



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:55 AM UTC

PDB ID : 7W7L / pdb_00007w7l
Title : Structure of NF-kB p52 homodimer bound to 13-mer A/T-centric P-Selectin
kB DNA fragment
Authors : Meshcheryakov, V.A.; Wang, V.Y.-F.
Deposited on : 2021-12-05
Resolution : 3.00 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

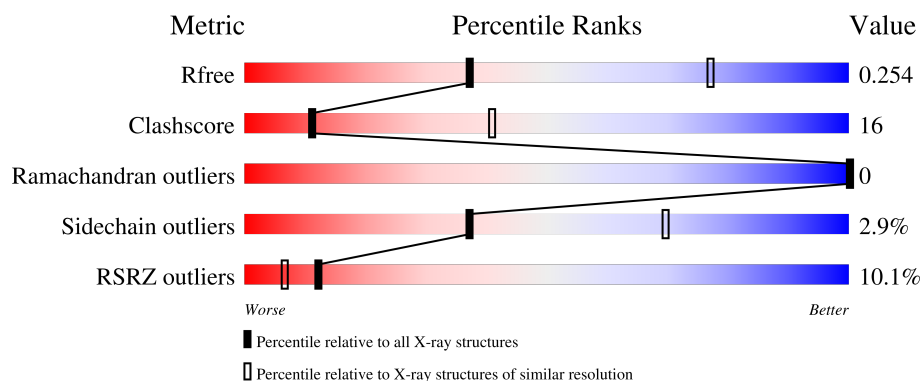
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	327	10% 64% 24% 10%
1	B	327	9% 64% 24% 10%
2	C	13	54% 31% 15%
3	D	13	38% 46% 15%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5191 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 Nuclear factor NF-kappa-B p52 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2321	1458	418	433	12			
1	B	294	Total	C	N	O	S	0	0	0
			2319	1458	418	431	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			262	125	49	76	12			

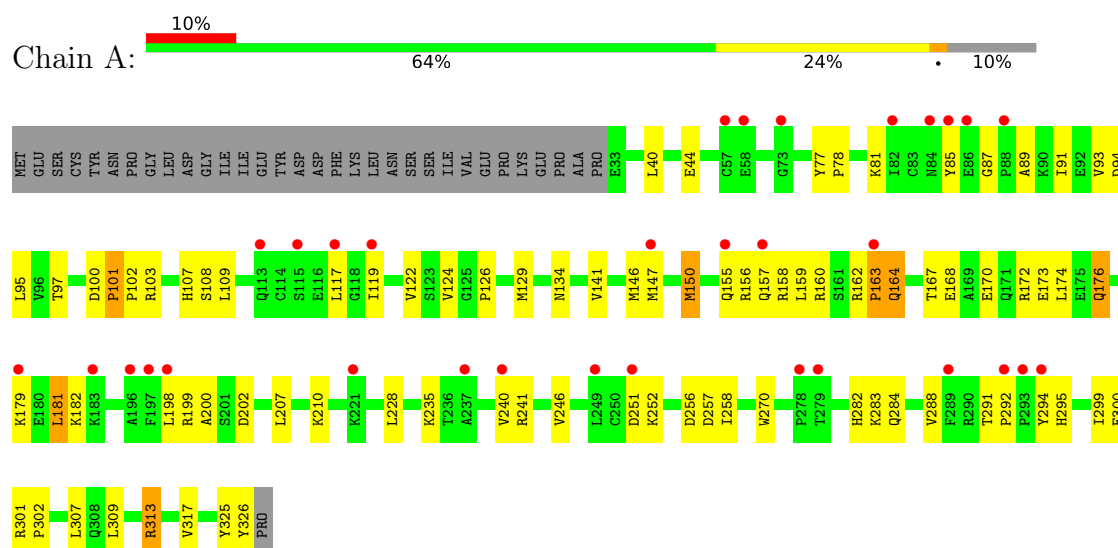
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	C	1	Total	O	0	0
			1	1		
4	B	6	Total	O	0	0
			6	6		

