



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:22 AM UTC

PDB ID : 6MUA / pdb_00006mua
Title : Crystal structure of Csm1-Csm4 subcomplex in the type III-A CRISPR-Csm interference complex
Authors : Jia, N.; Patel, D.J.
Deposited on : 2018-10-22
Resolution : 2.91 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

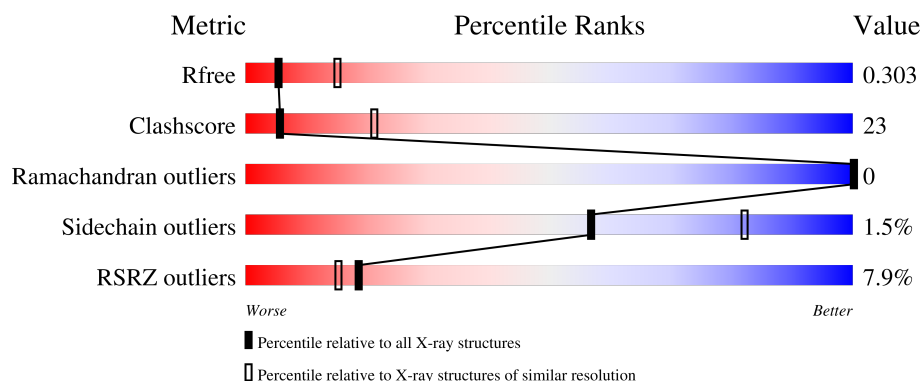
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	791	8% 58% 31% 10%
2	B	289	5% 60% 22% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7631 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 Uncharacterized protein Csm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	0	0	0
			5694	3662	979	1037	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP B6YWB8
A	-12	GLY	-	expression tag	UNP B6YWB8
A	-11	SER	-	expression tag	UNP B6YWB8
A	-10	SER	-	expression tag	UNP B6YWB8
A	-9	HIS	-	expression tag	UNP B6YWB8
A	-8	HIS	-	expression tag	UNP B6YWB8
A	-7	HIS	-	expression tag	UNP B6YWB8
A	-6	HIS	-	expression tag	UNP B6YWB8
A	-5	HIS	-	expression tag	UNP B6YWB8
A	-4	HIS	-	expression tag	UNP B6YWB8
A	-3	SER	-	expression tag	UNP B6YWB8
A	-2	GLN	-	expression tag	UNP B6YWB8
A	-1	ASP	-	expression tag	UNP B6YWB8
A	0	PRO	-	expression tag	UNP B6YWB8

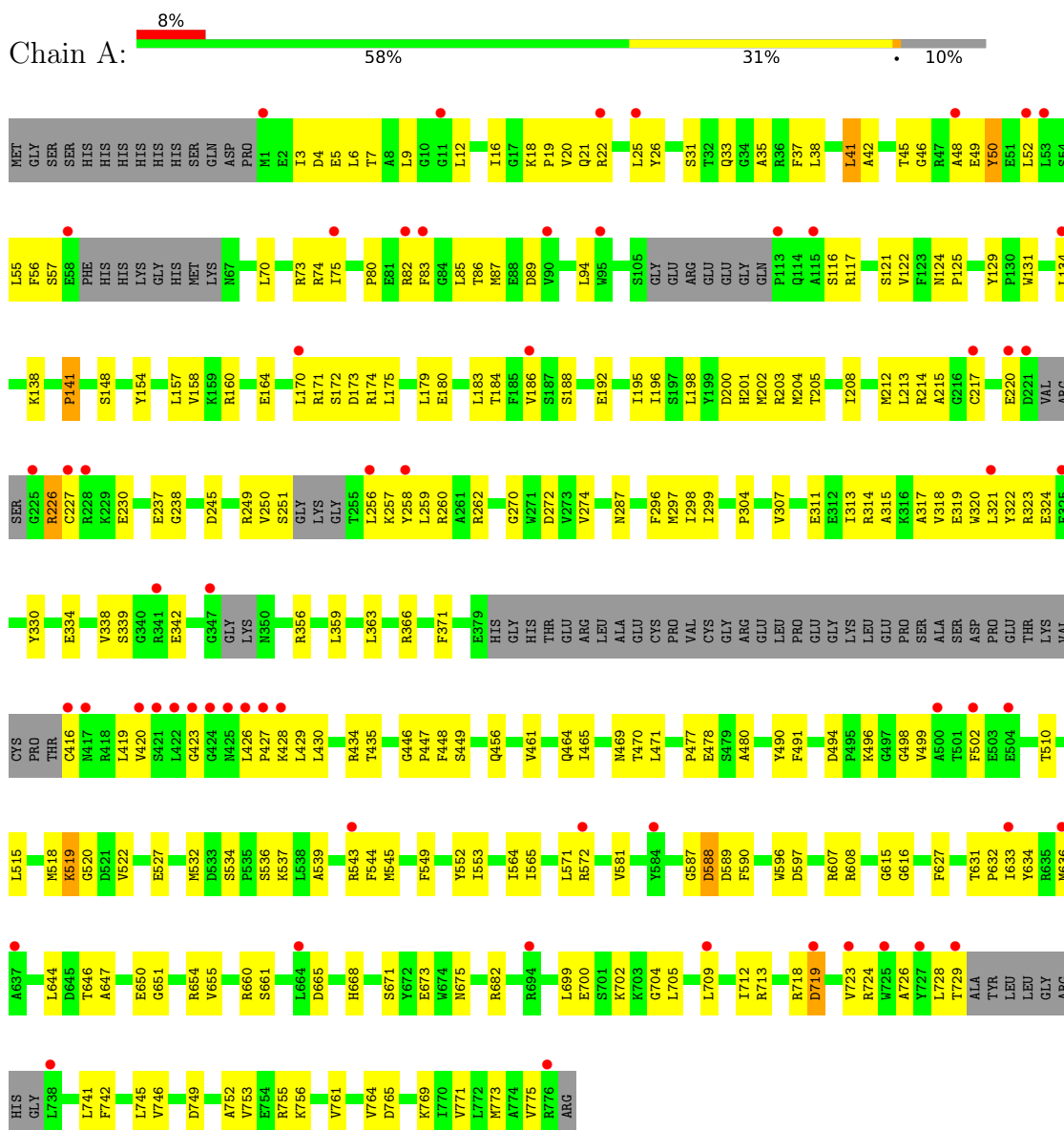
- Molecule 2 is a protein called Uncharacterized protein Csm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1937	1262	320	351	4			

3 Residue-property plots [i](#)

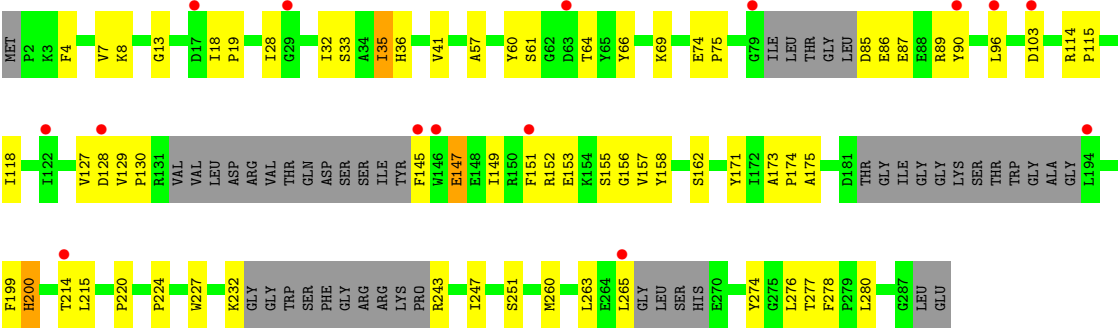
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein Csm1



• Molecule 2: Uncharacterized protein Csm4





