



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2025 – 04:17 pm BST

PDB ID : 9FBM / pdb_00009fbm
Title : Structure of human protein kinase ck2 catalytic subunit (ck2alpha, csnk2a1 gene product) in complex with the cyclic peptidomimetic compound fmp37 discovered by high-throughput screening
Authors : Werner, C.; Niefind, K.; Pietsch, M.; Eimermacher, S.; Lindenblatt, D.
Deposited on : 2024-05-14
Resolution : 2.05 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

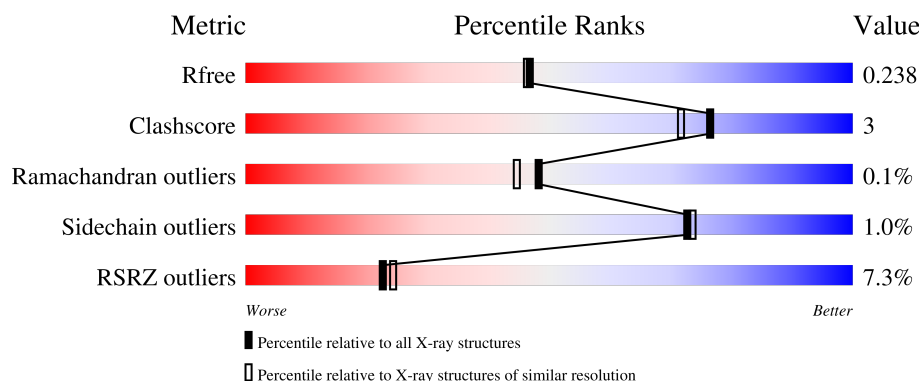
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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	349	<div> <div>6%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	B	349	<div> <div>7%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	C	349	<div> <div>7%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
2	F	5	<div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
2	G	5	<div> <div>20%</div> <div>60%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	5	<p>40%</p> <p>20% 80%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9450 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	3	0
			2819	1804	498	506	11			
1	B	332	Total	C	N	O	S	0	1	0
			2811	1800	495	504	12			
1	C	331	Total	C	N	O	S	0	2	0
			2805	1795	493	506	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P68400
A	-12	GLY	-	expression tag	UNP P68400
A	-11	SER	-	expression tag	UNP P68400
A	-10	SER	-	expression tag	UNP P68400
A	-9	HIS	-	expression tag	UNP P68400
A	-8	HIS	-	expression tag	UNP P68400
A	-7	HIS	-	expression tag	UNP P68400
A	-6	HIS	-	expression tag	UNP P68400
A	-5	HIS	-	expression tag	UNP P68400
A	-4	HIS	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLN	-	expression tag	UNP P68400
A	-1	ASP	-	expression tag	UNP P68400
A	0	PRO	-	expression tag	UNP P68400
B	-13	MET	-	initiating methionine	UNP P68400
B	-12	GLY	-	expression tag	UNP P68400
B	-11	SER	-	expression tag	UNP P68400
B	-10	SER	-	expression tag	UNP P68400
B	-9	HIS	-	expression tag	UNP P68400
B	-8	HIS	-	expression tag	UNP P68400
B	-7	HIS	-	expression tag	UNP P68400
B	-6	HIS	-	expression tag	UNP P68400
B	-5	HIS	-	expression tag	UNP P68400

