



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:25 PM GMT

PDB ID : 5A9J
Title : Crystal structure of the Helicase domain of human DNA polymerase theta, apo-form
Authors : Newman, J.A.; Cooper, C.D.O.; Aitkenhead, H.; Pinkas, D.M.; Kupinska, K.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2015-07-21
Resolution : 3.55 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

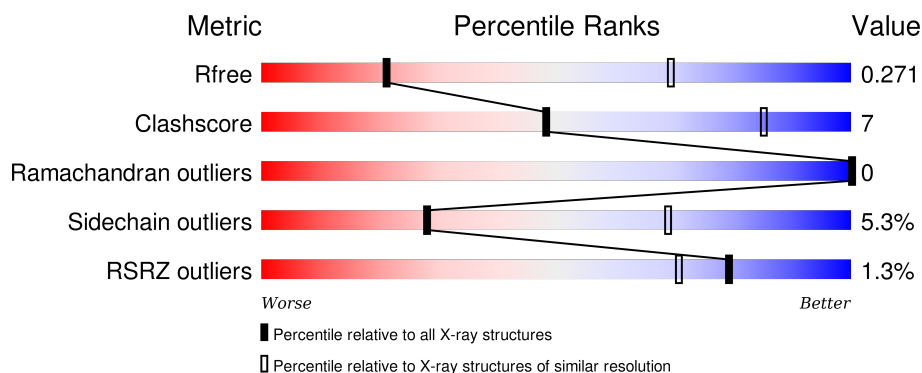
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.55 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	896	 71% 16% • 10%
1	B	896	 75% 13% • 11%
1	C	896	 72% 14% • 13%
1	D	896	 70% 15% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24408 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 DNA POLYMERASE THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	0	0
			6215	3974	1067	1134	40			
1	B	801	Total	C	N	O	S	0	0	0
			6168	3944	1058	1126	40			
1	C	780	Total	C	N	O	S	0	0	0
			6048	3870	1039	1102	37			
1	D	772	Total	C	N	O	S	0	0	0
			5977	3827	1025	1089	36			

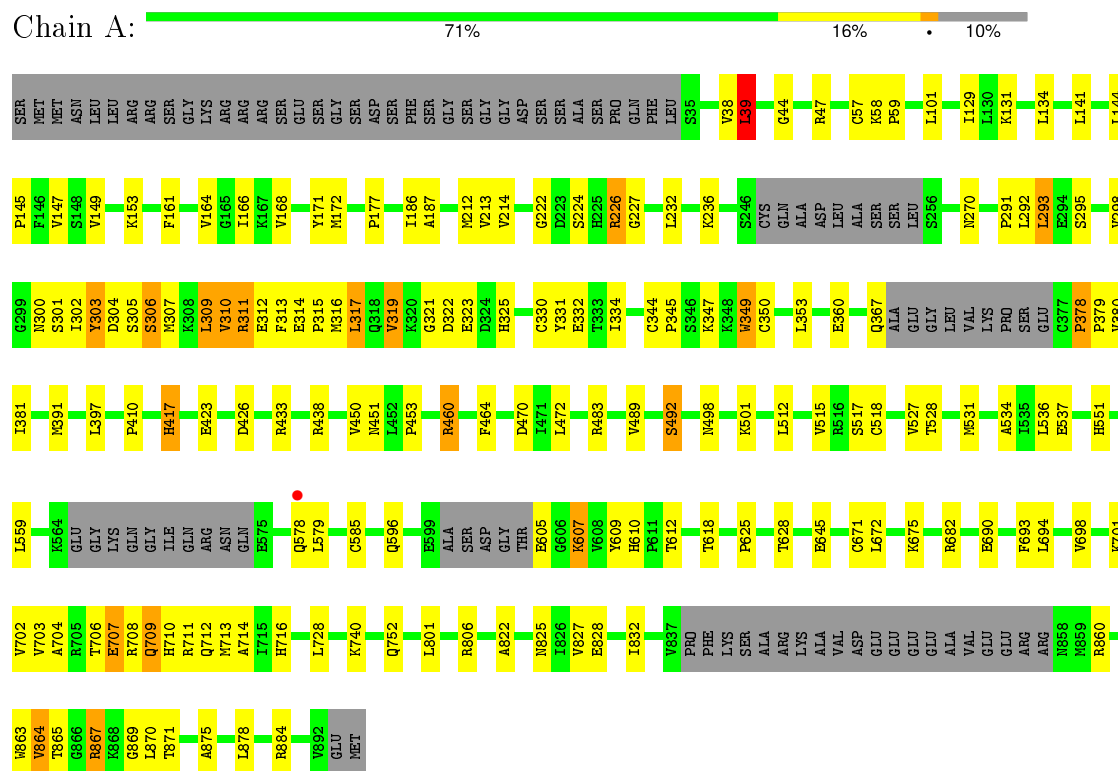
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP O75417
A	0	MET	-	EXPRESSION TAG	UNP O75417
B	-1	SER	-	EXPRESSION TAG	UNP O75417
B	0	MET	-	EXPRESSION TAG	UNP O75417
C	-1	SER	-	EXPRESSION TAG	UNP O75417
C	0	MET	-	EXPRESSION TAG	UNP O75417
D	-1	SER	-	EXPRESSION TAG	UNP O75417
D	0	MET	-	EXPRESSION TAG	UNP O75417

