



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 2PSQ / pdb_00002psq
Title : Crystal Structure of Unphosphorylated Unactivated Wild Type FGF Receptor 2 (FGFR2) Kinase Domain
Authors : Chen, H.; Mohammadi, M.
Deposited on : 2007-05-07
Resolution : 2.40 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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

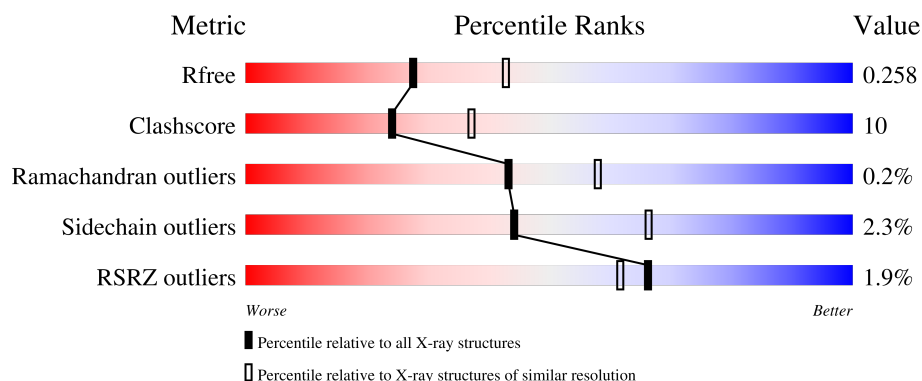
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	370	
1	B	370	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4725 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2269	1445	385	418	21			
1	B	286	Total	C	N	O	S	0	0	0
			2248	1430	382	415	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	MET	-	expression tag	UNP P21802
A	400	GLY	-	expression tag	UNP P21802
A	401	SER	-	expression tag	UNP P21802
A	402	SER	-	expression tag	UNP P21802
A	403	HIS	-	expression tag	UNP P21802
A	404	HIS	-	expression tag	UNP P21802
A	405	HIS	-	expression tag	UNP P21802
A	406	HIS	-	expression tag	UNP P21802
A	407	HIS	-	expression tag	UNP P21802
A	408	HIS	-	expression tag	UNP P21802
A	409	SER	-	expression tag	UNP P21802
A	410	GLN	-	expression tag	UNP P21802
A	411	ASP	-	expression tag	UNP P21802
A	412	PRO	-	expression tag	UNP P21802
B	399	MET	-	expression tag	UNP P21802
B	400	GLY	-	expression tag	UNP P21802
B	401	SER	-	expression tag	UNP P21802
B	402	SER	-	expression tag	UNP P21802
B	403	HIS	-	expression tag	UNP P21802
B	404	HIS	-	expression tag	UNP P21802
B	405	HIS	-	expression tag	UNP P21802
B	406	HIS	-	expression tag	UNP P21802
B	407	HIS	-	expression tag	UNP P21802
B	408	HIS	-	expression tag	UNP P21802
B	409	SER	-	expression tag	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	410	GLN	-	expression tag	UNP P21802
B	411	ASP	-	expression tag	UNP P21802
B	412	PRO	-	expression tag	UNP P21802

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

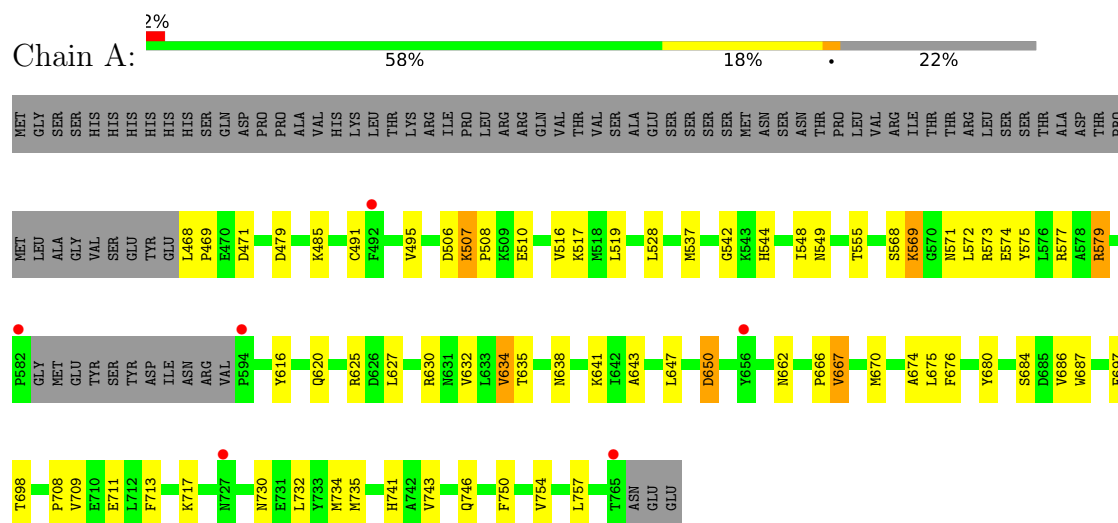
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	98	Total	O	0	0
			98	98		