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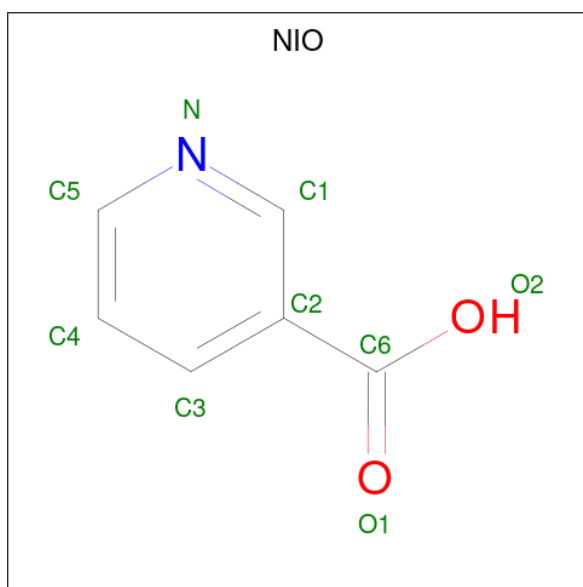
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLN	-	expression tag	UNP P68400
B	-1	ASP	-	expression tag	UNP P68400
B	0	PRO	-	expression tag	UNP P68400
C	-13	MET	-	initiating methionine	UNP P68400
C	-12	GLY	-	expression tag	UNP P68400
C	-11	SER	-	expression tag	UNP P68400
C	-10	SER	-	expression tag	UNP P68400
C	-9	HIS	-	expression tag	UNP P68400
C	-8	HIS	-	expression tag	UNP P68400
C	-7	HIS	-	expression tag	UNP P68400
C	-6	HIS	-	expression tag	UNP P68400
C	-5	HIS	-	expression tag	UNP P68400
C	-4	HIS	-	expression tag	UNP P68400
C	-3	SER	-	expression tag	UNP P68400
C	-2	GLN	-	expression tag	UNP P68400
C	-1	ASP	-	expression tag	UNP P68400
C	0	PRO	-	expression tag	UNP P68400

- Molecule 2 is a protein called Cyclic peptidomimetic compound FMP37.

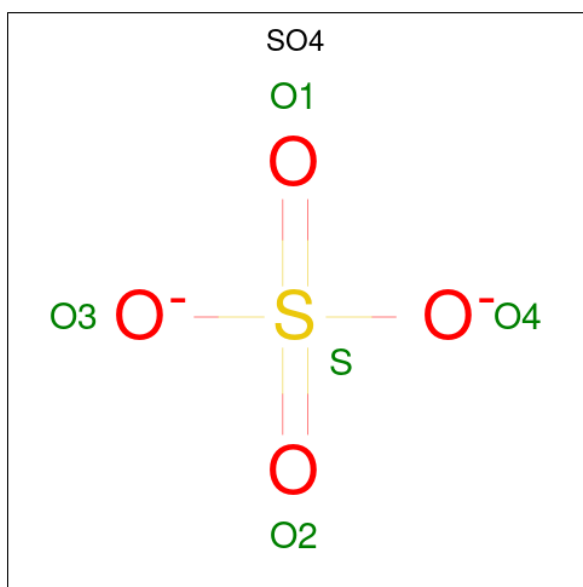
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	5	Total	C	Cl	N	O	S	0	0	0
			49	35	1	6	6	1			
2	G	5	Total	C	Cl	N	O	S	0	0	0
			49	35	1	6	6	1			
2	H	5	Total	C	Cl	N	O	S	0	0	0
			49	35	1	6	6	1			

- Molecule 3 is NICOTINIC ACID (CCD ID: NIO) (formula: C₆H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

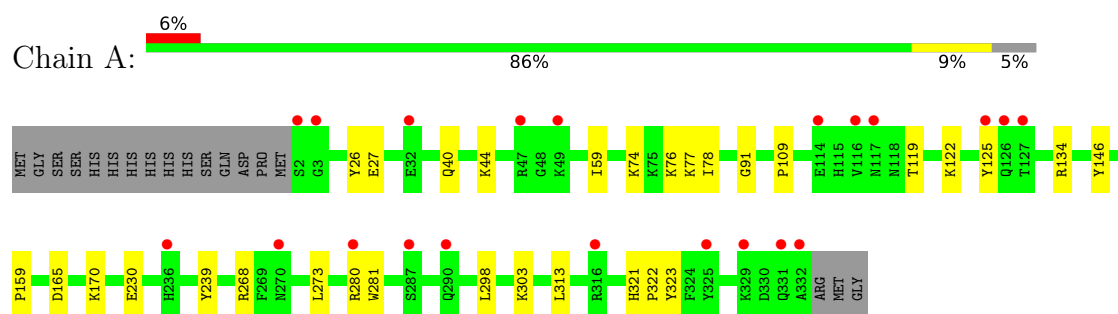
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	236	Total O 244 244	0	8
6	B	254	Total O 261 261	0	7
6	C	263	Total O 271 271	0	8
6	F	7	Total O 7 7	0	0
6	G	5	Total O 6 6	0	1

