



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 06:11 PM JST

PDB ID : 7VUP  
Title : Structure of NF-kB p52 homodimer bound to +1/-1 swap P-Selectin kB DNA fragment  
Authors : Meshcheryakov, V.A.; Wang, V.Y.-F.  
Deposited on : 2021-11-04  
Resolution : 3.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

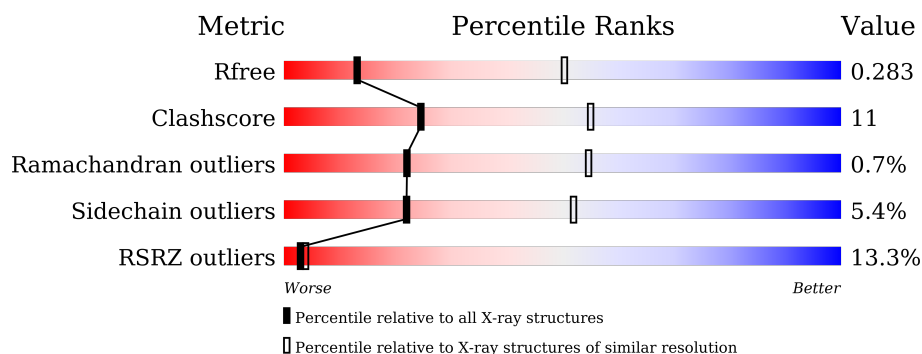
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	398	
1	B	398	
2	C	18	
3	D	18	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5359 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	296	Total	C	N	O	S	0	0	0
			2334	1469	420	433	12			
1	B	296	Total	C	N	O	S	0	0	0
			2334	1469	420	433	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			341	163	62	100	16			

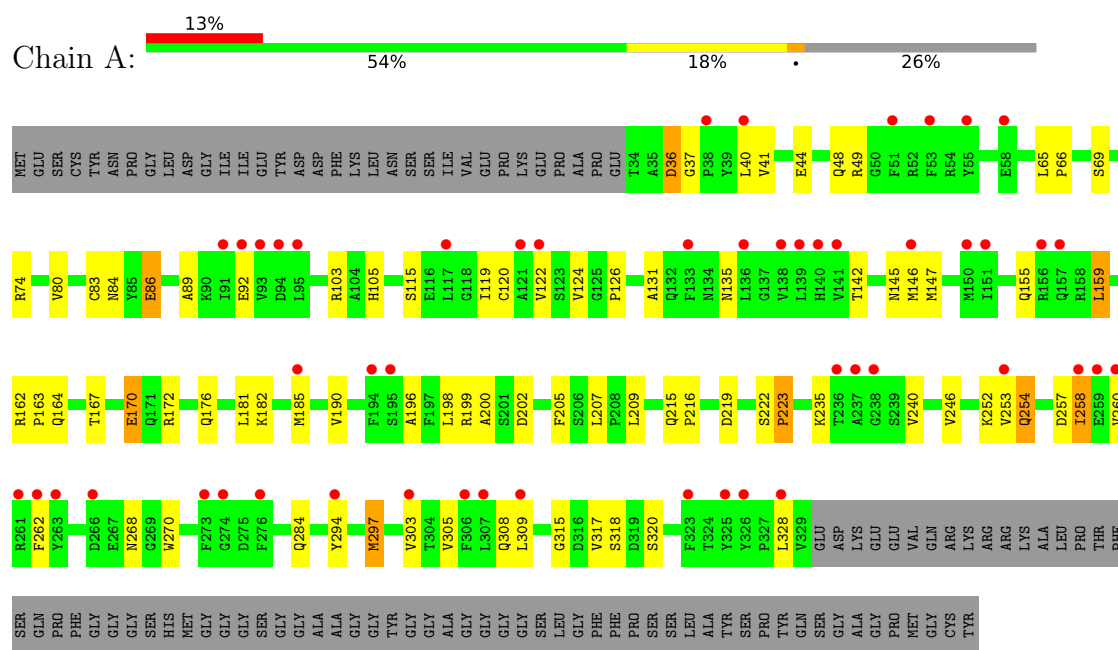
- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*AP\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*CP\*CP\*CP\*TP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

