



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:10 PM UTC

PDB ID : 6K4S / pdb_00006k4s
Title : Crystal structure of xCas9 in complex with sgRNA and DNA (TGC PAM)
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on : 2019-05-26
Resolution : 3.01 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

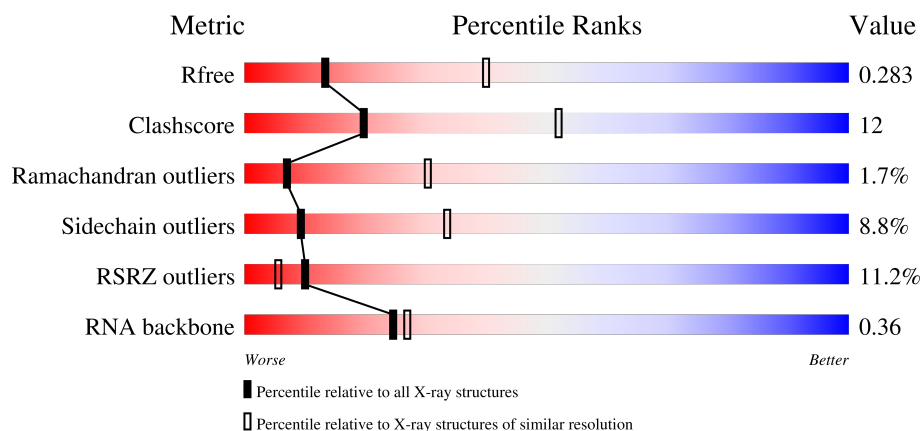
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)
RNA backbone	3983	1139 (3.24-2.80)

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	B	1368	11% 67% 25% • •
2	A	83	% 40% 37% 14% 5% •
3	C	28	11% 57% 39% •
4	D	12	25% 42% 50% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12412 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1308	Total	C	N	O	S	0	0	0
			9924	6324	1730	1854	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	80	LEU	CYS	engineered mutation	UNP Q99ZW2
B	262	THR	ALA	engineered mutation	UNP Q99ZW2
B	324	LEU	ARG	engineered mutation	UNP Q99ZW2
B	409	ILE	SER	engineered mutation	UNP Q99ZW2
B	480	LYS	GLU	engineered mutation	UNP Q99ZW2
B	543	ASP	GLU	engineered mutation	UNP Q99ZW2
B	574	GLU	CYS	engineered mutation	UNP Q99ZW2
B	694	ILE	MET	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	80	Total	C	N	O	P	0	0	0
			1710	768	313	549	80			

- Molecule 3 is a DNA chain called targeted DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	P	0	0	0
			554	268	95	164	27			

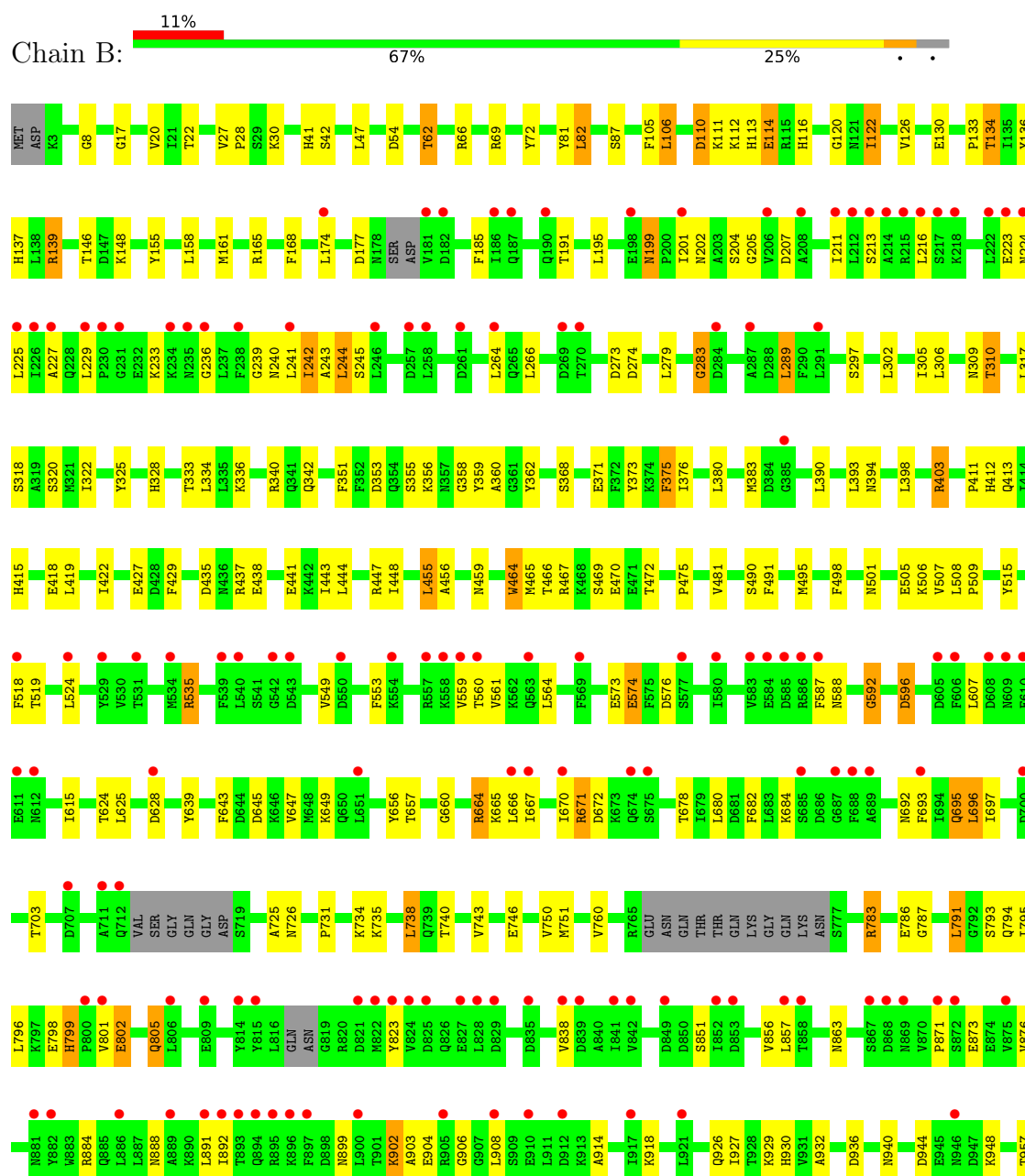
- Molecule 4 is a DNA chain called non-targeted DNA.

