W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 02:15 AM EDT

PDB ID	:	3OJ2
Title	:	Crystal structure of FGF1 complexed with the ectodomain of FGFR2b harboring the A172F Pfeiffer syndrome mutation
Authors	:	Beenken, A.; Mohammadi, M.
Deposited on	:	2010-08-20
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

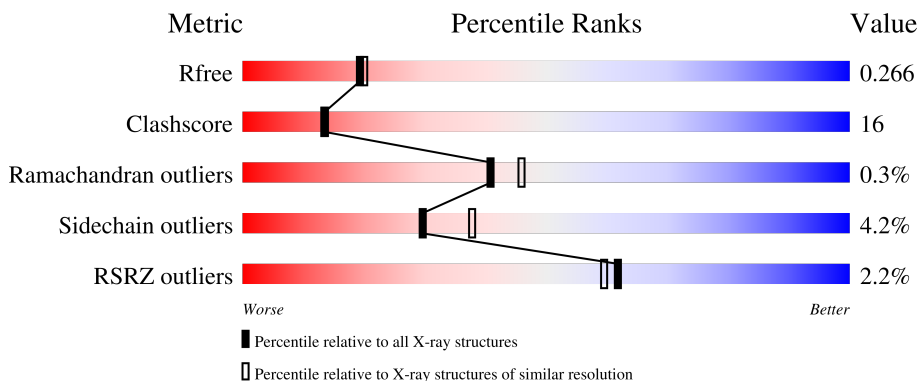|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
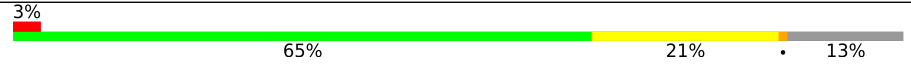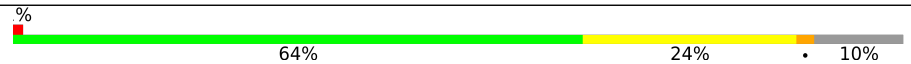*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		16
Ramachandran outliers		0.3%
Sidechain outliers		4.2%
RSRZ outliers		2.2%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	155	3% / 59% 26% •• 13%
1	B	155	3% / 65% 21% • 13%
2	C	231	% / 64% 24% • 10%
2	D	231	% / 67% 22% • 10%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5523 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 Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total 1057	C 669	N 184	O 200	S 4	0	0	0
1	B	135	Total 1057	C 669	N 184	O 200	S 4	0	0	0

