:332:ASN:HD22	1:B:335:ASP:CB	2.06	0.69
1:C:181:LEU:HB2	1:C:184:ASN:ND2	2.08	0.68
1:B:308:SER:CB	1:C:257:ASN:CG	2.61	0.68
1:B:308:SER:HB3	1:C:257:ASN:OD1	1.92	0.68
1:C:44:GLU:HG2	1:C:207:THR:HG22	1.76	0.68
1:C:163:LYS:HE3	1:C:188:LYS:O	1.93	0.67
1:B:188:LYS:HE3	1:B:188:LYS:N	2.08	0.67
1:B:315:LEU:CD2	1:C:229:LYS:HE3	2.24	0.67
1:B:207:THR:HG1	1:B:210:LYS:HB2	1.56	0.67
1:C:324:ILE:HG12	1:C:386:TRP:CZ2	2.30	0.67
1:D:44:GLU:HG2	1:D:207:THR:HG22	1.77	0.67
1:D:324:ILE:HG12	1:D:386:TRP:CZ2	2.29	0.66
1:B:44:GLU:HG2	1:B:207:THR:HG22	1.78	0.66
1:A:324:ILE:HG12	1:A:386:TRP:CZ2	2.30	0.66
1:C:300:ILE:HD13	1:C:392:GLY:HA2	1.78	0.65
1:A:207:THR:HG1	1:A:210:LYS:HB2	1.60	0.65
1:B:302:TYR:HD1	1:B:390:MET:CE	2.09	0.65
1:A:300:ILE:HD13	1:A:392:GLY:HA2	1.78	0.65
1:C:188:LYS:HE3	1:C:188:LYS:N	2.12	0.64
1:B:324:ILE:HG12	1:B:386:TRP:CZ2	2.33	0.64
1:A:194:VAL:HG13	1:A:198:LEU:HD23	1.77	0.64
1:D:300:ILE:HD13	1:D:392:GLY:HA2	1.80	0.64
1:D:163:LYS:HE3	1:D:189:GLU:HB2	1.79	0.63
1:A:166:TYR:OH	1:A:192:LYS:NZ	2.32	0.63
1:D:289:MET:HE2	1:D:338:LEU:HD22	1.81	0.63
1:A:302:TYR:HD1	1:A:390:MET:CE	2.12	0.62
1:B:300:ILE:HD13	1:B:392:GLY:HA2	1.79	0.62
1:A:208:PRO:HD2	2:A:426:HOH:O	1.99	0.62
1:A:48:LYS:HE3	1:A:201:GLU:O	2.00	0.62
1:A:95:GLY:HA2	1:A:198:LEU:HD13	1.82	0.61
1:B:46:ASN:HD21	1:B:155:ASN:HD22	1.46	0.61
1:B:78:LYS:O	1:B:107:LYS:NZ	2.30	0.61
1:C:302:TYR:HD1	1:C:390:MET:CE	2.14	0.61
1:B:74:GLN:NE2	1:B:225:GLU:HG3	2.16	0.61
1:D:302:TYR:CA	1:D:390:MET:HE1	2.31	0.60
1:C:46:ASN:HD21	1:C:155:ASN:HD22	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLN:NE2	1:D:225:GLU:HG3	2.17	0.59
1:C:84:LEU:HD22	1:C:103:TYR:HB3	1.84	0.59
1:A:79:THR:CG2	1:A:80:GLY:H	2.15	0.59
1:C:299:ASP:OD2	1:C:301:HIS:NE2	2.31	0.59
1:D:302:TYR:HD1	1:D:390:MET:CE	2.16	0.59
1:A:79:THR:CG2	1:A:80:GLY:N	2.66	0.59
1:C:188:LYS:H	1:C:188:LYS:CD	2.15	0.59
1:D:299:ASP:OD2	1:D:301:HIS:NE2	2.33	0.59
1:D:46:ASN:HD21	1:D:155:ASN:HD22	1.50	0.58
1:D:335:ASP:N	1:D:336:PRO:HD3	2.19	0.58
1:A:84:LEU:HD22	1:A:103:TYR:HB3	1.86	0.58
1:B:130:GLU:HG2	2:B:434:HOH:O	2.04	0.58