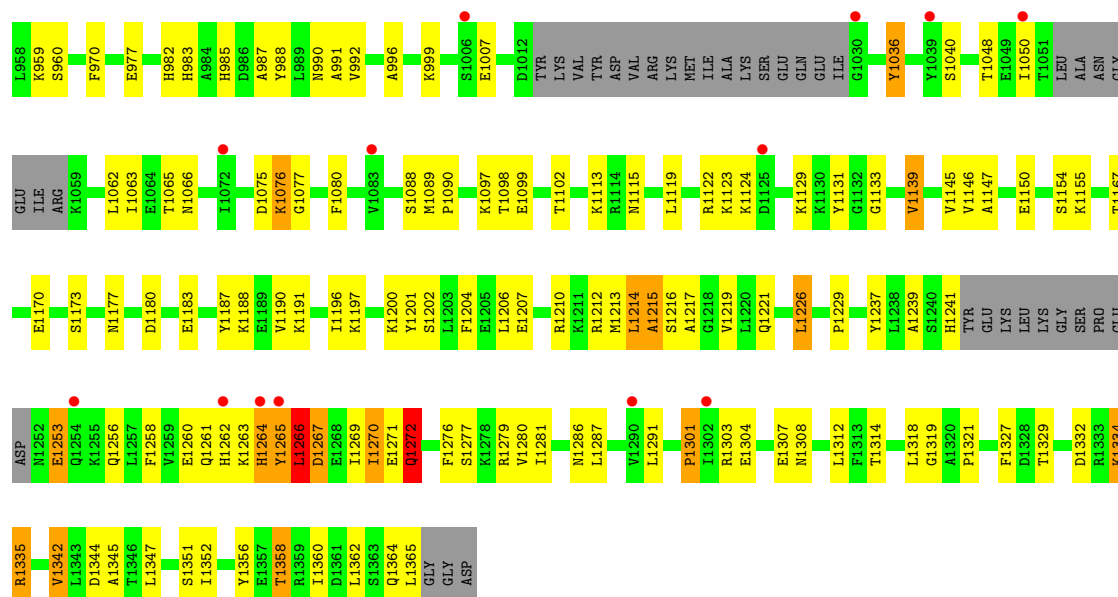
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total 224	C 109	N 41	O 64	P 10	0	0	0

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: CRISPR-associated endonuclease Cas9/Csn1

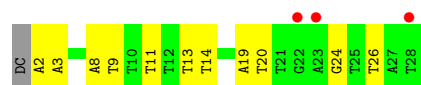




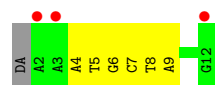
- Molecule 2: sgRNA



- Molecule 3: targeted DNA



- Molecule 4: non-targeted DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.46Å 70.36Å 188.90Å 90.00° 110.42° 90.00°	Depositor
Resolution (Å)	49.25 – 3.01 49.25 – 3.01	Depositor EDS
% Data completeness (in resolution range)	87.0 (49.25-3.01) 87.2 (49.25-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.285 0.237 , 0.283	Depositor DCC
R_{free} test set	1913 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12412	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [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	B	1.14	1/10093 (0.0%)	1.55	31/13650 (0.2%)
2	A	0.91	10/1917 (0.5%)	1.11	15/2984 (0.5%)
3	C	0.75	3/620 (0.5%)	0.89	0/955
4	D	0.72	1/251 (0.4%)	0.93	1/386 (0.3%)
All	All	1.09	15/12881 (0.1%)	1.44	47/17975 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	12	U	O3'-P	-7.60	1.49	1.61
3	C	8	DA	O3'-P	-7.27	1.50	1.61
2	A	46	A	O3'-P	-6.92	1.50	1.61
2	A	45	U	O3'-P	-6.83	1.50	1.61
2	A	49	A	O3'-P	-6.82	1.50	1.61
2	A	61	C	O3'-P	-6.81	1.50	1.61
2	A	25	U	O3'-P	-6.75	1.51	1.61
2	A	42	A	O3'-P	-6.18	1.51	1.61
3	C	9	DT	O3'-P	-5.94	1.52	1.61
2	A	47	A	O3'-P	-5.93	1.52	1.61
2	A	24	U	O3'-P	-5.92	1.52	1.61
4	D	5	DT	O3'-P	-5.88	1.52	1.61
2	A	62	G	O3'-P	-5.73	1.52	1.61
1	B	1197	LYS	C-O	-5.44	1.17	1.24
3	C	11	DT	O3'-P	-5.29	1.53	1.61