- Molecule 2 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total 1633	C 1036	N 292	O 297	S 8	0	0	0
2	D	209	Total 1625	C 1031	N 291	O 295	S 8	0	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	MET	-	initiating methionine	UNP P21802
C	172	PHE	ALA	engineered mutation	UNP P21802
C	314	HIS	-	SEE REMARK 999	UNP P21802
C	315	SER	-	SEE REMARK 999	UNP P21802
C	316	GLY	-	SEE REMARK 999	UNP P21802
C	317	ILE	-	SEE REMARK 999	UNP P21802
C	318	ASN	-	SEE REMARK 999	UNP P21802
C	319	SER	-	SEE REMARK 999	UNP P21802
C	320	SER	-	SEE REMARK 999	UNP P21802
C	321	ASN	-	SEE REMARK 999	UNP P21802
C	322	ALA	-	SEE REMARK 999	UNP P21802
C	323	GLU	-	SEE REMARK 999	UNP P21802
C	324	VAL	-	SEE REMARK 999	UNP P21802
C	325	LEU	-	SEE REMARK 999	UNP P21802
C	326	ALA	-	SEE REMARK 999	UNP P21802
C	327	LEU	-	SEE REMARK 999	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
C	328	PHE	-	SEE REMARK 999	UNP P21802
C	329	ASN	-	SEE REMARK 999	UNP P21802
C	330	VAL	-	SEE REMARK 999	UNP P21802
C	331	THR	-	SEE REMARK 999	UNP P21802
C	332	GLU	-	SEE REMARK 999	UNP P21802
C	333	ALA	-	SEE REMARK 999	UNP P21802
C	334	ASP	-	SEE REMARK 999	UNP P21802
C	335	ALA	-	SEE REMARK 999	UNP P21802
C	336	GLY	-	SEE REMARK 999	UNP P21802
C	337	GLU	-	SEE REMARK 999	UNP P21802
C	338	TYR	-	SEE REMARK 999	UNP P21802
C	339	ILE	-	SEE REMARK 999	UNP P21802
C	340	CYS	-	SEE REMARK 999	UNP P21802
C	341	LYS	-	SEE REMARK 999	UNP P21802
C	342	VAL	-	SEE REMARK 999	UNP P21802
C	343	SER	-	SEE REMARK 999	UNP P21802
C	344	ASN	-	SEE REMARK 999	UNP P21802
C	345	TYR	-	SEE REMARK 999	UNP P21802
C	346	ILE	-	SEE REMARK 999	UNP P21802
C	347	GLY	-	SEE REMARK 999	UNP P21802
C	348	GLN	-	SEE REMARK 999	UNP P21802
C	349	ALA	-	SEE REMARK 999	UNP P21802
C	350	ASN	-	SEE REMARK 999	UNP P21802
C	351	GLN	-	SEE REMARK 999	UNP P21802
C	352	SER	-	SEE REMARK 999	UNP P21802
C	353	ALA	-	SEE REMARK 999	UNP P21802
C	354	TRP	-	SEE REMARK 999	UNP P21802
C	355	LEU	-	SEE REMARK 999	UNP P21802
C	356	THR	-	SEE REMARK 999	UNP P21802
C	357	VAL	-	SEE REMARK 999	UNP P21802
C	358	LEU	-	SEE REMARK 999	UNP P21802
C	359	PRO	-	SEE REMARK 999	UNP P21802
C	360	LYS	-	SEE REMARK 999	UNP P21802
C	361	GLN	-	SEE REMARK 999	UNP P21802
C	362	GLN	-	SEE REMARK 999	UNP P21802
C	363	ALA	-	SEE REMARK 999	UNP P21802
C	364	PRO	-	SEE REMARK 999	UNP P21802
C	365	GLY	-	SEE REMARK 999	UNP P21802
C	366	ARG	-	SEE REMARK 999	UNP P21802
C	367	GLU	-	SEE REMARK 999	UNP P21802
C	368	LYS	-	SEE REMARK 999	UNP P21802
C	369	GLU	-	SEE REMARK 999	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
D	139	MET	-	initiating methionine	UNP P21802
D	172	PHE	ALA	engineered mutation	UNP P21802
D	314	HIS	-	SEE REMARK 999	UNP P21802
D	315	SER	-	SEE REMARK 999	UNP P21802
D	316	GLY	-	SEE REMARK 999	UNP P21802
D	317	ILE	-	SEE REMARK 999	UNP P21802
D	318	ASN	-	SEE REMARK 999	UNP P21802
D	319	SER	-	SEE REMARK 999	UNP P21802
D	320	SER	-	SEE REMARK 999	UNP P21802
D	321	ASN	-	SEE REMARK 999	UNP P21802
D	322	ALA	-	SEE REMARK 999	UNP P21802
D	323	GLU	-	SEE REMARK 999	UNP P21802
D	324	VAL	-	SEE REMARK 999	UNP P21802
D	325	LEU	-	SEE REMARK 999	UNP P21802
D	326	ALA	-	SEE REMARK 999	UNP P21802
D	327	LEU	-	SEE REMARK 999	UNP P21802
D	328	PHE	-	SEE REMARK 999	UNP P21802
D	329	ASN	-	SEE REMARK 999	UNP P21802
D	330	VAL	-	SEE REMARK 999	UNP P21802
D	331	THR	-	SEE REMARK 999	UNP P21802
D	332	GLU	-	SEE REMARK 999	UNP P21802
D	333	ALA	-	SEE REMARK 999	UNP P21802
D	334	ASP	-	SEE REMARK 999	UNP P21802
D	335	ALA	-	SEE REMARK 999	UNP P21802
D	336	GLY	-	SEE REMARK 999	UNP P21802
D	337	GLU	-	SEE REMARK 999	UNP P21802
D	338	TYR	-	SEE REMARK 999	UNP P21802
D	339	ILE	-	SEE REMARK 999	UNP P21802
D	340	CYS	-	SEE REMARK 999	UNP P21802
D	341	LYS	-	SEE REMARK 999	UNP P21802
D	342	VAL	-	SEE REMARK 999	UNP P21802
D	343	SER	-	SEE REMARK 999	UNP P21802
D	344	ASN	-	SEE REMARK 999	UNP P21802
D	345	TYR	-	SEE REMARK 999	UNP P21802
D	346	ILE	-	SEE REMARK 999	UNP P21802
D	347	GLY	-	SEE REMARK 999	UNP P21802
D	348	GLN	-	SEE REMARK 999	UNP P21802
D	349	ALA	-	SEE REMARK 999	UNP P21802
D	350	ASN	-	SEE REMARK 999	UNP P21802
D	351	GLN	-	SEE REMARK 999	UNP P21802
D	352	SER	-	SEE REMARK 999	UNP P21802
D	353	ALA	-	SEE REMARK 999	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
D	354	TRP	-	SEE REMARK 999	UNP P21802
D	355	LEU	-	SEE REMARK 999	UNP P21802
D	356	THR	-	SEE REMARK 999	UNP P21802
D	357	VAL	-	SEE REMARK 999	UNP P21802
D	358	LEU	-	SEE REMARK 999	UNP P21802
D	359	PRO	-	SEE REMARK 999	UNP P21802
D	360	LYS	-	SEE REMARK 999	UNP P21802
D	361	GLN	-	SEE REMARK 999	UNP P21802
D	362	GLN	-	SEE REMARK 999	UNP P21802
D	363	ALA	-	SEE REMARK 999	UNP P21802
D	364	PRO	-	SEE REMARK 999	UNP P21802
D	365	GLY	-	SEE REMARK 999	UNP P21802
D	366	ARG	-	SEE REMARK 999	UNP P21802
D	367	GLU	-	SEE REMARK 999	UNP P21802
D	368	LYS	-	SEE REMARK 999	UNP P21802
D	369	GLU	-	SEE REMARK 999	UNP P21802

