



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 4CRX / pdb_00004crx
Title : ASYMMETRIC DNA-BENDING IN THE CRE-LOXP SITE-SPECIFIC RE-COMBINATION SYNAPSE
Authors : Guo, F.; Gopaul, D.N.; Van Duyne, G.D.
Deposited on : 1999-04-20
Resolution : 2.20 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

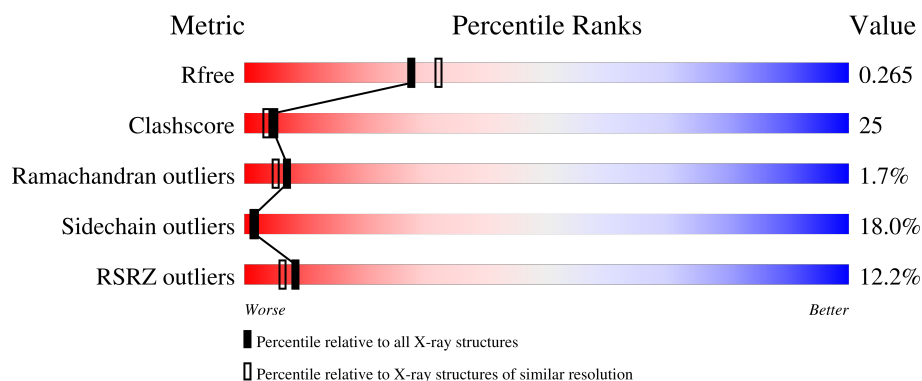
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	C	35	3% 69% 31%
1	D	35	3% 54% 37% 6%
2	A	322	12% 57% 31% 11%
2	B	322	14% 55% 35% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6999 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 DNA chain called DNA (35 NUCLEOTIDE CRE RECOGNITION SITE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	35	Total	C	N	O	P	0	0	0
			714	345	126	209	34			
1	D	35	Total	C	N	O	P	0	0	0
			714	345	126	209	34			

- Molecule 2 is a protein called PROTEIN (CRE RECOMBINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	322	Total	C	N	O	S	0	0	0
			2549	1584	484	466	15			
2	B	322	Total	C	N	O	S	0	0	0
			2549	1584	484	466	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	LYS	ARG	engineered mutation	UNP P06956
B	173	LYS	ARG	engineered mutation	UNP P06956

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	71	Total	O	0	0
			71	71		
3	D	87	Total	O	0	0
			87	87		
3	A	149	Total	O	0	0
			149	149		
3	B	166	Total	O	0	0
			166	166		

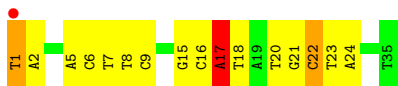
3 Residue-property plots

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.

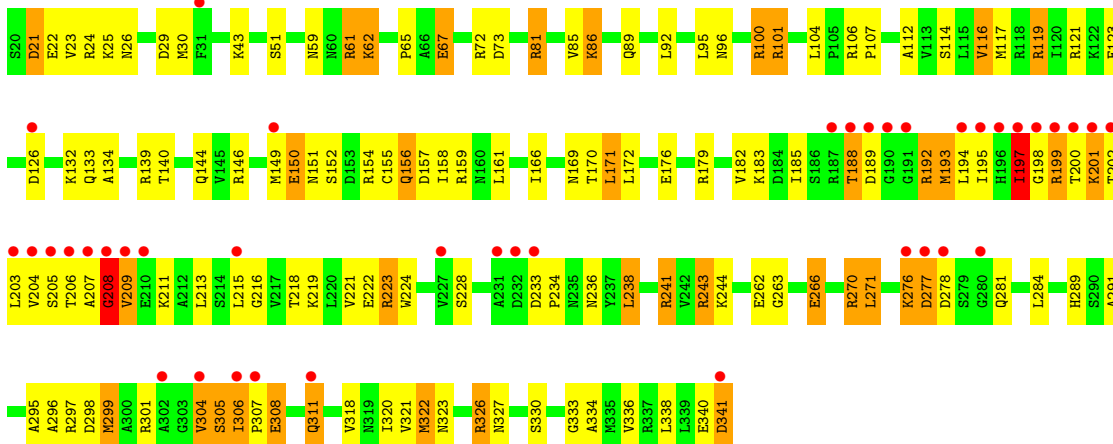
- Molecule 1: DNA (35 NUCLEOTIDE CRE RECOGNITION SITE)



- Molecule 1: DNA (35 NUCLEOTIDE CRE RECOGNITION SITE)

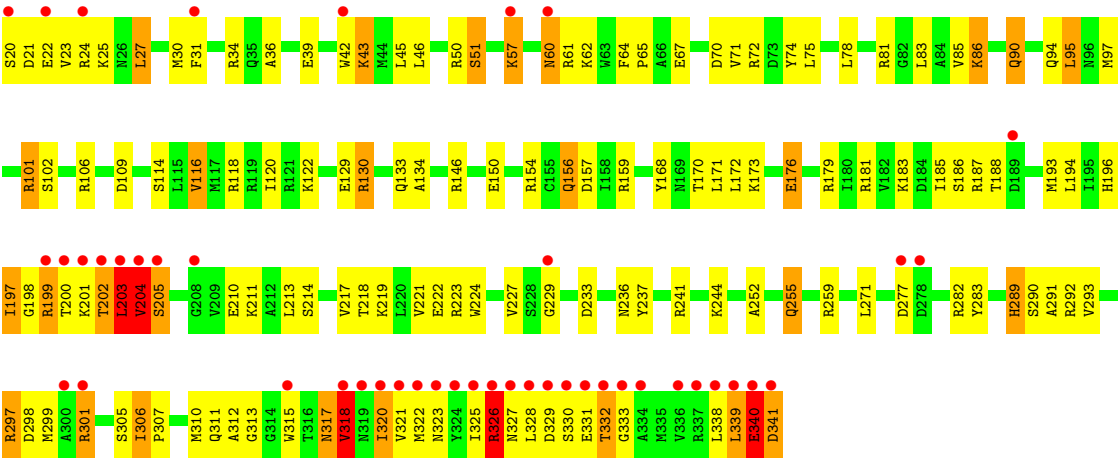


- Molecule 2: PROTEIN (CRE RECOMBINASE)