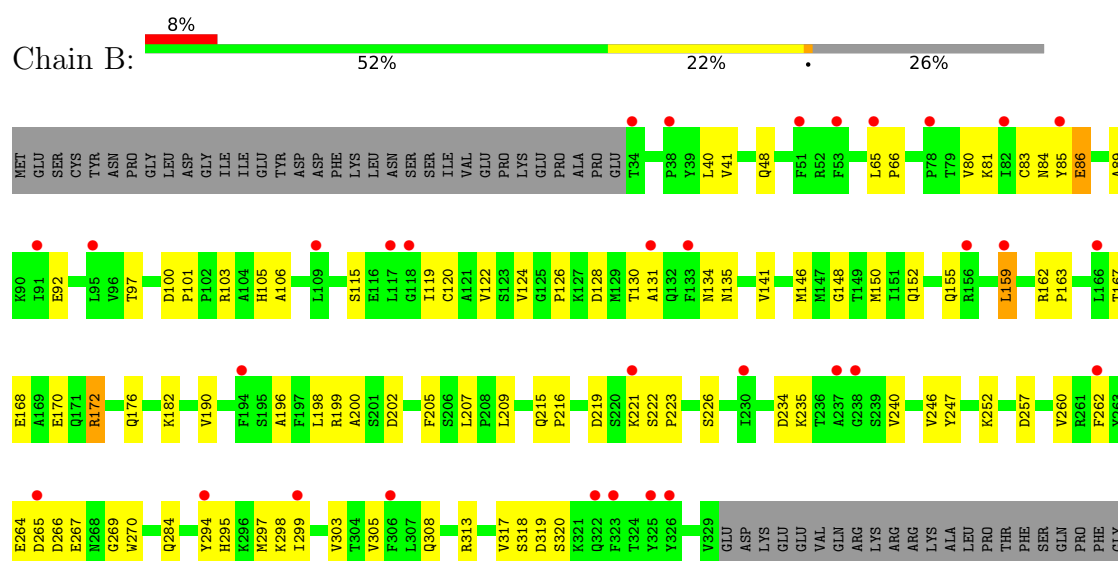
### 3 Residue-property plots

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: Nuclear factor NF-kappa-B p52 subunit

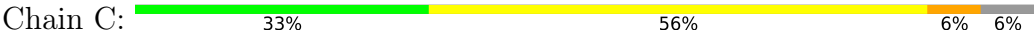


#### • Molecule 1: Nuclear factor NF-kappa-B p52 subunit



GLY	GLY	SER	HIS	MET	GLY	GLY	GLY	SER	GLY	GLY	ALA	ALA	GLY	GLY	TYR	GLY	GLY	ALA	GLY	GLY	GLY	SER	SER	LEU	GLY	PHE	PRO	SER	SER	LEU	ALA	TYR	SER	PRO	TYR	GLN	SER	GLY	ALA	GLY	PRO	MET	GLY	CYS	TYR
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● Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*GP\*GP\*GP\*GP\*AP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*T)-3')



C1	A2	A3	C4	G5	G6	G7	A8	C9	T10	C11	C12	C13	C14	C15	T16	T17	DC
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● Molecule 3: DNA (5'-D(\*AP\*AP\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*CP\*CP\*CP\*TP\*TP\*G)-3')