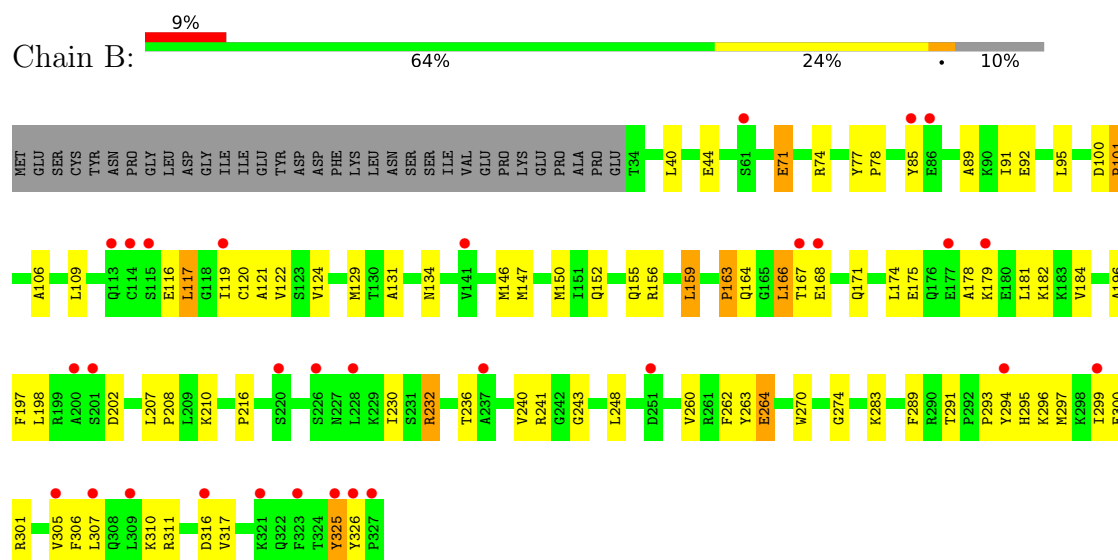
3 Residue-property plots [i](#)

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: Nuclear factor NF-kappa-B p52 subunit

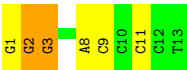


- Molecule 1: Nuclear factor NF-kappa-B p52 subunit

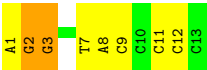
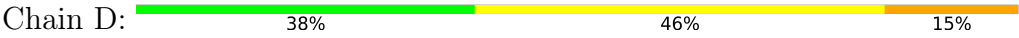


- Molecule 2: DNA (5'-D(*GP*GP*GP*GP*GP*TP*AP*AP*CP*CP*CP*CP*T)-3')