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.43Å 156.43Å 187.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.44 – 2.91 49.44 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.44-2.91) 99.9 (49.44-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.229 , 0.278 0.264 , 0.303	Depositor DCC
R_{free} test set	1499 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.9	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	0.92	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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	0.70	1/5817 (0.0%)	1.07	13/7844 (0.2%)
2	B	0.69	0/1985	1.09	3/2682 (0.1%)
All	All	0.70	1/7802 (0.0%)	1.07	16/10526 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	LEU	C-O	-5.18	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	GLY	CA-C-N	9.21	129.15	120.03
2	B	13	GLY	C-N-CA	9.21	129.15	120.03
1	A	427	PRO	N-CA-C	8.15	124.86	113.53
1	A	719	ASP	CA-C-N	8.10	128.19	119.28
1	A	719	ASP	C-N-CA	8.10	128.19	119.28
1	A	616	GLY	N-CA-C	-7.41	103.50	114.90
1	A	141	PRO	CB-CA-C	-6.14	104.87	111.56
1	A	534	SER	CA-C-N	5.78	125.91	119.32
1	A	534	SER	C-N-CA	5.78	125.91	119.32
1	A	138	LYS	CA-C-O	-5.52	115.02	120.82
1	A	50	TYR	CA-C-N	-5.36	112.16	120.31
1	A	50	TYR	C-N-CA	-5.36	112.16	120.31
1	A	700	GLU	N-CA-C	-5.34	101.95	109.96
2	B	19	PRO	N-CA-C	5.28	119.47	111.19
1	A	46	GLY	CA-C-N	-5.04	115.85	122.85
1	A	46	GLY	C-N-CA	-5.04	115.85	122.85

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	5694	0	5698	286	0
2	B	1937	0	1935	76	0
All	All	7631	0	7633	357	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 23.