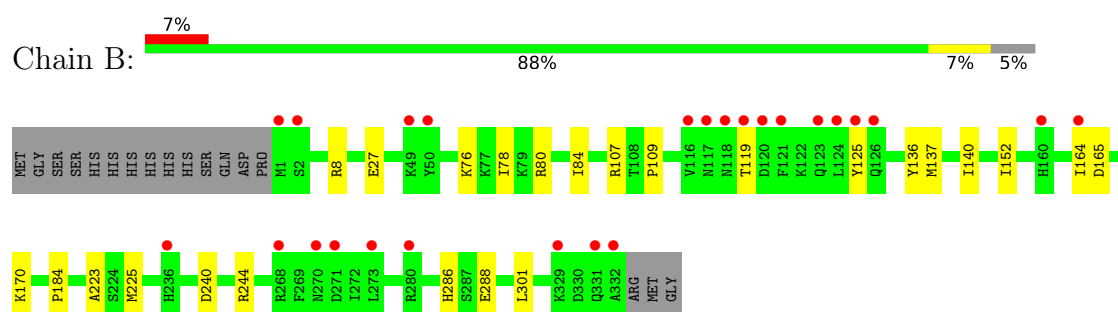
3 Residue-property plots [i](#)

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.

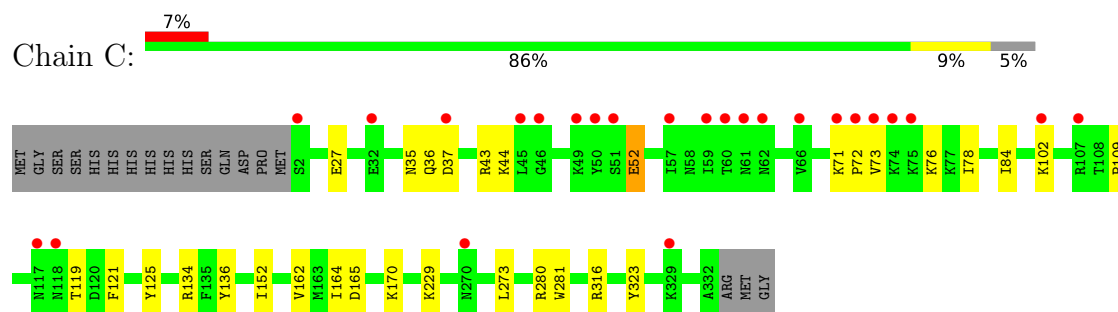
- Molecule 1: Casein kinase II subunit alpha



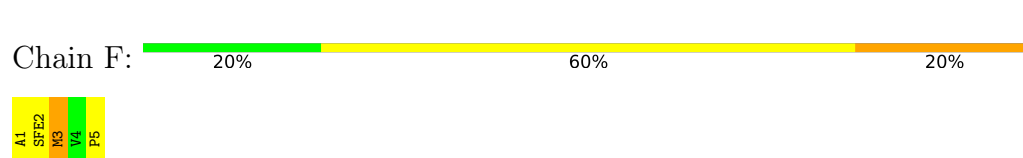
- Molecule 1: Casein kinase II subunit alpha



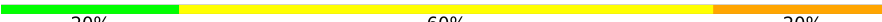
- Molecule 1: Casein kinase II subunit alpha