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
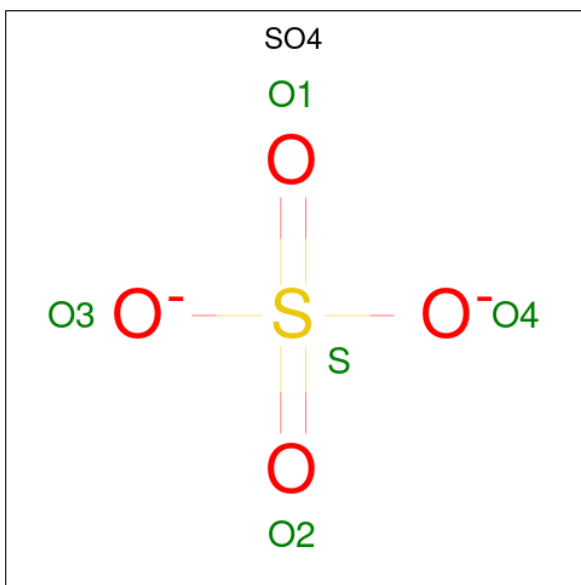
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total O S			0	0
			5	4	1		
3	C	1	Total O S			0	0
			5	4	1		

- Molecule 4 is water.

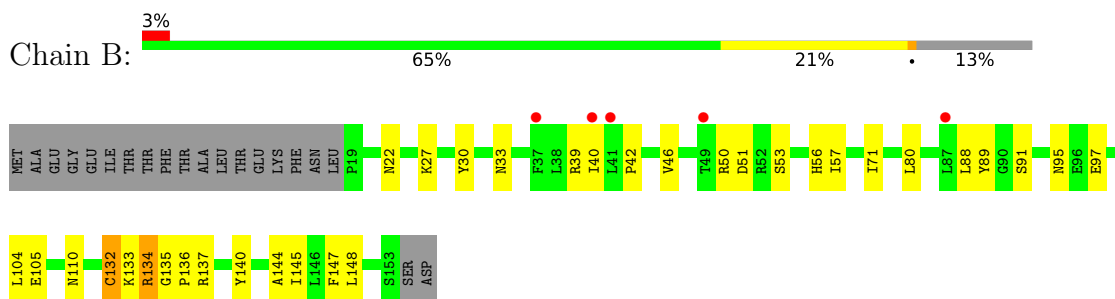| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total O		0	0
			13	13		
4	B	11	Total O		0	0
			11	11		
4	C	50	Total O		0	0
			50	50		
4	D	52	Total O		0	0
			52	52		