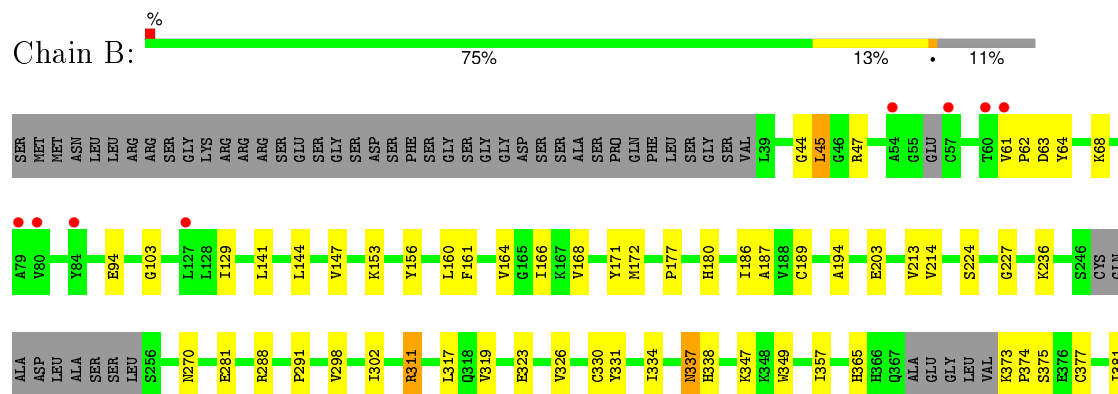
3 Residue-property plots

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

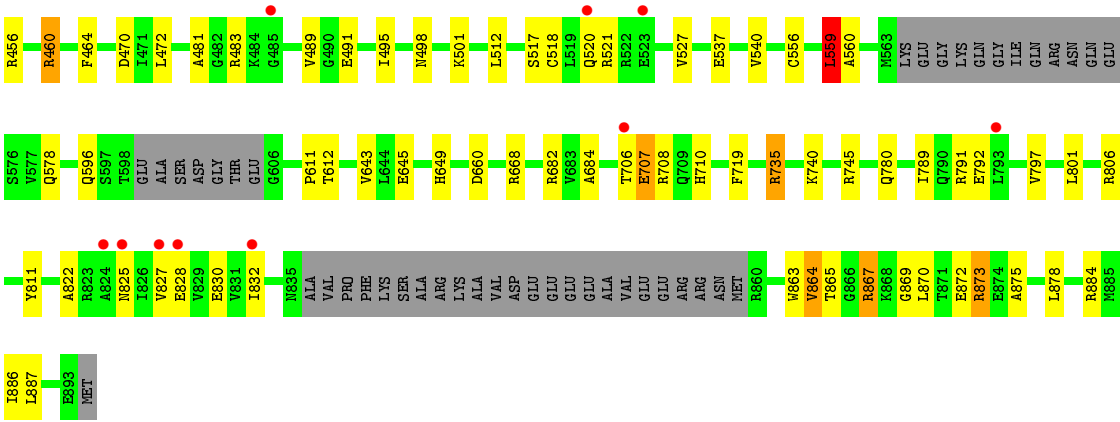
• Molecule 1: DNA POLYMERASE THETA



• Molecule 1: DNA POLYMERASE THETA







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.02Å 130.53Å 160.91Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	48.86 – 3.55 48.86 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.86-3.55) 99.1 (48.86-3.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.265 0.234 , 0.271	Depositor DCC
R_{free} test set	3060 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	130.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 71.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62486 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24408	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/6324	0.56	3/8563 (0.0%)
1	B	0.25	0/6278	0.50	1/8507 (0.0%)
1	C	0.26	0/6154	0.52	2/8333 (0.0%)
1	D	0.26	0/6082	0.53	3/8236 (0.0%)
All	All	0.28	0/24838	0.53	9/33639 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	887	LEU	CA-CB-CG	7.30	132.08	115.30
1	C	559	LEU	CA-CB-CG	6.75	130.81	115.30
1	A	319	VAL	N-CA-C	-6.73	92.84	111.00
1	B	559	LEU	CA-CB-CG	6.54	130.35	115.30
1	D	559	LEU	CA-CB-CG	6.46	130.15	115.30
1	D	378	PRO	N-CA-CB	5.44	109.82	103.30
1	A	378	PRO	N-CA-CB	5.42	109.80	103.30
1	C	378	PRO	N-CA-CB	5.18	109.52	103.30
1	A	39	LEU	CA-CB-CG	5.00	126.81	115.30

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	6215	0	6282	155	0
1	B	6168	0	6197	60	0
1	C	6048	0	6114	68	0
1	D	5977	0	6030	89	0
All	All	24408	0	24623	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 7.

