



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 9BDX / pdb_00009bdx
Title : NF-kappaB RelA homo-dimer bound to CG-centric kappaB DNA
Authors : Biswas, T.; Shahabi, S.; Tsodikov, O.V.; Ghosh, G.
Deposited on : 2024-04-12
Resolution : 3.60 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

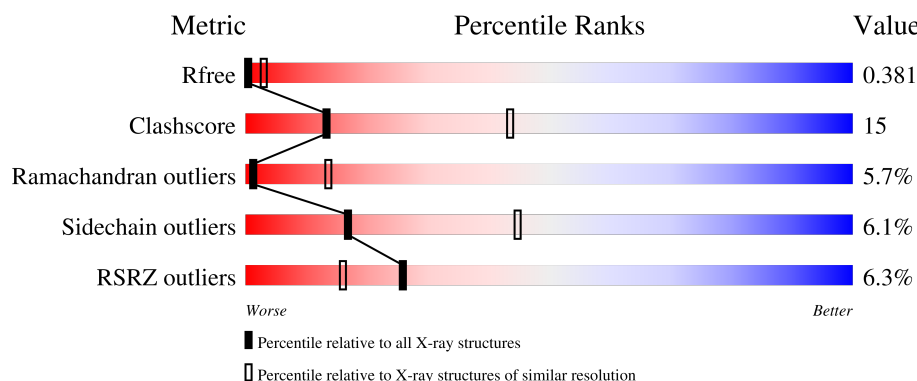
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	4% 53% 35% 8% .
1	B	287	9% 52% 37% 6% 5%
2	C	19	74% 16% 11%
3	D	19	63% 26% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5080 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 Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2197	1369	404	413	11			
1	B	274	Total	C	N	O	S	0	0	0
			2185	1363	402	408	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q04207
B	18	MET	-	initiating methionine	UNP Q04207

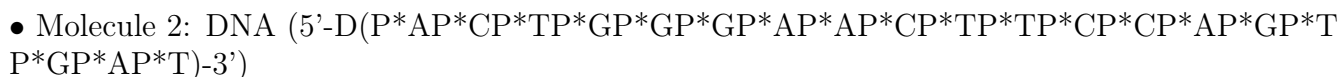
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*TP*GP*GP*GP*AP*AP*CP*TP*TP*CP*CP*AP*GP*TP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*TP*CP*AP*CP*TP*GP*GP*AP*AP*GP*TP*TP*CP*CP*CP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			347	165	63	102	17			

- Molecule 1: Transcription factor p65



Chain C:  74% 16% 11%



- Molecule 3: DNA (5'-D(*AP*TP*CP*AP*CP*TP*GP*GP*AP*AP*GP*TP*TP*CP*CP*CP*AP*GP*T)-3')

Chain D:  63% 26% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.95Å 132.18Å 66.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.60 29.75 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.75-3.60) 96.5 (29.75-3.60)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.65Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.321 , 0.374 0.332 , 0.381	Depositor DCC
R_{free} test set	585 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 15.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	5080	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	0/2250	1.37	11/3053 (0.4%)
1	B	0.87	0/2238	1.37	11/3036 (0.4%)
2	C	0.63	0/393	0.91	0/603
3	D	0.55	0/388	0.89	0/596
All	All	0.86	0/5269	1.31	22/7288 (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	A	0	8
1	B	0	5
All	All	0	13

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	NE-CZ-NH2	7.32	125.79	119.20
1	A	125	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	134	ILE	O-C-N	6.05	127.83	121.91
1	B	172	PRO	N-CA-CB	-6.03	96.92	103.25
1	A	291	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	88	HIS	CA-CB-CG	5.82	119.62	113.80
1	B	277	ASP	CA-CB-CG	5.75	118.34	112.60
1	A	94	ASP	CB-CA-C	5.73	119.54	111.86
1	B	275	PRO	N-CA-C	5.61	124.03	112.47
1	A	292	THR	N-CA-C	-5.58	106.06	112.92
1	A	45	SER	CA-C-N	-5.45	118.03	123.04
1	A	45	SER	C-N-CA	-5.45	118.03	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	83	HIS	CA-C-O	5.32	126.58	120.84
1	B	81	PRO	N-CA-C	5.30	117.16	110.70
1	A	96	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	115	ASN	CB-CA-C	5.21	120.07	111.31
1	B	28	LYS	O-C-N	5.12	129.47	122.82
1	B	24	ILE	CB-CA-C	5.11	119.67	111.29
1	A	242	ALA	N-CA-C	-5.11	107.33	113.21
1	A	185	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	142	HIS	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PHE	Peptide
1	A	122	LYS	Peptide
1	A	124	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	177	PRO	Peptide
1	A	186	ASN	Peptide
1	A	246	ARG	Sidechain
1	A	41	ARG	Peptide
1	B	122	LYS	Peptide
1	B	171	ARG	Sidechain
1	B	18	MET	Peptide
1	B	237	GLY	Peptide
1	B	264	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2197	0	2153	70	0
1	B	2185	0	2148	72	0
2	C	351	0	192	3	0
3	D	347	0	192	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5080	0	4685	144	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 15.