1:C:188:LYS:H	1:C:188:LYS:HD2	1.69	0.57
1:D:84:LEU:HD22	1:D:103:TYR:HB3	1.84	0.57
1:A:204:THR:HG22	1:A:205:THR:N	2.12	0.57
1:C:334:ASN:C	1:C:336:PRO:HD3	2.25	0.57
1:B:84:LEU:HD22	1:B:103:TYR:HB3	1.86	0.56
1:B:308:SER:OG	1:C:230:ASN:OD1	2.21	0.56
1:B:302:TYR:CA	1:B:390:MET:HE1	2.32	0.56
1:C:42:GLN:OE1	1:C:209:THR:HG21	2.06	0.56
1:D:42:GLN:OE1	1:D:209:THR:HG21	2.06	0.56
1:C:294:LYS:HB2	2:C:438:HOH:O	2.06	0.55
1:A:42:GLN:OE1	1:A:209:THR:HG21	2.05	0.55
1:B:195:SER:HB3	1:B:197:GLN:CG	2.22	0.55
1:B:46:ASN:ND2	1:B:155:ASN:HD22	2.04	0.54
1:D:184:ASN:HB3	2:D:424:HOH:O	2.07	0.54
1:B:311:GLN:HG3	1:C:229:LYS:HG3	1.89	0.54
1:B:42:GLN:OE1	1:B:209:THR:HG21	2.08	0.54
1:A:46:ASN:HD21	1:A:155:ASN:HD22	1.54	0.54
1:A:122:LYS:HE2	1:A:329:VAL:HG13	1.90	0.53
1:B:48:LYS:HD2	2:B:422:HOH:O	2.09	0.53
1:C:177:LYS:HE2	2:C:419:HOH:O	2.08	0.53
1:D:46:ASN:ND2	1:D:155:ASN:HD22	2.06	0.53
1:B:181:LEU:HB2	1:B:184:ASN:ND2	2.23	0.53
1:A:303:GLN:HG3	1:D:319:ASN:HB2	1.91	0.53
1:D:189:GLU:HG3	1:D:192:LYS:NZ	2.24	0.53
1:A:289:MET:SD	1:A:323:MET:CE	2.98	0.52
1:A:289:MET:HE1	1:A:338:LEU:HD22	1.91	0.52
1:A:311:GLN:HG3	1:D:229:LYS:HG3	1.90	0.52
1:A:211:VAL:HG12	2:A:418:HOH:O	2.09	0.52
1:B:308:SER:CA	1:C:257:ASN:OD1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLN:OE1	1:B:336:PRO:HA	2.10	0.52
1:C:46:ASN:ND2	1:C:155:ASN:HD22	2.06	0.52
1:A:302:TYR:CA	1:A:390:MET:HE1	2.36	0.52
1:B:335:ASP:CG	1:B:335:ASP:O	2.48	0.52
1:C:95:GLY:HA2	1:C:198:LEU:HD13	1.91	0.52
1:D:325:LEU:HD22	1:D:338:LEU:HD13	1.92	0.51
1:D:327:GLN:HG2	1:D:387:TYR:CD2	2.45	0.51
1:A:73:LYS:NZ	1:A:225:GLU:HB3	2.26	0.51
1:B:161:ASP:OD2	1:B:192:LYS:NZ	2.34	0.51
1:B:327:GLN:HG2	1:B:387:TYR:CD2	2.46	0.51
1:A:336:PRO:HD2	1:D:397:PRO:CB	2.36	0.51
1:D:289:MET:SD	1:D:323:MET:CE	2.99	0.51
1:A:185:ILE:HG23	1:A:186:LYS:N	2.25	0.50
1:C:302:TYR:CA	1:C:390:MET:HE1	2.39	0.50
1:B:302:TYR:CD1	1:B:390:MET:CE	2.94	0.50
1:C:327:GLN:HG2	1:C:387:TYR:CD2	2.46	0.50
1:A:55:LYS:HE2	2:A:442:HOH:O	2.11	0.50
1:B:79:THR:CG2	1:B:80:GLY:H	2.16	0.50
1:B:332:ASN:ND2	1:B:335:ASP:HB3	2.14	0.50