- Molecule 2: PROTEIN (CRE RECOMBINASE)





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.80Å 122.10Å 181.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.30 – 2.20 32.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.7 (32.30-2.20) 91.0 (32.30-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.213 , 0.251 0.232 , 0.265	Depositor DCC
R_{free} test set	2822 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 85.4	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	0.93	EDS
Total number of atoms	6999	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	C	0.37	0/800	0.86	0/1233
1	D	0.46	0/800	0.97	5/1233 (0.4%)
2	A	0.71	2/2590 (0.1%)	1.21	11/3490 (0.3%)
2	B	4.68	5/2589 (0.2%)	1.70	15/3487 (0.4%)
All	All	2.93	7/6779 (0.1%)	1.35	31/9443 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	A	0	3
2	B	0	2
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	ASP	C-OXT	226.32	5.76	1.23
2	B	340	GLU	C-N	-44.40	0.71	1.33
2	B	204	VAL	C-N	35.84	1.83	1.33
2	B	326	ARG	C-N	32.83	1.77	1.33
2	A	208	GLY	C-N	-28.31	0.95	1.33
2	B	198	GLY	C-N	-19.82	1.04	1.33
2	A	306	ILE	CA-CB	5.23	1.56	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	GLU	O-C-N	-70.92	29.51	123.12
2	A	208	GLY	O-C-N	-30.95	82.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	VAL	O-C-N	-27.70	87.95	122.57
2	A	197	ILE	O-C-N	-27.61	92.30	122.95
2	B	326	ARG	O-C-N	17.32	145.62	122.59
2	B	198	GLY	O-C-N	-16.44	101.32	122.70
2	B	204	VAL	CA-C-N	-11.15	100.23	121.54
2	B	204	VAL	C-N-CA	-11.15	100.23	121.54
1	D	1	DT	C1'-O4'-C4'	-10.78	93.53	109.70
2	A	341	ASP	CA-C-O	9.67	150.00	121.00
2	B	198	GLY	CA-C-N	7.64	132.93	122.77
2	B	198	GLY	C-N-CA	7.64	132.93	122.77
2	A	197	ILE	CA-C-N	-6.73	108.21	121.41
2	A	197	ILE	C-N-CA	-6.73	108.21	121.41
2	A	134	ALA	N-CA-C	6.63	119.58	110.24
2	A	81	ARG	N-CA-C	-6.35	105.50	113.18
2	B	290	SER	N-CA-C	6.22	118.86	111.33
2	A	192	ARG	N-CA-C	-6.20	101.34	110.52
2	A	21	ASP	N-CA-C	-6.15	104.69	111.82
2	A	333	GLY	N-CA-C	5.76	121.34	112.81
2	A	243	ARG	N-CA-C	5.74	117.31	110.19
2	B	36	ALA	N-CA-C	-5.73	105.54	112.54
2	B	134	ALA	N-CA-C	5.71	117.67	110.24
1	D	1	DT	C2-N1-C1'	-5.53	111.06	119.35
1	D	17	DA	N9-C1'-C2'	-5.36	105.45	113.50
2	B	199	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	D	1	DT	O4'-C1'-N1	5.18	116.17	108.40
2	B	185	ILE	N-CA-C	5.17	115.76	108.36
2	B	21	ASP	N-CA-C	-5.16	106.50	112.89
1	D	22	DC	O3'-P-O5'	-5.08	96.38	104.00
2	B	298	ASP	N-CA-C	-5.01	105.49	112.45

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	197	ILE	Mainchain
2	A	208	GLY	Mainchain,Peptide
2	B	340	GLU	Mainchain,Peptide
1	D	17	DA	Sidechain

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	C	714	0	400	16	0
1	D	714	0	400	28	2
2	A	2549	0	2568	146	3
2	B	2549	0	2566	158	7
3	A	149	0	0	13	0
3	B	166	0	0	12	7
3	C	71	0	0	6	0
3	D	87	0	0	1	0
All	All	6999	0	5934	314	10

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 25.