● Molecule 3: DNA (5'-D(*AP*GP*GP*GP*GP*TP*TP*AP*CP*CP*CP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	225.28Å 225.28Å 96.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.77 – 3.00 48.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.77-3.00) 99.9 (48.77-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.258 0.240 , 0.254	Depositor DCC
R_{free} test set	1529 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 135.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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	1.01	4/2370 (0.2%)	1.39	9/3190 (0.3%)
1	B	1.01	1/2369 (0.0%)	1.36	10/3190 (0.3%)
2	C	0.72	0/297	1.36	4/457 (0.9%)
3	D	0.72	0/293	1.37	6/450 (1.3%)
All	All	0.98	5/5329 (0.1%)	1.38	29/7287 (0.4%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	C-O	-6.96	1.17	1.24
1	B	197	PHE	C-O	6.51	1.31	1.24
1	A	150	MET	C-O	-5.54	1.17	1.24
1	A	91	ILE	C-O	-5.25	1.18	1.24
1	A	241	ARG	C-O	5.07	1.30	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLN	N-CA-C	9.26	121.37	111.28
2	C	1	DG	P-O3'-C3'	-7.28	109.28	120.20
1	A	174	LEU	N-CA-C	-7.04	103.68	111.36
1	A	176	GLN	O-C-N	6.64	128.94	122.03
1	B	181	LEU	N-CA-C	-6.55	105.42	113.41
1	B	101	PRO	N-CA-C	-6.45	102.83	110.70
3	D	3	DG	P-O3'-C3'	-6.28	110.78	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	LEU	N-CA-C	-6.24	103.06	112.04
3	D	1	DA	C4'-C3'-O3'	-6.23	100.65	110.00
1	B	216	PRO	N-CA-C	5.95	120.33	111.41
1	A	181	LEU	N-CA-C	-5.91	106.20	113.41
1	A	163	PRO	N-CA-C	5.89	119.76	111.33
3	D	12	DC	P-O3'-C3'	-5.87	111.40	120.20
2	C	3	DG	P-O3'-C3'	-5.86	111.41	120.20
1	B	163	PRO	N-CA-C	5.81	121.60	113.53
1	A	210	LYS	CA-C-N	5.68	126.12	119.99
1	A	210	LYS	C-N-CA	5.68	126.12	119.99
3	D	7	DT	P-O3'-C3'	-5.65	111.72	120.20
2	C	11	DC	C4'-C3'-O3'	-5.64	101.54	110.00
1	B	210	LYS	CA-C-N	5.64	126.08	119.99
1	B	210	LYS	C-N-CA	5.64	126.08	119.99
1	A	101	PRO	N-CA-C	-5.54	103.94	110.70
3	D	11	DC	C4'-C3'-O3'	-5.52	101.72	110.00
1	B	155	GLN	N-CA-C	-5.41	105.03	111.03
2	C	2	DG	O3'-P-O5'	-5.33	96.01	104.00
3	D	2	DG	O3'-P-O5'	-5.32	96.02	104.00
1	B	326	TYR	CB-CA-C	5.26	117.03	109.09
1	B	325	TYR	CA-C-O	-5.22	114.58	120.43
1	A	155	GLN	O-C-N	5.19	127.64	122.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	LYS	Mainchain