1:C:289:MET:SD	1:C:323:MET:CE	3.00	0.50
1:A:46:ASN:ND2	1:A:155:ASN:HD22	2.10	0.49
1:B:204:THR:HG22	1:B:205:THR:N	2.18	0.49
1:A:289:MET:SD	1:A:323:MET:HE1	2.52	0.49
2:B:426:HOH:O	1:C:257:ASN:HB2	2.11	0.49
1:B:301:HIS:ND1	1:C:318:ASP:OD1	2.46	0.49
1:A:327:GLN:HG2	1:A:387:TYR:CD2	2.47	0.49
1:C:74:GLN:NE2	1:C:225:GLU:HG3	2.28	0.49
1:D:285:PHE:C	1:D:289:MET:HE3	2.31	0.49
1:B:74:GLN:NE2	1:B:225:GLU:CG	2.75	0.49
1:B:74:GLN:HE21	1:B:225:GLU:HG3	1.77	0.49
1:D:309:TYR:CD1	1:D:354:GLU:HB3	2.48	0.49
1:B:147:ASP:O	1:B:150:LYS:HG2	2.13	0.48
1:C:335:ASP:O	1:C:337:HIS:N	2.46	0.48
1:D:334:ASN:C	1:D:336:PRO:HD3	2.33	0.48
1:A:284:THR:O	1:A:338:LEU:HD23	2.13	0.48
1:D:223:GLN:NE2	2:D:460:HOH:O	2.33	0.48
1:B:308:SER:HA	1:C:257:ASN:OD1	2.12	0.48
1:D:204:THR:CG2	1:D:205:THR:H	2.15	0.48
1:D:122:LYS:NZ	1:D:333:PRO:HG3	2.29	0.48
1:D:147:ASP:O	1:D:150:LYS:HG2	2.14	0.48
1:A:211:VAL:HG11	2:A:423:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HD2	1:B:259:ASP:OD1	2.14	0.47
1:C:309:TYR:CD1	1:C:354:GLU:HB3	2.49	0.47
1:A:329:VAL:HG12	1:A:329:VAL:O	2.15	0.47
1:D:204:THR:HG22	1:D:205:THR:N	2.18	0.47
1:D:337:HIS:HB3	2:D:451:HOH:O	2.13	0.47
1:C:289:MET:SD	1:C:323:MET:HE3	2.54	0.47
1:D:207:THR:HG1	1:D:210:LYS:HB2	1.75	0.47
1:C:297:GLY:HA2	1:C:395:GLU:CD	2.34	0.47
1:D:248:MET:CE	1:D:289:MET:HG2	2.45	0.47
1:B:289:MET:SD	1:B:323:MET:CE	3.03	0.47
1:B:308:SER:HB3	1:C:257:ASN:ND2	2.29	0.47
1:D:279:LEU:N	1:D:280:PRO:CD	2.78	0.47
1:C:279:LEU:N	1:C:280:PRO:CD	2.78	0.47
1:B:309:TYR:CD1	1:B:354:GLU:HB3	2.49	0.46
1:D:365:GLU:HB3	2:D:459:HOH:O	2.15	0.46
1:A:144:LYS:HA	1:A:144:LYS:CE	2.43	0.46
1:A:261:TYR:HA	2:A:462:HOH:O	2.15	0.46
1:C:207:THR:HG1	1:C:210:LYS:HB2	1.79	0.46
1:D:119:PRO:HG3	1:D:132:MET:SD	2.55	0.46
1:A:48:LYS:HZ3	1:A:203:LYS:HE2	1.81	0.46
1:A:98:ASP:HB3	2:A:421:HOH:O	2.16	0.46
1:A:130:GLU:HB3	2:A:429:HOH:O	2.15	0.46
1:A:302:TYR:CD1	1:A:390:MET:CE	2.95	0.46
1:A:93:PHE:HD1	2:A:432:HOH:O	1.97	0.46
1:A:166:TYR:CZ	1:A:192:LYS:NZ	2.81	0.46
1:A:194:VAL:HB	1:A:199:LYS:HE3	1.97	0.46
1:C:188:LYS:HE3	1:C:188:LYS:H	1.78	0.46
1:D:183:ASN:O	1:D:187:GLU:HG3	2.16	0.45