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9	A	C2'-C3'-O3'	-7.27	102.79	113.70
2	A	73	G	C1'-C2'-O2'	7.10	119.05	108.40
1	B	1102	THR	CA-CB-OG1	-7.00	99.11	109.60
2	A	47	A	C1'-C2'-O2'	-6.88	98.08	108.40
2	A	81	G	C2'-C3'-O3'	6.85	119.78	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	59	U	C3'-C2'-O2'	6.67	120.71	110.70
1	B	199	ASN	CB-CA-C	6.63	116.40	110.44
1	B	283	GLY	CA-C-O	-6.59	117.32	122.52
1	B	1098	THR	CA-CB-OG1	6.41	119.22	109.60
1	B	443	ILE	N-CA-C	-6.24	104.25	110.62
2	A	51	A	C2'-C3'-O3'	-6.21	104.39	113.70
1	B	72	TYR	CA-C-O	-6.00	114.52	120.82
1	B	1183	GLU	CA-C-N	5.99	129.13	120.38
1	B	1183	GLU	C-N-CA	5.99	129.13	120.38
1	B	509	PRO	CB-CA-C	-5.96	103.28	111.21
1	B	1358	THR	CB-CA-C	5.95	120.02	109.72
1	B	443	ILE	CA-C-O	-5.75	114.97	120.95
2	A	61	C	C2'-C3'-O3'	-5.73	105.11	113.70
1	B	22	THR	CA-CB-OG1	-5.69	101.07	109.60
1	B	731	PRO	N-CA-C	-5.69	106.75	113.86
2	A	62	G	C2'-C3'-O3'	-5.66	105.22	113.70
1	B	957	THR	CB-CA-C	5.65	119.07	109.80
2	A	51	A	C4'-C3'-O3'	-5.55	104.68	113.00
1	B	1265	TYR	N-CA-C	-5.51	106.40	113.01
1	B	1197	LYS	CA-C-O	-5.37	114.56	120.69
2	A	24	U	C1'-C2'-O2'	-5.34	100.39	108.40
1	B	927	ILE	N-CA-C	-5.31	104.71	110.23
2	A	78	A	C3'-C2'-O2'	5.29	118.63	110.70
2	A	72	U	C3'-C2'-O2'	5.26	118.59	110.70
2	A	74	A	C3'-C2'-O2'	5.22	118.53	110.70
4	D	4	DA	C2'-C3'-O3'	-5.22	103.67	111.50
1	B	1214	LEU	CB-CA-C	5.21	118.33	109.84
1	B	427	GLU	CA-C-N	5.21	127.98	120.38
1	B	427	GLU	C-N-CA	5.21	127.98	120.38
1	B	1215	ALA	N-CA-C	-5.19	107.08	113.41
1	B	1360	ILE	CA-C-O	-5.19	114.59	120.66
2	A	9	A	C1'-C2'-O2'	5.19	116.18	108.40
1	B	783	ARG	CA-C-N	5.17	128.14	120.74
1	B	783	ARG	C-N-CA	5.17	128.14	120.74
1	B	746	GLU	CA-C-O	-5.17	115.02	120.55
1	B	1272	GLN	CA-C-N	5.16	127.14	120.70
1	B	1272	GLN	C-N-CA	5.16	127.14	120.70
1	B	66	ARG	N-CA-C	-5.08	105.63	111.07
2	A	16	A	C1'-C2'-O2'	5.06	115.99	108.40
1	B	81	TYR	CA-C-O	-5.06	115.49	120.90
1	B	41	HIS	N-CA-C	-5.04	106.54	113.30
1	B	411	PRO	CA-C-O	-5.02	115.89	122.12

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	B	9924	0	9432	238	0
2	A	1710	0	858	37	0
3	C	554	0	310	13	0
4	D	224	0	127	2	0
All	All	12412	0	10727	266	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 12.