All (144) 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:B:149:ARG:O	1:B:150:GLY:O	1.96	0.84
1:A:72:VAL:HG23	1:A:163:VAL:HG22	1.65	0.78
1:A:134:ILE:HD11	1:A:148:GLN:HE22	1.52	0.73
1:A:96:ARG:HH12	1:A:101:GLU:HB3	1.52	0.73
1:A:70:GLY:HA3	1:A:104:LEU:HD12	1.74	0.69
1:A:212:ILE:HD12	1:A:254:THR:HG21	1.75	0.69
1:A:228:PHE:HB2	1:A:235:ALA:HB3	1.74	0.69
1:B:81:PRO:HA	1:B:82:PRO:C	2.19	0.68
1:B:122:LYS:O	1:B:125:ASP:N	2.26	0.68
2:C:107:DA:H2''	2:C:108:DA:C8	2.30	0.66
1:B:245:HIS:O	1:B:246:ARG:HB2	1.94	0.66
1:A:212:ILE:HD12	1:A:254:THR:CG2	2.25	0.66
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.62	0.65
1:B:230:GLY:O	1:B:232:GLY:N	2.29	0.65
1:B:90:LEU:HD12	1:B:117:GLY:O	1.97	0.64
1:B:19:PRO:HB3	1:B:65:GLY:O	1.96	0.64
1:B:212:ILE:HB	1:B:252:PHE:CE1	2.34	0.63
1:B:180:SER:O	1:B:181:HIS:C	2.41	0.63
1:A:194:LEU:O	1:A:281:SER:HB2	2.00	0.62
1:A:21:VAL:HG22	1:A:63:ILE:HG23	1.82	0.62
1:A:35:ARG:O	1:A:119:GLN:HG3	2.00	0.61
1:B:60:THR:HG22	1:B:112:SER:OG	1.99	0.61
1:B:45:SER:HA	1:B:116:LEU:O	2.01	0.61
1:B:27:PRO:HG3	1:B:183:ILE:HD11	1.82	0.61
1:B:206:CYS:HA	1:B:288:TYR:CD1	2.36	0.60
1:B:58:HIS:O	1:B:60:THR:HG23	2.01	0.59
1:A:65:GLY:O	1:A:66:TYR:CB	2.51	0.59
3:D:216:DC:H2''	3:D:217:DA:C8	2.37	0.59
1:A:105:CYS:SG	1:A:107:ASP:OD2	2.60	0.59
1:B:65:GLY:O	1:B:66:TYR:HB2	2.02	0.58
1:B:220:GLN:HA	1:B:247:GLN:HE21	1.68	0.58
1:A:180:SER:O	1:A:181:HIS:C	2.47	0.57
1:A:127:GLU:OE2	1:A:127:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLU:C	1:B:149:ARG:H	2.12	0.57
1:A:79:LYS:NZ	1:A:153:ASP:OD2	2.38	0.57
1:A:223:ASP:O	1:A:224:ILE:HB	2.03	0.57
3:D:217:DA:H2'	3:D:218:DG:C8	2.40	0.57
1:B:221:LYS:HB3	1:B:244:VAL:HG11	1.87	0.56
1:A:86:HIS:NE2	1:A:157:VAL:HG12	2.20	0.56
1:A:267:ARG:HH11	1:A:267:ARG:CG	2.18	0.56
1:B:85:PRO:HD3	1:B:139:ASN:OD1	2.05	0.56
1:A:58:HIS:HB3	1:A:59:PRO:CD	2.36	0.56
1:B:167:ASP:HB3	1:B:173:LEU:HD11	1.88	0.55
1:B:63:ILE:HB	1:B:109:SER:HB2	1.88	0.55
1:A:122:LYS:O	1:A:124:ARG:N	2.39	0.55
1:B:211:GLU:HA	1:B:252:PHE:O	2.06	0.55
1:B:221:LYS:HE3	1:B:222:GLU:OE2	2.06	0.54
1:B:136:THR:O	1:B:137:ASN:HB2	2.07	0.54
1:B:141:PHE:O	1:B:143:VAL:N	2.41	0.54
1:A:267:ARG:CG	1:A:267:ARG:NH1	2.70	0.54
1:A:212:ILE:CD1	1:A:254:THR:HG21	2.37	0.54
1:B:194:LEU:HD21	1:B:274:ARG:NH1	2.23	0.53
1:A:233:TRP:CH2	1:A:235:ALA:HB2	2.44	0.53
1:B:180:SER:O	1:B:181:HIS:O	2.26	0.52
1:A:36:TYR:CE1	1:A:120:CYS:SG	3.02	0.52
1:A:206:CYS:SG	1:A:262:LEU:HD12	2.50	0.52
1:B:277:ASP:O	1:B:278:ARG:HB2	2.08	0.52
1:A:95:CYS:HA	1:A:99:TYR:O	2.10	0.52
1:A:84:ARG:HB3	1:A:85:PRO:HD2	1.91	0.51
1:B:125:ASP:O	1:B:128:GLN:NE2	2.44	0.51
1:B:93:LYS:HB2	1:B:115:ASN:HD22	1.76	0.51
1:A:71:THR:HG22	1:A:103:ASP:OD1	2.11	0.51
1:B:60:THR:HA	1:B:111:HIS:O	2.10	0.51
1:A:219:VAL:O	1:A:247:GLN:HB3	2.11	0.51
1:B:233:TRP:CD1	1:B:258:ALA:HB2	2.46	0.50
1:A:220:GLN:HA	1:A:247:GLN:NE2	2.27	0.50
1:A:214:LEU:HD23	1:A:214:LEU:C	2.36	0.50
1:A:205:SER:HB2	1:A:210:ASP:OD2	2.10	0.50
1:B:89:GLU:HB2	1:B:119:GLN:HE21	1.76	0.50
1:A:226:VAL:HG11	1:A:252:PHE:CE2	2.47	0.50
1:A:74:ILE:HD13	1:A:161:PHE:HE1	1.78	0.49
1:B:232:GLY:O	1:B:233:TRP:HB2	2.12	0.49
1:A:81:PRO:HA	1:A:82:PRO:C	2.38	0.49