1:B:279:LEU:N	1:B:280:PRO:CD	2.79	0.45
1:C:279:LEU:HB3	1:C:280:PRO:HD3	1.98	0.45
1:A:73:LYS:HZ1	1:A:225:GLU:HB3	1.80	0.45
1:C:248:MET:CE	1:C:289:MET:HG2	2.46	0.45
1:C:302:TYR:CD1	1:C:390:MET:CE	2.98	0.45
1:A:342:LEU:N	1:A:342:LEU:HD12	2.31	0.45
1:A:110:LYS:HA	1:A:150:LYS:HZ3	1.82	0.45
1:A:309:TYR:CD1	1:A:354:GLU:HB3	2.51	0.45
1:B:81:LYS:O	1:B:107:LYS:HA	2.17	0.45
1:D:289:MET:SD	1:D:323:MET:HE3	2.56	0.45
1:A:147:ASP:O	1:A:150:LYS:HG2	2.16	0.45
1:B:297:GLY:HA2	1:B:395:GLU:OE1	2.16	0.45
1:C:144:LYS:HA	1:C:144:LYS:CE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LYS:HD2	1:D:201:GLU:HB3	1.98	0.45
1:D:298:ARG:NE	2:D:415:HOH:O	2.49	0.45
1:C:79:THR:HG22	1:C:82:TYR:OH	2.17	0.45
1:A:396:VAL:HA	1:A:397:PRO:HD3	1.72	0.45
1:C:147:ASP:O	1:C:150:LYS:HG2	2.17	0.45
1:D:279:LEU:HB3	1:D:280:PRO:HD3	1.99	0.45
1:A:48:LYS:NZ	1:A:203:LYS:HE2	2.31	0.44
1:A:299:ASP:OD2	1:A:301:HIS:NE2	2.43	0.44
1:C:110:LYS:HA	1:C:150:LYS:HZ3	1.81	0.44
1:B:342:LEU:HD12	1:B:342:LEU:N	2.32	0.44
1:D:74:GLN:NE2	1:D:225:GLU:CG	2.81	0.44
1:D:145:ASP:CG	1:D:176:VAL:HG13	2.37	0.44
1:A:279:LEU:HB3	1:A:280:PRO:HD3	1.99	0.44
1:D:289:MET:HE2	1:D:338:LEU:CD2	2.46	0.44
1:A:130:GLU:OE2	1:B:260:THR:OG1	2.21	0.44
1:B:64:PHE:CG	1:B:84:LEU:HG	2.53	0.44
1:D:289:MET:SD	1:D:323:MET:HE1	2.58	0.44
1:A:279:LEU:N	1:A:280:PRO:CD	2.80	0.44
1:A:335:ASP:N	1:A:336:PRO:HD3	2.33	0.44
1:A:130:GLU:HG3	1:B:261:TYR:CZ	2.53	0.43
1:B:122:LYS:HE2	1:B:329:VAL:HG13	1.99	0.43
1:C:188:LYS:H	1:C:188:LYS:CE	2.31	0.43
1:B:279:LEU:HB3	1:B:280:PRO:HD3	1.99	0.43
1:C:139:SER:HB2	2:C:447:HOH:O	2.18	0.43
1:D:144:LYS:HA	1:D:144:LYS:CE	2.46	0.43
1:A:336:PRO:CD	1:D:397:PRO:HB3	2.38	0.43
1:C:342:LEU:N	1:C:342:LEU:HD12	2.33	0.43
1:D:151:ASP:HB2	2:D:461:HOH:O	2.18	0.43
1:A:82:TYR:HA	1:A:106:ILE:O	2.19	0.43
1:C:110:LYS:HA	1:C:150:LYS:NZ	2.34	0.43
1:B:69:LYS:HA	1:B:69:LYS:HD2	1.90	0.43
1:D:342:LEU:HD12	1:D:342:LEU:N	2.34	0.43
1:B:48:LYS:HE3	1:B:201:GLU:O	2.19	0.43
1:C:332:ASN:HB2	1:C:335:ASP:HB3	2.01	0.43
1:B:82:TYR:HA	1:B:106:ILE:O	2.19	0.43
1:C:168:GLU:OE2	1:C:194:VAL:HB	2.18	0.43