DC	A2	A3	C4	G5	G8	A9	C12	C13	C14	C15	T16	T17	G18
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.99Å 84.29Å 140.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.40 45.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.45-3.40) 99.7 (45.41-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.271 , 0.286 0.271 , 0.283	Depositor DCC
$R_{free}$ test set	690 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.0	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 108.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1259e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.66	0/2384	0.86	0/3211
1	B	0.65	0/2384	0.86	0/3211
2	C	0.92	0/381	1.45	6/585 (1.0%)
3	D	0.95	0/393	1.44	3/606 (0.5%)
All	All	0.70	0/5542	0.97	9/7613 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	DA	P-O3'-C3'	-12.41	104.81	119.70
2	C	5	DG	P-O3'-C3'	-8.39	109.63	119.70
3	D	9	DA	P-O3'-C3'	-6.88	111.44	119.70
3	D	8	DG	P-O3'-C3'	-6.34	112.09	119.70
2	C	4	DG	P-O3'-C3'	-5.93	112.58	119.70
3	D	5	DG	P-O3'-C3'	-5.79	112.75	119.70
2	C	2	DA	P-O3'-C3'	-5.47	113.13	119.70
2	C	10	DT	C1'-O4'-C4'	-5.41	104.69	110.10
2	C	11	DC	C1'-O4'-C4'	-5.20	104.90	110.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2334	0	2345	48	2
1	B	2334	0	2345	57	2
2	C	341	0	192	7	0
3	D	350	0	192	5	0
All	All	5359	0	5074	113	2

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 11.