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.
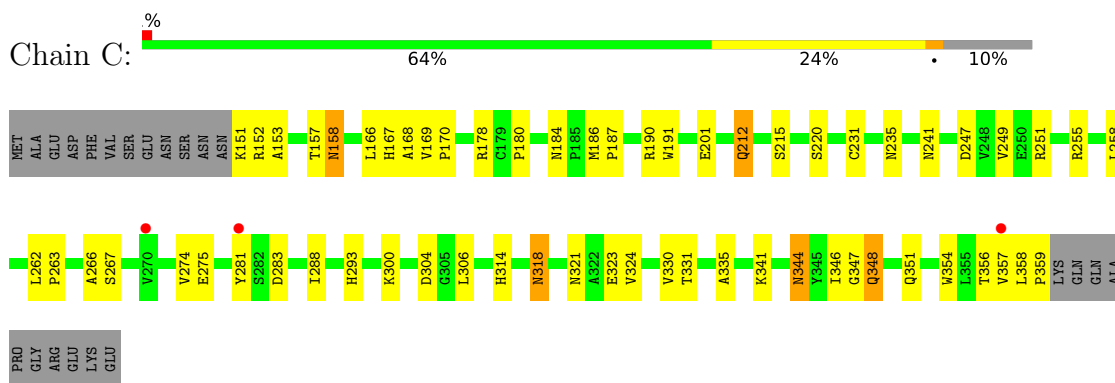
• Molecule 1: Heparin-binding growth factor 1
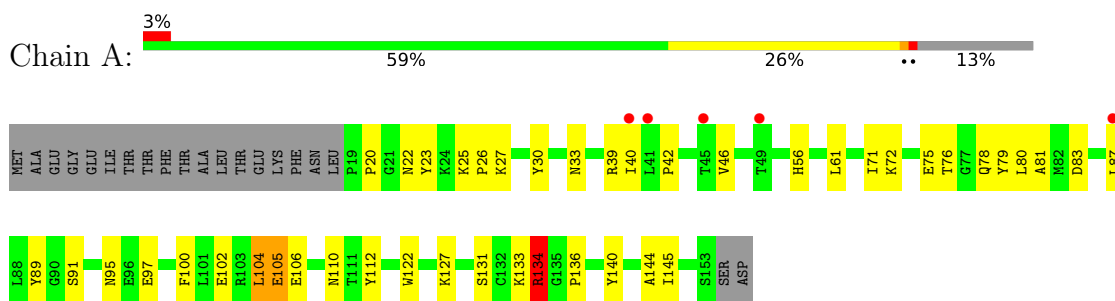
• Molecule 1: Heparin-binding growth factor 1

• Molecule 2: Fibroblast growth factor receptor 2

• Molecule 2: Fibroblast growth factor receptor 2

MET ALA GLU ASP PHE VAL SER GLU ASN SER ASN ASN K151 R152 W156 T159 M162 E163 L166 P170 N173 K176 F177 R178 C179 N184 R190 W191 K199 H202 Q212 H213 W214 S215 L216 I217 S220 C231 V232 E236 Y237 I240 H245