All (357) 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:217:CYS:SG	1:A:227:CYS:SG	1.40	1.35
1:A:12:LEU:HD23	1:A:175:LEU:HD23	1.06	1.05
2:B:151:PHE:HZ	2:B:157:VAL:HG23	1.23	1.03
2:B:151:PHE:CZ	2:B:157:VAL:HG23	1.97	0.99
1:A:50:TYR:CZ	1:A:170:LEU:HD21	1.99	0.98
2:B:96:LEU:HD23	2:B:118:ILE:HG13	1.46	0.97
1:A:237:GLU:HB3	1:A:363:LEU:HD11	1.45	0.97
1:A:12:LEU:CD2	1:A:175:LEU:HD23	1.94	0.97
1:A:416:CYS:O	1:A:420:VAL:HG23	1.65	0.96
2:B:18:ILE:HG13	2:B:149:ILE:CD1	1.97	0.95
1:A:515:LEU:HD23	1:A:636:MET:HE1	1.48	0.94
1:A:258:TYR:CE1	1:A:262:ARG:HD3	2.03	0.92
1:A:769:LYS:O	1:A:773:MET:HG3	1.70	0.92
1:A:80:PRO:HB2	1:A:85:LEU:O	1.70	0.92
1:A:226:ARG:HB2	1:A:226:ARG:CZ	1.98	0.90
1:A:75:ILE:HD11	1:A:94:LEU:HD11	1.54	0.89
2:B:28:ILE:O	2:B:32:ILE:HG12	1.70	0.89
1:A:477:PRO:HG2	1:A:480:ALA:HB2	1.54	0.87
1:A:510:THR:OG1	1:A:572:ARG:HD2	1.74	0.87
1:A:22:ARG:HH21	1:A:186:VAL:HG11	1.37	0.87
1:A:25:LEU:CD1	1:A:158:VAL:HG11	2.04	0.86
1:A:469:ASN:O	1:A:470:THR:HG23	1.75	0.85
1:A:4:ASP:HB2	1:A:214:ARG:NH2	1.91	0.85
2:B:18:ILE:HG13	2:B:149:ILE:HD13	1.58	0.85
1:A:217:CYS:CB	1:A:227:CYS:SG	2.65	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:HD23	2:B:118:ILE:CG1	2.08	0.84
2:B:215:LEU:HD11	2:B:280:LEU:HD11	1.60	0.84
1:A:745:LEU:HD22	1:A:761:VAL:HA	1.59	0.84
1:A:26:TYR:HB2	1:A:33:GLN:HG3	1.58	0.84
1:A:12:LEU:HD23	1:A:175:LEU:CD2	2.01	0.84
1:A:179:LEU:HD22	1:A:202:MET:HE1	1.58	0.84
1:A:21:GLN:HA	1:A:33:GLN:OE1	1.77	0.83
1:A:502:PHE:HD1	1:A:515:LEU:CD2	1.92	0.83
1:A:250:VAL:HB	1:A:633:ILE:HD11	1.60	0.82
1:A:502:PHE:HD1	1:A:515:LEU:HD21	1.42	0.81
1:A:226:ARG:O	1:A:230:GLU:HB3	1.80	0.81
1:A:745:LEU:HD11	1:A:764:VAL:HG21	1.62	0.81
2:B:220:PRO:HG3	2:B:247:ILE:HD11	1.63	0.81
1:A:70:LEU:HD23	1:A:74:ARG:NH1	1.95	0.81
1:A:510:THR:HG1	1:A:572:ARG:HD2	1.46	0.81
1:A:75:ILE:HD11	1:A:94:LEU:CD1	2.12	0.80
1:A:18:LYS:HB3	1:A:22:ARG:HH12	1.47	0.79
1:A:22:ARG:NH2	1:A:186:VAL:HG11	1.98	0.79
1:A:70:LEU:HD12	1:A:73:ARG:NH2	1.97	0.79
1:A:338:VAL:HG13	1:A:342:GLU:OE1	1.83	0.79
1:A:665:ASP:OD1	1:A:668:HIS:HD2	1.65	0.78
2:B:96:LEU:CD2	2:B:118:ILE:CG1	2.61	0.78
1:A:70:LEU:CD1	1:A:73:ARG:NH2	2.48	0.77
2:B:151:PHE:HZ	2:B:157:VAL:CG2	1.98	0.76
1:A:122:VAL:HA	1:A:195:ILE:HG23	1.67	0.75
1:A:226:ARG:O	1:A:230:GLU:CB	2.34	0.75
2:B:224:PRO:HG2	2:B:227:TRP:CE3	2.21	0.75
1:A:502:PHE:CD1	1:A:515:LEU:HD21	2.21	0.74
1:A:469:ASN:O	1:A:470:THR:CG2	2.36	0.74
1:A:477:PRO:HG2	1:A:480:ALA:CB	2.18	0.73
1:A:571:LEU:CD1	1:A:596:TRP:CH2	2.72	0.72
1:A:419:LEU:HD12	1:A:419:LEU:H	1.53	0.72
2:B:35:ILE:HG22	2:B:36:HIS:CD2	2.24	0.72
1:A:25:LEU:HD11	1:A:158:VAL:HG11	1.71	0.72
1:A:334:GLU:HB2	1:A:363:LEU:HD23	1.71	0.72
1:A:82:ARG:HH21	1:A:83:PHE:HE2	1.34	0.71
1:A:334:GLU:HB2	1:A:363:LEU:CD2	2.20	0.71
1:A:70:LEU:HD12	1:A:73:ARG:HH21	1.55	0.71
1:A:709:LEU:HA	1:A:712:ILE:HD12	1.73	0.71
1:A:122:VAL:HA	1:A:195:ILE:CG2	2.21	0.71
1:A:171:ARG:NH2	1:A:478:GLU:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:PHE:HA	1:A:553:ILE:CD1	2.21	0.70