All (314) 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)
2:B:340:GLU:CA	2:B:341:ASP:N	1.76	1.45
2:B:326:ARG:C	2:B:327:ASN:N	1.77	1.41
2:B:204:VAL:C	2:B:205:SER:N	1.83	1.34
2:A:306:ILE:CG2	2:A:307:PRO:HD3	1.58	1.33
2:A:207:ALA:CB	2:B:130:ARG:HG2	1.56	1.33
2:A:207:ALA:HB2	2:B:130:ARG:CG	1.67	1.25
2:A:207:ALA:CA	2:B:130:ARG:HG2	1.67	1.24
2:B:340:GLU:O	2:B:341:ASP:CB	1.92	1.17
2:B:330:SER:O	3:B:499:HOH:O	1.59	1.16
2:B:340:GLU:O	2:B:341:ASP:HA	1.39	1.12
2:B:297:ARG:CG	2:B:328:LEU:HD11	1.73	1.11
2:A:207:ALA:HB2	2:B:130:ARG:HG2	1.11	1.09
2:B:297:ARG:CB	2:B:328:LEU:HD11	1.82	1.09
2:B:340:GLU:O	2:B:341:ASP:C	1.95	1.08
2:A:207:ALA:HB2	2:B:130:ARG:CB	1.83	1.07
1:D:1:DT:H1'	1:D:2:DA:OP2	1.53	1.06
2:A:193:MET:HE1	2:A:221:VAL:HB	1.36	1.06
1:D:17:DA:H5'	1:D:17:DA:H8	1.21	1.05
2:B:340:GLU:O	2:B:341:ASP:CA	0.76	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:306:ILE:HG23	2:A:307:PRO:HD3	1.08	1.05
2:B:326:ARG:HG2	2:B:327:ASN:N	1.72	1.04
2:B:332:THR:C	2:B:333:GLY:N	2.17	1.03
2:A:306:ILE:HG23	2:A:307:PRO:CD	1.87	1.02
2:B:203:LEU:HD12	2:B:204:VAL:H	1.23	1.02
2:B:332:THR:C	2:B:333:GLY:CA	2.35	0.99
2:A:146:ARG:O	2:A:150:GLU:HB2	1.63	0.99
2:B:204:VAL:O	2:B:205:SER:O	1.80	0.98
2:A:306:ILE:HD11	2:A:318:VAL:HG11	1.43	0.98
2:A:197:ILE:HG12	2:A:198:GLY:N	1.75	0.97
2:B:297:ARG:HB2	2:B:328:LEU:HD11	1.43	0.97
2:A:197:ILE:CG1	2:A:198:GLY:N	2.28	0.95
1:C:5:DA:H2''	1:C:6:DC:H5''	1.49	0.92
1:D:17:DA:H5'	1:D:17:DA:C8	2.05	0.92
2:A:306:ILE:CG2	2:A:307:PRO:CD	2.46	0.92
2:B:173:LYS:HZ3	2:B:201:LYS:HD3	1.35	0.91
2:A:156:GLN:HE21	2:A:156:GLN:H	1.18	0.90
2:A:306:ILE:HG22	2:A:307:PRO:HD3	1.51	0.89
2:B:173:LYS:NZ	2:B:201:LYS:HD3	1.87	0.89
2:B:197:ILE:HD13	2:B:211:LYS:HG3	1.53	0.89
2:B:297:ARG:NH1	2:B:328:LEU:CD2	2.33	0.89
2:B:326:ARG:CA	2:B:327:ASN:N	2.35	0.88
2:A:197:ILE:CG1	2:A:198:GLY:H	1.84	0.87
1:D:20:DT:H2''	1:D:21:DG:H5'	1.56	0.86
2:A:276:LYS:HD2	2:A:284:LEU:HB2	1.56	0.86
2:B:332:THR:C	2:B:333:GLY:HA2	2.01	0.85
2:B:202:THR:O	2:B:203:LEU:HB2	1.76	0.85
2:B:129:GLU:O	2:B:130:ARG:HD3	1.78	0.84
2:B:326:ARG:CG	2:B:327:ASN:N	2.43	0.82
2:B:297:ARG:CG	2:B:328:LEU:CD1	2.55	0.81
2:B:204:VAL:C	2:B:205:SER:CA	2.54	0.81
1:D:17:DA:H2''	1:D:18:DT:O5'	1.80	0.81
2:B:340:GLU:C	2:B:341:ASP:N	0.71	0.81
3:D:61:HOH:O	2:A:241:ARG:HD3	1.80	0.80
2:A:207:ALA:HB2	2:B:130:ARG:HB2	1.63	0.80
2:B:176:GLU:OE1	2:B:200:THR:CB	2.30	0.79
2:A:199:ARG:HD2	2:A:209:VAL:HG21	1.63	0.79
2:B:340:GLU:HA	2:B:341:ASP:N	1.94	0.79
1:C:24:DA:H5'	3:C:79:HOH:O	1.81	0.78
2:A:172:LEU:HD22	2:A:197:ILE:HD13	1.64	0.78
2:B:321:VAL:HG23	3:B:480:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:O	2:B:205:SER:N	2.18	0.77
2:B:203:LEU:HD12	2:B:204:VAL:N	1.98	0.77
2:B:297:ARG:NH1	2:B:328:LEU:HD23	1.99	0.76
2:A:193:MET:HE2	2:A:218:THR:HG23	1.66	0.76
2:A:172:LEU:CD2	2:A:197:ILE:HD13	2.16	0.76
1:D:5:DA:H2"	1:D:6:DC:H5"	1.66	0.75
2:A:172:LEU:HD22	2:A:197:ILE:CD1	2.16	0.75
2:B:199:ARG:NH1	3:B:492:HOH:O	2.18	0.75
2:B:297:ARG:HH11	2:B:328:LEU:CD2	1.98	0.75
2:A:208:GLY:C	2:A:209:VAL:HG23	2.10	0.75
2:A:207:ALA:HA	2:B:130:ARG:HG2	1.64	0.75
1:D:17:DA:H3'	2:A:202:THR:HG21	1.68	0.74
2:A:207:ALA:HA	2:B:130:ARG:NE	2.03	0.74
2:B:326:ARG:CB	2:B:327:ASN:N	2.51	0.73
2:B:176:GLU:OE1	2:B:200:THR:HB	1.89	0.73
1:D:24:DA:C5'	2:B:201:LYS:HG3	2.20	0.72
2:A:207:ALA:N	2:B:130:ARG:HG2	2.05	0.72
2:B:325:ILE:HG22	2:B:331:GLU:HG3	1.72	0.71
2:B:176:GLU:OE1	2:B:200:THR:HG22	1.90	0.71
2:B:214:SER:O	2:B:218:THR:HG23	1.90	0.71