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:708:ARG:NH2	1:D:708:ARG:CB	1.73	1.47
1:A:708:ARG:NH2	1:D:708:ARG:HB2	1.16	1.42
1:A:708:ARG:HH22	1:D:708:ARG:N	1.21	1.34
1:A:708:ARG:NH2	1:D:708:ARG:H	1.25	1.34
1:A:708:ARG:HH21	1:D:708:ARG:CB	1.33	1.25
1:A:708:ARG:NH2	1:D:708:ARG:CA	2.13	1.12
1:C:830:GLU:OE1	1:C:873:ARG:HD3	1.50	1.11
1:A:708:ARG:NH2	1:D:708:ARG:N	1.85	1.08
1:A:708:ARG:HH21	1:D:708:ARG:HB3	1.21	1.04
1:A:708:ARG:HH22	1:D:708:ARG:CA	1.72	1.01
1:A:707:GLU:N	1:A:707:GLU:OE1	1.93	0.99
1:A:693:PHE:HE1	1:A:710:HIS:CE1	1.85	0.93
1:A:309:LEU:HD12	1:A:310:VAL:N	1.83	0.92
1:C:830:GLU:OE1	1:C:873:ARG:CD	2.17	0.91
1:A:298:VAL:HG11	1:A:501:LYS:HD3	1.50	0.91
1:A:693:PHE:HE1	1:A:710:HIS:HE1	1.20	0.88
1:D:338:HIS:HD2	1:D:455:ARG:HH11	1.23	0.86
1:A:693:PHE:CE1	1:A:710:HIS:CE1	2.63	0.86
1:A:711:ARG:O	1:A:714:ALA:N	2.12	0.82
1:A:559:LEU:HD21	1:A:578:GLN:HG2	1.61	0.82
1:A:693:PHE:CE1	1:A:710:HIS:HE1	1.98	0.80
1:A:317:LEU:O	1:A:317:LEU:HD23	1.82	0.80
1:C:498:ASN:HA	1:C:501:LYS:HG3	1.62	0.79
1:D:521:ARG:H	1:D:578:GLN:HE22	1.31	0.79
1:B:801:LEU:O	1:B:806:ARG:NH1	2.15	0.78
1:B:298:VAL:HG11	1:B:501:LYS:HD3	1.64	0.78
1:A:708:ARG:CZ	1:D:708:ARG:HB2	2.10	0.77
1:D:801:LEU:O	1:D:806:ARG:NH1	2.19	0.76
1:D:288:ARG:NH2	1:D:481:ALA:O	2.19	0.75
1:A:293:LEU:N	1:A:293:LEU:HD23	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:LEU:O	1:A:806:ARG:NH1	2.22	0.73
1:C:801:LEU:HD11	1:C:878:LEU:HD22	1.69	0.72
1:B:801:LEU:HD11	1:B:878:LEU:HD22	1.71	0.72
1:C:41:PRO:HB3	1:C:101:LEU:HD21	1.72	0.71
1:A:609:TYR:O	1:A:610:HIS:CG	2.44	0.71
1:D:801:LEU:HD11	1:D:878:LEU:HD22	1.72	0.70
1:A:708:ARG:HH22	1:D:708:ARG:H	0.80	0.69
1:D:298:VAL:HG11	1:D:501:LYS:HD3	1.75	0.69
1:A:314:GLU:OE1	1:A:314:GLU:HA	1.93	0.68
1:C:319:VAL:HB	1:C:323:GLU:HG3	1.75	0.68
1:A:317:LEU:HD23	1:A:317:LEU:C	2.14	0.68
1:C:801:LEU:O	1:C:806:ARG:NH1	2.27	0.68
1:A:304:ASP:OD2	1:A:306:SER:OG	2.11	0.68
1:A:607:LYS:HD2	1:A:607:LYS:N	2.09	0.68
1:A:236:LYS:NZ	1:A:537:GLU:OE1	2.25	0.68
1:A:708:ARG:CZ	1:D:708:ARG:H	2.04	0.67
1:D:830:GLU:OE1	1:D:873:ARG:NH1	2.28	0.67
1:A:306:SER:O	1:A:307:MET:HB2	1.93	0.66
1:A:309:LEU:HD12	1:A:309:LEU:C	2.16	0.66
1:B:168:VAL:HG22	1:B:186:ILE:HB	1.76	0.66
1:A:321:GLY:O	1:A:323:GLU:N	2.29	0.66
1:A:291:PRO:HG2	1:A:489:VAL:HG12	1.78	0.66
1:B:319:VAL:HB	1:B:323:GLU:HG3	1.77	0.65
1:A:321:GLY:O	1:A:322:ASP:C	2.33	0.65
1:C:396:ARG:HE	1:C:837:VAL:HG13	1.61	0.65
1:A:300:ASN:O	1:A:313:PHE:HB3	1.96	0.65
1:A:309:LEU:HD11	1:A:311:ARG:C	2.17	0.65
1:A:145:PRO:O	1:A:226:ARG:NH2	2.29	0.64
1:C:288:ARG:NH2	1:C:481:ALA:O	2.30	0.64
1:A:607:LYS:HD2	1:A:607:LYS:H	1.63	0.64
1:A:498:ASN:HA	1:A:501:LYS:HG3	1.79	0.64
1:A:161:PHE:HB3	1:A:166:ILE:HB	1.79	0.64
1:D:559:LEU:HD22	1:D:578:GLN:HG2	1.81	0.63
1:C:236:LYS:NZ	1:C:537:GLU:OE1	2.31	0.63
1:A:311:ARG:NH2	1:A:332:GLU:OE1	2.32	0.63
1:A:472:LEU:HD13	1:A:512:LEU:HD21	1.79	0.63
1:D:171:TYR:CZ	1:D:177:PRO:HG3	2.34	0.63
1:C:806:ARG:NH2	1:C:863:TRP:O	2.32	0.63
1:A:292:LEU:C	1:A:293:LEU:HD23	2.19	0.62
1:B:302:ILE:HD12	1:B:311:ARG:HD2	1.79	0.62
1:A:311:ARG:HG2	1:A:312:GLU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:VAL:HG13	1:A:702:VAL:O	1.98	0.61
1:A:801:LEU:HD23	1:A:864:VAL:HG21	1.81	0.61