1:A:82:ARG:NH2	1:A:83:PHE:CZ	2.60	0.70
1:A:315:ALA:O	1:A:319:GLU:HG3	1.90	0.70
1:A:549:PHE:CD1	1:A:553:ILE:HD11	2.27	0.70
1:A:571:LEU:HD11	1:A:596:TRP:CH2	2.27	0.70
1:A:564:ILE:N	1:A:564:ILE:HD12	2.06	0.69
1:A:204:MET:HE1	1:A:299:ILE:HD12	1.74	0.69
1:A:491:PHE:HB2	1:A:499:VAL:HG23	1.73	0.69
1:A:319:GLU:O	1:A:323:ARG:HG3	1.93	0.69
2:B:96:LEU:CD2	2:B:118:ILE:HG12	2.22	0.69
2:B:57:ALA:HB1	2:B:157:VAL:CG1	2.22	0.69
1:A:70:LEU:CD1	1:A:73:ARG:HH21	2.06	0.68
1:A:771:VAL:O	1:A:775:VAL:HG23	1.93	0.68
2:B:18:ILE:CG1	2:B:149:ILE:HD13	2.24	0.68
1:A:41:LEU:HD12	1:A:41:LEU:O	1.93	0.68
2:B:85:ASP:O	2:B:89:ARG:HG3	1.95	0.67
1:A:70:LEU:CG	1:A:73:ARG:HH21	2.08	0.66
1:A:527:GLU:OE1	2:B:87:GLU:HG2	1.95	0.66
1:A:45:THR:HG22	1:A:45:THR:O	1.94	0.66
1:A:416:CYS:HA	1:A:419:LEU:HD13	1.77	0.66
1:A:502:PHE:CD1	1:A:515:LEU:CD2	2.76	0.66
1:A:522:VAL:HG21	1:A:545:MET:CE	2.24	0.66
2:B:33:SER:OG	2:B:41:VAL:HG21	1.95	0.66
1:A:571:LEU:HD12	1:A:597:ASP:CB	2.26	0.66
1:A:749:ASP:O	1:A:753:VAL:CG2	2.44	0.66
2:B:263:LEU:HD13	2:B:265:LEU:HG	1.76	0.65
1:A:430:LEU:HD11	1:A:456:GLN:HA	1.78	0.65
1:A:212:MET:O	1:A:215:ALA:HB3	1.98	0.64
1:A:116:SER:HB2	1:A:148:SER:HB2	1.80	0.64
1:A:435:THR:HG21	1:A:461:VAL:HG12	1.79	0.64
1:A:702:LYS:HB3	1:A:705:LEU:HD12	1.78	0.64
1:A:196:ILE:HD11	1:A:537:LYS:HG3	1.79	0.64
1:A:70:LEU:HG	1:A:73:ARG:NH2	2.13	0.64
2:B:127:VAL:O	2:B:147:GLU:HB2	1.97	0.63
2:B:171:TYR:O	2:B:174:PRO:HD2	1.98	0.63
1:A:201:HIS:O	1:A:205:THR:HG23	1.98	0.63
1:A:22:ARG:NH2	1:A:186:VAL:CG1	2.61	0.63
2:B:32:ILE:HD11	2:B:175:ALA:HB2	1.80	0.63
1:A:122:VAL:CA	1:A:195:ILE:HG23	2.29	0.63
1:A:543:ARG:NH1	1:A:544:PHE:HE1	1.96	0.63
1:A:204:MET:CE	1:A:299:ILE:HD12	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TYR:HE1	1:A:262:ARG:HD3	1.60	0.63
1:A:632:PRO:CD	2:B:145:PHE:HE2	2.11	0.63
1:A:171:ARG:HB3	1:A:173:ASP:OD1	1.99	0.62
1:A:627:PHE:HB2	1:A:636:MET:HE2	1.80	0.62
1:A:654:ARG:NH2	1:A:673:GLU:HG3	2.13	0.62
1:A:134:LEU:HB2	1:A:184:THR:HG21	1.80	0.62
1:A:200:ASP:HA	1:A:203:ARG:HD3	1.81	0.62
2:B:69:LYS:HE2	2:B:96:LEU:O	2.00	0.62
1:A:52:LEU:HD22	1:A:83:PHE:CD2	2.35	0.62
1:A:188:SER:HB3	1:A:198:LEU:HA	1.81	0.62
2:B:215:LEU:HD11	2:B:280:LEU:CD1	2.28	0.61
2:B:247:ILE:CG2	2:B:251:SER:OG	2.47	0.61
1:A:515:LEU:HD23	1:A:636:MET:CE	2.27	0.61
1:A:317:ALA:O	1:A:321:LEU:HG	2.01	0.61
1:A:565:ILE:O	1:A:608:ARG:HD2	2.00	0.61
1:A:549:PHE:HD1	1:A:553:ILE:HD11	1.64	0.61
1:A:718:ARG:O	1:A:719:ASP:OD1	2.19	0.61
2:B:220:PRO:HG3	2:B:247:ILE:CD1	2.31	0.61
1:A:18:LYS:HB3	1:A:22:ARG:NH1	2.16	0.60
1:A:477:PRO:CG	1:A:480:ALA:HB2	2.27	0.60
1:A:723:VAL:HG12	1:A:723:VAL:O	2.01	0.60
1:A:749:ASP:OD2	1:A:752:ALA:HB2	2.01	0.60
1:A:519:LYS:HD3	1:A:644:LEU:HD23	1.82	0.60
2:B:220:PRO:CG	2:B:247:ILE:HD11	2.31	0.60
1:A:627:PHE:CD2	1:A:636:MET:HG2	2.37	0.59
1:A:21:GLN:HA	1:A:33:GLN:CD	2.26	0.59
1:A:257:LYS:HG2	1:A:499:VAL:HG12	1.84	0.59
1:A:141:PRO:HD3	1:A:552:TYR:CZ	2.37	0.59