V249 E250 R251 H254 R255 L262 P263 A266 V270 V274 E275 I288 H314 N318 N321 A322 E323 V324 V330 T331 A335 K341 V342 S343 N344 Y345 I346 G347 Q348 W354 V357 L358 P359 LYS GLN GLN ALA PRO GLY ARG GLU LYS GLU
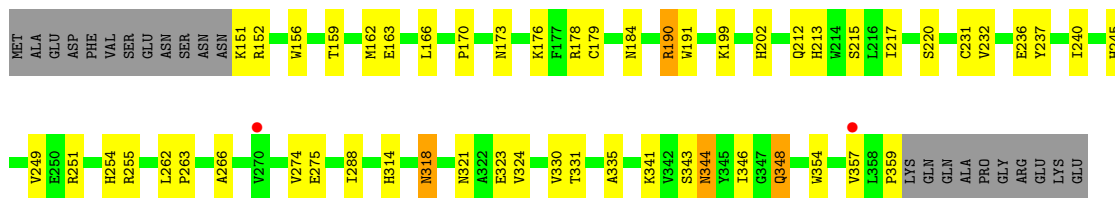
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	77.94Å 77.94Å 137.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.20 29.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.20) 96.7 (29.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.98 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.294 0.262 , 0.266	Depositor DCC
R_{free} test set	3494 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.488 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.38	0/1082	0.69	0/1462
1	B	0.36	0/1082	0.64	0/1462
2	C	0.42	0/1678	0.67	1/2282 (0.0%)
2	D	0.44	0/1670	0.67	1/2273 (0.0%)
All	All	0.41	0/5512	0.67	2/7479 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	359	PRO	N-CA-CB	5.81	110.27	103.30
2	D	359	PRO	N-CA-CB	5.73	110.17	103.30

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	1057	0	1031	51	0
1	B	1057	0	1031	28	0
2	C	1633	0	1579	49	0
2	D	1625	0	1564	44	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	5	0	0	0	0
4	A	13	0	0	0	0
4	B	11	0	0	0	0
4	C	50	0	0	4	0
4	D	52	0	0	1	0
All	All	5523	0	5205	166	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 16.

The worst 5 of 166 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:134:ARG:HD3	1:A:134:ARG:H	1.18	1.02
2:D:199:LYS:H	2:D:202:HIS:CD2	1.80	1.00
2:C:157:THR:C	2:C:158:ASN:HD22	1.65	0.99
2:C:212:GLN:NE2	2:C:212:GLN:H	1.67	0.91
1:A:134:ARG:HB2	1:A:134:ARG:HH11	1.38	0.86

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	133/155 (86%)	122 (92%)	10 (8%)	1 (1%)	19	19
1	B	133/155 (86%)	121 (91%)	11 (8%)	1 (1%)	19	19
2	C	207/231 (90%)	198 (96%)	9 (4%)	0	100	100
2	D	207/231 (90%)	198 (96%)	9 (4%)	0	100	100
All	All	680/772 (88%)	639 (94%)	39 (6%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	B	134	ARG

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	114/135 (84%)	111 (97%)	3 (3%)	46	58
1	B	114/135 (84%)	112 (98%)	2 (2%)	59	72
2	C	173/198 (87%)	161 (93%)	12 (7%)	15	16
2	D	171/198 (86%)	164 (96%)	7 (4%)	30	39
All	All	572/666 (86%)	548 (96%)	24 (4%)	30	38

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	344	ASN
2	D	190	ARG
2	C	354	TRP
2	D	220	SER
2	C	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	318	ASN
2	D	173	ASN
2	D	318	ASN
2	C	350	ASN
2	D	184	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#|Z| > 2$
3	SO4	B	304	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	B	303	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	300	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	C	370	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	A	301	-	4,4,4	0.28	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	135/155 (87%)	0.43	5 (3%)	41	39	36, 58, 73, 77	0
1	B	135/155 (87%)	0.42	5 (3%)	41	39	35, 58, 73, 76	0
2	C	209/231 (90%)	0.19	3 (1%)	75	73	28, 41, 58, 68	0
2	D	209/231 (90%)	0.21	2 (0%)	82	81	26, 41, 57, 68	0
All	All	688/772 (89%)	0.29	15 (2%)	62	59	26, 46, 70, 77	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	270	VAL	4.0
2	D	357	VAL	3.8
2	D	270	VAL	3.4
1	B	41	LEU	3.1
1	A	40	ILE	2.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
3	SO4	C	370	5/5	0.90	0.12	99,99,100,100	0
3	SO4	B	303	5/5	0.95	0.16	99,100,100,100	0
3	SO4	A	300	5/5	0.95	0.13	97,97,97,97	0
3	SO4	A	301	5/5	0.98	0.11	74,74,74,74	0
3	SO4	B	304	5/5	0.99	0.12	69,69,69,69	0

6.5   Other polymers ⓘ

There are no such residues in this entry.