All (113) 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:44:GLU:OE2	1:A:69:SER:OG	1.64	1.14
1:B:40:LEU:HD12	1:B:196:ALA:HB2	1.52	0.90
1:A:40:LEU:HD12	1:A:196:ALA:HB2	1.53	0.90
1:B:40:LEU:HD21	1:B:80:VAL:HB	1.56	0.88
1:A:40:LEU:HD21	1:A:80:VAL:HB	1.57	0.85
2:C:7:DG:O6	1:B:221:LYS:NZ	2.13	0.81
1:B:155:GLN:O	1:B:159:LEU:HB2	1.81	0.81
1:B:167:THR:HG23	1:B:170:GLU:H	1.48	0.78
1:A:167:THR:HG23	1:A:170:GLU:H	1.50	0.76
1:A:253:VAL:HB	1:A:258:ILE:HG13	1.69	0.74
1:A:199:ARG:HA	1:A:205:PHE:HA	1.70	0.73
1:B:270:TRP:HZ3	1:B:305:VAL:HG11	1.51	0.73
1:B:199:ARG:HA	1:B:205:PHE:HA	1.71	0.72
1:B:270:TRP:CZ3	1:B:305:VAL:HG11	2.27	0.69
1:B:222:SER:HB2	1:B:223:PRO:HD2	1.73	0.69
1:B:48:GLN:HG3	1:B:216:PRO:O	1.92	0.68
2:C:14:DC:H2''	2:C:15:DC:O5'	1.95	0.67
1:B:269:GLY:O	1:B:270:TRP:C	2.33	0.67
1:A:222:SER:HB2	1:A:223:PRO:HD2	1.78	0.66
1:A:48:GLN:HG3	1:A:216:PRO:O	1.99	0.63
1:B:317:VAL:HG12	1:B:318:SER:O	1.99	0.62
1:B:92:GLU:HA	1:B:120:CYS:O	2.00	0.61
1:A:92:GLU:HA	1:A:120:CYS:O	2.01	0.61
1:A:317:VAL:HG12	1:A:318:SER:O	2.00	0.60
1:B:270:TRP:CD1	1:B:295:HIS:HB3	2.37	0.60
1:B:200:ALA:HB2	1:B:207:LEU:CD2	2.32	0.60
1:B:198:LEU:O	1:B:207:LEU:HB2	2.03	0.59
1:A:198:LEU:O	1:A:207:LEU:HB2	2.04	0.58
2:C:13:DC:H2'	2:C:14:DC:C6	2.38	0.58
1:B:270:TRP:CG	1:B:295:HIS:HD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG23	1:B:294:TYR:HB3	1.86	0.56
1:B:162:ARG:HH12	1:B:167:THR:HG22	1.71	0.56
1:A:122:VAL:HG21	1:A:131:ALA:HB1	1.88	0.55
1:A:240:VAL:HG23	1:A:294:TYR:HB3	1.87	0.55
1:B:219:ASP:HB3	1:B:222:SER:HB3	1.88	0.55
1:A:40:LEU:CD2	1:A:80:VAL:HB	2.33	0.55
1:A:162:ARG:HH12	1:A:167:THR:HG22	1.72	0.55
1:B:234:ASP:CG	1:B:247:TYR:H	2.11	0.55
1:A:142:THR:OG1	1:A:145:ASN:HB2	2.07	0.55
1:B:122:VAL:HG21	1:B:131:ALA:HB1	1.88	0.54
1:A:200:ALA:HB2	1:A:207:LEU:CD2	2.38	0.53
1:A:40:LEU:HD23	1:A:41:VAL:N	2.23	0.53
1:B:40:LEU:HD23	1:B:41:VAL:N	2.23	0.53
1:B:40:LEU:CD2	1:B:80:VAL:HB	2.33	0.53
2:C:14:DC:H2'	2:C:15:DC:C6	2.44	0.53
1:A:36:ASP:OD1	1:A:37:GLY:N	2.40	0.52
1:A:270:TRP:HZ3	1:A:305:VAL:HG11	1.75	0.52
1:B:235:LYS:HB2	1:B:246:VAL:HG22	1.92	0.52
1:A:235:LYS:HB2	1:A:246:VAL:HG22	1.92	0.51
1:B:106:ALA:HB2	1:B:150:MET:HE1	1.92	0.51
1:B:270:TRP:CG	1:B:295:HIS:CD2	2.98	0.50
3:D:14:DC:H2'	3:D:15:DC:C6	2.46	0.50
1:A:103:ARG:HD2	1:A:181:LEU:HD21	1.93	0.50
1:B:146:MET:HB3	1:B:182:LYS:HE2	1.92	0.50
1:B:294:TYR:CZ	1:B:303:VAL:HG11	2.46	0.50
1:B:65:LEU:HD12	1:B:66:PRO:HD2	1.93	0.50