1:A:320:TRP:CZ3	1:A:447:PRO:HD3	2.38	0.59
1:A:426:LEU:O	1:A:429:LEU:HD22	2.03	0.59
1:A:608:ARG:NH2	1:A:682:ARG:HH21	2.01	0.59
1:A:518:MET:HE3	1:A:590:PHE:CE1	2.37	0.58
1:A:257:LYS:HG2	1:A:499:VAL:CG1	2.33	0.58
1:A:654:ARG:HE	1:A:671:SER:HB2	1.69	0.58
1:A:20:VAL:HG23	1:A:33:GLN:HG2	1.84	0.58
1:A:322:TYR:HB2	1:A:371:PHE:CE1	2.38	0.58
1:A:70:LEU:CG	1:A:73:ARG:NH2	2.67	0.58
1:A:184:THR:OG1	1:A:543:ARG:NH2	2.35	0.58
2:B:64:THR:HG23	2:B:103:ASP:OD2	2.03	0.58
1:A:270:GLY:O	1:A:274:VAL:HG23	2.04	0.58
2:B:32:ILE:CD1	2:B:175:ALA:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LYS:HD3	1:A:644:LEU:CD2	2.34	0.57
2:B:263:LEU:CD1	2:B:265:LEU:HG	2.34	0.57
1:A:359:LEU:O	1:A:363:LEU:HG	2.04	0.57
2:B:220:PRO:HB3	2:B:247:ILE:CD1	2.34	0.57
1:A:314:ARG:O	1:A:318:VAL:HG23	2.03	0.57
1:A:6:LEU:HD22	1:A:85:LEU:HD13	1.86	0.57
1:A:171:ARG:O	1:A:172:SER:C	2.48	0.57
1:A:272:ASP:OD1	1:A:434:ARG:NH1	2.37	0.57
1:A:125:PRO:HG3	1:A:195:ILE:CD1	2.35	0.56
1:A:200:ASP:O	1:A:203:ARG:HG2	2.05	0.56
1:A:237:GLU:HB3	1:A:363:LEU:CD1	2.30	0.56
1:A:416:CYS:CA	1:A:419:LEU:HD13	2.35	0.56
2:B:215:LEU:HD12	2:B:278:PHE:CD1	2.40	0.56
1:A:745:LEU:HD22	1:A:761:VAL:CA	2.33	0.56
1:A:70:LEU:HG	1:A:73:ARG:HH21	1.71	0.56
1:A:220:GLU:OE1	1:A:226:ARG:NH2	2.39	0.55
1:A:226:ARG:HG3	1:A:230:GLU:OE1	2.06	0.55
2:B:152:ARG:HG2	2:B:153:GLU:H	1.70	0.55
1:A:82:ARG:NH2	1:A:83:PHE:CE2	2.61	0.55
1:A:571:LEU:HD12	1:A:597:ASP:HB3	1.88	0.55
1:A:565:ILE:O	1:A:608:ARG:CD	2.55	0.55
1:A:646:THR:O	1:A:650:GLU:HG3	2.06	0.55
2:B:130:PRO:HA	2:B:145:PHE:HB2	1.89	0.55
1:A:125:PRO:HG3	1:A:195:ILE:HD11	1.88	0.55
1:A:226:ARG:O	1:A:230:GLU:HB2	2.07	0.55
1:A:179:LEU:HD13	1:A:202:MET:HE3	1.89	0.54
1:A:212:MET:HE2	1:A:227:CYS:HB3	1.89	0.54
1:A:338:VAL:HG12	1:A:339:SER:N	2.21	0.54
1:A:564:ILE:HD12	1:A:564:ILE:H	1.70	0.54
1:A:741:LEU:HG	1:A:742:PHE:CD2	2.42	0.54
1:A:45:THR:O	1:A:45:THR:CG2	2.56	0.54
1:A:502:PHE:HD1	1:A:515:LEU:HD22	1.72	0.54
2:B:74:GLU:HB2	2:B:75:PRO:HD3	1.90	0.54
2:B:220:PRO:CG	2:B:247:ILE:CD1	2.85	0.54
1:A:571:LEU:HD11	1:A:596:TRP:CZ3	2.43	0.53
1:A:749:ASP:O	1:A:753:VAL:HG23	2.08	0.53
1:A:131:TRP:CH2	1:A:157:LEU:HD13	2.44	0.53
1:A:608:ARG:HH22	1:A:682:ARG:NH2	2.05	0.53
1:A:50:TYR:CE2	1:A:170:LEU:HD21	2.43	0.53
1:A:313:ILE:HG23	1:A:448:PHE:CZ	2.44	0.53
1:A:543:ARG:NH1	1:A:544:PHE:CE1	2.75	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CZ	1:A:170:LEU:CD2	2.84	0.53
1:A:180:GLU:OE1	1:A:471:LEU:HD11	2.09	0.53
1:A:564:ILE:N	1:A:564:ILE:CD1	2.72	0.53
1:A:704:GLY:O	1:A:705:LEU:C	2.52	0.53
2:B:60:TYR:CE2	2:B:156:GLY:HA3	2.44	0.52
1:A:632:PRO:CG	2:B:145:PHE:HE2	2.21	0.52
1:A:7:THR:OG1	1:A:213:LEU:HD22	2.09	0.52
1:A:212:MET:HE2	1:A:227:CYS:CB	2.40	0.52
1:A:322:TYR:HD2	1:A:371:PHE:CD1	2.27	0.52
1:A:469:ASN:C	1:A:470:THR:HG23	2.34	0.52
1:A:660:ARG:HD2	1:A:765:ASP:OD2	2.09	0.52
1:A:665:ASP:OD1	1:A:668:HIS:CD2	2.55	0.52
1:A:712:ILE:HG12	1:A:728:LEU:CD1	2.40	0.52
1:A:117:ARG:HH22	1:A:192:GLU:N	2.07	0.52