1:A:313:PHE:HE2	1:A:325:HIS:HB3	1.65	0.61
1:D:498:ASN:HA	1:D:501:LYS:HG3	1.81	0.61
1:C:707:GLU:H	1:C:707:GLU:CD	2.04	0.61
1:B:870:LEU:HD13	1:B:875:ALA:HA	1.83	0.61
1:C:161:PHE:HB3	1:C:166:ILE:HB	1.82	0.61
1:B:161:PHE:HB3	1:B:166:ILE:HB	1.83	0.60
1:A:309:LEU:HD12	1:A:311:ARG:N	2.17	0.60
1:A:147:VAL:HG13	1:A:172:MET:HB3	1.81	0.60
1:B:334:ILE:HD12	1:B:438:ARG:HB3	1.82	0.60
1:B:291:PRO:HG2	1:B:489:VAL:HG12	1.82	0.60
1:D:291:PRO:HG2	1:D:489:VAL:HG12	1.84	0.60
1:A:860:ARG:HG2	1:A:871:THR:HG22	1.84	0.59
1:D:453:PRO:O	1:D:483:ARG:NH1	2.36	0.59
1:D:399:SER:O	1:D:735:ARG:NH1	2.36	0.59
1:A:303:TYR:CD1	1:A:303:TYR:N	2.71	0.59
1:A:703:VAL:HG13	1:A:704:ALA:N	2.17	0.58
1:A:596:GLN:HG3	1:A:612:THR:HG22	1.85	0.58
1:D:342:LEU:HD21	1:D:353:LEU:HD23	1.85	0.58
1:A:312:GLU:HG3	1:A:313:PHE:N	2.18	0.58
1:A:690:GLU:OE1	1:A:712:GLN:NE2	2.36	0.58
1:C:298:VAL:HG11	1:C:501:LYS:HD3	1.84	0.58
1:A:870:LEU:HD13	1:A:875:ALA:HA	1.86	0.58
1:B:671:CYS:O	1:B:675:LYS:HD3	2.04	0.58
1:A:301:SER:CB	1:A:303:TYR:HE1	2.17	0.58
1:D:355:ASP:OD1	1:D:407:LYS:NZ	2.36	0.57
1:B:396:ARG:HE	1:B:837:VAL:HG12	1.69	0.57
1:A:708:ARG:HH22	1:D:708:ARG:HB2	1.38	0.57
1:A:319:VAL:O	1:A:321:GLY:N	2.35	0.57
1:D:168:VAL:HG22	1:D:186:ILE:HB	1.86	0.57
1:D:222:GLY:O	1:D:518:CYS:HB2	2.05	0.57
1:C:144:LEU:HD13	1:C:150:ALA:HA	1.87	0.57
1:D:870:LEU:HD13	1:D:875:ALA:HA	1.87	0.56
1:D:806:ARG:NH2	1:D:863:TRP:O	2.38	0.56
1:A:301:SER:CB	1:A:303:TYR:CE1	2.88	0.56
1:A:311:ARG:HD3	1:A:312:GLU:O	2.04	0.56
1:D:433:ARG:NH1	1:D:451:ASN:O	2.39	0.56
1:C:546:THR:HG22	1:C:608:VAL:HG12	1.88	0.56
1:B:129:ILE:HD11	1:B:214:VAL:HG21	1.87	0.56
1:B:830:GLU:OE1	1:B:873:ARG:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:GLN:HG3	1:B:612:THR:HG22	1.88	0.56
1:B:559:LEU:HD22	1:B:578:GLN:HG2	1.88	0.55
1:A:806:ARG:NH2	1:A:863:TRP:O	2.38	0.55
1:D:472:LEU:HB2	1:D:512:LEU:HD21	1.88	0.55
1:B:288:ARG:NH2	1:B:481:ALA:O	2.39	0.55
1:D:129:ILE:HD11	1:D:214:VAL:HG21	1.89	0.55
1:A:301:SER:HB2	1:A:303:TYR:HE1	1.72	0.55
1:A:171:TYR:CZ	1:A:177:PRO:HG3	2.42	0.55
1:D:297:LYS:HZ1	1:D:325:HIS:HB2	1.70	0.55
1:A:711:ARG:C	1:A:713:MET:N	2.60	0.54
1:A:311:ARG:HG2	1:A:312:GLU:N	2.23	0.54
1:B:224:SER:HB3	1:B:227:GLY:H	1.72	0.54
1:A:303:TYR:N	1:A:303:TYR:HD1	2.05	0.54
1:A:309:LEU:HD11	1:A:311:ARG:O	2.08	0.54
1:A:645:GLU:OE2	1:A:682:ARG:NH1	2.40	0.54
1:D:596:GLN:HG3	1:D:612:THR:HG22	1.90	0.54
1:C:559:LEU:O	1:C:562:SER:OG	2.21	0.53
1:A:319:VAL:HG13	1:A:360:GLU:HG3	1.90	0.53
1:D:329:LEU:HD12	1:D:495:ILE:HD11	1.91	0.53
1:D:141:LEU:HD12	1:D:187:ALA:HB3	1.89	0.53
1:B:863:TRP:HD1	1:B:867:ARG:HE	1.57	0.53
1:B:433:ARG:NH1	1:B:451:ASN:O	2.42	0.53
1:D:144:LEU:HD13	1:D:150:ALA:HA	1.91	0.53
1:A:309:LEU:CD1	1:A:311:ARG:N	2.72	0.53
1:D:326:VAL:HG21	1:D:460:ARG:NE	2.24	0.53
1:A:301:SER:HB3	1:A:303:TYR:CE1	2.44	0.52
1:A:141:LEU:HB3	1:A:213:VAL:HG12	1.91	0.52
1:C:645:GLU:OE2	1:C:682:ARG:NH1	2.43	0.52
1:B:396:ARG:HD2	1:B:861:THR:HB	1.91	0.52
1:C:311:ARG:HH22	1:C:332:GLU:CD	2.12	0.52
1:B:860:ARG:HG2	1:B:871:THR:HG22	1.92	0.52
1:B:147:VAL:HG13	1:B:172:MET:HB2	1.91	0.52
1:D:300:ASN:O	1:D:313:PHE:HB3	2.10	0.51
1:B:496:CYS:HB3	1:B:500:GLU:HG3	1.92	0.51
1:A:702:VAL:HG22	1:A:704:ALA:HB2	1.92	0.51
