



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 AM UTC

PDB ID : 1JFI / pdb_00001jfi
Title : Crystal Structure of the NC2-TBP-DNA Ternary Complex
Authors : Kamada, K.; Shu, F.; Chen, H.; Malik, S.; Stelzer, G.; Roeder, R.G.; Meisterernst, M.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2001-06-20
Resolution : 2.62 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

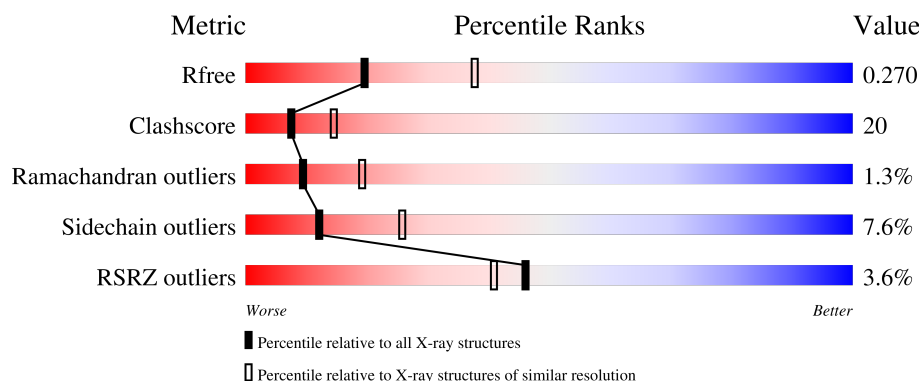
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	D	19	11% 26% 53% 11% 5% 5%
2	E	19	5% 42% 42% 11% 5%
3	A	98	4% 36% 21% 7% 36%
4	B	179	3% 47% 26% •• 25%
5	C	185	2% 62% 32% 5% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3743 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 5'-D(*TP*TP*GP*GP*CP*TP*AP*TP*AP*AP*AP*A P*GP*GP*GP*CP*TP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	18	Total	C	N	O	P	0	0	0
			369	177	69	106	17			

- Molecule 2 is a DNA chain called 5'-D(*G*GP*AP*GP*CP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			363	175	65	106	17			

- Molecule 3 is a protein called Transcription Regulator NC2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	63	Total	C	N	O	S	0	0	0
			490	311	87	88	4			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	cloning artifact	UNP Q14919
A	79	ASP	-	cloning artifact	UNP Q14919
A	80	PRO	-	cloning artifact	UNP Q14919
A	81	ALA	-	cloning artifact	UNP Q14919
A	82	ALA	-	cloning artifact	UNP Q14919
A	83	ASN	-	cloning artifact	UNP Q14919
A	84	LYS	-	cloning artifact	UNP Q14919
A	85	ALA	-	cloning artifact	UNP Q14919
A	86	ARG	-	cloning artifact	UNP Q14919
A	87	LYS	-	cloning artifact	UNP Q14919
A	88	GLU	-	cloning artifact	UNP Q14919
A	89	ALA	-	cloning artifact	UNP Q14919

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Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLU	-	cloning artifact	UNP Q14919
A	91	LEU	-	cloning artifact	UNP Q14919
A	92	ALA	-	cloning artifact	UNP Q14919
A	93	ALA	-	cloning artifact	UNP Q14919
A	94	ALA	-	cloning artifact	UNP Q14919
A	95	THR	-	cloning artifact	UNP Q14919
A	96	ALA	-	cloning artifact	UNP Q14919
A	97	GLU	-	cloning artifact	UNP Q14919
A	98	GLN	-	cloning artifact	UNP Q14919

- Molecule 4 is a protein called Transcription Regulator NC2 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	135	Total	C	N	O	S	0	0	0
			1059	655	190	209	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	GLY	-	cloning artifact	UNP Q01658
B	99	PRO	-	cloning artifact	UNP Q01658
B	100	HIS	-	cloning artifact	UNP Q01658

- Molecule 5 is a protein called TATA-BOX-BINDING PROTEIN (TBP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	183	Total	C	N	O	S	0	0	0
			1453	941	257	247	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	355	GLY	-	cloning artifact	UNP P20226
C	356	SER	-	cloning artifact	UNP P20226
C	357	HIS	-	cloning artifact	UNP P20226
C	358	MET	-	cloning artifact	UNP P20226

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O	0	0
			1	1		

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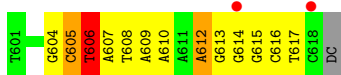
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	O 1	0	0
6	B	1	Total 1	O 1	0	0
6	C	6	Total 6	O 6	0	0

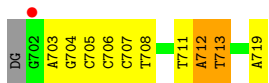
3 Residue-property plots

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.