1:A:258:TYR:CE1	1:A:262:ARG:CD	2.87	0.52
2:B:220:PRO:HB3	2:B:247:ILE:HD12	1.92	0.52
1:A:245:ASP:HA	1:A:249:ARG:HD2	1.90	0.51
1:A:87:MET:SD	1:A:87:MET:C	2.94	0.51
1:A:522:VAL:HG21	1:A:545:MET:HE2	1.93	0.51
1:A:338:VAL:CG1	1:A:342:GLU:HB2	2.41	0.51
1:A:545:MET:HE3	1:A:549:PHE:HE2	1.76	0.51
1:A:608:ARG:NH2	1:A:682:ARG:NH2	2.59	0.50
2:B:152:ARG:HG2	2:B:153:GLU:N	2.25	0.50
1:A:755:ARG:O	1:A:756:LYS:HB2	2.11	0.50
1:A:272:ASP:CG	1:A:449:SER:OG	2.55	0.50
1:A:632:PRO:HG2	2:B:145:PHE:CE2	2.46	0.50
1:A:572:ARG:HD2	1:A:597:ASP:OD2	2.11	0.50
1:A:35:ALA:HB2	1:A:57:SER:OG	2.12	0.50
1:A:171:ARG:O	1:A:173:ASP:N	2.44	0.50
2:B:129:VAL:HG13	2:B:130:PRO:HD2	1.92	0.50
1:A:745:LEU:CD2	1:A:761:VAL:HA	2.37	0.50
1:A:549:PHE:HA	1:A:553:ILE:HD12	1.90	0.49
2:B:60:TYR:CZ	2:B:156:GLY:HA3	2.47	0.49
1:A:571:LEU:HD12	1:A:597:ASP:HB2	1.93	0.49
1:A:56:PHE:CE1	1:A:94:LEU:HD23	2.47	0.49
2:B:128:ASP:HA	2:B:147:GLU:CB	2.42	0.49
2:B:64:THR:HG22	2:B:66:TYR:CE1	2.48	0.49
2:B:247:ILE:HG22	2:B:251:SER:OG	2.12	0.49
1:A:256:LEU:HD21	1:A:581:VAL:HG11	1.95	0.49
1:A:307:VAL:O	1:A:311:GLU:HG3	2.13	0.49
1:A:198:LEU:O	1:A:202:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.78	0.48
1:A:16:ILE:O	1:A:19:PRO:HD2	2.13	0.48
1:A:134:LEU:HD23	1:A:134:LEU:C	2.38	0.48
1:A:589:ASP:OD1	1:A:590:PHE:N	2.47	0.48
1:A:4:ASP:CB	1:A:214:ARG:NH2	2.71	0.48
1:A:121:SER:HA	1:A:129:TYR:CE2	2.48	0.48
1:A:48:ALA:HB1	1:A:82:ARG:NH2	2.29	0.48
1:A:322:TYR:CD2	1:A:371:PHE:CD1	3.02	0.48
2:B:64:THR:HG23	2:B:103:ASP:CG	2.39	0.48
2:B:173:ALA:HB3	2:B:174:PRO:HD3	1.95	0.48
1:A:25:LEU:HD12	1:A:158:VAL:HG11	1.92	0.48
1:A:320:TRP:CH2	1:A:446:GLY:HA2	2.49	0.48
1:A:429:LEU:HD23	1:A:429:LEU:O	2.14	0.48
1:A:564:ILE:H	1:A:564:ILE:CD1	2.26	0.47
1:A:70:LEU:HA	1:A:73:ARG:HE	1.79	0.47
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.78	0.47
1:A:435:THR:CG2	1:A:461:VAL:HG12	2.43	0.47
1:A:26:TYR:HE2	1:A:37:PHE:HA	1.79	0.47
1:A:338:VAL:CG1	1:A:339:SER:N	2.77	0.47
1:A:174:ARG:NH2	1:A:480:ALA:O	2.44	0.47
1:A:250:VAL:O	1:A:251:SER:C	2.57	0.47
2:B:171:TYR:C	2:B:174:PRO:HD2	2.39	0.47
2:B:263:LEU:HD13	2:B:265:LEU:CG	2.45	0.46
1:A:20:VAL:CG2	1:A:33:GLN:HG2	2.45	0.46
2:B:57:ALA:HB1	2:B:157:VAL:HG12	1.95	0.46
2:B:60:TYR:CE2	2:B:156:GLY:C	2.94	0.46
1:A:49:GLU:O	1:A:52:LEU:HB3	2.15	0.46
2:B:57:ALA:HA	2:B:158:TYR:O	2.15	0.46
1:A:21:GLN:CA	1:A:33:GLN:OE1	2.57	0.46
1:A:82:ARG:CZ	1:A:83:PHE:CZ	2.98	0.46
1:A:274:VAL:HG13	1:A:298:ILE:HD11	1.96	0.46
1:A:338:VAL:HG13	1:A:342:GLU:HB2	1.96	0.46
1:A:769:LYS:O	1:A:773:MET:CG	2.55	0.46
1:A:520:GLY:HA3	1:A:590:PHE:CZ	2.51	0.46
1:A:70:LEU:HD23	1:A:74:ARG:CZ	2.46	0.46
1:A:50:TYR:CE1	1:A:170:LEU:HD21	2.50	0.46
1:A:25:LEU:HD11	1:A:158:VAL:CG1	2.45	0.45
1:A:183:LEU:HD12	1:A:202:MET:HE1	1.98	0.45
1:A:571:LEU:HD13	1:A:596:TRP:CH2	2.51	0.45
2:B:152:ARG:CG	2:B:153:GLU:H	2.30	0.45
1:A:5:GLU:O	1:A:9:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:SER:CB	1:A:148:SER:HB2	2.46	0.45
1:A:587:GLY:O	1:A:588:ASP:OD1	2.34	0.45