1:A:34:PHE:CZ	1:A:185:ASP:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:HD3	1:B:139:ASN:CG	2.37	0.49
1:A:199:VAL:HG21	1:A:284:MET:HE1	1.93	0.49
1:B:257:TYR:C	1:B:259:ASP:H	2.22	0.48
1:A:26:GLN:O	1:A:48:GLY:HA2	2.13	0.48
3:D:207:DG:H2''	3:D:208:DG:C8	2.49	0.47
1:B:188:ALA:O	1:B:192:ALA:HB2	2.15	0.47
1:A:194:LEU:HD12	1:A:279:GLU:HG3	1.97	0.47
1:B:233:TRP:NE1	1:B:258:ALA:HB2	2.29	0.47
1:A:171:ARG:HG3	1:A:172:PRO:HD2	1.97	0.46
1:A:189:PRO:HB2	1:A:220:GLN:HG3	1.98	0.46
1:B:73:ARG:NH2	1:B:99:TYR:CZ	2.83	0.46
1:B:141:PHE:O	1:B:142:HIS:C	2.58	0.46
1:A:90:LEU:HD23	1:A:117:GLY:O	2.16	0.46
1:A:90:LEU:H	1:A:98:GLY:HA2	1.80	0.46
1:B:105:CYS:SG	1:B:108:ARG:NH1	2.89	0.46
1:A:243:ASP:OD1	1:B:198:ARG:NH2	2.37	0.45
1:B:214:LEU:C	1:B:214:LEU:HD23	2.40	0.45
1:A:241:GLN:C	1:A:243:ASP:H	2.24	0.45
1:A:86:HIS:C	1:A:88:HIS:H	2.23	0.45
1:A:122:LYS:O	1:A:125:ASP:N	2.48	0.44
1:B:180:SER:C	1:B:181:HIS:O	2.60	0.44
1:B:230:GLY:O	1:B:231:PRO:C	2.61	0.44
1:B:26:GLN:HB3	1:B:27:PRO:HD2	2.00	0.44
1:A:26:GLN:HB3	1:A:27:PRO:HD2	2.00	0.44
1:B:246:ARG:HH12	2:C:106:DG:P	2.41	0.44
1:A:66:TYR:CE2	1:A:165:VAL:HB	2.53	0.44
1:B:51:SER:O	1:B:52:THR:HG23	2.18	0.44
1:B:240:SER:C	1:B:242:ALA:H	2.26	0.43
1:A:28:LYS:HB2	1:A:47:PRO:HG2	2.00	0.43
1:A:86:HIS:O	1:A:88:HIS:N	2.43	0.43
1:A:58:HIS:HB3	1:A:59:PRO:HD3	2.00	0.43
1:A:205:SER:CB	1:A:210:ASP:OD2	2.66	0.43
1:B:143:VAL:CG1	1:B:144:PRO:HD2	2.49	0.43
1:A:264:ALA:O	1:A:290:PRO:HG3	2.19	0.43
1:B:248:VAL:HG23	1:B:248:VAL:O	2.18	0.43
1:A:244:VAL:HA	1:A:249:ALA:O	2.19	0.43
1:B:100:TYR:CD1	1:B:100:TYR:C	2.96	0.42
1:B:226:VAL:HG11	1:B:252:PHE:CE2	2.53	0.42
1:B:235:ALA:HB1	1:B:255:PRO:CG	2.50	0.42
1:A:97:ASP:HB2	1:A:99:TYR:CE2	2.55	0.42
1:B:34:PHE:CE2	1:B:185:ASP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ASP:C	1:B:169:ALA:H	2.28	0.42
1:B:221:LYS:NZ	2:C:107:DA:H5'	2.34	0.42
1:A:167:ASP:HB2	1:A:168:PRO:HD2	2.02	0.41
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.94	0.41
1:B:219:VAL:HG22	1:B:247:GLN:O	2.20	0.41
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.33	0.41
1:A:264:ALA:HB1	1:A:265:PRO:CD	2.51	0.41
1:A:290:PRO:O	1:A:292:THR:HG23	2.21	0.41
1:A:223:ASP:OD1	1:A:274:ARG:HG2	2.20	0.41
1:A:30:ARG:O	1:A:31:GLY:C	2.64	0.41
1:B:224:ILE:HD11	1:B:272:LEU:HD22	2.03	0.41
1:A:251:VAL:HB	1:B:198:ARG:NH2	2.35	0.41
1:B:214:LEU:HD23	1:B:215:LEU:N	2.35	0.41
1:B:222:GLU:HA	1:B:241:GLN:NE2	2.35	0.41
1:A:63:ILE:HD12	1:A:63:ILE:N	2.36	0.41
1:B:129:ALA:O	1:B:133:ARG:HG2	2.21	0.41
1:B:200:ASN:HB3	1:B:213:PHE:HB2	2.02	0.41
1:B:206:CYS:HA	1:B:288:TYR:CE1	2.55	0.41
1:A:176:THR:HA	1:A:177:PRO:HD3	1.80	0.41
1:A:187:ARG:HG3	1:A:187:ARG:NH1	2.36	0.41
1:A:274:ARG:HA	1:A:275:PRO:HD3	1.81	0.41
1:B:76:LEU:HD11	1:B:90:LEU:HD13	2.03	0.41
1:B:271:GLN:HE22	1:B:280:LEU:HD13	1.86	0.41
1:A:275:PRO:O	1:A:276:SER:C	2.64	0.40
1:B:239:PHE:CD1	1:B:239:PHE:N	2.88	0.40
1:B:77:VAL:HA	1:B:84:ARG:O	2.21	0.40
1:A:277:ASP:O	1:A:278:ARG:C	2.64	0.40
1:B:35:ARG:O	1:B:119:GLN:HA	2.21	0.40
1:B:136:THR:O	1:B:137:ASN:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	274/287 (96%)	219 (80%)	43 (16%)	12 (4%)	2	18
1	B	272/287 (95%)	211 (78%)	42 (15%)	19 (7%)	1	10
All	All	546/574 (95%)	430 (79%)	85 (16%)	31 (6%)	1	13