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	2321	0	2324	68	1
1	B	2319	0	2325	97	0
2	C	265	0	147	2	0
3	D	262	0	147	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	0	0	0
4	B	6	0	0	0	0
4	C	1	0	0	0	0
All	All	5191	0	4943	165	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 16.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HA	1:A:207:LEU:HD23	1.41	1.01
1:A:198:LEU:HB2	1:A:207:LEU:HD11	1.50	0.94
1:B:171:GLN:O	1:B:175:GLU:HG3	1.70	0.91
1:A:167:THR:OG1	1:A:170:GLU:HG2	1.71	0.89
1:B:260:VAL:CG2	1:B:274:GLY:HA3	2.02	0.89
1:A:168:GLU:OE2	1:A:172:ARG:HG3	1.73	0.88
1:A:207:LEU:HD12	1:A:207:LEU:O	1.73	0.87
1:B:296:LYS:HB3	1:B:299:ILE:HD11	1.60	0.84
1:B:147:MET:HE3	1:B:178:ALA:HB1	1.61	0.82
1:A:240:VAL:HG13	1:A:294:TYR:HB3	1.64	0.78
1:A:173:GLU:O	1:A:176:GLN:HB2	1.84	0.78
1:A:240:VAL:HG22	1:A:325:TYR:HB3	1.67	0.76
1:B:122:VAL:CG2	1:B:131:ALA:HB1	2.16	0.76
1:B:262:PHE:CE1	1:B:307:LEU:HD13	2.23	0.74
1:A:288:VAL:HG11	1:B:232:ARG:NH1	2.03	0.73
1:B:122:VAL:HG21	1:B:131:ALA:HB1	1.73	0.71
1:B:116:GLU:OE2	1:B:116:GLU:N	2.22	0.70
1:A:93:VAL:O	1:A:119:ILE:HG13	1.92	0.70
2:C:2:DG:H2''	2:C:3:DG:H5''	1.74	0.70
3:D:2:DG:H2''	3:D:3:DG:H5''	1.72	0.70
1:B:163:PRO:O	1:B:167:THR:HG23	1.92	0.70
1:B:241:ARG:HA	1:B:293:PRO:HB3	1.75	0.69
1:B:230:ILE:CG2	1:B:248:LEU:HD11	2.22	0.69
3:D:8:DA:H2''	3:D:9:DC:O5'	1.93	0.68
1:B:74:ARG:O	1:B:74:ARG:HG2	1.92	0.68
1:B:146:MET:HE2	1:B:182:LYS:HA	1.76	0.68
1:A:100:ASP:O	1:A:102:PRO:HD3	1.96	0.66
1:A:158:ARG:NH1	1:A:170:GLU:OE1	2.28	0.66
1:B:117:LEU:HD12	1:B:119:ILE:H	1.61	0.66
1:B:230:ILE:HG23	1:B:248:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:HA	1:B:120:CYS:O	1.96	0.65
2:C:8:DA:H2''	2:C:9:DC:O5'	1.96	0.65
1:B:260:VAL:HG23	1:B:274:GLY:H	1.61	0.65
1:A:200:ALA:CA	1:A:207:LEU:HD23	2.23	0.65
1:B:240:VAL:HB	1:B:325:TYR:HB3	1.79	0.64
1:B:152:GLN:O	1:B:156:ARG:HG3	1.98	0.64
1:B:184:VAL:HG12	1:B:184:VAL:O	1.96	0.63
1:B:168:GLU:OE2	1:B:168:GLU:N	2.31	0.63
1:A:126:PRO:HA	1:A:129:MET:HE3	1.79	0.63
1:B:260:VAL:HG23	1:B:274:GLY:HA3	1.81	0.63
1:B:240:VAL:HG23	1:B:294:TYR:HB2	1.80	0.62
1:B:260:VAL:HG21	1:B:274:GLY:HA3	1.81	0.62
1:B:117:LEU:CD1	1:B:119:ILE:HB	2.30	0.62
1:A:299:ILE:HD11	1:A:326:TYR:HB2	1.80	0.62
1:A:117:LEU:O	1:A:117:LEU:HD23	1.99	0.62
1:A:198:LEU:O	1:A:207:LEU:HG	2.00	0.61
1:B:166:LEU:C	1:B:166:LEU:HD23	2.24	0.61
1:B:230:ILE:HD13	1:B:248:LEU:HD11	1.83	0.61
1:A:258:ILE:HD11	1:A:309:LEU:HD22	1.81	0.61
1:A:159:LEU:CD1	1:A:164:GLN:HA	2.30	0.61
1:B:240:VAL:HG23	1:B:294:TYR:CB	2.31	0.61