1:A:70:LEU:HA	1:A:73:ARG:HH21	1.81	0.45
2:B:260:MET:HE3	2:B:274:TYR:HA	1.99	0.45
1:A:4:ASP:HA	1:A:213:LEU:CD2	2.46	0.45
1:A:647:ALA:O	1:A:651:GLY:O	2.34	0.45
1:A:238:GLY:HA3	1:A:296:PHE:CZ	2.52	0.45
2:B:33:SER:OG	2:B:41:VAL:CG2	2.63	0.45
2:B:4:PHE:CD1	2:B:162:SER:HB3	2.52	0.45
1:A:502:PHE:CD1	1:A:515:LEU:HD22	2.49	0.44
1:A:4:ASP:HB2	1:A:214:ARG:HH22	1.76	0.44
1:A:55:LEU:HD13	1:A:75:ILE:HG12	1.98	0.44
2:B:86:GLU:O	2:B:90:TYR:CD2	2.70	0.44
1:A:297:MET:HE1	1:A:356:ARG:NH1	2.33	0.44
1:A:82:ARG:NE	1:A:83:PHE:CZ	2.85	0.44
1:A:712:ILE:HG12	1:A:728:LEU:CD2	2.48	0.44
1:A:430:LEU:CD1	1:A:456:GLN:HA	2.47	0.44
1:A:607:ARG:HH12	1:A:675:ASN:HD21	1.64	0.44
1:A:632:PRO:CG	2:B:145:PHE:CE2	3.01	0.44
2:B:114:ARG:HB3	2:B:115:PRO:HD2	1.99	0.44
2:B:7:VAL:HA	2:B:199:PHE:HB3	2.00	0.44
2:B:35:ILE:HG22	2:B:36:HIS:CG	2.53	0.44
1:A:196:ILE:HD13	1:A:536:SER:OG	2.18	0.44
2:B:263:LEU:HD11	2:B:265:LEU:HD12	2.00	0.44
1:A:258:TYR:CZ	1:A:262:ARG:HD3	2.52	0.44
2:B:263:LEU:CD1	2:B:265:LEU:CD1	2.96	0.44
1:A:48:ALA:HB1	1:A:82:ARG:CZ	2.47	0.43
2:B:232:LYS:C	2:B:243:ARG:HA	2.43	0.43
1:A:70:LEU:CD1	1:A:73:ARG:HH22	2.30	0.43
1:A:330:TYR:OH	1:A:366:ARG:HD2	2.18	0.43
1:A:745:LEU:HD21	1:A:764:VAL:CG2	2.48	0.43
1:A:22:ARG:HH21	1:A:186:VAL:CG1	2.15	0.43
1:A:322:TYR:HD2	1:A:371:PHE:CE1	2.37	0.43
1:A:572:ARG:CD	1:A:597:ASP:OD2	2.66	0.43
1:A:607:ARG:HH12	1:A:675:ASN:ND2	2.16	0.43
1:A:729:THR:HG21	1:A:746:VAL:HA	2.00	0.43
1:A:122:VAL:HG23	1:A:195:ILE:CG2	2.49	0.43
1:A:661:SER:OG	1:A:713:ARG:NH2	2.52	0.43
1:A:631:THR:HB	1:A:636:MET:HE3	2.01	0.43
1:A:297:MET:HE1	1:A:356:ARG:HH11	1.83	0.43
1:A:633:ILE:HG13	1:A:634:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:CD1	1:A:728:LEU:HD21	2.49	0.42
1:A:22:ARG:HB3	1:A:154:TYR:CD2	2.55	0.42
1:A:31:SER:O	1:A:57:SER:HB2	2.19	0.42
1:A:334:GLU:HB2	1:A:363:LEU:HD21	2.00	0.42
1:A:416:CYS:N	1:A:419:LEU:CD1	2.82	0.42
1:A:203:ARG:NH1	1:A:539:ALA:HB1	2.34	0.42
2:B:60:TYR:CE2	2:B:156:GLY:CA	3.02	0.42
2:B:152:ARG:O	2:B:155:SER:HB2	2.20	0.42
1:A:38:LEU:O	1:A:42:ALA:N	2.48	0.42
1:A:160:ARG:O	1:A:164:GLU:HG2	2.19	0.42
1:A:171:ARG:NH1	1:A:173:ASP:OD1	2.52	0.42
1:A:532:MET:HE3	1:A:537:LYS:HB3	2.00	0.42
1:A:338:VAL:HG12	1:A:339:SER:O	2.20	0.42
1:A:728:LEU:C	1:A:728:LEU:HD23	2.45	0.42
1:A:3:ILE:HG13	1:A:4:ASP:N	2.34	0.41
1:A:124:ASN:CB	1:A:615:GLY:HA3	2.50	0.41
1:A:226:ARG:HB2	1:A:226:ARG:NH1	2.31	0.41
2:B:214:THR:HG22	2:B:277:THR:HB	2.01	0.41
1:A:262:ARG:HD2	1:A:419:LEU:CD2	2.50	0.41
1:A:320:TRP:CD2	1:A:447:PRO:HA	2.56	0.41
1:A:259:LEU:HD12	1:A:633:ILE:HD12	2.01	0.41
1:A:549:PHE:HA	1:A:553:ILE:HD11	2.02	0.41
1:A:655:VAL:O	1:A:655:VAL:HG13	2.20	0.41
2:B:69:LYS:CE	2:B:96:LEU:O	2.68	0.41
2:B:220:PRO:CB	2:B:247:ILE:CD1	2.98	0.41
2:B:274:TYR:CZ	2:B:276:LEU:HB2	2.55	0.41
1:A:121:SER:HA	1:A:129:TYR:HE2	1.86	0.41
1:A:496:LYS:C	1:A:498:GLY:H	2.29	0.41
1:A:86:THR:HB	1:A:89:ASP:CG	2.46	0.41
1:A:464:GLN:O	1:A:465:ILE:HD13	2.21	0.41
2:B:8:LYS:HD3	2:B:200:HIS:CE1	2.55	0.41