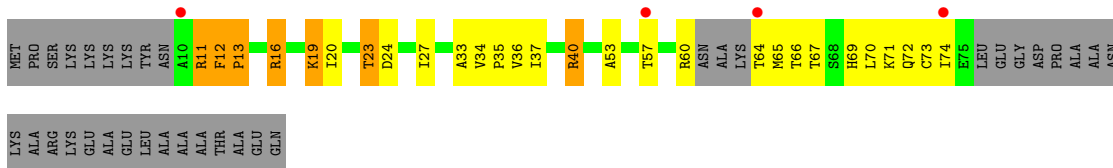
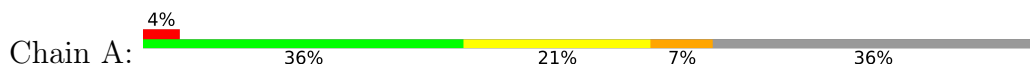
- Molecule 1: 5'-D(*TP*TP*GP*GP*CP*TP*AP*TP*AP*AP*AP*GP*GP*GP*CP*TP*CP*P*C)-3'



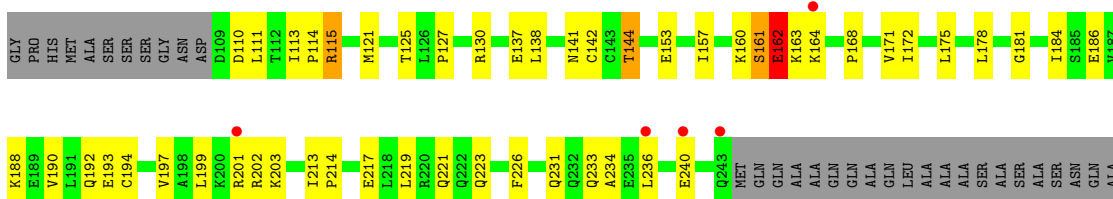
- Molecule 2: 5'-D(*G*GP*AP*GP*CP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*CP*AP*A)-3'



- Molecule 3: Transcription Regulator NC2 alpha chain

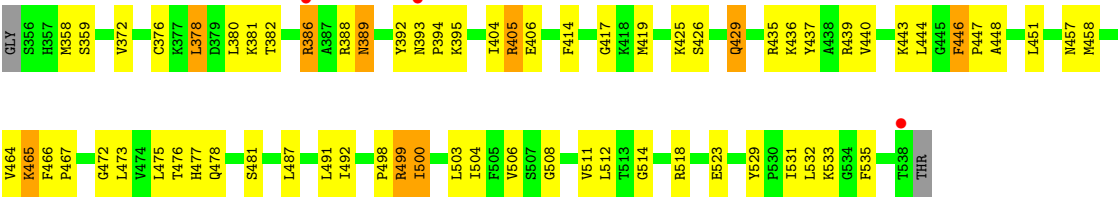


- Molecule 4: Transcription Regulator NC2 beta chain



GLY
SER
SER
GLN
ASP
GLU
GLU
ASP
ASP
ASP
ASP
ILE

● Molecule 5: TATA-BOX-BINDING PROTEIN (TBP)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.68Å 119.08Å 155.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.62 19.84 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.84-2.62) 98.5 (19.84-2.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.63Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.233 , 0.277 0.230 , 0.270	Depositor DCC
R_{free} test set	1499 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	D	0.34	0/414	1.07	1/638 (0.2%)
2	E	0.32	0/406	0.83	0/624
3	A	0.47	0/494	0.99	3/662 (0.5%)
4	B	0.45	0/1068	0.87	0/1437
5	C	0.46	0/1480	0.99	4/1991 (0.2%)
All	All	0.43	0/3862	0.95	8/5352 (0.1%)