1:B:45:LEU:HG	1:B:68:LYS:HB3	1.91	0.51
1:C:830:GLU:OE1	1:C:873:ARG:HD2	2.09	0.51
1:C:596:GLN:HG3	1:C:612:THR:HG22	1.92	0.51
1:D:453:PRO:HB2	1:D:483:ARG:HG2	1.92	0.51
1:C:302:ILE:HD12	1:C:311:ARG:HD3	1.92	0.51
1:A:149:VAL:HG12	1:A:450:VAL:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:NZ	1:C:135:GLU:OE2	2.41	0.51
1:C:860:ARG:HB3	1:C:869:GLY:O	2.11	0.51
1:B:236:LYS:NZ	1:B:537:GLU:OE1	2.42	0.50
1:A:391:MET:SD	1:A:410:PRO:HG3	2.51	0.50
1:A:607:LYS:CD	1:A:607:LYS:N	2.73	0.50
1:D:242:ARG:HD2	1:D:556:CYS:SG	2.51	0.50
1:A:39:LEU:HG	1:A:131:LYS:HD2	1.94	0.50
1:A:302:ILE:C	1:A:303:TYR:CD1	2.85	0.50
1:A:144:LEU:HD11	1:A:153:LYS:HG2	1.94	0.50
1:D:668:ARG:HD3	1:D:740:LYS:O	2.11	0.50
1:A:380:VAL:C	1:A:381:ILE:HG13	2.32	0.50
1:D:540:VAL:HG22	1:D:611:PRO:HB3	1.94	0.49
1:C:171:TYR:CZ	1:C:177:PRO:HG3	2.47	0.49
1:A:706:THR:HG23	1:A:707:GLU:N	2.28	0.49
1:A:453:PRO:HB2	1:A:483:ARG:HG2	1.94	0.49
1:A:300:ASN:O	1:A:313:PHE:N	2.46	0.49
1:A:870:LEU:HB3	1:A:875:ALA:HB2	1.94	0.49
1:D:79:ALA:HB3	1:D:164:VAL:HG22	1.95	0.49
1:A:301:SER:HB2	1:A:303:TYR:CE1	2.48	0.49
1:C:828:GLU:O	1:C:832:ILE:HG13	2.13	0.49
1:A:822:ALA:HB1	1:A:884:ARG:HG2	1.94	0.49
1:C:224:SER:HB3	1:C:227:GLY:HA3	1.94	0.49
1:B:144:LEU:HD11	1:B:153:LYS:HG2	1.94	0.49
1:A:433:ARG:NH1	1:A:451:ASN:O	2.45	0.49
1:C:129:ILE:HD11	1:C:214:VAL:HG21	1.93	0.49
1:C:711:ARG:HE	1:C:715:ILE:HD11	1.77	0.48
1:C:37:SER:HA	1:C:135:GLU:OE1	2.12	0.48
1:A:559:LEU:CD2	1:A:578:GLN:HG2	2.38	0.48
1:C:218:LEU:H	1:C:265:SER:HB3	1.78	0.48
1:B:643:VAL:H	1:B:649:HIS:HD2	1.58	0.48
1:D:707:GLU:H	1:D:707:GLU:HG3	1.39	0.48
1:C:643:VAL:H	1:C:649:HIS:HD2	1.60	0.48
1:A:129:ILE:HD11	1:A:214:VAL:HG21	1.95	0.48
1:B:270:ASN:HD21	1:B:515:VAL:H	1.62	0.48
1:A:302:ILE:C	1:A:303:TYR:HD1	2.17	0.48
1:D:867:ARG:HG2	1:D:869:GLY:H	1.79	0.48
1:B:64:TYR:OH	1:B:94:GLU:OE1	2.31	0.48
1:A:345:PRO:HA	1:A:464:PHE:CD2	2.49	0.48
1:A:347:LYS:HB3	1:A:417:HIS:CD2	2.49	0.47
1:A:706:THR:HG23	1:A:707:GLU:CD	2.34	0.47
1:D:224:SER:HB3	1:D:227:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD12	1:A:438:ARG:HB3	1.96	0.47
1:D:402:ASP:OD1	1:D:745:ARG:NH2	2.41	0.47
1:A:423:GLU:N	1:A:423:GLU:OE2	2.47	0.47
1:A:706:THR:HG23	1:A:707:GLU:HG3	1.95	0.47
1:B:44:GLY:HA2	1:B:47:ARG:HD3	1.96	0.47
1:A:708:ARG:HD2	1:D:708:ARG:HB3	1.96	0.47
1:D:792:GLU:HB3	1:D:811:TYR:CE1	2.49	0.47
1:A:825:ASN:OD1	1:A:827:VAL:HG12	2.15	0.47
1:A:44:GLY:HA2	1:A:47:ARG:HG3	1.97	0.47
1:B:801:LEU:HD23	1:B:864:VAL:HG21	1.97	0.47
1:D:780:GLN:HE22	1:D:791:ARG:HD3	1.78	0.47
1:A:618:THR:OG1	1:A:628:THR:HG21	2.15	0.46
1:A:224:SER:HB3	1:A:227:GLY:HA3	1.96	0.46
1:D:643:VAL:H	1:D:649:HIS:HD2	1.63	0.46
1:A:708:ARG:C	1:A:710:HIS:H	2.19	0.46
1:D:559:LEU:HD12	1:D:560:ALA:N	2.30	0.46
1:B:331:TYR:OH	1:B:377:CYS:HB3	2.15	0.46
1:C:224:SER:HB3	1:C:227:GLY:H	1.79	0.46
1:B:298:VAL:HG21	1:B:501:LYS:HG2	1.98	0.46
1:A:531:MET:HG2	1:A:585:CYS:SG	2.55	0.46
1:D:326:VAL:HG21	1:D:460:ARG:CZ	2.46	0.46
1:B:171:TYR:CZ	1:B:177:PRO:HG3	2.51	0.45
1:A:291:PRO:CG	1:A:489:VAL:HG12	2.44	0.45
1:D:218:LEU:H	1:D:265:SER:HB3	1.81	0.45
1:C:222:GLY:O	1:C:518:CYS:HB3	2.16	0.45
1:B:867:ARG:HG2	1:B:869:GLY:H	1.81	0.45
1:A:330:CYS:O	1:A:334:ILE:HG12	2.15	0.45
1:C:342:LEU:HD21	1:C:353:LEU:HD23	1.97	0.45