- Molecule 2: Cyclic peptidomimetic compound FMP37



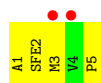
- Molecule 2: Cyclic peptidomimetic compound FMP37

Chain G:  20% 60% 20%



- Molecule 2: Cyclic peptidomimetic compound FMP37

Chain H:  20% 40% 80%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.02Å 208.36Å 76.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.70 – 2.05 54.70 – 2.05	Depositor EDS
% Data completeness (in resolution range)	87.4 (54.70-2.05) 81.7 (54.70-2.05)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	0.56	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.185 , 0.239 0.184 , 0.238	Depositor DCC
R_{free} test set	67930 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9450	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.81% 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: NA, SO4, A1ICB, NIO, SFE

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	0.31	0/2896	0.50	0/3917
1	B	0.32	0/2887	0.51	0/3904
1	C	0.29	0/2880	0.48	0/3895
2	F	2.77	1/18 (5.6%)	1.91	1/21 (4.8%)
2	G	2.80	1/18 (5.6%)	1.39	0/21
2	H	3.01	1/18 (5.6%)	1.98	1/21 (4.8%)
All	All	0.38	3/8717 (0.0%)	0.51	2/11779 (0.0%)

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
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	MET	C-N	10.40	1.48	1.33
2	G	3	MET	C-N	9.85	1.47	1.33
2	F	3	MET	C-N	9.51	1.46	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	MET	CG-SD-CE	5.34	112.65	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	MET	CG-SD-CE	5.28	112.51	100.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	1	ALA	Peptide
2	G	1	ALA	Peptide
2	H	1	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	2819	0	2751	18	0
1	B	2811	0	2753	14	0
1	C	2805	0	2743	15	0
2	F	49	0	32	2	0
2	G	49	0	33	1	0
2	H	49	0	32	0	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
3	C	9	0	4	0	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	244	0	0	0	0
6	B	261	0	0	2	0
6	C	271	0	0	3	0
6	F	7	0	0	0	0
6	G	6	0	0	0	0
All	All	9450	0	8356	47	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 3.

All (47) 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:137:MET:HE3	1:B:225:MET:HE1	1.56	0.87
1:B:136:TYR:CZ	1:B:164:ILE:HD11	2.30	0.67
1:B:165:ASP:HB3	1:B:170:LYS:HG2	1.82	0.62
1:B:136:TYR:CE2	1:B:164:ILE:HD11	2.38	0.58
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.87	0.57
1:A:74:LYS:HE3	1:A:77:LYS:HE3	1.87	0.56
1:C:44:LYS:NZ	1:C:52:GLU:HG2	2.20	0.56
1:C:121:PHE:HB2	1:C:162:VAL:HB	1.88	0.55
1:A:26:TYR:OH	1:A:76:LYS:HE2	2.06	0.55
1:C:27:GLU:OE2	1:C:76:LYS:HE3	2.08	0.53
1:C:136:TYR:CZ	1:C:164:ILE:HD11	2.43	0.53
1:A:165:ASP:HB3	1:A:170:LYS:HG2	1.90	0.53
1:A:280:ARG:HH11	1:A:281:TRP:H	1.56	0.52
1:A:78:ILE:HD13	1:A:109:PRO:HG2	1.92	0.52
1:A:239:TYR:CZ	1:A:268:ARG:HD2	2.46	0.51
1:A:59:ILE:HG21	2:F:3:MET:SD	2.52	0.50
1:A:40:GLN:NE2	2:F:3:MET:HE2	2.27	0.49
1:A:281:TRP:HB3	1:A:298:LEU:HD22	1.94	0.48
1:A:303:LYS:HB3	1:A:313:LEU:HG	1.96	0.46
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.49	0.46
1:B:78:ILE:HD13	1:B:109:PRO:HG2	1.98	0.46
1:A:321:HIS:CG	1:A:322:PRO:HD2	2.51	0.46
1:C:78:ILE:HD13	1:C:109:PRO:HG3	1.98	0.46
1:C:229:LYS:NZ	6:C:514:HOH:O	2.49	0.46
1:B:8:ARG:HD2	1:B:184:PRO:HB3	1.97	0.45
1:C:280:ARG:NH1	1:C:281:TRP:HD1	2.13	0.45
1:C:316:ARG:HG2	6:C:726:HOH:O	2.16	0.45
1:C:84:ILE:HG23	1:C:152:ILE:HD13	1.99	0.45
1:A:122:LYS:HB2	1:A:159:PRO:HB2	1.99	0.45
1:B:137:MET:HE2	1:B:140:ILE:HD12	1.98	0.45
1:B:286:HIS:CE1	1:B:288:GLU:HB2	2.52	0.44
1:C:35:ASN:OD1	1:C:37:ASP:HB2	2.17	0.44
1:C:43:ARG:HD3	6:C:717:HOH:O	2.19	0.43
1:C:134:ARG:HG2	1:C:323:TYR:CZ	2.54	0.43
1:C:71:LYS:O	1:C:73:VAL:N	2.52	0.43
1:B:27:GLU:HG2	1:B:76:LYS:HG3	2.02	0.42
6:B:648:HOH:O	2:G:3:MET:HG3	2.18	0.42
1:A:27:GLU:CD	1:A:76:LYS:HE3	2.44	0.42
1:B:240:ASP:O	1:B:244:ARG:HG2	2.20	0.41
1:C:273:LEU:HA	1:C:273:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HZ3	1:B:107:ARG:HD2	1.85	0.41
1:A:122:LYS:NZ	1:A:230:GLU:OE2	2.40	0.41
1:B:80:ARG:NH1	6:B:523:HOH:O	2.53	0.41
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.56	0.40
1:C:165:ASP:HB3	1:C:170:LYS:HG2	2.02	0.40
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.95	0.40
1:B:223:ALA:HB2	1:B:301:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