2:B:299:MET:HE1	2:B:312:ALA:HB2	1.73	0.70
2:A:197:ILE:HG13	2:A:198:GLY:H	1.54	0.70
2:A:270:ARG:HH11	2:A:270:ARG:HG3	1.57	0.70
2:A:192:ARG:HE	2:A:215:LEU:HG	1.57	0.69
2:B:332:THR:O	2:B:333:GLY:N	2.24	0.69
2:B:31:PHE:CE1	2:B:34:ARG:NH1	2.61	0.69
2:A:188:THR:OG1	2:A:194:LEU:HD22	1.92	0.69
2:A:207:ALA:CA	2:B:130:ARG:CG	2.60	0.69
2:A:112:ALA:O	2:A:116:VAL:HG22	1.93	0.68
2:B:51:SER:HB3	2:B:74:TYR:OH	1.93	0.68
2:A:65:PRO:HB3	2:A:104:LEU:HD13	1.76	0.68
2:B:146:ARG:O	2:B:150:GLU:HB2	1.93	0.67
2:A:119:ARG:O	2:A:123:GLU:HG3	1.95	0.67
2:A:277:ASP:HB2	2:A:284:LEU:HD13	1.75	0.67
2:A:216:GLY:HA2	2:A:219:LYS:HE3	1.77	0.67
2:A:341:ASP:OD1	3:A:460:HOH:O	2.12	0.66
2:B:133:GLN:CD	2:B:326:ARG:NH2	2.54	0.66
2:A:72:ARG:HG3	2:A:116:VAL:HG21	1.78	0.65
2:A:121:ARG:NH1	3:A:482:HOH:O	2.30	0.65
2:B:233:ASP:O	2:B:236:ASN:HB2	1.96	0.65
1:D:15:DG:O6	2:A:86:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:PHE:O	2:B:34:ARG:HG3	1.98	0.64
2:B:176:GLU:OE1	2:B:200:THR:CG2	2.45	0.64
2:B:42:TRP:O	2:B:46:LEU:HG	1.97	0.64
1:C:5:DA:C2'	1:C:6:DC:H5''	2.24	0.64
1:C:16:DC:C5'	2:B:201:LYS:HE2	2.27	0.64
2:A:152:SER:O	2:A:223:ARG:NH2	2.31	0.63
2:A:156:GLN:H	2:A:156:GLN:NE2	1.94	0.63
1:D:24:DA:H5''	2:B:201:LYS:HG3	1.79	0.63
2:A:277:ASP:OD1	2:A:277:ASP:N	2.32	0.62
2:B:67:GLU:HG3	3:B:349:HOH:O	1.99	0.62
2:B:299:MET:HE1	2:B:312:ALA:CB	2.30	0.62
1:C:16:DC:H5'	2:B:201:LYS:HE2	1.82	0.61
2:A:193:MET:HE1	2:A:221:VAL:CB	2.24	0.61
2:A:271:LEU:HD22	2:A:271:LEU:O	2.00	0.61
2:A:276:LYS:HG3	2:A:277:ASP:H	1.65	0.61
2:B:297:ARG:HG3	2:B:328:LEU:HD11	1.79	0.61
2:A:59:ASN:O	2:A:61:ARG:HD3	1.99	0.61
2:B:133:GLN:CD	2:B:326:ARG:HH22	2.08	0.61
2:A:176:GLU:HB3	2:A:197:ILE:HD11	1.81	0.61
2:B:193:MET:H	2:B:218:THR:HG21	1.65	0.61
2:A:24:ARG:HG3	2:A:24:ARG:HH11	1.65	0.61
2:B:223:ARG:O	2:B:227:VAL:HG23	2.01	0.61
1:D:1:DT:H1'	1:D:2:DA:P	2.41	0.60
2:B:332:THR:O	2:B:333:GLY:CA	2.48	0.60
2:A:305:SER:OG	2:A:308:GLU:HG3	2.01	0.60
2:B:306:ILE:N	2:B:307:PRO:HD2	2.15	0.60
1:D:17:DA:H3'	2:A:202:THR:CG2	2.32	0.60
1:D:17:DA:C3'	2:A:202:THR:HG21	2.31	0.60
2:A:144:GLN:NE2	3:A:472:HOH:O	2.34	0.59
2:B:50:ARG:NH2	3:B:396:HOH:O	2.35	0.59
2:A:185:ILE:CG2	2:A:193:MET:HG2	2.32	0.59
2:B:204:VAL:C	2:B:205:SER:O	2.44	0.59
2:B:170:THR:O	2:B:171:LEU:HB2	2.02	0.59
1:D:17:DA:H4'	2:A:201:LYS:NZ	2.18	0.59
2:A:193:MET:HE2	2:A:218:THR:HA	1.83	0.59
2:A:30:MET:HE2	2:A:101:ARG:HB3	1.84	0.59
2:B:173:LYS:HG2	2:B:289:HIS:HE1	1.68	0.59
2:B:176:GLU:OE1	2:B:200:THR:HA	2.03	0.59
2:B:326:ARG:HG2	2:B:327:ASN:CA	2.33	0.59
2:A:299:MET:HG2	2:A:304:VAL:HG21	1.85	0.58
2:A:192:ARG:NE	2:A:215:LEU:HG	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:299:MET:O	2:A:304:VAL:HG23	2.03	0.58
1:D:17:DA:C3'	2:A:202:THR:CG2	2.80	0.58
1:D:24:DA:H4'	2:B:201:LYS:HD2	1.84	0.58
2:A:62:LYS:HE2	2:A:67:GLU:OE2	2.04	0.58
2:B:297:ARG:HB2	2:B:328:LEU:CD1	2.26	0.58
2:A:208:GLY:C	2:A:209:VAL:CG2	2.73	0.57
2:B:159:ARG:HB2	2:B:224:TRP:CZ3	2.38	0.57
2:B:196:HIS:HD2	3:B:474:HOH:O	1.86	0.57
2:A:185:ILE:HG22	2:A:193:MET:HG2	1.85	0.57
2:A:263:GLY:HA2	2:A:266:GLU:HG3	1.87	0.57
2:B:310:MET:SD	2:B:318:VAL:HG13	2.44	0.57
2:A:100:ARG:NH1	3:A:400:HOH:O	2.36	0.57
2:A:203:LEU:HD11	2:B:85:VAL:HB	1.87	0.57
2:B:204:VAL:C	2:B:205:SER:C	2.73	0.57
1:D:1:DT:H4'	1:D:2:DA:OP2	2.05	0.57
2:A:318:VAL:HA	2:A:321:VAL:HG12	1.86	0.56
2:B:282:ARG:O	2:B:283:TYR:HB2	2.05	0.56
2:A:24:ARG:HG3	2:A:24:ARG:NH1	2.19	0.56
2:B:213:LEU:HB2	2:B:218:THR:HG22	1.86	0.56
1:D:20:DT:H2''	1:D:21:DG:C5'	2.33	0.56