1:A:58:LYS:HG3	1:A:59:PRO:HD2	1.98	0.45
1:D:828:GLU:O	1:D:832:ILE:HG13	2.17	0.45
1:A:313:PHE:HE2	1:A:325:HIS:CB	2.29	0.45
1:B:156:TYR:O	1:B:160:LEU:HD13	2.17	0.45
1:A:864:VAL:HG22	1:A:865:THR:H	1.82	0.45
1:A:708:ARG:O	1:A:708:ARG:HG2	2.17	0.45
1:A:319:VAL:C	1:A:321:GLY:H	2.20	0.45
1:A:706:THR:HG23	1:A:707:GLU:CG	2.47	0.44
1:C:232:LEU:O	1:C:236:LYS:HB2	2.17	0.44
1:B:357:ILE:HD13	1:B:439:VAL:HG11	1.98	0.44
1:C:396:ARG:HD3	1:C:861:THR:HB	1.99	0.44
1:A:344:CYS:HB2	1:A:350:CYS:SG	2.58	0.44
1:A:801:LEU:HD11	1:A:878:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:LEU:HA	1:D:353:LEU:HD12	1.78	0.44
1:D:472:LEU:HD13	1:D:512:LEU:HD11	1.99	0.44
1:C:733:PRO:HB2	1:C:736:GLU:HG3	1.99	0.44
1:C:531:MET:HG2	1:C:585:CYS:SG	2.57	0.44
1:D:338:HIS:CD2	1:D:455:ARG:HH11	2.16	0.44
1:D:521:ARG:H	1:D:578:GLN:NE2	2.09	0.44
1:A:349:TRP:HZ3	1:A:460:ARG:HD2	1.82	0.44
1:D:234:LEU:HD22	1:D:261:ILE:HD13	1.99	0.44
1:B:141:LEU:HD12	1:B:187:ALA:HB3	1.98	0.44
1:D:645:GLU:OE2	1:D:682:ARG:NH1	2.50	0.44
1:A:300:ASN:O	1:A:313:PHE:CB	2.64	0.44
1:C:559:LEU:HD12	1:C:560:ALA:N	2.32	0.44
1:B:61:VAL:HA	1:B:62:PRO:HD2	1.84	0.44
1:C:864:VAL:HG22	1:C:865:THR:H	1.82	0.44
1:D:864:VAL:HG22	1:D:865:THR:H	1.83	0.44
1:A:703:VAL:CG1	1:A:704:ALA:N	2.81	0.44
1:D:643:VAL:H	1:D:649:HIS:CD2	2.36	0.44
1:D:236:LYS:NZ	1:D:537:GLU:OE1	2.40	0.44
1:C:366:HIS:O	1:C:366:HIS:ND1	2.51	0.44
1:A:671:CYS:O	1:A:675:LYS:HD3	2.18	0.44
1:A:694:LEU:O	1:A:698:VAL:HG23	2.18	0.44
1:C:330:CYS:O	1:C:334:ILE:HG12	2.18	0.43
1:A:168:VAL:HG22	1:A:186:ILE:HB	2.00	0.43
1:C:873:ARG:HH11	1:C:873:ARG:HG2	1.84	0.43
1:A:141:LEU:HD12	1:A:187:ALA:HB3	2.01	0.43
1:A:728:LEU:HD21	1:A:752:GLN:HB3	1.99	0.43
1:B:707:GLU:HG3	1:B:707:GLU:H	1.46	0.43
1:A:426:ASP:OD2	1:A:863:TRP:NE1	2.50	0.43
1:B:559:LEU:HD12	1:B:560:ALA:N	2.33	0.43
1:B:224:SER:HB3	1:B:227:GLY:HA3	2.00	0.43
1:C:464:PHE:CD1	1:C:469:LEU:HD13	2.53	0.43
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.82	0.43
1:C:141:LEU:HD12	1:C:187:ALA:HB3	2.00	0.43
1:A:222:GLY:O	1:A:518:CYS:HB2	2.18	0.43
1:A:867:ARG:HG2	1:A:869:GLY:H	1.82	0.43
1:B:337:ASN:HA	1:B:438:ARG:NH2	2.33	0.43
1:C:345:PRO:HA	1:C:464:PHE:CD2	2.53	0.43
1:A:536:LEU:HD22	1:A:625:PRO:HG3	2.00	0.43
1:C:783:LYS:HB2	1:C:783:LYS:HE3	1.86	0.43
1:A:38:VAL:HG21	1:A:134:LEU:HD12	1.99	0.43
1:B:792:GLU:HB3	1:B:811:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:HIS:CD2	1:D:455:ARG:HD3	2.54	0.43
1:A:551:HIS:ND1	1:A:579:LEU:HD11	2.34	0.43
1:A:609:TYR:O	1:A:610:HIS:CD2	2.71	0.43
1:D:337:ASN:HA	1:D:438:ARG:NH2	2.33	0.43
1:C:396:ARG:CD	1:C:861:THR:HB	2.48	0.43
1:B:655:THR:HA	1:B:656:PRO:HD3	1.79	0.43
1:D:360:GLU:O	1:D:364:LEU:HD23	2.18	0.43
1:C:408:THR:HB	1:C:413:VAL:HB	2.01	0.43
1:A:312:GLU:HG3	1:A:313:PHE:H	1.80	0.43
1:D:347:LYS:HG2	1:D:417:HIS:CD2	2.54	0.43
1:A:316:MET:HE2	1:A:331:TYR:CD2	2.54	0.43
1:B:531:MET:HG2	1:B:585:CYS:SG	2.59	0.43
1:D:393:GLN:O	1:D:397:LEU:HD13	2.19	0.43
1:D:121:LYS:HB3	1:D:264:MET:HE3	2.01	0.43
1:B:189:CYS:HB2	1:B:194:ALA:HB2	2.01	0.43
1:C:387:LEU:HD21	1:C:409:VAL:O	2.18	0.43
1:D:330:CYS:O	1:D:334:ILE:HG12	2.19	0.42
1:D:822:ALA:HB1	1:D:884:ARG:HG2	2.01	0.42
1:A:315:PRO:HG3	1:A:325:HIS:CE1	2.54	0.42
1:D:801:LEU:HD22	1:D:864:VAL:HG21	2.01	0.42