All (266) 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)
3:C:19:DA:H2''	3:C:20:DT:C5'	1.64	1.27
3:C:19:DA:H2''	3:C:20:DT:H5''	1.13	1.10
3:C:19:DA:C2'	3:C:20:DT:H5''	1.88	1.03
1:B:241:LEU:HD11	1:B:289:LEU:HD13	1.44	0.99
3:C:19:DA:H2''	3:C:20:DT:H5'	1.51	0.92
1:B:1263:LYS:O	1:B:1264:HIS:HB2	1.74	0.87
1:B:241:LEU:CD1	1:B:289:LEU:HD13	2.08	0.83
2:A:42:A:H8	2:A:42:A:H5''	1.46	0.81
1:B:1265:TYR:O	1:B:1269:ILE:HG13	1.82	0.80
1:B:105:PHE:CD1	2:A:24:U:O2	2.36	0.79
1:B:191:THR:HG22	1:B:289:LEU:HD23	1.67	0.77
3:C:19:DA:C2'	3:C:20:DT:C5'	2.55	0.76
1:B:241:LEU:HD11	1:B:289:LEU:CD1	2.16	0.76
1:B:8:GLY:HA3	1:B:987:ALA:O	1.86	0.75
1:B:823:TYR:CB	1:B:863:ASN:HD22	2.01	0.74
1:B:725:ALA:O	1:B:734:LYS:NZ	2.20	0.74
1:B:876:VAL:HG21	1:B:903:ALA:HB3	1.68	0.73
1:B:1266:LEU:N	1:B:1266:LEU:HD23	2.01	0.73
1:B:518:PHE:CD1	1:B:667:ILE:HD12	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:NH2	2:A:41:A:OP2	2.22	0.71
2:A:46:A:H2'	2:A:47:A:C8	2.25	0.71
1:B:692:ASN:HD21	3:C:26:DT:H2''	1.58	0.68
1:B:936:ASP:OD1	1:B:940:ASN:ND2	2.27	0.67
1:B:926:GLN:O	1:B:930:HIS:ND1	2.26	0.66
1:B:1113:LYS:HB2	1:B:1129:LYS:O	1.96	0.66
1:B:191:THR:CG2	1:B:289:LEU:HD23	2.26	0.65
1:B:368:SER:OG	1:B:371:GLU:HG3	1.96	0.65
1:B:106:LEU:O	1:B:111:LYS:NZ	2.22	0.65
1:B:871:PRO:O	1:B:903:ALA:HB2	1.96	0.65
1:B:549:VAL:HA	1:B:553:PHE:HB2	1.79	0.65
1:B:838:VAL:HA	1:B:857:LEU:HA	1.77	0.65
1:B:1226:LEU:C	1:B:1226:LEU:HD12	2.22	0.64
1:B:1263:LYS:O	1:B:1264:HIS:CB	2.46	0.64
1:B:69:ARG:HD2	2:A:62:G:N7	2.12	0.63
1:B:795:ILE:O	1:B:799:HIS:HB2	1.98	0.63
2:A:42:A:H8	2:A:42:A:C5'	2.11	0.62
1:B:1196:ILE:HD11	1:B:1364:GLN:HE22	1.65	0.62
1:B:244:LEU:HD22	1:B:266:LEU:HD12	1.83	0.61
1:B:1266:LEU:O	1:B:1269:ILE:N	2.33	0.61
1:B:553:PHE:CG	1:B:559:VAL:HG21	2.35	0.61
1:B:191:THR:HG22	1:B:289:LEU:CD2	2.31	0.60
1:B:491:PHE:O	1:B:495:MET:HE3	2.01	0.60
1:B:884:ARG:O	1:B:888:ASN:ND2	2.34	0.60
2:A:42:A:H5''	2:A:42:A:C8	2.33	0.59
1:B:1287:LEU:O	1:B:1291:LEU:HG	2.02	0.59
2:A:42:A:C5'	2:A:42:A:C8	2.85	0.59
1:B:1335:ARG:CG	1:B:1335:ARG:HH11	2.14	0.59
2:A:33:G:N2	2:A:36:A:OP2	2.35	0.59
1:B:1260:GLU:O	1:B:1263:LYS:HB2	2.04	0.58
1:B:518:PHE:CD1	1:B:667:ILE:CD1	2.86	0.58
1:B:114:GLU:OE2	1:B:116:HIS:HB2	2.03	0.58
1:B:114:GLU:HG3	1:B:120:GLY:O	2.04	0.58
1:B:1258:PHE:O	1:B:1261:GLN:O	2.22	0.58
1:B:419:LEU:HD13	1:B:444:LEU:HD12	1.85	0.58
1:B:899:ASN:O	1:B:902:LYS:HB3	2.04	0.57
1:B:105:PHE:HD1	2:A:24:U:O2	1.86	0.57
1:B:412:HIS:CE1	1:B:413:GLN:HE22	2.22	0.57
1:B:185:PHE:HE1	1:B:242:ILE:HD11	1.69	0.57
1:B:306:LEU:O	1:B:306:LEU:HD12	2.04	0.57
1:B:592:GLY:O	1:B:596:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1215:ALA:HB3	1:B:1219:VAL:HG23	1.87	0.56
1:B:1139:VAL:HA	1:B:1167:THR:HA	1.88	0.56
1:B:1204:PHE:CD1	1:B:1342:VAL:HG13	2.42	0.55
2:A:46:A:H2'	2:A:47:A:H8	1.69	0.55
1:B:309:ASN:O	1:B:310:THR:HG22	2.07	0.55
1:B:353:ASP:CG	1:B:355:SER:HG	2.14	0.55
2:A:58:G:C2	2:A:60:C:O2	2.59	0.55
1:B:740:THR:O	1:B:743:VAL:HB	2.07	0.55
1:B:110:ASP:OD2	1:B:1131:TYR:OH	2.21	0.55
1:B:1206:LEU:HD13	1:B:1210:ARG:NH2	2.22	0.55
1:B:390:LEU:O	1:B:394:ASN:ND2	2.40	0.54
1:B:535:ARG:HG3	1:B:535:ARG:HH11	1.72	0.54
1:B:264:LEU:HD22	1:B:274:ASP:HB3	1.89	0.54
1:B:672:ASP:OD2	1:B:703:THR:N	2.38	0.54
1:B:302:LEU:HA	1:B:305:ILE:HG12	1.90	0.54
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.54
1:B:615:ILE:HG23	1:B:639:TYR:CE1	2.43	0.53
1:B:524:LEU:HD12	1:B:587:PHE:HE2	1.73	0.53
1:B:760:VAL:HG11	1:B:990:ASN:O	2.09	0.53
4:D:6:DG:C4	4:D:7:DC:C5	2.96	0.53
1:B:518:PHE:CG	1:B:667:ILE:HD12	2.43	0.53
1:B:680:LEU:O	1:B:684:LYS:HG3	2.09	0.53
1:B:1308:ASN:OD1	1:B:1327:PHE:N	2.39	0.53
2:A:54:G:C6	2:A:55:C:N4	2.77	0.53
1:B:279:LEU:O	1:B:283:GLY:N	2.40	0.53
1:B:1150:GLU:HB2	1:B:1155:LYS:HA	1.90	0.53
1:B:1269:ILE:O	1:B:1270:ILE:C	2.51	0.53
1:B:1145:VAL:HG21	1:B:1187:TYR:CZ	2.44	0.52
1:B:588:ASN:OD1	3:C:24:DG:N2	2.43	0.52
1:B:970:PHE:CD1	1:B:1080:PHE:HZ	2.27	0.52
1:B:1146:VAL:HG13	1:B:1191:LYS:HB2	1.91	0.52