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	TYR
1	A	181	HIS
1	A	224	ILE
1	B	142	HIS
1	B	150	GLY
1	B	181	HIS
1	B	224	ILE
1	B	231	PRO
1	B	263	GLN
1	A	278	ARG
1	A	291	ASP
1	B	138	ASN
1	B	232	GLY
1	B	233	TRP
1	B	249	ALA
1	A	42	SER
1	A	262	LEU
1	B	148	GLN
1	B	278	ARG
1	A	231	PRO
1	A	265	PRO
1	B	40	GLY
1	B	66	TYR
1	B	165	VAL
1	B	171	ARG
1	B	264	ALA
1	B	275	PRO
1	A	168	PRO
1	A	165	VAL
1	A	177	PRO
1	B	172	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	
1	A	245/257 (95%)	228 (93%)	17 (7%)	14	41
1	B	244/257 (95%)	231 (95%)	13 (5%)	20	48
All	All	489/514 (95%)	459 (94%)	30 (6%)	17	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	32	MET
1	A	63	ILE
1	A	76	LEU
1	A	79	LYS
1	A	88	HIS
1	A	113	PHE
1	A	127	GLU
1	A	128	GLN
1	A	130	ILE
1	A	146	GLU
1	A	187	ARG
1	A	200	ASN
1	A	203	SER
1	A	240	SER
1	A	269	SER
1	A	270	MET
1	B	28	LYS
1	B	78	THR
1	B	96	ARG
1	B	108	ARG
1	B	124	ARG
1	B	128	GLN
1	B	146	GLU
1	B	157	VAL
1	B	231	PRO
1	B	239	PHE