1:A:319:VAL:C	1:A:321:GLY:N	2.73	0.42
1:B:860:ARG:HB3	1:B:869:GLY:O	2.19	0.42
1:A:708:ARG:HH21	1:D:708:ARG:CA	2.00	0.42
1:D:517:SER:OG	1:D:559:LEU:HB3	2.19	0.42
1:B:864:VAL:HG22	1:B:865:THR:H	1.85	0.42
1:D:345:PRO:HA	1:D:464:PHE:CD2	2.53	0.42
1:A:709:GLN:O	1:A:709:GLN:HG3	2.19	0.42
1:D:456:ARG:NH2	1:D:491:GLU:OE1	2.52	0.42
1:A:706:THR:CG2	1:A:707:GLU:CD	2.88	0.42
1:D:405:LEU:O	1:D:409:VAL:HB	2.19	0.42
1:D:789:ILE:HD13	1:D:797:VAL:HG11	2.01	0.42
1:C:423:GLU:OE2	1:C:423:GLU:N	2.53	0.42
1:C:809:VAL:O	1:C:813:SER:OG	2.34	0.42
1:B:822:ALA:HB1	1:B:884:ARG:HG2	2.01	0.42
1:C:629:LEU:HA	1:C:629:LEU:HD23	1.89	0.42
1:B:752:GLN:NE2	1:B:785:LEU:O	2.51	0.42
1:D:297:LYS:NZ	1:D:299:GLY:O	2.51	0.42
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.78	0.42
1:D:470:ASP:OD1	1:D:472:LEU:N	2.46	0.42
1:A:470:ASP:OD1	1:A:472:LEU:N	2.47	0.42
1:A:712:GLN:O	1:A:716:HIS:ND1	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:CE	1:A:331:TYR:CE2	3.03	0.42
1:B:399:SER:O	1:B:735:ARG:NH1	2.53	0.42
1:C:867:ARG:HG2	1:C:869:GLY:H	1.85	0.41
1:A:708:ARG:C	1:A:710:HIS:N	2.73	0.41
1:B:330:CYS:O	1:B:334:ILE:HG12	2.21	0.41
1:A:129:ILE:HA	1:A:212:MET:SD	2.60	0.41
1:C:433:ARG:NH1	1:C:451:ASN:O	2.53	0.41
1:B:103:GLY:HA3	1:B:281:GLU:OE1	2.20	0.41
1:A:517:SER:OG	1:A:559:LEU:HB2	2.21	0.41
1:C:42:PRO:HG2	1:C:68:LYS:O	2.19	0.41
1:B:792:GLU:HB3	1:B:811:TYR:CZ	2.55	0.41
1:B:326:VAL:HG21	1:B:460:ARG:NE	2.36	0.41
1:B:338:HIS:ND1	1:B:455:ARG:HD3	2.36	0.41
1:C:168:VAL:HG22	1:C:186:ILE:HB	2.02	0.41
1:D:423:GLU:N	1:D:423:GLU:OE2	2.54	0.41
1:A:309:LEU:C	1:A:309:LEU:CD1	2.86	0.41
1:A:672:LEU:HD11	1:A:740:LYS:HG2	2.03	0.41
1:B:423:GLU:OE2	1:B:423:GLU:N	2.54	0.41
1:D:825:ASN:OD1	1:D:827:VAL:HG12	2.21	0.41
1:A:295:SER:OG	1:A:492:SER:O	2.35	0.41
1:C:655:THR:HA	1:C:656:PRO:HD3	1.81	0.41
1:C:518:CYS:SG	1:C:519:LEU:HD12	2.61	0.41
1:C:79:ALA:HB3	1:C:164:VAL:HG22	2.03	0.41
1:C:219:HIS:ND1	1:C:265:SER:HB2	2.36	0.41
1:C:643:VAL:H	1:C:649:HIS:CD2	2.38	0.41
1:C:353:LEU:HA	1:C:353:LEU:HD12	1.83	0.41
1:B:373:LYS:N	1:B:374:PRO:HD2	2.36	0.41
1:C:357:ILE:HD13	1:C:439:VAL:HG11	2.03	0.41
1:A:347:LYS:HB3	1:A:417:HIS:HD2	1.85	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.85	0.41
1:C:304:ASP:HB3	1:C:310:VAL:HG11	2.01	0.40
1:D:298:VAL:HG21	1:D:501:LYS:HG2	2.04	0.40
1:A:232:LEU:HG	1:A:534:ALA:HB2	2.02	0.40
1:D:684:ALA:HB2	1:D:719:PHE:CZ	2.57	0.40
1:C:423:GLU:HG3	1:C:863:TRP:CH2	2.56	0.40
1:A:270:ASN:HD21	1:A:515:VAL:H	1.67	0.40
1:A:863:TRP:HD1	1:A:867:ARG:HE	1.69	0.40
1:A:319:VAL:HG13	1:A:360:GLU:CD	2.42	0.40
1:A:828:GLU:O	1:A:832:ILE:HG13	2.22	0.40
1:C:676:LEU:HA	1:C:677:PRO:HD3	1.95	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	793/896 (88%)	754 (95%)	39 (5%)	0	100	100
1	B	787/896 (88%)	746 (95%)	41 (5%)	0	100	100
1	C	766/896 (86%)	726 (95%)	40 (5%)	0	100	100
1	D	758/896 (85%)	720 (95%)	38 (5%)	0	100	100
All	All	3104/3584 (87%)	2946 (95%)	158 (5%)	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	668/768 (87%)	641 (96%)	27 (4%)	38	76
1	B	659/768 (86%)	622 (94%)	37 (6%)	26	67
1	C	652/768 (85%)	614 (94%)	38 (6%)	25	66
1	D	642/768 (84%)	605 (94%)	37 (6%)	25	66
All	All	2621/3072 (85%)	2482 (95%)	139 (5%)	28	69