1:C:6:DC:H2'	1:C:7:DT:H72	1.87	0.56
2:A:201:LYS:HD2	3:A:469:HOH:O	2.05	0.55
2:B:297:ARG:HH11	2:B:328:LEU:HD22	1.72	0.55
1:D:5:DA:C2'	1:D:6:DC:H5''	2.34	0.55
2:B:318:VAL:O	2:B:322:MET:HG2	2.07	0.55
2:A:188:THR:OG1	2:A:194:LEU:HB2	2.07	0.55
1:C:34:DA:H2''	1:C:35:DT:OP2	2.08	0.54
2:A:183:LYS:HG3	2:A:183:LYS:O	2.08	0.54
2:B:197:ILE:CD1	2:B:211:LYS:HG3	2.31	0.54
2:B:301:ARG:HD3	2:B:330:SER:HB3	1.89	0.54
2:A:262:GLU:O	2:A:266:GLU:HG2	2.08	0.54
2:B:181:ARG:NH2	2:B:252:ALA:O	2.41	0.54
2:B:202:THR:O	2:B:203:LEU:CB	2.53	0.54
2:A:89:GLN:HG2	2:A:117:MET:CE	2.39	0.53
1:D:16:DC:H4'	1:D:16:DC:OP1	2.08	0.53
2:A:318:VAL:O	2:A:322:MET:HB2	2.08	0.53
2:B:154:ARG:HD3	2:B:157:ASP:OD2	2.08	0.53
2:A:96:ASN:OD1	2:A:107:PRO:HD2	2.09	0.53
2:A:207:ALA:N	2:B:130:ARG:CG	2.70	0.53
2:B:305:SER:HB2	2:B:307:PRO:HD2	1.91	0.52
2:A:171:LEU:HD11	2:A:295:ALA:HB1	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:O	2:B:75:LEU:HG	2.10	0.52
2:A:170:THR:O	2:A:171:LEU:HB2	2.09	0.52
2:A:61:ARG:NH2	2:A:73:ASP:OD2	2.43	0.52
2:B:176:GLU:OE1	2:B:200:THR:CA	2.57	0.52
1:D:24:DA:H5'	2:B:201:LYS:HG3	1.91	0.52
2:A:295:ALA:O	2:A:299:MET:HB2	2.10	0.52
2:A:72:ARG:HG3	2:A:116:VAL:CG2	2.40	0.51
1:D:6:DC:H2'	1:D:7:DT:C6	2.45	0.51
2:A:26:ASN:O	2:A:29:ASP:HB2	2.10	0.51
2:A:62:LYS:H	2:A:62:LYS:CD	2.23	0.51
2:B:72:ARG:NH2	3:B:420:HOH:O	2.43	0.51
1:D:1:DT:H2''	1:D:1:DT:O2	2.11	0.51
2:A:154:ARG:HH11	2:A:157:ASP:CG	2.19	0.51
2:A:326:ARG:HG3	2:A:327:ASN:H	1.74	0.51
2:B:60:ASN:ND2	3:B:440:HOH:O	2.43	0.50
2:B:173:LYS:HZ1	2:B:201:LYS:HD3	1.75	0.50
2:B:229:GLY:HA2	3:B:391:HOH:O	2.11	0.50
1:C:15:DG:O6	2:B:86:LYS:NZ	2.41	0.50
1:C:11:DT:OP2	2:B:50:ARG:NH1	2.44	0.50
2:B:313:GLY:HA3	2:B:315:TRP:CZ3	2.47	0.50
2:A:24:ARG:NH1	3:A:399:HOH:O	2.45	0.50
2:A:276:LYS:HG3	2:A:277:ASP:N	2.27	0.50
2:A:334:ALA:O	2:A:338:LEU:HD13	2.11	0.49
2:A:193:MET:CE	2:A:218:THR:HG23	2.40	0.49
2:A:203:LEU:CD1	2:B:85:VAL:HB	2.42	0.49
2:B:106:ARG:O	2:B:109:ASP:HB2	2.13	0.49
1:D:6:DC:H2''	1:D:7:DT:O5'	2.12	0.49
1:D:21:DG:H2''	1:D:22:DC:O5'	2.12	0.49
2:A:158:ILE:HG23	2:A:223:ARG:HG2	1.95	0.49
2:B:193:MET:HB2	2:B:218:THR:HG22	1.94	0.49
2:A:291:ALA:HB3	3:A:344:HOH:O	2.13	0.49
2:B:20:SER:N	2:B:22:GLU:OE1	2.46	0.48
1:C:17:DA:H8	3:C:94:HOH:O	1.96	0.48
2:A:233:ASP:O	2:A:236:ASN:HB2	2.12	0.48
2:B:81:ARG:NH1	3:B:453:HOH:O	2.46	0.48
2:A:156:GLN:HE21	2:A:156:GLN:N	1.98	0.48
2:B:317:ASN:C	2:B:318:VAL:HG22	2.38	0.48
2:B:188:THR:HG22	2:B:194:LEU:HD11	1.96	0.48
1:D:22:DC:H2''	1:D:23:DT:C6	2.49	0.47
2:B:133:GLN:NE2	2:B:326:ARG:NH2	2.61	0.47
2:B:297:ARG:HG3	2:B:328:LEU:CD1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:GLU:C	2:B:341:ASP:C	2.62	0.47
2:A:207:ALA:HA	2:B:130:ARG:CG	2.39	0.47
2:B:325:ILE:HA	2:B:328:LEU:HG	1.97	0.47
1:C:16:DC:OP2	2:B:320:ILE:HG21	2.15	0.47
1:D:8:DT:H2''	1:D:9:DC:H5'	1.97	0.47
2:A:158:ILE:CG2	2:A:223:ARG:HG2	2.44	0.47
2:A:326:ARG:HG3	2:A:327:ASN:N	2.29	0.47
2:B:64:PHE:HA	2:B:65:PRO:C	2.40	0.47
2:B:200:THR:OG1	2:B:201:LYS:N	2.48	0.46
2:B:27:LEU:HD12	2:B:30:MET:HE2	1.97	0.46
2:B:305:SER:C	2:B:307:PRO:HD2	2.41	0.46
2:A:72:ARG:HG3	2:A:116:VAL:HG11	1.98	0.46
2:B:156:GLN:HB2	3:B:356:HOH:O	2.15	0.46
2:A:219:LYS:O	2:A:222:GLU:HB2	2.15	0.46
2:B:197:ILE:HD13	2:B:211:LYS:CG	2.36	0.46
2:B:340:GLU:O	2:B:341:ASP:N	0.71	0.46
2:A:172:LEU:HD21	2:A:197:ILE:HD13	1.94	0.46
2:B:90:GLN:HE22	2:B:94:GLN:HE21	1.63	0.46
2:A:243:ARG:NH1	3:A:393:HOH:O	2.48	0.45
1:C:24:DA:C5'	3:C:79:HOH:O	2.51	0.45
2:A:323:ASN:O	2:A:326:ARG:HG2	2.16	0.45