1:A:208:ILE:O	1:A:212:MET:HG3	2.22	0.40
1:A:724:ARG:O	1:A:726:ALA:N	2.54	0.40
2:B:96:LEU:HD22	2:B:118:ILE:HD11	2.03	0.40
1:A:125:PRO:HG3	1:A:195:ILE:HD13	2.04	0.40
1:A:141:PRO:CD	1:A:552:TYR:CZ	3.04	0.40
1:A:260:ARG:NH2	1:A:490:TYR:O	2.54	0.40
1:A:423:GLY:O	1:A:426:LEU:HB3	2.21	0.40
1:A:122:VAL:HA	1:A:195:ILE:HG21	2.01	0.40
1:A:131:TRP:CZ2	1:A:157:LEU:HD13	2.55	0.40
1:A:287:ASN:O	1:A:298:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HA	1:A:702:LYS:HB2	2.02	0.40
1:A:712:ILE:HG12	1:A:728:LEU:HD11	2.03	0.40
2:B:64:THR:CG2	2:B:66:TYR:CE1	3.03	0.40
1:A:124:ASN:HB2	1:A:615:GLY:HA3	2.04	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	693/791 (88%)	668 (96%)	25 (4%)	0	100	100
2	B	230/289 (80%)	221 (96%)	9 (4%)	0	100	100
All	All	923/1080 (86%)	889 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	519/665 (78%)	512 (99%)	7 (1%)	61	84
2	B	204/240 (85%)	200 (98%)	4 (2%)	48	77
All	All	723/905 (80%)	712 (98%)	11 (2%)	57	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ARG
1	A	304	PRO
1	A	324	GLU
1	A	428	LYS
1	A	494	ASP
1	A	519	LYS
1	A	588	ASP
2	B	35	ILE
2	B	61	SER
2	B	147	GLU
2	B	200	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	287	ASN
1	A	668	HIS
1	A	675	ASN
2	B	106	ASN
2	B	200	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	709/791 (89%)	0.57	60 (8%)	16 14	30, 90, 139, 191	0
2	B	242/289 (83%)	0.39	15 (6%)	26 21	56, 82, 133, 148	0
All	All	951/1080 (88%)	0.52	75 (7%)	18 15	30, 88, 135, 191	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	CYS	5.7
1	A	426	LEU	4.8
1	A	425	ASN	4.6
2	B	63	ASP	4.3
2	B	103	ASP	4.0
1	A	424	GLY	4.0
1	A	727	TYR	4.0
1	A	227	CYS	3.8
2	B	151	PHE	3.8
2	B	214	THR	3.8
1	A	321	LEU	3.7
1	A	347	GLY	3.7
1	A	417	ASN	3.7
1	A	11	GLY	3.6
2	B	146	TRP	3.6
1	A	729	THR	3.5
2	B	96	LEU	3.4
1	A	113	PRO	3.3
1	A	738	LEU	3.3
2	B	17	ASP	3.2
2	B	90	TYR	3.1
1	A	22	ARG	3.1
1	A	502	PHE	3.0
1	A	416	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	637	ALA	2.9
2	B	128	ASP	2.9
2	B	79	GLY	2.8
1	A	428	LYS	2.8
1	A	170	LEU	2.8
2	B	194	LEU	2.8
1	A	75	ILE	2.8
1	A	1	MET	2.8
1	A	500	ALA	2.8
1	A	633	ILE	2.8
1	A	543	ARG	2.7
1	A	258	TYR	2.7
1	A	221	ASP	2.7
1	A	225	GLY	2.7
1	A	90	VAL	2.7
1	A	341	ARG	2.6
1	A	256	LEU	2.6
1	A	325	PHE	2.6
1	A	25	LEU	2.6
1	A	422	LEU	2.6
1	A	228	ARG	2.5
2	B	145	PHE	2.5
1	A	220	GLU	2.5
1	A	52	LEU	2.4
1	A	421	SER	2.4
1	A	82	ARG	2.4
1	A	186	VAL	2.4
1	A	83	PHE	2.4
1	A	723	VAL	2.4
1	A	694	ARG	2.4
1	A	53	LEU	2.4
1	A	95	TRP	2.3
1	A	427	PRO	2.3
1	A	423	GLY	2.3
1	A	58	GLU	2.2
1	A	776	ARG	2.2
1	A	48	ALA	2.2
2	B	265	LEU	2.2
1	A	420	VAL	2.2
1	A	584	TYR	2.2
1	A	636	MET	2.2
2	B	122	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	725	TRP	2.2
1	A	664	LEU	2.2
1	A	709	LEU	2.1
1	A	115	ALA	2.1
1	A	504	GLU	2.1
1	A	719	ASP	2.1
1	A	134	LEU	2.1
1	A	572	ARG	2.0
2	B	29	GLY	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 oligosaccharides 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.