1:B:695:GLN:O	1:B:697:ILE:N	2.43	0.52
1:B:475:PRO:HG3	2:A:59:U:O4	2.09	0.52
1:B:1145:VAL:HG21	1:B:1187:TYR:CE1	2.45	0.52
1:B:1271:GLU:HA	1:B:1271:GLU:OE1	2.09	0.52
1:B:1321:PRO:HG2	1:B:1335:ARG:HA	1.92	0.52
1:B:1206:LEU:HD23	1:B:1345:ALA:HB2	1.93	0.51
1:B:1253:GLU:O	1:B:1256:GLN:HB3	2.10	0.51
1:B:645:ASP:O	1:B:649:LYS:N	2.43	0.51
1:B:1301:PRO:HD2	1:B:1304:GLU:CD	2.36	0.51
1:B:342:GLN:HE22	1:B:383:MET:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:TYR:CB	1:B:863:ASN:ND2	2.73	0.51
1:B:1266:LEU:N	1:B:1266:LEU:CD2	2.72	0.50
1:B:1200:LYS:O	1:B:1201:TYR:HB2	2.11	0.50
1:B:105:PHE:CD1	2:A:24:U:C2	2.99	0.50
1:B:191:THR:O	1:B:195:LEU:HG	2.12	0.50
1:B:472:THR:HG23	2:A:59:U:OP2	2.11	0.49
1:B:615:ILE:HG23	1:B:639:TYR:CZ	2.47	0.49
1:B:376:ILE:HG22	1:B:380:LEU:HG	1.95	0.49
1:B:507:VAL:CB	1:B:660:GLY:O	2.61	0.49
1:B:553:PHE:HZ	1:B:587:PHE:CD2	2.30	0.49
1:B:1210:ARG:HE	1:B:1212:ARG:HH12	1.60	0.49
1:B:403:ARG:NH1	2:A:20:A:OP1	2.46	0.49
1:B:158:LEU:HA	1:B:161:MET:HE3	1.94	0.49
1:B:1097:LYS:HE3	1:B:1099:GLU:CD	2.38	0.48
1:B:201:ILE:HG23	1:B:229:LEU:HD12	1.94	0.48
1:B:750:VAL:HG22	1:B:1356:TYR:OH	2.13	0.48
1:B:501:ASN:HD22	1:B:666:LEU:CD1	2.25	0.48
1:B:643:PHE:HB3	1:B:647:VAL:HB	1.94	0.48
1:B:318:SER:OG	1:B:418:GLU:OE1	2.23	0.48
1:B:447:ARG:O	1:B:448:ILE:C	2.56	0.48
1:B:111:LYS:NZ	2:A:25:U:O2'	2.27	0.48
1:B:515:TYR:OH	2:A:5:C:OP1	2.30	0.48
1:B:678:THR:O	1:B:682:PHE:HB2	2.13	0.48
1:B:795:ILE:HG22	1:B:796:LEU:HD23	1.96	0.48
1:B:1207:GLU:OE2	1:B:1210:ARG:NH1	2.47	0.48
1:B:1237:TYR:CE1	1:B:1241:HIS:CE1	3.01	0.48
1:B:139:ARG:HH12	1:B:415:HIS:HD2	1.61	0.48
1:B:1256:GLN:OE1	1:B:1256:GLN:HA	2.14	0.48
2:A:40:C:H2'	2:A:41:A:C8	2.49	0.48
1:B:122:ILE:O	1:B:126:VAL:HG23	2.13	0.47
1:B:403:ARG:HD2	2:A:20:A:OP1	2.14	0.47
1:B:692:ASN:O	1:B:696:LEU:HD13	2.14	0.47
1:B:666:LEU:C	1:B:666:LEU:HD23	2.39	0.47
1:B:1196:ILE:HD11	1:B:1364:GLN:NE2	2.28	0.47
1:B:982:HIS:HE2	1:B:983:HIS:CE1	2.33	0.47
1:B:1239:ALA:O	1:B:1303:ARG:HA	2.15	0.46
1:B:165:ARG:NH1	2:A:18:A:OP1	2.47	0.46
1:B:105:PHE:CE1	2:A:24:U:H1'	2.51	0.46
1:B:553:PHE:HA	1:B:559:VAL:CG2	2.46	0.46
1:B:1075:ASP:O	1:B:1077:GLY:N	2.48	0.46
1:B:1210:ARG:HE	1:B:1212:ARG:NH1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:HG23	1:B:137:HIS:CE1	2.51	0.46
1:B:738:LEU:O	1:B:738:LEU:HD22	2.16	0.46
1:B:1308:ASN:N	1:B:1308:ASN:HD22	2.13	0.46
1:B:1356:TYR:HB3	2:A:81:G:N1	2.30	0.46
4:D:8:DT:H2''	4:D:9:DA:C5'	2.46	0.46
1:B:988:TYR:O	1:B:991:ALA:N	2.47	0.46
1:B:161:MET:HE1	1:B:422:ILE:HD12	1.98	0.46
1:B:464:TRP:CD1	1:B:464:TRP:C	2.94	0.45
1:B:146:THR:O	1:B:146:THR:OG1	2.33	0.45
1:B:223:GLU:O	1:B:227:ALA:HB3	2.16	0.45
2:A:38:A:N6	2:A:39:G:C6	2.84	0.45
1:B:317:LEU:O	1:B:320:SER:N	2.50	0.45
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.49	0.45
1:B:1221:GLN:HB2	1:B:1319:GLY:O	2.15	0.45
1:B:393:LEU:HD23	1:B:393:LEU:O	2.17	0.45
1:B:802:GLU:HB2	1:B:805:GLN:HB2	1.99	0.45
1:B:805:GLN:HE21	1:B:805:GLN:HB3	1.60	0.45
1:B:1122:ARG:HD3	1:B:1133:GLY:HA2	1.98	0.45
1:B:467:ARG:NH2	2:A:59:U:OP1	2.50	0.45
1:B:573:GLU:O	1:B:574:GLU:C	2.60	0.45
1:B:787:GLY:O	1:B:791:LEU:HB2	2.16	0.45
1:B:467:ARG:HD3	1:B:470:GLU:HA	1.98	0.44
1:B:560:THR:O	1:B:564:LEU:CB	2.65	0.44
1:B:982:HIS:NE2	1:B:983:HIS:NE2	2.65	0.44
1:B:1048:THR:HG22	1:B:1076:LYS:HD3	1.98	0.44
1:B:1226:LEU:HB3	1:B:1276:PHE:CZ	2.52	0.44
1:B:1036:TYR:HD1	1:B:1036:TYR:C	2.26	0.44
1:B:1062:LEU:HD23	1:B:1063:ILE:HG13	1.98	0.44
1:B:1202:SER:O	1:B:1213:MET:HA	2.16	0.44
1:B:20:VAL:HG11	1:B:751:MET:HE2	2.00	0.44
1:B:560:THR:O	1:B:564:LEU:N	2.51	0.44
1:B:876:VAL:CG2	1:B:903:ALA:HB3	2.42	0.44
1:B:1269:ILE:O	1:B:1271:GLU:N	2.51	0.44
1:B:373:TYR:CE1	1:B:398:LEU:HB3	2.52	0.44
1:B:325:TYR:O	1:B:328:HIS:HB3	2.18	0.44
1:B:133:PRO:HG2	1:B:137:HIS:CE1	2.53	0.43
1:B:456:ALA:HA	2:A:58:G:O2'	2.18	0.43
1:B:1089:MET:HA	1:B:1090:PRO:HD3	1.87	0.43
1:B:1344:ASP:HA	1:B:1362:LEU:O	2.18	0.43
1:B:148:LYS:HA	1:B:429:PHE:CD2	2.53	0.43