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	4
2	E	0	2
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	23	THR	N-CA-C	-8.54	102.85	113.18
5	C	448	ALA	N-CA-C	7.27	119.94	108.67
1	D	606	DT	N1-C1'-C2'	-6.48	103.78	113.50
5	C	451	LEU	N-CA-C	6.01	119.50	109.95
3	A	12	PHE	CA-C-N	5.95	126.51	120.38
3	A	12	PHE	C-N-CA	5.95	126.51	120.38
5	C	446	PHE	CA-C-N	5.82	127.11	119.84
5	C	446	PHE	C-N-CA	5.82	127.11	119.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	604	DG	Sidechain
1	D	605	DC	Sidechain
1	D	606	DT	Sidechain
1	D	612	DA	Sidechain
2	E	712	DA	Sidechain
2	E	713	DT	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	D	369	0	205	17	0
2	E	363	0	205	11	0
3	A	490	0	529	38	0
4	B	1059	0	1073	45	0
5	C	1453	0	1542	54	1
6	A	1	0	0	1	0
6	B	1	0	0	0	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
All	All	3743	0	3554	148	1

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 20.

All (148) 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:A:33:ALA:O	3:A:36:VAL:HG22	1.78	0.83
1:D:613:DG:H2''	1:D:614:DG:C8	2.14	0.82
2:E:712:DA:H2''	2:E:713:DT:H5'	1.62	0.81
3:A:36:VAL:HG21	4:B:194:CYS:SG	2.20	0.81
4:B:115:ARG:HG2	4:B:115:ARG:HH11	1.45	0.81
3:A:53:ALA:O	3:A:57:THR:HG23	1.85	0.77
3:A:24:ASP:HB3	3:A:27:ILE:HD13	1.67	0.77
1:D:615:DG:H2''	1:D:616:DC:H5''	1.66	0.76
5:C:378:LEU:HD22	5:C:417:GLY:HA2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:473:LEU:HD12	5:C:491:LEU:HD11	1.67	0.75
4:B:201:ARG:HH21	4:B:202:ARG:HG3	1.51	0.74
5:C:499:ARG:HH11	5:C:499:ARG:HB2	1.53	0.73
4:B:172:ILE:HG23	4:B:184:ILE:HG23	1.69	0.73
5:C:500:ILE:HD11	5:C:512:LEU:HD23	1.72	0.70
3:A:57:THR:HG22	3:A:69:HIS:CD2	2.26	0.69
5:C:382:THR:O	5:C:386:ARG:HD3	1.93	0.69
4:B:121:MET:HE2	4:B:125:THR:OG1	1.94	0.67
5:C:476:THR:HB	5:C:477:HIS:HD2	1.58	0.67
5:C:382:THR:HG22	5:C:386:ARG:HE	1.56	0.67
1:D:615:DG:H2''	1:D:616:DC:C5'	2.24	0.67
1:D:615:DG:H5''	4:B:164:LYS:HD3	1.76	0.66
4:B:121:MET:HE3	4:B:121:MET:HA	1.76	0.66
1:D:606:DT:H2''	1:D:607:DA:H5'	1.78	0.65
4:B:184:ILE:O	4:B:188:LYS:HG3	1.97	0.65
4:B:217:GLU:HG3	4:B:221:GLN:HE21	1.61	0.65
3:A:16:ARG:HB2	3:A:16:ARG:NH1	2.12	0.65
3:A:66:THR:H	3:A:69:HIS:HD2	1.43	0.64
1:D:613:DG:H2''	1:D:614:DG:N7	2.12	0.64
3:A:16:ARG:HB2	3:A:16:ARG:HH11	1.63	0.64
3:A:11:ARG:HB2	3:A:11:ARG:HH11	1.63	0.63
2:E:705:DC:H2''	2:E:706:DC:H5'	1.82	0.62
4:B:181:GLY:O	4:B:184:ILE:HG13	2.00	0.61
5:C:491:LEU:HD23	5:C:492:ILE:N	2.16	0.61