1:A:339:GLY:HA2	2:A:459:HOH:O	2.18	0.42
1:D:189:GLU:HG3	1:D:192:LYS:HZ1	1.84	0.42
1:D:237:GLN:HB2	1:D:246:PHE:CD2	2.55	0.42
1:C:145:ASP:CG	1:C:176:VAL:HG13	2.38	0.42
1:B:334:ASN:C	1:B:336:PRO:HD3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ASP:N	1:D:336:PRO:CD	2.82	0.42
1:A:237:GLN:HB2	1:A:246:PHE:CD2	2.55	0.42
1:A:248:MET:CE	1:A:289:MET:HG2	2.49	0.42
1:C:64:PHE:CG	1:C:84:LEU:HG	2.54	0.42
1:D:194:VAL:HG13	1:D:198:LEU:HD23	2.00	0.42
1:A:92:LYS:HB3	2:A:431:HOH:O	2.19	0.42
1:A:145:ASP:CG	1:A:176:VAL:HG13	2.40	0.42
1:D:180:PRO:HD2	1:D:362:TRP:NE1	2.35	0.42
1:D:299:ASP:CG	1:D:301:HIS:HE2	2.21	0.42
1:A:289:MET:SD	1:A:323:MET:HE3	2.60	0.42
1:B:98:ASP:HB3	2:B:404:HOH:O	2.19	0.42
1:B:119:PRO:HG3	1:B:132:MET:SD	2.60	0.42
1:C:82:TYR:HA	1:C:106:ILE:O	2.20	0.42
1:D:180:PRO:HD2	1:D:362:TRP:CD1	2.54	0.42
1:A:64:PHE:CG	1:A:84:LEU:HG	2.55	0.42
1:A:341:ALA:C	1:A:342:LEU:HD12	2.41	0.41
1:B:87:ALA:HB2	1:B:103:TYR:CE2	2.55	0.41
1:B:341:ALA:C	1:B:342:LEU:HD12	2.41	0.41
1:B:110:LYS:HA	1:B:150:LYS:HZ3	1.85	0.41
1:B:144:LYS:HA	1:B:144:LYS:CE	2.45	0.41
1:B:289:MET:SD	1:B:323:MET:HE1	2.61	0.41
1:A:119:PRO:HG3	1:A:132:MET:SD	2.61	0.41
1:B:299:ASP:OD2	1:B:301:HIS:NE2	2.46	0.41
1:B:308:SER:CB	1:C:257:ASN:ND2	2.84	0.41
1:D:302:TYR:CD1	1:D:390:MET:CE	3.00	0.41
1:A:166:TYR:CD1	1:A:166:TYR:N	2.89	0.41
1:B:142:ILE:HG22	1:B:176:VAL:HG12	2.03	0.41
1:B:145:ASP:CG	1:B:176:VAL:HG13	2.41	0.41
1:C:98:ASP:HB3	2:C:402:HOH:O	2.20	0.41
1:C:142:ILE:HG22	1:C:176:VAL:HG12	2.03	0.41
1:C:166:TYR:CD1	1:C:166:TYR:N	2.89	0.41
1:B:74:GLN:HE22	1:B:225:GLU:CG	2.34	0.40
1:C:341:ALA:C	1:C:342:LEU:HD12	2.42	0.40
1:D:48:LYS:HZ1	1:D:201:GLU:HA	1.87	0.40
1:D:82:TYR:HA	1:D:106:ILE:O	2.21	0.40
1:D:166:TYR:CD1	1:D:166:TYR:N	2.89	0.40
1:D:300:ILE:HD13	1:D:392:GLY:CA	2.49	0.40
1:B:75:SER:O	1:B:76:ASN:HB2	2.21	0.40
1:B:166:TYR:CD1	1:B:166:TYR:N	2.89	0.40
1:C:299:ASP:CG	1:C:301:HIS:HE2	2.23	0.40
1:B:302:TYR:CB	1:B:390:MET:HE1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLN:HB2	1:C:246:PHE:CD2	2.56	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	342/367 (93%)	323 (94%)	16 (5%)	3 (1%)	17	31