1:B:234:ASP:OD1	1:B:247:TYR:N	2.37	0.50
1:B:81:LYS:HD3	1:B:130:THR:OG1	2.12	0.49
1:A:219:ASP:HB3	1:A:222:SER:HB3	1.92	0.49
1:A:40:LEU:HD12	1:A:196:ALA:CB	2.35	0.49
2:C:3:DA:H2''	2:C:4:DG:O5'	2.13	0.49
1:B:148:GLY:O	1:B:152:GLN:HG2	2.13	0.49
1:B:40:LEU:HD12	1:B:196:ALA:CB	2.35	0.48
1:A:65:LEU:HD12	1:A:66:PRO:HD2	1.96	0.47
1:B:159:LEU:O	1:B:163:PRO:HA	2.15	0.47
1:B:284:GLN:NE2	3:D:8:DG:OP1	2.44	0.47
1:A:294:TYR:CZ	1:A:303:VAL:HG11	2.50	0.47
1:A:252:LYS:HA	1:A:284:GLN:O	2.15	0.47
1:A:297:MET:HG2	1:A:328:LEU:HD11	1.96	0.46
1:A:308:GLN:NE2	1:A:317:VAL:HG11	2.30	0.46
1:A:181:LEU:O	1:A:185:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG12	1:A:262:PHE:HE1	1.80	0.45
1:A:159:LEU:O	1:A:163:PRO:HA	2.15	0.45
2:C:13:DC:H2'	2:C:14:DC:C5	2.50	0.45
1:B:222:SER:CB	1:B:223:PRO:HD2	2.44	0.45
1:B:252:LYS:HA	1:B:284:GLN:O	2.17	0.45
1:B:264:GLU:HG3	1:B:305:VAL:HG13	1.98	0.45
1:A:222:SER:CB	1:A:223:PRO:HD2	2.46	0.45
1:B:97:THR:HG23	1:B:103:ARG:O	2.17	0.45
1:B:308:GLN:NE2	1:B:317:VAL:HG11	2.31	0.45
3:D:4:DG:H2''	3:D:5:DG:O5'	2.16	0.44
1:A:135:ASN:O	1:A:135:ASN:CG	2.56	0.44
1:B:83:CYS:O	1:B:84:ASN:HB2	2.18	0.44
1:B:100:ASP:N	1:B:101:PRO:HD2	2.33	0.43
3:D:16:DT:O2	3:D:16:DT:H2'	2.17	0.43
1:A:254:GLN:HB2	1:A:257:ASP:OD1	2.18	0.43
1:B:115:SER:HB2	1:B:119:ILE:HG22	2.00	0.43
1:B:135:ASN:O	1:B:135:ASN:CG	2.57	0.43
1:B:198:LEU:HG	1:B:209:LEU:CD1	2.49	0.43
1:B:260:VAL:HG12	1:B:262:PHE:HE1	1.83	0.43
1:A:115:SER:HB2	1:A:119:ILE:HG22	2.00	0.43
1:A:146:MET:HB3	1:A:182:LYS:HE2	2.01	0.43
1:B:89:ALA:HB3	1:B:124:VAL:CG2	2.49	0.43
1:A:83:CYS:O	1:A:84:ASN:HB2	2.18	0.42
1:B:270:TRP:CD2	1:B:295:HIS:HD2	2.37	0.42
1:A:49:ARG:HA	1:A:49:ARG:HD3	1.93	0.42
1:B:105:HIS:CD2	1:B:190:VAL:HG12	2.55	0.42
1:B:215:GLN:HB2	1:B:216:PRO:HD2	2.02	0.42
1:A:258:ILE:HD11	1:A:309:LEU:HD22	2.02	0.41
1:A:44:GLU:OE2	1:A:69:SER:CB	2.64	0.41
1:A:89:ALA:HB3	1:A:124:VAL:CG2	2.50	0.41
1:A:198:LEU:HG	1:A:209:LEU:CD1	2.50	0.41
1:B:86:GLU:HG3	1:B:126:PRO:O	2.20	0.41
1:A:155:GLN:O	1:A:159:LEU:HB2	2.21	0.41
1:A:86:GLU:HG3	1:A:126:PRO:O	2.21	0.41
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.76	0.41
1:A:215:GLN:HB2	1:A:216:PRO:HD2	2.03	0.41
1:A:284:GLN:NE2	2:C:7:DG:OP1	2.54	0.41
1:B:264:GLU:HB3	1:B:266:ASP:OD1	2.21	0.41
1:B:257:ASP:OD2	1:B:313:ARG:HD2	2.21	0.40
1:A:105:HIS:CD2	1:A:190:VAL:HG12	2.56	0.40
1:B:106:ALA:HB1	1:B:141:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LYS:HZ2	3:D:12:DC:N4	2.20	0.40