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	57	CYS

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Mol	Chain	Res	Type
1	A	164	VAL
1	A	226	ARG
1	A	293	LEU
1	A	303	TYR
1	A	305	SER
1	A	306	SER
1	A	309	LEU
1	A	310	VAL
1	A	311	ARG
1	A	317	LEU
1	A	349	TRP
1	A	367	GLN
1	A	397	LEU
1	A	417	HIS
1	A	460	ARG
1	A	492	SER
1	A	527	VAL
1	A	528	THR
1	A	605	GLU
1	A	607	LYS
1	A	701	LYS
1	A	707	GLU
1	A	709	GLN
1	A	864	VAL
1	A	867	ARG
1	B	45	LEU
1	B	63	ASP
1	B	164	VAL
1	B	180	HIS
1	B	203	GLU
1	B	213	VAL
1	B	311	ARG
1	B	317	LEU
1	B	337	ASN
1	B	347	LYS
1	B	349	TRP
1	B	365	HIS
1	B	375	SER
1	B	381	ILE
1	B	382	LEU
1	B	388	LEU
1	B	391	MET

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Mol	Chain	Res	Type
1	B	397	LEU
1	B	417	HIS
1	B	460	ARG
1	B	492	SER
1	B	527	VAL
1	B	528	THR
1	B	548	GLN
1	B	559	LEU
1	B	587	MET
1	B	649	HIS
1	B	660	ASP
1	B	678	THR
1	B	699	LYS
1	B	706	THR
1	B	707	GLU
1	B	711	ARG
1	B	735	ARG
1	B	776	LEU
1	B	864	VAL
1	B	867	ARG
1	C	70	LEU
1	C	164	VAL
1	C	174	SER
1	C	203	GLU
1	C	213	VAL
1	C	217	GLU
1	C	220	MET
1	C	226	ARG
1	C	317	LEU
1	C	347	LYS
1	C	349	TRP
1	C	364	LEU
1	C	381	ILE
1	C	387	LEU
1	C	388	LEU
1	C	391	MET
1	C	397	LEU
1	C	417	HIS
1	C	455	ARG
1	C	460	ARG
1	C	492	SER
1	C	517	SER

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Mol	Chain	Res	Type
1	C	518	CYS
1	C	520	GLN
1	C	550	MET
1	C	559	LEU
1	C	660	ASP
1	C	678	THR
1	C	707	GLU
1	C	710	HIS
1	C	711	ARG
1	C	735	ARG
1	C	813	SER
1	C	818	VAL
1	C	864	VAL
1	C	867	ARG
1	C	870	LEU
1	C	889	GLN
1	D	39	LEU
1	D	70	LEU
1	D	164	VAL
1	D	172	MET
1	D	180	HIS
1	D	203	GLU
1	D	213	VAL
1	D	226	ARG
1	D	311	ARG
1	D	317	LEU
1	D	323	GLU
1	D	347	LYS
1	D	349	TRP
1	D	364	LEU
1	D	366	HIS
1	D	367	GLN
1	D	379	PRO
1	D	381	ILE
1	D	383	GLU
1	D	384	GLN
1	D	388	LEU
1	D	397	LEU
1	D	417	HIS
1	D	460	ARG
1	D	520	GLN
1	D	527	VAL

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Mol	Chain	Res	Type
1	D	559	LEU
1	D	660	ASP
1	D	706	THR
1	D	707	GLU
1	D	710	HIS
1	D	735	ARG
1	D	864	VAL
1	D	867	ARG
1	D	872	GLU
1	D	873	ARG
1	D	886	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	A	710	HIS
1	B	199	ASN
1	B	858	ASN
1	D	338	HIS
1	D	578	GLN
1	D	752	GLN

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 carbohydrates 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, 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	805/896 (89%)	-0.34	1 (0%) 95 95	70, 124, 178, 203	0
1	B	801/896 (89%)	-0.23	11 (1%) 78 69	88, 149, 211, 255	0
1	C	780/896 (87%)	-0.29	5 (0%) 90 85	78, 144, 195, 217	0
1	D	772/896 (86%)	-0.04	24 (3%) 52 43	78, 178, 243, 264	0
All	All	3158/3584 (88%)	-0.23	41 (1%) 79 71	70, 146, 218, 264	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	CYS	5.5
1	D	411	TRP	4.3
1	D	520	GLN	3.7
1	D	297	LYS	3.5
1	D	169	ASP	3.5
1	B	837	VAL	3.2
1	D	485	GLY	3.0
1	D	380	VAL	3.0
1	C	263	GLY	2.9
1	D	824	ALA	2.8
1	D	828	GLU	2.8
1	D	222	GLY	2.8
1	B	54	ALA	2.8
1	D	386	GLU	2.7
1	D	223	ASP	2.7
1	C	821	LEU	2.7
1	B	84	TYR	2.6
1	A	578	GLN	2.5
1	D	361	PHE	2.5
1	D	357	ILE	2.5
1	C	879	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	868	LYS	2.5
1	D	832	ILE	2.4
1	B	836	ALA	2.4
1	D	827	VAL	2.4
1	D	99	CYS	2.4
1	D	825	ASN	2.3
1	D	328	SER	2.3
1	B	60	THR	2.3
1	D	390	VAL	2.3
1	B	61	VAL	2.3
1	D	793	LEU	2.3
1	D	523	GLU	2.2
1	D	101	LEU	2.2
1	D	706	THR	2.2
1	C	543	VAL	2.2
1	B	127	LEU	2.1
1	B	80	VAL	2.1
1	B	79	ALA	2.1
1	C	868	LYS	2.1
1	D	246	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.