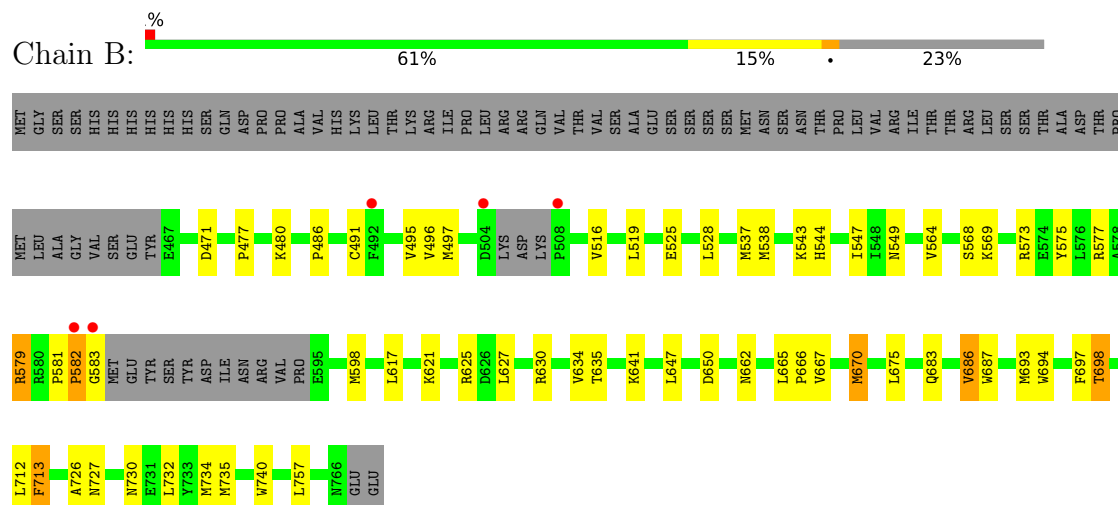
3 Residue-property plots

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: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.61Å 118.61Å 63.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.40) 96.4 (25.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.44 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.258 0.211 , 0.258	Depositor DCC
R_{free} test set	3199 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.7	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	0.93	EDS
Total number of atoms	4725	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.40	0/2317	0.95	13/3135 (0.4%)
1	B	0.40	0/2295	0.95	10/3107 (0.3%)
All	All	0.40	0/4612	0.95	23/6242 (0.4%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	667	VAL	N-CA-C	8.58	119.38	110.62
1	A	471	ASP	CA-C-N	7.61	128.00	119.32
1	A	471	ASP	C-N-CA	7.61	128.00	119.32
1	A	667	VAL	N-CA-C	7.50	118.28	110.62
1	B	568	SER	N-CA-C	7.39	120.21	111.71
1	A	650	ASP	N-CA-C	-6.87	99.34	110.20
1	B	698	THR	N-CA-C	-6.50	104.97	113.17
1	A	569	LYS	N-CA-C	6.45	121.15	113.16
1	B	712	LEU	N-CA-C	6.41	117.93	111.07
1	A	568	SER	N-CA-C	6.39	119.07	111.33
1	B	670	MET	N-CA-C	6.33	119.96	109.46
1	B	471	ASP	CA-C-N	6.14	127.52	119.84
1	B	471	ASP	C-N-CA	6.14	127.52	119.84
1	A	507	LYS	CA-C-N	6.10	126.55	119.47
1	A	507	LYS	C-N-CA	6.10	126.55	119.47
1	A	485	LYS	CA-C-N	5.98	125.92	119.76
1	A	485	LYS	C-N-CA	5.98	125.92	119.76
1	B	497	MET	N-CA-C	-5.85	102.66	110.55
1	A	687	TRP	N-CA-C	-5.84	104.82	111.07
1	B	650	ASP	N-CA-C	-5.83	102.28	110.50
1	B	713	PHE	N-CA-C	5.64	118.37	111.82
1	A	572	LEU	N-CA-C	5.21	116.96	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	THR	N-CA-C	-5.11	106.64	112.92

There are no chirality outliers.

There are no planarity outliers.

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	2269	0	2256	43	0
1	B	2248	0	2217	49	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	90	0	0	1	0
3	B	98	0	0	1	0
All	All	4725	0	4473	90	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 10.