2:B:301:ARG:HD3	2:B:330:SER:CB	2.45	0.45
2:B:306:ILE:N	2:B:307:PRO:CD	2.78	0.45
2:B:27:LEU:HD13	2:B:102:SER:OG	2.17	0.45
2:B:237:TYR:CE2	2:B:255:GLN:HG2	2.51	0.45
2:A:296:ALA:HA	2:A:299:MET:HE3	1.98	0.45
1:C:8:DT:O4	2:B:259:ARG:HG2	2.17	0.45
2:A:185:ILE:HD11	2:A:238:LEU:HG	1.99	0.45
1:C:35:DT:H1'	2:A:244:LYS:HD3	1.99	0.45
2:A:62:LYS:H	2:A:62:LYS:HD2	1.81	0.45
2:A:85:VAL:O	2:A:89:GLN:HG3	2.16	0.45
2:B:97:MET:HG2	2:B:101:ARG:HD2	1.99	0.45
2:A:30:MET:HE2	2:A:101:ARG:CB	2.47	0.45
2:A:202:THR:OG1	2:A:205:SER:HB3	2.16	0.45
2:B:95:LEU:HD12	2:B:95:LEU:HA	1.78	0.45
2:A:197:ILE:HG12	2:A:198:GLY:C	2.42	0.44
2:A:200:THR:C	2:A:201:LYS:HG3	2.41	0.44
2:B:237:TYR:CZ	2:B:255:GLN:HG2	2.52	0.44
2:B:193:MET:HE3	2:B:222:GLU:HG3	2.00	0.44
2:B:97:MET:O	2:B:101:ARG:HB2	2.18	0.44
2:A:140:THR:HG23	3:A:415:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ARG:HD3	2:B:70:ASP:OD2	2.17	0.44
2:B:204:VAL:O	2:B:205:SER:C	2.57	0.44
2:B:43:LYS:HA	2:B:43:LYS:HD3	1.38	0.44
2:A:185:ILE:HA	2:A:194:LEU:O	2.18	0.44
2:A:86:LYS:HE2	3:A:391:HOH:O	2.17	0.43
2:B:217:VAL:O	2:B:221:VAL:HG23	2.18	0.43
2:A:192:ARG:HH21	2:A:215:LEU:CD1	2.31	0.43
2:B:179:ARG:NH2	2:B:199:ARG:O	2.52	0.43
2:A:179:ARG:HG3	3:A:366:HOH:O	2.17	0.43
2:A:182:VAL:HG23	2:A:236:ASN:O	2.18	0.43
2:A:306:ILE:HG23	2:A:307:PRO:N	2.31	0.43
2:B:116:VAL:O	2:B:120:ILE:HG13	2.19	0.43
2:B:168:TYR:HA	2:B:291:ALA:HB1	2.01	0.43
2:B:193:MET:H	2:B:218:THR:CG2	2.30	0.43
2:A:199:ARG:NE	2:A:211:LYS:CE	2.82	0.43
2:B:27:LEU:CD1	2:B:102:SER:OG	2.67	0.43
2:A:336:VAL:O	2:A:340:GLU:HG3	2.18	0.42
3:C:98:HOH:O	2:A:204:VAL:HG21	2.18	0.42
2:A:298:ASP:OD1	2:A:301:ARG:NH1	2.53	0.42
2:B:172:LEU:HD11	2:B:197:ILE:HD11	2.01	0.42
2:A:159:ARG:HB2	2:A:224:TRP:CE3	2.55	0.42
2:A:207:ALA:CB	2:B:130:ARG:CG	2.42	0.42
2:A:318:VAL:CA	2:A:321:VAL:HG12	2.48	0.42
1:C:5:DA:H8	3:C:89:HOH:O	2.02	0.42
2:A:195:ILE:HD11	2:A:213:LEU:HD11	2.02	0.42
1:C:6:DC:H2'	1:C:7:DT:C7	2.49	0.42
2:A:149:MET:O	2:A:150:GLU:C	2.63	0.42
2:A:233:ASP:HA	2:A:234:PRO:HD3	1.93	0.42
2:A:121:ARG:HG3	2:A:121:ARG:HH11	1.85	0.42
2:A:311:GLN:OE1	2:B:331:GLU:O	2.38	0.42
2:B:325:ILE:CG2	2:B:331:GLU:HG3	2.45	0.42
2:B:173:LYS:HG2	2:B:289:HIS:CE1	2.52	0.41
2:A:297:ARG:HG2	2:A:297:ARG:HH11	1.85	0.41
2:A:270:ARG:HH11	2:A:270:ARG:CG	2.28	0.41
2:A:100:ARG:HA	3:A:429:HOH:O	2.20	0.41
2:A:139:ARG:NH1	2:B:339:LEU:HA	2.36	0.41
2:B:194:LEU:HB3	2:B:210:GLU:OE1	2.20	0.41
3:C:52:HOH:O	2:B:156:GLN:HG3	2.20	0.41
2:A:149:MET:O	2:A:151:ASN:N	2.53	0.41
2:A:266:GLU:HG2	3:A:419:HOH:O	2.21	0.41
2:B:57:LYS:HD3	3:B:417:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ILE:HD13	2:B:320:ILE:HA	1.90	0.41
2:A:224:TRP:CZ3	2:A:228:SER:HB3	2.56	0.41
2:A:270:ARG:HG3	2:A:270:ARG:NH1	2.30	0.41
1:D:16:DC:H2''	1:D:17:DA:H5''	2.03	0.41
2:A:183:LYS:HB3	2:A:234:PRO:O	2.20	0.41
2:A:271:LEU:HD22	2:A:271:LEU:C	2.46	0.40
2:A:320:ILE:O	2:A:323:ASN:HB2	2.21	0.40
2:B:78:LEU:HD22	2:B:83:LEU:HD12	2.02	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ASP:OD2	3:B:440:HOH:O[8_556]	0.72	1.48
1:D:1:DT:O5'	3:B:449:HOH:O[6_655]	0.86	1.34
2:A:126:ASP:OD1	2:B:199:ARG:NE[4_566]	1.47	0.73
2:B:329:ASP:CG	3:B:440:HOH:O[8_556]	1.48	0.72
2:A:126:ASP:OD1	2:B:199:ARG:CD[4_566]	1.94	0.26
1:D:1:DT:C5'	3:B:449:HOH:O[6_655]	1.96	0.24
3:B:455:HOH:O	3:B:462:HOH:O[8_556]	2.11	0.09
2:B:329:ASP:CB	3:B:440:HOH:O[8_556]	2.15	0.05
2:A:126:ASP:OD1	2:B:199:ARG:CZ[4_566]	2.16	0.04
2:B:330:SER:N	3:B:421:HOH:O[8_556]	2.16	0.04