All (2) 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:74:ARG:NH2	1:B:128:ASP:OD1[2_455]	1.65	0.55
1:A:74:ARG:NH2	1:B:128:ASP:CG[2_455]	2.13	0.07

## 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	294/398 (74%)	270 (92%)	21 (7%)	3 (1%)	15	46
1	B	294/398 (74%)	280 (95%)	13 (4%)	1 (0%)	41	72
All	All	588/796 (74%)	550 (94%)	34 (6%)	4 (1%)	22	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	B	85	TYR
1	A	223	PRO
1	A	315	GLY

### 5.3.2 Protein sidechains [i](#)

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	257/330 (78%)	244 (95%)	13 (5%)	24	54
1	B	257/330 (78%)	242 (94%)	15 (6%)	20	50
All	All	514/660 (78%)	486 (95%)	28 (5%)	22	52

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLU
1	A	147	MET
1	A	159	LEU
1	A	164	GLN
1	A	170	GLU
1	A	172	ARG
1	A	176	GLN
1	A	202	ASP
1	A	254	GLN
1	A	258	ILE
1	A	268	ASN
1	A	297	MET
1	A	320	SER
1	B	86	GLU
1	B	134	ASN
1	B	159	LEU
1	B	168	GLU
1	B	172	ARG
1	B	176	GLN
1	B	202	ASP
1	B	226	SER
1	B	265	ASP
1	B	267	GLU
1	B	297	MET
1	B	298	LYS
1	B	299	ILE
1	B	319	ASP
1	B	320	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	B	134	ASN
1	B	145	ASN
1	B	282	HIS
1	B	295	HIS

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/398 (74%)	0.73	51 (17%) 1 1	110, 160, 240, 289	0
1	B	296/398 (74%)	0.67	32 (10%) 5 7	102, 156, 229, 282	0
2	C	17/18 (94%)	0.10	0 100 100	142, 169, 213, 228	0
3	D	17/18 (94%)	0.28	0 100 100	146, 172, 212, 230	0
All	All	626/832 (75%)	0.67	83 (13%) 3 4	102, 160, 234, 289	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	GLY	5.6
1	A	260	VAL	5.2
1	B	322	GLN	4.8
1	A	325	TYR	4.7
1	A	262	PHE	4.6
1	A	237	ALA	4.5
1	B	159	LEU	4.1
1	A	141	VAL	3.9
1	B	117	LEU	3.8
1	A	263	TYR	3.7
1	A	150	MET	3.6
1	B	238	GLY	3.6
1	B	323	PHE	3.5
1	B	118	GLY	3.5
1	A	323	PHE	3.5
1	B	51	PHE	3.5
1	B	325	TYR	3.4
1	A	91	ILE	3.4
1	A	326	TYR	3.3
1	B	82	ILE	3.3
1	B	95	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	3.2
1	A	273	PHE	3.2
1	A	146	MET	3.1
1	A	92	GLU	3.1
1	A	259	GLU	3.1
1	A	38	PRO	3.1
1	A	236	THR	3.1
1	B	156	ARG	3.0
1	A	140	HIS	3.0
1	A	133	PHE	2.9
1	A	138	VAL	2.9
1	A	303	VAL	2.9
1	B	133	PHE	2.8
1	A	253	VAL	2.8
1	B	262	PHE	2.8
1	B	237	ALA	2.8
1	B	78	PRO	2.7
1	A	261	ARG	2.7
1	A	53	PHE	2.7
1	A	274	GLY	2.7
1	A	276	PHE	2.7
1	A	95	LEU	2.6
1	B	230	ILE	2.6
1	A	194	PHE	2.6
1	A	294	TYR	2.6
1	B	194	PHE	2.6
1	B	299	ILE	2.5
1	A	195	SER	2.4
1	A	306	PHE	2.4
1	A	122	VAL	2.4
1	B	38	PRO	2.4
1	B	294	TYR	2.4
1	A	151	ILE	2.4
1	A	94	ASP	2.4
1	A	157	GLN	2.3
1	B	131	ALA	2.3
1	B	91	ILE	2.3
1	A	185	MET	2.3
1	A	58	GLU	2.2
1	A	117	LEU	2.2
1	A	40	LEU	2.2
1	B	326	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	221	LYS	2.2
1	A	156	ARG	2.2
1	A	258	ILE	2.2
1	A	136	LEU	2.2
1	B	166	LEU	2.2
1	B	53	PHE	2.2
1	A	121	ALA	2.2
1	B	34	THR	2.1
1	A	55	TYR	2.1
1	B	109	LEU	2.1
1	B	85	TYR	2.1
1	A	266	ASP	2.1
1	B	306	PHE	2.1
1	B	265	ASP	2.1
1	A	93	VAL	2.0
1	A	307	LEU	2.0
1	A	309	LEU	2.0
1	A	51	PHE	2.0
1	A	328	LEU	2.0
1	B	65	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 monosaccharides 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.