All (90) 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:667:VAL:HG21	1:A:709:VAL:HB	1.51	0.92
1:A:544:HIS:H	1:A:549:ASN:HD21	1.17	0.90
1:A:735:MET:HE1	1:A:757:LEU:HD21	1.58	0.84
1:A:741:HIS:HD2	1:A:743:VAL:H	1.25	0.81
1:B:665:LEU:HD12	1:B:670:MET:HE3	1.65	0.76
1:B:575:TYR:O	1:B:579:ARG:HD3	1.90	0.72
1:B:735:MET:HE1	1:B:757:LEU:HD21	1.74	0.69
1:A:676:PHE:CZ	1:A:717:LYS:HE3	2.30	0.67
1:A:573:ARG:HH21	1:A:577:ARG:NH2	1.95	0.64
1:A:573:ARG:NH2	1:A:577:ARG:NH2	2.45	0.64
1:A:730:ASN:O	1:A:734:MET:HG3	1.97	0.64
1:B:625:ARG:HD3	1:B:647:LEU:O	1.97	0.64
1:B:569:LYS:HB2	1:B:634:VAL:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:VAL:HG22	1:A:517:LYS:HG2	1.81	0.62
1:A:575:TYR:O	1:A:579:ARG:HG2	2.00	0.61
1:A:708:PRO:HG2	1:A:711:GLU:HG2	1.83	0.61
1:B:683:GLN:HA	1:B:686:VAL:HG13	1.82	0.61
1:B:662:ASN:HB3	1:B:670:MET:CE	2.32	0.59
1:B:630:ARG:NH2	1:B:666:PRO:HG2	2.17	0.59
1:A:670:MET:HE2	1:A:674:ALA:HB3	1.85	0.58
1:B:726:ALA:O	1:B:727:ASN:HB2	2.03	0.57
1:A:507:LYS:HB3	1:A:510:GLU:HB2	1.87	0.55
1:A:625:ARG:HD3	1:A:647:LEU:O	2.07	0.55
1:A:675:LEU:HD22	1:A:713:PHE:CE1	2.41	0.55
1:B:735:MET:HE1	1:B:757:LEU:CD2	2.35	0.55
1:A:542:GLY:H	1:A:620:GLN:HE21	1.55	0.55
1:A:735:MET:HE1	1:A:757:LEU:CD2	2.34	0.54
1:B:547:ILE:CD1	1:B:617:LEU:HD13	2.38	0.54
1:B:573:ARG:NH2	1:B:577:ARG:NH2	2.56	0.54
1:B:735:MET:HE1	1:B:757:LEU:CG	2.38	0.54
1:A:569:LYS:HB2	1:A:634:VAL:HG22	1.89	0.53
1:A:571:ASN:HA	1:A:632:VAL:O	2.09	0.53
1:B:730:ASN:HD21	1:B:734:MET:HE3	1.74	0.52
1:A:741:HIS:CD2	1:A:743:VAL:H	2.16	0.51
1:B:573:ARG:NH2	1:B:577:ARG:HH22	2.07	0.51
1:B:693:MET:CE	1:B:735:MET:HE2	2.41	0.51
1:A:634:VAL:HG23	1:A:638:ASN:HA	1.92	0.51
1:B:581:PRO:C	1:B:583:GLY:H	2.18	0.51
1:B:630:ARG:HH21	1:B:666:PRO:HG2	1.74	0.51
1:A:548:ILE:HG13	1:A:643:ALA:HB2	1.91	0.51
1:A:675:LEU:HD11	1:B:525:GLU:OE1	2.11	0.50
1:B:575:TYR:O	1:B:579:ARG:CD	2.57	0.50
1:B:547:ILE:O	1:B:641:LYS:NZ	2.45	0.50
1:A:573:ARG:HH21	1:A:577:ARG:HH22	1.58	0.50
1:A:662:ASN:HB3	1:A:670:MET:HE3	1.94	0.49
1:A:542:GLY:HA3	1:A:616:TYR:OH	2.12	0.49
1:B:635:THR:CG2	1:B:641:LYS:HD2	2.43	0.49
1:A:630:ARG:NH2	1:A:666:PRO:HG2	2.27	0.49
1:A:519:LEU:HD11	1:A:528:LEU:HD13	1.95	0.48
1:A:743:VAL:HB	1:A:746:GLN:HB2	1.94	0.48
1:B:538:MET:HE1	1:B:564:VAL:HG11	1.95	0.48
1:B:694:TRP:O	1:B:698:THR:HG23	2.12	0.48
1:B:543:LYS:HZ3	1:B:549:ASN:HB3	1.76	0.48
1:A:697:PHE:CZ	1:A:732:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ASN:O	1:B:670:MET:HE1	2.14	0.48
1:A:495:VAL:HA	1:A:516:VAL:O	2.15	0.47
1:A:544:HIS:H	1:A:549:ASN:ND2	1.99	0.47
1:A:667:VAL:CG2	1:A:709:VAL:HB	2.36	0.47
1:B:543:LYS:NZ	1:B:549:ASN:HB3	2.30	0.47
1:B:519:LEU:HD11	1:B:528:LEU:HD13	1.97	0.46
1:A:468:LEU:HD23	1:A:555:THR:HB	1.98	0.45
1:B:547:ILE:HD13	1:B:617:LEU:HD13	1.99	0.45
1:B:581:PRO:O	1:B:583:GLY:N	2.42	0.45
1:B:665:LEU:HB2	1:B:670:MET:HE3	1.98	0.45
1:B:547:ILE:HD11	1:B:617:LEU:HD13	1.99	0.45
1:B:486:PRO:HA	1:B:496:VAL:HG12	1.98	0.45
1:A:627:LEU:HA	1:A:627:LEU:HD12	1.85	0.44
1:B:477:PRO:HB2	1:B:480:LYS:CG	2.48	0.44
1:B:581:PRO:HA	1:B:582:PRO:HD3	1.90	0.44
1:A:750:PHE:O	1:A:754:VAL:HG23	2.17	0.44
1:A:491:CYS:SG	1:B:491:CYS:SG	3.01	0.43
1:A:506:ASP:C	1:A:508:PRO:HD3	2.43	0.43
1:B:693:MET:HE1	1:B:735:MET:HE2	2.00	0.43
1:B:730:ASN:ND2	1:B:734:MET:HE3	2.33	0.43
1:B:569:LYS:HB2	1:B:634:VAL:O	2.18	0.43
1:A:735:MET:HG3	3:A:83:HOH:O	2.19	0.43
1:B:543:LYS:HA	1:B:543:LYS:HD3	1.87	0.42
1:B:544:HIS:H	1:B:549:ASN:HD21	1.67	0.42
1:B:687:TRP:CD1	1:B:687:TRP:C	2.98	0.42
1:A:635:THR:HG23	1:A:641:LYS:HD2	2.02	0.42
1:A:635:THR:CG2	1:A:641:LYS:HD2	2.49	0.42
1:B:697:PHE:CZ	1:B:732:LEU:HD13	2.55	0.42
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.90	0.42
1:A:680:TYR:CE2	1:A:684:SER:HB2	2.56	0.41
1:B:579:ARG:HG3	1:B:598:MET:HG2	2.03	0.41
1:B:621:LYS:HA	3:B:125:HOH:O	2.21	0.41
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.94	0.40
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.56	0.40
1:B:675:LEU:HD22	1:B:713:PHE:CE1	2.56	0.40
1:B:495:VAL:HA	1:B:516:VAL:O	2.21	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	283/370 (76%)	273 (96%)	10 (4%)	0	100	100
1	B	280/370 (76%)	266 (95%)	13 (5%)	1 (0%)	30	43
All	All	563/740 (76%)	539 (96%)	23 (4%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	582	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	245/328 (75%)	238 (97%)	7 (3%)	37	60
1	B	241/328 (74%)	237 (98%)	4 (2%)	53	74
All	All	486/656 (74%)	475 (98%)	11 (2%)	44	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	537	MET
1	A	574	GLU
1	A	579	ARG
1	A	634	VAL