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	332/349 (95%)	321 (97%)	11 (3%)	0	100	100
1	B	331/349 (95%)	321 (97%)	10 (3%)	0	100	100
1	C	331/349 (95%)	320 (97%)	10 (3%)	1 (0%)	37	31
2	F	2/5 (40%)	2 (100%)	0	0	100	100
2	G	2/5 (40%)	2 (100%)	0	0	100	100
2	H	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	1000/1062 (94%)	967 (97%)	32 (3%)	1 (0%)	48	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	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	307/320 (96%)	305 (99%)	2 (1%)	81	82
1	B	306/320 (96%)	304 (99%)	2 (1%)	81	82
1	C	306/320 (96%)	301 (98%)	5 (2%)	58	57
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	925/966 (96%)	916 (99%)	9 (1%)	73	73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	125	TYR
1	B	119	THR
1	B	125	TYR
1	C	36	GLN
1	C	52	GLU
1	C	102	LYS
1	C	119	THR
1	C	125	TYR

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	18	HIS
1	A	40	GLN
1	B	117	ASN
1	B	118	ASN
1	B	207	GLN
1	B	270	ASN
1	B	310	GLN
1	C	29	HIS

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Mol	Chain	Res	Type
1	C	115	HIS
1	C	117	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	SFE	H	2	2	11,11,12	1.10	1 (9%)	10,13,15	1.08	1 (10%)
2	A1ICB	H	5	2	16,19,20	3.87	6 (37%)	20,26,28	1.40	3 (15%)
2	A1ICB	F	5	2	16,19,20	3.70	7 (43%)	20,26,28	1.35	5 (25%)
2	A1ICB	G	5	2	16,19,20	3.81	7 (43%)	20,26,28	1.70	4 (20%)
2	SFE	G	2	2	11,11,12	1.16	2 (18%)	10,13,15	0.84	1 (10%)
2	SFE	F	2	2	11,11,12	1.27	1 (9%)	10,13,15	0.97	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SFE	H	2	2	-	3/7/7/8	0/1/1/1
2	A1ICB	H	5	2	-	0/8/19/21	0/2/2/2
2	A1ICB	F	5	2	-	0/8/19/21	0/2/2/2
2	A1ICB	G	5	2	-	0/8/19/21	0/2/2/2
2	SFE	G	2	2	-	2/7/7/8	0/1/1/1
2	SFE	F	2	2	-	0/7/7/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	A1ICB	CB-CA	-9.21	1.34	1.54
2	F	5	A1ICB	CB-CA	-9.13	1.34	1.54