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Mol	Chain	Res	Type
1	B	262	LEU
1	B	285	GLU
1	B	291	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	137	ASN
1	A	148	GLN
1	A	181	HIS
1	A	186	ASN
1	A	241	GLN
1	A	247	GLN
1	A	287	GLN
1	B	29	GLN
1	B	58	HIS
1	B	114	GLN
1	B	115	ASN
1	B	119	GLN
1	B	128	GLN
1	B	135	GLN
1	B	137	ASN
1	B	148	GLN
1	B	155	ASN
1	B	162	GLN
1	B	190	ASN
1	B	200	ASN
1	B	241	GLN
1	B	247	GLN
1	B	271	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 ⓘ

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	276/287 (96%)	0.77	12 (4%) 40 22	61, 108, 182, 217	0
1	B	274/287 (95%)	0.84	25 (9%) 15 11	47, 117, 153, 186	0
2	C	17/19 (89%)	0.87	0 100 100	58, 84, 137, 156	0
3	D	17/19 (89%)	1.02	0 100 100	46, 84, 159, 195	0
All	All	584/612 (95%)	0.81	37 (6%) 26 16	46, 113, 173, 217	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	ALA	4.1
1	B	249	ALA	3.7
1	B	155	ASN	3.7
1	B	76	LEU	3.3
1	A	155	ASN	3.2
1	A	163	VAL	3.1
1	A	218	LYS	2.9
1	B	217	ASP	2.8
1	B	270	MET	2.8
1	A	276	SER	2.7
1	A	41	ARG	2.7
1	B	113	PHE	2.6
1	B	87	PRO	2.6
1	B	142	HIS	2.5
1	B	120	CYS	2.5
1	B	157	VAL	2.5
1	A	287	GLN	2.5
1	B	218	LYS	2.5
1	B	187	ARG	2.5
1	B	121	VAL	2.5
1	B	188	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	177	PRO	2.4
1	B	118	ILE	2.3
1	B	153	ASP	2.3
1	B	286	PHE	2.3
1	B	156	ALA	2.2
1	B	138	ASN	2.2
1	A	192	ALA	2.2
1	B	43	ALA	2.2
1	A	33	ARG	2.2
1	B	208	GLY	2.2
1	A	85	PRO	2.1
1	A	156	ALA	2.1
1	B	154	LEU	2.1
1	A	121	VAL	2.1
1	B	88	HIS	2.1
1	B	207	LEU	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.