1:B:147:MET:HE3	1:B:178:ALA:CB	2.31	0.60
1:A:162:ARG:HB3	1:A:163:PRO:HD2	1.84	0.59
1:B:240:VAL:HA	1:B:325:TYR:CD1	2.38	0.58
1:B:262:PHE:CZ	1:B:307:LEU:HD13	2.38	0.58
1:A:146:MET:HE2	1:A:182:LYS:HA	1.86	0.58
1:B:310:LYS:CB	1:B:317:VAL:HG12	2.34	0.58
1:B:167:THR:OG1	1:B:168:GLU:OE2	2.20	0.57
1:B:260:VAL:HG23	1:B:274:GLY:N	2.19	0.56
1:B:147:MET:HE1	1:B:179:LYS:N	2.20	0.56
1:B:117:LEU:HA	1:B:156:ARG:HH22	1.71	0.56
1:A:282:HIS:CE1	1:A:283:LYS:HG2	2.41	0.56
1:A:240:VAL:HG21	1:A:299:ILE:HD13	1.87	0.55
1:A:167:THR:O	1:A:170:GLU:HB2	2.06	0.55
1:B:260:VAL:CG2	1:B:274:GLY:CA	2.82	0.55
1:B:147:MET:HE1	1:B:178:ALA:C	2.32	0.55
1:B:260:VAL:HG23	1:B:274:GLY:CA	2.36	0.55
1:B:159:LEU:HD21	1:B:167:THR:HG22	1.88	0.54
1:A:117:LEU:HD22	1:A:156:ARG:HH12	1.72	0.54
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.72	0.54
1:B:311:ARG:HB2	1:B:316:ASP:OD1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:O	1:B:121:ALA:HA	2.08	0.54
1:B:230:ILE:HG21	1:B:248:LEU:HD11	1.89	0.54
1:A:251:ASP:OD1	1:B:283:LYS:HE2	2.08	0.54
1:B:243:GLY:HA2	1:B:291:THR:O	2.07	0.54
1:A:159:LEU:HD13	1:A:164:GLN:HA	1.91	0.53
1:B:310:LYS:HA	1:B:317:VAL:HG12	1.90	0.53
1:A:301:ARG:HG3	1:A:302:PRO:HD2	1.91	0.53
1:A:301:ARG:CG	1:A:302:PRO:HD2	2.39	0.52
1:A:159:LEU:HG	1:A:159:LEU:O	2.09	0.52
1:B:77:TYR:CD1	1:B:134:ASN:HA	2.44	0.52
1:A:77:TYR:CD1	1:A:134:ASN:HA	2.44	0.51
1:B:270:TRP:CD1	1:B:295:HIS:HB3	2.44	0.51
1:B:95:LEU:HD21	1:B:109:LEU:HD21	1.93	0.50
1:B:305:VAL:HG12	1:B:306:PHE:N	2.27	0.50
1:A:95:LEU:HG	1:A:109:LEU:HG	1.92	0.50
1:A:158:ARG:HH12	1:A:170:GLU:HB3	1.76	0.50
1:B:264:GLU:HG3	1:B:270:TRP:HE3	1.76	0.50
1:A:95:LEU:HD21	1:A:109:LEU:HD21	1.94	0.49
1:A:235:LYS:HB2	1:A:246:VAL:HG22	1.93	0.49
1:A:291:THR:HG23	1:A:292:PRO:HD2	1.93	0.49
1:A:200:ALA:HA	1:A:207:LEU:CD2	2.28	0.49
1:B:124:VAL:HG22	1:B:129:MET:HA	1.94	0.49
1:A:240:VAL:CG2	1:A:299:ILE:HD13	2.42	0.49
1:A:107:HIS:ND1	1:A:141:VAL:HG12	2.28	0.48
1:A:288:VAL:HG11	1:B:232:ARG:HH11	1.77	0.48
1:B:40:LEU:HD11	1:B:196:ALA:HB2	1.94	0.48
1:B:166:LEU:C	1:B:166:LEU:CD2	2.87	0.48
1:B:241:ARG:HG2	1:B:297:MET:SD	2.53	0.48
1:B:240:VAL:CG2	1:B:294:TYR:CB	2.91	0.48
1:B:147:MET:HE1	1:B:179:LYS:HA	1.96	0.47
1:A:182:LYS:O	1:A:182:LYS:HG3	2.13	0.47
1:B:243:GLY:CA	1:B:291:THR:O	2.62	0.47
1:A:89:ALA:HB3	1:A:124:VAL:CG2	2.44	0.47
1:B:116:GLU:H	1:B:116:GLU:CD	2.19	0.47
1:B:146:MET:HE3	1:B:150:MET:CE	2.44	0.47
1:B:147:MET:HE1	1:B:179:LYS:CA	2.45	0.47
1:B:92:GLU:HB3	1:B:119:ILE:CG2	2.45	0.46
1:B:310:LYS:HB2	1:B:317:VAL:HG12	1.98	0.46
1:B:116:GLU:N	1:B:116:GLU:CD	2.74	0.46