1:D:615:DG:C5'	4:B:164:LYS:HD3	2.30	0.61
5:C:382:THR:CG2	5:C:386:ARG:HE	2.14	0.61
5:C:529:TYR:CE2	5:C:533:LYS:HD2	2.36	0.61
3:A:34:VAL:O	3:A:37:ILE:HG12	2.01	0.60
4:B:115:ARG:HH11	4:B:115:ARG:CG	2.10	0.60
2:E:712:DA:H2''	2:E:713:DT:C5'	2.32	0.60
3:A:66:THR:H	3:A:69:HIS:CD2	2.19	0.60
4:B:219:LEU:O	4:B:223:GLN:HG3	2.02	0.60
5:C:457:ASN:HD21	5:C:514:GLY:H	1.47	0.59
3:A:65:MET:HE3	3:A:70:LEU:HD11	1.83	0.59
5:C:372:VAL:HG12	5:C:419:MET:HE2	1.83	0.59
4:B:193:GLU:O	4:B:197:VAL:HG23	2.02	0.59
5:C:458:MET:HE1	5:C:518:ARG:HB3	1.83	0.59
5:C:393:ASN:C	5:C:395:LYS:H	2.09	0.59
4:B:236:LEU:O	4:B:236:LEU:HD23	2.03	0.59
5:C:436:LYS:O	5:C:440:VAL:HG23	2.03	0.59
3:A:53:ALA:HB1	3:A:70:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:382:THR:CG2	5:C:386:ARG:HH21	2.16	0.58
5:C:393:ASN:C	5:C:395:LYS:N	2.56	0.58
1:D:613:DG:H1	2:E:707:DC:H42	1.51	0.58
5:C:386:ARG:HD3	5:C:386:ARG:H	1.67	0.57
3:A:60:ARG:HG3	3:A:69:HIS:CE1	2.38	0.57
1:D:615:DG:C2'	1:D:616:DC:H5''	2.34	0.57
3:A:57:THR:HG22	3:A:69:HIS:CG	2.39	0.57
2:E:704:DG:H2''	2:E:705:DC:OP2	2.04	0.57
3:A:60:ARG:HG3	3:A:69:HIS:HE1	1.70	0.57
5:C:473:LEU:O	5:C:473:LEU:HD13	2.04	0.56
2:E:719:DA:H2'	4:B:115:ARG:HG3	1.87	0.55
5:C:372:VAL:CG1	5:C:419:MET:HE2	2.36	0.55
3:A:34:VAL:HB	3:A:35:PRO:HD3	1.88	0.55
5:C:405:ARG:HD2	5:C:406:GLU:H	1.69	0.55
4:B:115:ARG:HG2	4:B:115:ARG:NH1	2.20	0.55
4:B:236:LEU:O	4:B:240:GLU:HG3	2.07	0.55
3:A:16:ARG:HH11	3:A:16:ARG:CB	2.19	0.55
2:E:707:DC:H2'	2:E:708:DT:H71	1.88	0.54
5:C:473:LEU:HD12	5:C:491:LEU:CD1	2.37	0.54
4:B:115:ARG:CG	4:B:115:ARG:NH1	2.66	0.53
2:E:719:DA:C2'	4:B:115:ARG:HG3	2.38	0.53
4:B:161:SER:C	4:B:162:GLU:HG3	2.34	0.52
3:A:24:ASP:CB	3:A:27:ILE:HD13	2.36	0.52
4:B:125:THR:C	4:B:127:PRO:HD3	2.35	0.52
4:B:125:THR:O	4:B:127:PRO:HD3	2.09	0.52
5:C:464:VAL:HG22	5:C:508:GLY:O	2.09	0.52
5:C:389:ASN:HD22	5:C:389:ASN:N	2.07	0.52
5:C:439:ARG:O	5:C:443:LYS:HG3	2.10	0.51
1:D:605:DC:H2'	1:D:606:DT:C7	2.40	0.51
1:D:607:DA:H2''	1:D:608:DT:H5'	1.92	0.51
4:B:190:VAL:O	4:B:193:GLU:HG2	2.11	0.50
5:C:440:VAL:O	5:C:444:LEU:HD13	2.12	0.50
3:A:19:LYS:HB3	4:B:111:LEU:HD13	1.93	0.50
5:C:389:ASN:N	5:C:389:ASN:ND2	2.59	0.50
5:C:405:ARG:HD2	5:C:405:ARG:N	2.27	0.50
3:A:71:LYS:C	3:A:73:CYS:H	2.19	0.50
5:C:467:PRO:HA	5:C:506:VAL:O	2.11	0.50
3:A:16:ARG:NH1	6:A:1001:HOH:O	2.45	0.50
5:C:386:ARG:HD3	5:C:386:ARG:N	2.27	0.49
2:E:703:DA:H2''	2:E:704:DG:O5'	2.12	0.49