1:B:1036:TYR:C	1:B:1036:TYR:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:HA	1:B:243:ALA:HB3	1.99	0.43
1:B:322:ILE:O	1:B:325:TYR:HB3	2.18	0.43
1:B:333:THR:O	1:B:336:LYS:HB2	2.19	0.43
1:B:787:GLY:O	1:B:791:LEU:HD22	2.19	0.43
3:C:19:DA:C8	3:C:20:DT:H71	2.53	0.43
1:B:1123:LYS:O	1:B:1124:LYS:C	2.61	0.43
1:B:1262:HIS:O	1:B:1265:TYR:CD2	2.72	0.43
1:B:211:ILE:HD12	1:B:225:LEU:HA	2.00	0.43
1:B:671:ARG:NH2	1:B:678:THR:HG23	2.33	0.43
1:B:1204:PHE:CE1	1:B:1342:VAL:HG13	2.53	0.43
1:B:1216:SER:OG	1:B:1217:ALA:N	2.51	0.43
1:B:342:GLN:NE2	1:B:383:MET:HA	2.33	0.43
1:B:871:PRO:O	1:B:903:ALA:CB	2.66	0.43
1:B:929:LYS:O	1:B:932:ALA:HB3	2.19	0.43
2:A:38:A:C6	2:A:39:G:C6	3.06	0.43
1:B:1286:ASN:ND2	1:B:1332:ASP:O	2.52	0.43
1:B:168:PHE:CD2	1:B:412:HIS:CE1	3.06	0.43
1:B:1279:ARG:HG2	1:B:1280:VAL:HG13	2.00	0.43
3:C:2:DA:H2''	3:C:3:DA:C8	2.54	0.43
1:B:1266:LEU:HD23	1:B:1266:LEU:H	1.78	0.43
1:B:914:ALA:HB2	1:B:1036:TYR:HB2	2.01	0.42
1:B:239:GLY:O	1:B:243:ALA:N	2.49	0.42
1:B:469:SER:CB	1:B:481:VAL:HG23	2.49	0.42
1:B:1351:SER:HB3	1:B:1356:TYR:HB2	2.02	0.42
2:A:38:A:C6	2:A:39:G:C5	3.07	0.42
1:B:977:GLU:H	1:B:977:GLU:CD	2.28	0.42
1:B:136:TYR:HE1	1:B:139:ARG:NH2	2.17	0.42
1:B:918:LYS:NZ	1:B:1007:GLU:OE2	2.52	0.42
2:A:6:U:H2'	2:A:7:C:C6	2.55	0.42
1:B:358:GLY:HA2	1:B:375:PHE:CE1	2.55	0.42
1:B:359:TYR:O	1:B:362:TYR:HB3	2.20	0.42
1:B:1065:THR:OG1	1:B:1066:ASN:N	2.52	0.42
2:A:42:A:C6	2:A:43:G:C6	3.08	0.42
1:B:116:HIS:CE1	1:B:122:ILE:HD13	2.55	0.42
1:B:236:GLY:O	1:B:240:ASN:ND2	2.53	0.42
1:B:351:PHE:C	1:B:360:ALA:HB2	2.44	0.42
1:B:245:SER:HA	1:B:297:SER:CB	2.50	0.42
1:B:1097:LYS:HE3	1:B:1099:GLU:OE2	2.19	0.42
1:B:625:LEU:HD12	1:B:625:LEU:HA	1.91	0.42
1:B:944:ASP:OD2	1:B:948:LYS:HB2	2.20	0.42
1:B:1264:HIS:C	1:B:1266:LEU:H	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD13	1:B:155:TYR:CE1	2.55	0.42
2:A:42:A:N6	2:A:43:G:C6	2.88	0.42
1:B:1036:TYR:HD1	1:B:1036:TYR:O	2.03	0.41
3:C:19:DA:H5''	3:C:19:DA:H8	1.85	0.41
1:B:985:HIS:O	1:B:988:TYR:HB3	2.19	0.41
1:B:1229:PRO:HD3	1:B:1272:GLN:NE2	2.35	0.41
1:B:1334:LYS:NZ	3:C:3:DA:OP2	2.49	0.41
1:B:666:LEU:HD21	1:B:693:PHE:HE1	1.83	0.41
1:B:1147:ALA:HB2	1:B:1190:VAL:HA	2.02	0.41
1:B:1277:SER:HA	1:B:1281:ILE:HB	2.02	0.41
1:B:1335:ARG:CG	1:B:1335:ARG:NH1	2.81	0.41
1:B:28:PRO:HG2	1:B:47:LEU:HD12	2.02	0.41
1:B:465:MET:HE3	1:B:467:ARG:HG3	2.02	0.41
1:B:1147:ALA:HB1	1:B:1188:LYS:O	2.20	0.41
3:C:13:DT:H2'	3:C:14:DT:H6	1.85	0.41
1:B:873:GLU:HG3	1:B:904:GLU:HA	2.02	0.41
1:B:1264:HIS:C	1:B:1266:LEU:N	2.76	0.41
1:B:1266:LEU:HB2	1:B:1267:ASP:H	1.75	0.41
2:A:19:A:H2'	2:A:20:A:O4'	2.20	0.41
1:B:624:THR:HA	1:B:656:TYR:O	2.20	0.41
1:B:1177:ASN:ND2	1:B:1180:ASP:OD2	2.53	0.41
1:B:62:THR:HG22	2:A:63:U:O2'	2.21	0.41
1:B:1170:GLU:O	1:B:1173:SER:HB3	2.21	0.41
1:B:553:PHE:CD2	1:B:559:VAL:HG21	2.56	0.41
1:B:113:HIS:C	1:B:114:GLU:O	2.64	0.41
1:B:325:TYR:CD1	2:A:44:U:C2	3.08	0.41
1:B:437:ARG:O	1:B:441:GLU:HG3	2.20	0.41
1:B:498:PHE:HB3	1:B:505:GLU:O	2.21	0.41
1:B:501:ASN:HD22	1:B:666:LEU:HD11	1.85	0.41
1:B:508:LEU:HD21	1:B:664:ARG:HB2	2.02	0.41
1:B:996:ALA:O	1:B:999:LYS:N	2.53	0.41
1:B:317:LEU:O	1:B:318:SER:C	2.65	0.40
1:B:665:LYS:O	1:B:666:LEU:C	2.64	0.40
1:B:403:ARG:HH11	2:A:20:A:P	2.45	0.40
1:B:419:LEU:HD13	1:B:444:LEU:CD1	2.51	0.40
1:B:692:ASN:ND2	3:C:26:DT:H2''	2.32	0.40
1:B:1210:ARG:HG3	1:B:1280:VAL:HA	2.03	0.40
1:B:1351:SER:O	1:B:1352:ILE:C	2.64	0.40
1:B:459:ASN:ND2	2:A:56:U:H1'	2.37	0.40
1:B:17:GLY:HA3	1:B:983:HIS:O	2.22	0.40
1:B:356:LYS:C	1:B:358:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1303:ARG:HD2	1:B:1307:GLU:OE2	2.21	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	B	1292/1368 (94%)	1144 (88%)	126 (10%)	22 (2%)	7	30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	LEU
1	B	607	LEU
1	B	114	GLU
1	B	696	LEU
1	B	906	GLY
1	B	908	LEU
1	B	992	VAL
1	B	30	LYS
1	B	204	SER
1	B	205	GLY
1	B	576	ASP
1	B	695	GLN
1	B	1076	LYS
1	B	1266	LEU
1	B	87	SER
1	B	464	TRP
1	B	574	GLU
1	B	1267	ASP
1	B	1301	PRO
1	B	1270	ILE