1:B:236:THR:O	1:B:236:THR:HG22	2.15	0.46
1:B:310:LYS:CA	1:B:317:VAL:HG12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD11	1:B:196:ALA:CB	2.46	0.46
1:B:159:LEU:HD13	1:B:163:PRO:HB3	1.97	0.46
1:A:100:ASP:N	1:A:101:PRO:HD2	2.31	0.46
1:A:252:LYS:HA	1:A:284:GLN:O	2.16	0.46
1:A:87:GLY:O	1:A:129:MET:HE1	2.16	0.46
1:B:77:TYR:CG	1:B:134:ASN:HA	2.51	0.46
1:A:240:VAL:HG21	1:A:299:ILE:CD1	2.46	0.45
1:B:270:TRP:HZ3	1:B:305:VAL:HG11	1.81	0.45
1:B:184:VAL:O	1:B:184:VAL:CG1	2.62	0.45
1:B:296:LYS:O	1:B:299:ILE:HD11	2.16	0.45
1:B:95:LEU:HG	1:B:109:LEU:HG	1.98	0.45
1:A:258:ILE:HD11	1:A:309:LEU:CD2	2.47	0.45
1:A:40:LEU:HD12	1:A:81:LYS:O	2.17	0.45
1:A:288:VAL:CG1	1:B:232:ARG:NH1	2.75	0.45
1:A:240:VAL:HG13	1:A:294:TYR:CB	2.42	0.44
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.47	0.44
1:A:94:ASP:HB3	1:A:119:ILE:HG12	1.99	0.44
1:A:307:LEU:HD12	1:A:307:LEU:C	2.43	0.44
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.00	0.44
1:B:124:VAL:CG2	1:B:129:MET:HA	2.47	0.43
1:B:262:PHE:CD1	1:B:307:LEU:HD13	2.53	0.43
1:A:207:LEU:HD12	1:A:207:LEU:C	2.42	0.43
1:B:100:ASP:N	1:B:101:PRO:CD	2.81	0.43
1:B:270:TRP:HZ3	1:B:305:VAL:CG1	2.30	0.43
1:A:100:ASP:N	1:A:101:PRO:CD	2.82	0.43
1:A:157:GLN:O	1:A:160:ARG:HB3	2.18	0.43
1:B:146:MET:CE	1:B:182:LYS:HA	2.47	0.43
1:B:240:VAL:CG2	1:B:294:TYR:HB3	2.48	0.43
1:A:109:LEU:HB2	1:A:119:ILE:HD11	2.00	0.43
1:B:270:TRP:CZ3	1:B:305:VAL:HG11	2.54	0.43
1:B:85:TYR:CE2	1:B:198:LEU:HD13	2.54	0.43
1:B:248:LEU:HB2	1:B:289:PHE:HE1	1.84	0.43
1:A:270:TRP:CD1	1:A:295:HIS:HB3	2.53	0.42
1:B:106:ALA:HB2	1:B:150:MET:HE1	2.01	0.42
1:B:207:LEU:HD12	1:B:208:PRO:CD	2.49	0.42
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.92	0.42
1:B:117:LEU:HD12	1:B:119:ILE:N	2.30	0.42
1:B:264:GLU:CG	1:B:270:TRP:HE3	2.32	0.42
1:A:44:GLU:O	1:A:78:PRO:HA	2.20	0.42
1:A:85:TYR:CD1	1:A:85:TYR:C	2.98	0.42
1:A:257:ASP:OD1	1:A:313:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:O	1:B:207:LEU:HB3	2.19	0.41
1:B:263:TYR:CD1	1:B:263:TYR:C	2.98	0.41
1:B:44:GLU:O	1:B:78:PRO:HA	2.19	0.41
1:B:71:GLU:O	1:B:74:ARG:O	2.38	0.41
1:A:100:ASP:O	1:A:102:PRO:CD	2.68	0.41
1:B:117:LEU:H	1:B:117:LEU:HG	1.63	0.41
1:A:77:TYR:CG	1:A:134:ASN:HA	2.56	0.41
1:A:97:THR:HG23	1:A:103:ARG:O	2.21	0.41
1:A:199:ARG:O	1:A:207:LEU:HD21	2.21	0.40
1:A:157:GLN:HG2	1:A:160:ARG:HE	1.87	0.40
1:A:228:LEU:HD12	1:A:317:VAL:HA	2.03	0.40
1:B:300:GLU:HG2	1:B:301:ARG:HG2	2.04	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)
1:A:326:TYR:O	1:A:326:TYR:O[10_444]	1.84	0.36