1	B	342/367 (93%)	321 (94%)	18 (5%)	3 (1%)	17	31
1	C	342/367 (93%)	321 (94%)	15 (4%)	6 (2%)	8	14
1	D	342/367 (93%)	322 (94%)	18 (5%)	2 (1%)	25	43
All	All	1368/1468 (93%)	1287 (94%)	67 (5%)	14 (1%)	15	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	LYS
1	A	336	PRO
1	B	190	SER
1	C	190	SER
1	C	336	PRO
1	B	79	THR
1	A	79	THR
1	C	79	THR
1	C	338	LEU
1	D	190	SER
1	A	142	ILE
1	B	142	ILE
1	C	142	ILE
1	D	142	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	309/328 (94%)	301 (97%)	8 (3%)	46	72
1	B	309/328 (94%)	299 (97%)	10 (3%)	39	65
1	C	309/328 (94%)	297 (96%)	12 (4%)	32	57
1	D	309/328 (94%)	300 (97%)	9 (3%)	42	69
All	All	1236/1312 (94%)	1197 (97%)	39 (3%)	39	65

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	84	LEU
1	A	117	LEU
1	A	168	GLU
1	A	188	LYS
1	A	193	THR
1	A	223	GLN
1	A	375	LEU
1	B	48	LYS
1	B	117	LEU
1	B	168	GLU
1	B	188	LYS
1	B	197	GLN
1	B	204	THR
1	B	223	GLN
1	B	335	ASP
1	B	375	LEU
1	B	397	PRO
1	C	48	LYS
1	C	79	THR
1	C	117	LEU
1	C	168	GLU
1	C	188	LYS
1	C	193	THR

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Mol	Chain	Res	Type
1	C	200	GLN
1	C	204	THR
1	C	223	GLN
1	C	327	GLN
1	C	336	PRO
1	C	375	LEU
1	D	48	LYS
1	D	117	LEU
1	D	168	GLU
1	D	188	LYS
1	D	204	THR
1	D	223	GLN
1	D	336	PRO
1	D	375	LEU
1	D	396	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	126	ASN
1	A	155	ASN
1	A	223	GLN
1	A	257	ASN
1	A	303	GLN
1	A	311	GLN
1	A	327	GLN
1	B	74	GLN
1	B	76	ASN
1	B	126	ASN
1	B	155	ASN
1	B	197	GLN
1	B	223	GLN
1	B	257	ASN
1	B	303	GLN
1	B	311	GLN
1	B	327	GLN
1	B	332	ASN
1	C	74	GLN
1	C	126	ASN
1	C	155	ASN
1	C	223	GLN

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Mol	Chain	Res	Type
1	C	303	GLN
1	C	311	GLN
1	C	327	GLN
1	D	74	GLN
1	D	76	ASN
1	D	126	ASN
1	D	155	ASN
1	D	223	GLN
1	D	257	ASN
1	D	277	GLN
1	D	303	GLN
1	D	311	GLN
1	D	327	GLN
1	D	337	HIS

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 monosaccharides 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	346/367 (94%)	0.30	21 (6%)	21	22	19, 33, 64, 108	0