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Mol	Chain	Res	Type
1	A	650	ASP
1	A	686	VAL
1	B	537	MET
1	B	579	ARG
1	B	627	LEU
1	B	686	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	620	GLN
1	A	631	ASN
1	A	653	ASN
1	A	683	GLN
1	A	741	HIS
1	B	546	ASN
1	B	549	ASN
1	B	631	ASN
1	B	637	ASN
1	B	653	ASN
1	B	683	GLN
1	B	730	ASN
1	B	766	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 [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	304	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	B	304	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	A	303	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	B	303	-	4,4,4	0.39	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	287/370 (77%)	-0.06	6 (2%) 63 59	13, 28, 53, 71	0
1	B	286/370 (77%)	-0.18	5 (1%) 69 65	14, 26, 49, 63	0
All	All	573/740 (77%)	-0.12	11 (1%) 66 62	13, 27, 50, 71	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	THR	4.3
1	B	582	PRO	4.0
1	A	594	PRO	4.0
1	B	583	GLY	3.2
1	A	582	PRO	3.0
1	B	504	ASP	2.9
1	A	492	PHE	2.9
1	B	492	PHE	2.8
1	A	727	ASN	2.4
1	B	508	PRO	2.3
1	A	656	TYR	2.3

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	303	5/5	0.70	0.20	71,71,73,74	0
2	SO4	A	303	5/5	0.82	0.21	85,85,86,86	0
2	SO4	B	304	5/5	0.87	0.18	87,87,87,88	0
2	SO4	A	304	5/5	0.89	0.13	67,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.