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	
2	A	320/322 (99%)	302 (94%)	14 (4%)	4 (1%)	9	8
2	B	318/322 (99%)	297 (93%)	14 (4%)	7 (2%)	5	3
All	All	638/644 (99%)	599 (94%)	28 (4%)	11 (2%)	7	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	150	GLU
2	A	209	VAL
2	B	203	LEU
2	B	205	SER
2	B	318	VAL
2	B	326	ARG
2	A	278	ASP
2	B	202	THR
2	B	277	ASP
2	B	204	VAL
2	A	189	ASP

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	
2	A	269/269 (100%)	219 (81%)	50 (19%)	1	1
2	B	269/269 (100%)	222 (82%)	47 (18%)	2	1
All	All	538/538 (100%)	441 (82%)	97 (18%)	2	1

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	21	ASP
2	A	22	GLU
2	A	23	VAL
2	A	25	LYS
2	A	43	LYS
2	A	51	SER
2	A	61	ARG
2	A	62	LYS
2	A	67	GLU
2	A	81	ARG
2	A	86	LYS
2	A	92	LEU

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Mol	Chain	Res	Type
2	A	95	LEU
2	A	100	ARG
2	A	101	ARG
2	A	106	ARG
2	A	114	SER
2	A	116	VAL
2	A	119	ARG
2	A	132	LYS
2	A	133	GLN
2	A	155	CYS
2	A	156	GLN
2	A	161	LEU
2	A	166	ILE
2	A	169	ASN
2	A	171	LEU
2	A	188	THR
2	A	193	MET
2	A	199	ARG
2	A	201	LYS
2	A	206	THR
2	A	223	ARG
2	A	238	LEU
2	A	241	ARG
2	A	266	GLU
2	A	270	ARG
2	A	271	LEU
2	A	276	LYS
2	A	277	ASP
2	A	281	GLN
2	A	289	HIS
2	A	299	MET
2	A	304	VAL
2	A	305	SER
2	A	308	GLU
2	A	311	GLN
2	A	322	MET
2	A	326	ARG
2	A	330	SER
2	B	23	VAL
2	B	24	ARG
2	B	25	LYS
2	B	27	LEU