3:A:74:ILE:HD11	4:B:142:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:13:PRO:HB2	3:A:16:ARG:HB3	1.94	0.49
3:A:40:ARG:NH1	4:B:186:GLU:HB3	2.28	0.48
5:C:473:LEU:HD13	5:C:473:LEU:C	2.39	0.48
5:C:393:ASN:O	5:C:395:LYS:N	2.47	0.48
3:A:53:ALA:CB	3:A:70:LEU:HD12	2.44	0.48
4:B:231:GLN:O	4:B:234:ALA:HB3	2.13	0.48
4:B:226:PHE:HA	5:C:531:ILE:HD11	1.94	0.48
3:A:65:MET:CE	3:A:70:LEU:HD11	2.43	0.48
5:C:498:PRO:HD3	5:C:523:GLU:CD	2.39	0.48
1:D:605:DC:H2'	1:D:606:DT:H72	1.97	0.47
3:A:16:ARG:O	3:A:20:ILE:HG13	2.14	0.47
4:B:184:ILE:HG22	4:B:188:LYS:HE3	1.97	0.47
4:B:141:ASN:O	4:B:144:THR:HG23	2.14	0.47
5:C:376:CYS:O	5:C:378:LEU:HD13	2.14	0.47
4:B:168:PRO:O	4:B:172:ILE:HG13	2.15	0.47
3:A:67:THR:OG1	3:A:71:LYS:HE3	2.14	0.47
4:B:192:GLN:HA	4:B:192:GLN:OE1	2.14	0.47
5:C:481:SER:HB3	5:C:491:LEU:HD21	1.96	0.46
5:C:491:LEU:HD23	5:C:491:LEU:C	2.41	0.46
5:C:404:ILE:HG23	5:C:437:TYR:CE1	2.51	0.45
1:D:612:DA:H1'	5:C:414:PHE:CZ	2.51	0.45
4:B:161:SER:O	4:B:163:LYS:HG3	2.17	0.45
1:D:615:DG:H5''	4:B:164:LYS:CD	2.43	0.45
3:A:37:ILE:HD11	4:B:171:VAL:HB	1.99	0.45
4:B:153:GLU:O	4:B:157:ILE:HG13	2.17	0.45
5:C:503:LEU:HB2	5:C:511:VAL:HB	2.00	0.44
5:C:381:LYS:HD2	5:C:392:TYR:HE2	1.84	0.43
5:C:472:GLY:O	5:C:475:LEU:HB2	2.18	0.43
3:A:11:ARG:HH11	3:A:11:ARG:CB	2.30	0.43
5:C:386:ARG:N	5:C:386:ARG:CD	2.82	0.43
4:B:113:ILE:HG23	4:B:114:PRO:HD2	2.00	0.43
1:D:609:DA:H2''	1:D:610:DA:H5'	2.01	0.43
3:A:74:ILE:CD1	4:B:142:CYS:SG	3.07	0.42
5:C:405:ARG:HD2	5:C:405:ARG:H	1.83	0.42
3:A:19:LYS:HB3	4:B:111:LEU:CD1	2.48	0.42
3:A:70:LEU:HB3	4:B:138:LEU:HD23	2.00	0.42
2:E:711:DT:H6	2:E:711:DT:H2'	1.53	0.42
4:B:160:LYS:C	4:B:162:GLU:H	2.27	0.42
3:A:64:THR:HA	4:B:130:ARG:O	2.19	0.42
5:C:393:ASN:O	5:C:394:PRO:C	2.61	0.41
5:C:435:ARG:O	5:C:439:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:476:THR:OG1	5:C:535:PHE:HZ	2.02	0.41
4:B:199:LEU:HG	4:B:203:LYS:HE2	2.02	0.41
1:D:616:DC:C2'	1:D:617:DT:H71	2.49	0.41
2:E:706:DC:H2''	2:E:707:DC:C6	2.56	0.41
5:C:358:MET:O	5:C:359:SER:C	2.63	0.41
5:C:465:LYS:O	5:C:466:PHE:HB3	2.21	0.41
5:C:405:ARG:H	5:C:405:ARG:CD	2.33	0.41
3:A:12:PHE:HA	3:A:13:PRO:HD3	1.81	0.41
5:C:504:ILE:HD13	5:C:532:LEU:HD21	2.02	0.41
4:B:213:ILE:O	4:B:214:PRO:C	2.63	0.41
5:C:529:TYR:CZ	5:C:533:LYS:HD2	2.55	0.41
3:A:34:VAL:CB	3:A:35:PRO:HD3	2.50	0.40
5:C:426:SER:OG	5:C:429:GLN:HB2	2.21	0.40
1:D:605:DC:H2''	1:D:606:DT:O5'	2.21	0.40
3:A:11:ARG:HG3	3:A:12:PHE:N	2.37	0.40
5:C:446:PHE:HA	5:C:447:PRO:HD3	1.77	0.40