1	B	346/367 (94%)	0.26	20 (5%)	23	24	19, 34, 63, 100	0
1	C	346/367 (94%)	0.34	31 (8%)	9	9	20, 35, 65, 100	0
1	D	346/367 (94%)	0.33	29 (8%)	11	11	19, 35, 64, 94	0
All	All	1384/1468 (94%)	0.31	101 (7%)	15	15	19, 34, 64, 108	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ASP	13.0
1	B	333	PRO	12.1
1	B	334	ASN	11.7
1	A	332	ASN	11.6
1	D	396	VAL	10.5
1	A	333	PRO	10.5
1	D	397	PRO	9.6
1	A	334	ASN	9.2
1	B	336	PRO	8.9
1	C	334	ASN	8.0
1	A	338	LEU	7.8
1	B	335	ASP	6.2
1	D	186	LYS	5.8
1	A	337	HIS	5.6
1	C	335	ASP	5.5
1	D	273	GLU	5.5
1	A	336	PRO	5.0
1	C	332	ASN	4.8
1	B	332	ASN	4.6
1	C	336	PRO	4.6
1	B	331	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	187	GLU	4.4
1	B	41	LYS	4.1
1	D	189	GLU	4.1
1	D	76	ASN	4.0
1	D	188	LYS	4.0
1	C	223	GLN	4.0
1	C	333	PRO	4.0
1	D	190	SER	4.0
1	C	285	PHE	3.9
1	B	79	THR	3.9
1	D	281	ASN	3.9
1	D	184	ASN	3.8
1	A	397	PRO	3.8
1	C	185	ILE	3.8
1	A	188	LYS	3.8
1	D	185	ILE	3.8
1	D	223	GLN	3.7
1	D	334	ASN	3.6
1	C	273	GLU	3.6
1	C	186	LYS	3.5
1	A	285	PHE	3.5
1	D	287	ASN	3.4
1	C	281	ASN	3.3
1	D	395	GLU	3.3
1	C	76	ASN	3.3
1	A	223	GLN	3.2
1	C	190	SER	3.2
1	D	393	TYR	3.2
1	A	331	GLN	3.2
1	B	170	ASP	3.2
1	C	277	GLN	3.2
1	C	337	HIS	3.2
1	A	330	SER	3.1
1	C	42	GLN	3.1
1	B	200	GLN	3.1
1	D	41	LYS	3.0
1	A	273	GLU	3.0
1	D	277	GLN	3.0
1	A	41	LYS	3.0
1	A	78	LYS	3.0
1	C	257	ASN	2.9
1	A	79	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	289	MET	2.9
1	D	285	PHE	2.8
1	B	229	LYS	2.8
1	B	61	GLN	2.8
1	C	283	ALA	2.8
1	C	126	ASN	2.7
1	C	396	VAL	2.7
1	C	272	PRO	2.7
1	D	392	GLY	2.7
1	B	76	ASN	2.6
1	C	338	LEU	2.6
1	A	186	LYS	2.6
1	A	200	GLN	2.6
1	B	78	LYS	2.5
1	D	123	ASP	2.5
1	C	288	GLN	2.5
1	D	62	GLN	2.4
1	D	394	LEU	2.4
1	D	304	GLU	2.4
1	B	287	ASN	2.3
1	C	48	LYS	2.3
1	C	331	GLN	2.3
1	B	337	HIS	2.3
1	D	77	ALA	2.2
1	B	153	ASN	2.2
1	D	182	ALA	2.2
1	B	223	GLN	2.2
1	D	148	GLN	2.2
1	C	78	LYS	2.2
1	A	277	GLN	2.2
1	C	233	ILE	2.1
1	C	329	VAL	2.0
1	A	229	LYS	2.0
1	C	41	LYS	2.0
1	C	188	LYS	2.0
1	B	188	LYS	2.0
1	B	282	CYS	2.0
1	C	287	ASN	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.