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Mol	Chain	Res	Type
2	B	39	GLU
2	B	43	LYS
2	B	45	LEU
2	B	51	SER
2	B	57	LYS
2	B	60	ASN
2	B	62	LYS
2	B	86	LYS
2	B	90	GLN
2	B	95	LEU
2	B	101	ARG
2	B	114	SER
2	B	116	VAL
2	B	118	ARG
2	B	122	LYS
2	B	130	ARG
2	B	156	GLN
2	B	176	GLU
2	B	183	LYS
2	B	186	SER
2	B	187	ARG
2	B	197	ILE
2	B	203	LEU
2	B	219	LYS
2	B	241	ARG
2	B	244	LYS
2	B	255	GLN
2	B	271	LEU
2	B	289	HIS
2	B	292	ARG
2	B	293	VAL
2	B	297	ARG
2	B	301	ARG
2	B	306	ILE
2	B	311	GLN
2	B	317	ASN
2	B	318	VAL
2	B	320	ILE
2	B	323	ASN
2	B	326	ARG
2	B	332	THR
2	B	338	LEU

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Mol	Chain	Res	Type
2	B	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	89	GLN
2	A	133	GLN
2	A	144	GLN
2	A	151	ASN
2	A	156	GLN
2	A	255	GLN
2	A	269	HIS
2	A	323	ASN
2	B	90	GLN
2	B	133	GLN
2	B	196	HIS
2	B	255	GLN
2	B	323	ASN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	5
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	332:THR	C	333:GLY	N	2.17
1	B	204:VAL	C	205:SER	N	1.83
1	B	326:ARG	C	327:ASN	N	1.77
1	B	198:GLY	C	199:ARG	N	1.04
1	A	208:GLY	C	209:VAL	N	0.95
1	B	340:GLU	C	341:ASP	N	0.71

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	C	35/35 (100%)	0.00	1 (2%) 53 50	22, 36, 68, 92	0
1	D	35/35 (100%)	0.11	1 (2%) 53 50	22, 31, 48, 63	0
2	A	322/322 (100%)	0.96	40 (12%) 8 6	19, 40, 77, 99	0
2	B	322/322 (100%)	0.85	45 (13%) 6 4	16, 33, 70, 97	0
All	All	714/714 (100%)	0.82	87 (12%) 8 6	16, 36, 75, 99	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	207	ALA	15.7
2	B	200	THR	14.7
2	B	202	THR	12.0
2	A	198	GLY	11.7
2	B	330	SER	11.3
2	B	331	GLU	11.1
2	A	200	THR	11.0
2	B	327	ASN	10.9
2	B	201	LYS	10.3
2	A	206	THR	10.1
2	B	328	LEU	9.9
2	A	208	GLY	9.4
2	A	205	SER	9.2
2	B	329	ASP	9.0
2	B	199	ARG	8.3
2	A	204	VAL	7.3
2	B	204	VAL	7.3
2	A	199	ARG	7.2
2	A	201	LYS	7.1
2	B	332	THR	7.0
2	B	203	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
2	A	203	LEU	6.7
1	D	1	DT	6.7
2	A	202	THR	6.5
2	B	341	ASP	6.3
2	B	333	GLY	5.9
2	B	300	ALA	5.7
2	B	189	ASP	4.6
2	A	197	ILE	4.6
2	B	326	ARG	4.6
2	B	319	ASN	4.5
2	B	320	ILE	4.5
2	A	188	THR	4.3
2	A	306	ILE	4.3
2	B	318	VAL	4.0
2	B	42	TRP	4.0
2	A	190	GLY	3.9
2	A	191	GLY	3.9
2	A	311	GLN	3.8
2	A	304	VAL	3.6
2	B	339	LEU	3.6
2	B	325	ILE	3.5
2	B	20	SER	3.3
2	A	209	VAL	3.3
2	A	341	ASP	3.2
2	A	231	ALA	3.2
2	A	196	HIS	3.2
2	B	338	LEU	3.1
2	A	210	GLU	3.1
2	A	302	ALA	3.1
2	B	205	SER	2.9
2	A	187	ARG	2.9
2	B	334	ALA	2.9
2	B	301	ARG	2.8
2	A	149	MET	2.8
2	B	340	GLU	2.7
1	C	1	DT	2.6
2	B	278	ASP	2.6
2	B	337	ARG	2.6
2	A	31	PHE	2.6
2	B	60	ASN	2.6
2	A	277	ASP	2.5
2	B	277	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	307	PRO	2.4
2	A	189	ASP	2.4
2	B	208	GLY	2.4
2	B	324	TYR	2.4
2	B	323	ASN	2.4
2	B	57	LYS	2.3
2	B	336	VAL	2.3
2	A	195	ILE	2.3
2	B	321	VAL	2.3
2	B	31	PHE	2.3
2	A	232	ASP	2.2
2	A	233	ASP	2.2
2	B	322	MET	2.2
2	A	227	VAL	2.2
2	A	278	ASP	2.2
2	B	229	GLY	2.2
2	A	194	LEU	2.2
2	B	24	ARG	2.2
2	B	22	GLU	2.1
2	A	126	ASP	2.1
2	A	280	GLY	2.1
2	A	215	LEU	2.0
2	B	315	TRP	2.0
2	A	276	LYS	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.