All (1) 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)
5:C:386:ARG:NH2	5:C:386:ARG:NH2[3_755]	1.88	0.32

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	
3	A	59/98 (60%)	56 (95%)	1 (2%)	2 (3%)	3	4
4	B	133/179 (74%)	123 (92%)	8 (6%)	2 (2%)	8	16
5	C	181/185 (98%)	170 (94%)	10 (6%)	1 (1%)	21	39
All	All	373/462 (81%)	349 (94%)	19 (5%)	5 (1%)	9	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	388	ARG
4	B	162	GLU
4	B	161	SER
3	A	72	GLN
3	A	13	PRO

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	
3	A	55/80 (69%)	50 (91%)	5 (9%)	9	18
4	B	117/151 (78%)	109 (93%)	8 (7%)	14	30
5	C	158/159 (99%)	146 (92%)	12 (8%)	12	26
All	All	330/390 (85%)	305 (92%)	25 (8%)	12	26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	ARG
3	A	16	ARG
3	A	19	LYS
3	A	23	THR
3	A	40	ARG
4	B	110	ASP
4	B	115	ARG
4	B	137	GLU
4	B	144	THR
4	B	162	GLU
4	B	175	LEU
4	B	178	LEU
4	B	233	GLN
5	C	378	LEU
5	C	380	LEU
5	C	386	ARG

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Mol	Chain	Res	Type
5	C	389	ASN
5	C	405	ARG
5	C	425	LYS
5	C	429	GLN
5	C	465	LYS
5	C	478	GLN
5	C	487	LEU
5	C	499	ARG
5	C	500	ILE

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

Mol	Chain	Res	Type
3	A	58	GLN
3	A	69	HIS
3	A	72	GLN
4	B	141	ASN
4	B	159	ASN
4	B	173	GLN
4	B	223	GLN
4	B	239	GLN
5	C	366	GLN
5	C	389	ASN
5	C	429	GLN
5	C	442	GLN
5	C	457	ASN
5	C	477	HIS
5	C	478	GLN
5	C	479	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	D	18/19 (94%)	0.29	2 (11%) 10 8	37, 51, 100, 110	0
2	E	18/19 (94%)	0.38	1 (5%) 30 25	42, 53, 120, 139	0
3	A	63/98 (64%)	0.39	4 (6%) 26 21	39, 58, 109, 128	0
4	B	135/179 (75%)	0.30	5 (3%) 45 40	36, 60, 114, 132	0
5	C	183/185 (98%)	-0.03	3 (1%) 70 67	30, 52, 76, 98	0
All	All	417/500 (83%)	0.17	15 (3%) 46 41	30, 56, 100, 139	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	243	GLN	6.5
2	E	702	DG	4.6
4	B	164	LYS	3.9
3	A	74	ILE	3.7
1	D	618	DC	3.2
3	A	10	ALA	3.1
3	A	64	THR	3.0
3	A	57	THR	3.0
5	C	538	THR	2.8
4	B	240	GLU	2.4
5	C	393	ASN	2.3
4	B	201	ARG	2.2
4	B	236	LEU	2.2
1	D	614	DG	2.1
5	C	386	ARG	2.1

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.