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/327 (89%)	272 (93%)	20 (7%)	0	100	100
1	B	292/327 (89%)	272 (93%)	20 (7%)	0	100	100
All	All	584/654 (89%)	544 (93%)	40 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	255/285 (90%)	248 (97%)	7 (3%)	39	71
1	B	255/285 (90%)	247 (97%)	8 (3%)	35	68
All	All	510/570 (90%)	495 (97%)	15 (3%)	37	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	147	MET
1	A	150	MET
1	A	202	ASP
1	A	256	ASP
1	A	300	GLU
1	A	313	ARG
1	B	71	GLU
1	B	117	LEU
1	B	159	LEU
1	B	164	GLN
1	B	166	LEU
1	B	202	ASP
1	B	232	ARG
1	B	264	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	113	GLN
1	A	140	HIS
1	A	152	GLN
1	A	282	HIS
1	A	308	GLN
1	B	140	HIS

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	164	GLN
1	B	227	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 [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	294/327 (89%)	0.76	32 (10%) 10 6	60, 117, 196, 242	0
1	B	294/327 (89%)	0.89	30 (10%) 12 6	73, 130, 198, 238	0
2	C	13/13 (100%)	-0.72	0 100 100	74, 80, 87, 88	0
3	D	13/13 (100%)	-0.64	0 100 100	74, 78, 84, 90	0
All	All	614/680 (90%)	0.76	62 (10%) 12 7	60, 120, 197, 242	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	4.8
1	A	221	LYS	3.7
1	B	61	SER	3.6
1	A	58	GLU	3.5
1	A	293	PRO	3.5
1	B	307	LEU	3.5
1	A	157	GLN	3.4
1	A	117	LEU	3.3
1	A	85	TYR	3.2
1	A	147	MET	3.1
1	B	305	VAL	3.1
1	A	88	PRO	3.1
1	A	86	GLU	3.1
1	A	279	THR	3.0
1	B	113	GLN	3.0
1	B	323	PHE	3.0
1	A	179	LYS	2.9
1	A	278	PRO	2.9
1	B	326	TYR	2.8
1	B	85	TYR	2.8
1	B	115	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	2.6
1	A	237	ALA	2.6
1	B	294	TYR	2.6
1	A	249	LEU	2.6
1	A	84	ASN	2.5
1	A	82	ILE	2.5
1	B	321	LYS	2.5
1	A	155	GLN	2.5
1	A	240	VAL	2.5
1	B	141	VAL	2.4
1	B	299	ILE	2.4
1	A	163	PRO	2.4
1	A	289	PHE	2.4
1	B	226	SER	2.4
1	B	316	ASP	2.4
1	B	168	GLU	2.4
1	A	198	LEU	2.3
1	B	86	GLU	2.3
1	A	183	LYS	2.3
1	A	119	ILE	2.3
1	A	197	PHE	2.3
1	A	113	GLN	2.3
1	A	115	SER	2.2
1	B	114	CYS	2.2
1	B	177	GLU	2.2
1	A	57	CYS	2.2
1	B	179	LYS	2.2
1	B	325	TYR	2.2
1	B	220	SER	2.2
1	B	119	ILE	2.2
1	A	292	PRO	2.2
1	B	200	ALA	2.2
1	B	251	ASP	2.2
1	A	196	ALA	2.2
1	B	167	THR	2.1
1	A	251	ASP	2.1
1	B	309	LEU	2.1
1	B	327	PRO	2.1
1	A	73	GLY	2.1
1	B	201	SER	2.0
1	B	228	LEU	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.