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Mol	Chain	Res	Type
1	B	592	GLY
1	B	670	ILE

5.3.2 Protein sidechains ⓘ

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	B	969/1226 (79%)	884 (91%)	85 (9%)	9 33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	42	SER
1	B	62	THR
1	B	82	LEU
1	B	106	LEU
1	B	110	ASP
1	B	112	LYS
1	B	122	ILE
1	B	130	GLU
1	B	134	THR
1	B	139	ARG
1	B	174	LEU
1	B	177	ASP
1	B	199	ASN
1	B	202	ASN
1	B	207	ASP
1	B	213	SER
1	B	216	LEU
1	B	224	ASN
1	B	233	LYS
1	B	242	ILE
1	B	244	LEU
1	B	273	ASP
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	310	THR
1	B	334	LEU
1	B	375	PHE
1	B	403	ARG
1	B	435	ASP
1	B	438	GLU
1	B	455	LEU
1	B	466	THR
1	B	490	SER
1	B	506	LYS
1	B	519	THR
1	B	535	ARG
1	B	561	VAL
1	B	596	ASP
1	B	628	ASP
1	B	657	THR
1	B	664	ARG
1	B	671	ARG
1	B	726	ASN
1	B	738	LEU
1	B	783	ARG
1	B	786	GLU
1	B	791	LEU
1	B	793	SER
1	B	794	GLN
1	B	798	GLU
1	B	799	HIS
1	B	801	VAL
1	B	802	GLU
1	B	805	GLN
1	B	851	SER
1	B	856	VAL
1	B	891	LEU
1	B	892	ILE
1	B	902	LYS
1	B	959	LYS
1	B	960	SER
1	B	1036	TYR
1	B	1040	SER
1	B	1050	ILE
1	B	1088	SER
1	B	1115	ASN

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Mol	Chain	Res	Type
1	B	1119	LEU
1	B	1139	VAL
1	B	1154	SER
1	B	1214	LEU
1	B	1226	LEU
1	B	1253	GLU
1	B	1264	HIS
1	B	1266	LEU
1	B	1272	GLN
1	B	1312	LEU
1	B	1314	THR
1	B	1318	LEU
1	B	1329	THR
1	B	1334	LYS
1	B	1335	ARG
1	B	1342	VAL
1	B	1347	LEU
1	B	1358	THR
1	B	1365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	342	GLN
1	B	413	GLN
1	B	415	HIS
1	B	459	ASN
1	B	501	ASN
1	B	504	ASN
1	B	511	HIS
1	B	556	ASN
1	B	692	ASN
1	B	805	GLN
1	B	863	ASN
1	B	888	ASN
1	B	1041	ASN
1	B	1115	ASN
1	B	1311	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	79/83 (95%)	19 (24%)	4 (5%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	A
2	A	10	U
2	A	24	U
2	A	26	A
2	A	28	A
2	A	29	G
2	A	32	A
2	A	35	A
2	A	39	G
2	A	42	A
2	A	43	G
2	A	44	U
2	A	45	U
2	A	51	A
2	A	59	U
2	A	63	U
2	A	68	A
2	A	74	A
2	A	81	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	8	A
2	A	9	A
2	A	28	A
2	A	42	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	1308/1368 (95%)	0.70	152 (11%) 9 5	25, 82, 155, 229	0
2	A	80/83 (96%)	-0.05	1 (1%) 75 53	26, 43, 122, 147	0
3	C	27/28 (96%)	0.63	3 (11%) 10 6	40, 71, 145, 186	0
4	D	11/12 (91%)	1.22	3 (27%) 1 1	63, 85, 159, 164	0
All	All	1426/1491 (95%)	0.67	159 (11%) 10 5	25, 78, 155, 229	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	LEU	7.5
1	B	893	THR	6.8
1	B	586	ARG	5.5
1	B	226	ILE	5.5
1	B	229	LEU	4.6
1	B	224	ASN	4.6
1	B	806	LEU	4.4
1	B	892	ILE	4.4
1	B	867	SER	4.4
1	B	238	PHE	4.4
1	B	897	PHE	4.2
1	B	214	ALA	4.2
1	B	801	VAL	4.1
1	B	872	SER	4.1
1	B	583	VAL	4.0
1	B	868	ASP	4.0
1	B	559	VAL	3.9
1	B	385	GLY	3.9
1	B	1264	HIS	3.9
1	B	524	LEU	3.9
1	B	821	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	529	TYR	3.8
1	B	611	GLU	3.8
1	B	609	ASN	3.7
1	B	261	ASP	3.6
1	B	585	ASP	3.5
1	B	917	ILE	3.5
1	B	875	VAL	3.4
1	B	1050	ILE	3.4
1	B	688	PHE	3.4
1	B	612	ASN	3.3
1	B	587	PHE	3.3
1	B	827	GLU	3.3
1	B	869	ASN	3.3
1	B	800	PRO	3.3
1	B	222	LEU	3.3
1	B	1083	VAL	3.2
1	B	241	LEU	3.2
1	B	908	LEU	3.2
1	B	858	THR	3.2
1	B	605	ASP	3.1
1	B	896	LYS	3.1
1	B	212	LEU	3.1
1	B	674	GLN	3.1
1	B	234	LYS	3.1
1	B	815	TYR	3.1
1	B	1006	SER	3.0
1	B	651	LEU	3.0
1	B	675	SER	3.0
1	B	900	LEU	3.0
1	B	822	MET	2.9
1	B	881	ASN	2.9
1	B	852	ILE	2.9
1	B	841	ILE	2.9
1	B	853	ASP	2.9
1	B	628	ASP	2.8
1	B	849	ASP	2.8
1	B	667	ILE	2.8
2	A	9	A	2.8
1	B	871	PRO	2.8
1	B	700	ASP	2.8
1	B	563	GLN	2.8
1	B	838	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	216	LEU	2.8
1	B	182	ASP	2.8
1	B	687	GLY	2.8
1	B	223	GLU	2.8
1	B	231	GLY	2.7
1	B	829	ASP	2.7
1	B	828	LEU	2.7
1	B	187	GLN	2.7
1	B	707	ASP	2.7
1	B	518	PHE	2.7
1	B	693	PHE	2.7
1	B	685	SER	2.7
1	B	206	VAL	2.6
1	B	889	ALA	2.6
1	B	1039	TYR	2.6
1	B	186	ILE	2.6
1	B	905	ARG	2.6
1	B	814	TYR	2.6
1	B	534	MET	2.6
1	B	543	ASP	2.6
1	B	946	ASN	2.6
3	C	28	DT	2.5
1	B	712	GLN	2.5
1	B	291	LEU	2.5
1	B	891	LEU	2.5
1	B	235	ASN	2.5
1	B	584	GLU	2.5
1	B	211	ILE	2.5
1	B	857	LEU	2.5
3	C	22	DG	2.5
1	B	882	TYR	2.5
1	B	540	LEU	2.5
1	B	208	ALA	2.5
1	B	711	ALA	2.5
1	B	246	LEU	2.5
4	D	3	DA	2.4
1	B	284	ASP	2.4
4	D	2	DA	2.4
1	B	227	ALA	2.4
1	B	554	LYS	2.4
1	B	539	PHE	2.4
1	B	912	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1262	HIS	2.4
1	B	201	ILE	2.4
1	B	823	TYR	2.4
1	B	230	PRO	2.4
1	B	270	THR	2.3
1	B	190	GLN	2.3
1	B	894	GLN	2.3
1	B	824	VAL	2.3
1	B	1302	ILE	2.3
1	B	1265	TYR	2.3
1	B	666	LEU	2.3
1	B	181	VAL	2.3
1	B	542	GLY	2.3
1	B	531	THR	2.3
1	B	825	ASP	2.3
1	B	670	ILE	2.3
1	B	689	ALA	2.3
1	B	560	THR	2.3
1	B	218	LYS	2.3
1	B	835	ASP	2.3
3	C	23	DA	2.2
1	B	217	SER	2.2
1	B	1290	VAL	2.2
1	B	264	LEU	2.2
1	B	569	PHE	2.2
1	B	213	SER	2.2
1	B	921	LEU	2.2
4	D	12	DG	2.2
1	B	1072	ILE	2.2
1	B	886	LEU	2.2
1	B	1030	GLY	2.2
1	B	557	ARG	2.1
1	B	606	PHE	2.1
1	B	550	ASP	2.1
1	B	608	ASP	2.1
1	B	236	GLY	2.1
1	B	577	SER	2.1
1	B	174	LEU	2.1
1	B	580	ILE	2.1
1	B	287	ALA	2.1
1	B	610	GLU	2.1
1	B	809	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	842	VAL	2.1
1	B	258	LEU	2.1
1	B	1254	GLN	2.1
1	B	895	ARG	2.1
1	B	257	ASP	2.1
1	B	269	ASP	2.0
1	B	1125	ASP	2.0
1	B	198	GLU	2.0
1	B	215	ARG	2.0
1	B	839	ASP	2.0
1	B	558	LYS	2.0
1	B	910	GLU	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.