2	H	5	A1ICB	CB-CA	-9.10	1.34	1.54
2	H	5	A1ICB	CB-CG	8.13	1.68	1.53
2	F	5	A1ICB	CB-CG	7.67	1.67	1.53
2	G	5	A1ICB	CB-CG	7.59	1.67	1.53
2	H	5	A1ICB	C09-N11	6.53	1.48	1.34
2	G	5	A1ICB	C09-N11	6.43	1.48	1.34
2	F	5	A1ICB	C09-N11	5.66	1.46	1.34
2	F	5	A1ICB	C04-C09	3.73	1.57	1.50
2	G	5	A1ICB	C05-CL06	3.70	1.82	1.73
2	H	5	A1ICB	C04-C09	3.68	1.57	1.50
2	H	5	A1ICB	C05-CL06	3.53	1.82	1.73
2	G	5	A1ICB	C04-C09	3.51	1.57	1.50
2	F	5	A1ICB	C05-CL06	3.28	1.81	1.73
2	H	5	A1ICB	CD-N	3.17	1.58	1.47
2	F	2	SFE	CA-C	2.96	1.57	1.49
2	H	2	SFE	CA-C	2.91	1.57	1.49
2	F	5	A1ICB	CD-N	2.71	1.56	1.47
2	G	5	A1ICB	CD-N	2.66	1.56	1.47
2	G	5	A1ICB	O10-C09	-2.61	1.18	1.23
2	G	2	SFE	CA-C	2.58	1.56	1.49
2	G	2	SFE	CG-CB	2.24	1.54	1.52
2	F	5	A1ICB	O10-C09	-2.04	1.19	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	A1ICB	CG-N11-C09	-3.48	117.72	122.55
2	G	5	A1ICB	C03-C04-C05	3.03	121.38	117.92
2	G	5	A1ICB	CB-CG-N11	-2.97	107.18	112.61
2	H	5	A1ICB	C03-C04-C05	2.64	120.94	117.92
2	F	2	SFE	CB-CA-C	-2.40	104.14	114.50
2	F	5	A1ICB	O-C-CA	-2.33	118.67	124.78
2	H	5	A1ICB	CA-CB-CG	2.27	107.00	103.89
2	F	5	A1ICB	CG-N11-C09	-2.27	119.41	122.55
2	G	5	A1ICB	C07-C05-C04	-2.26	118.75	121.36
2	F	5	A1ICB	C03-C04-C05	2.19	120.42	117.92
2	H	2	SFE	O-C-CA	-2.18	119.09	125.43
2	G	2	SFE	CB-CA-C	-2.15	105.20	114.50
2	H	5	A1ICB	CB-CG-N11	-2.14	108.70	112.61
2	F	5	A1ICB	CD-CG-N11	-2.12	108.21	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	A1ICB	C08-C02-C03	2.09	121.09	117.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	SFE	O-C-CA-CB
2	H	2	SFE	N-CB-CG-CD2
2	G	2	SFE	N-CB-CG-CD2
2	G	2	SFE	N-CB-CG-CD1
2	H	2	SFE	N-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	$\# Z > 2$
4	SO4	B	402	-	4,4,4	0.59	0	6,6,6	0.25	0
4	SO4	A	403	-	4,4,4	0.70	0	6,6,6	0.47	0
3	NIO	B	401	-	9,9,9	0.96	0	11,11,11	0.96	1 (9%)
3	NIO	C	401	-	9,9,9	0.93	1 (11%)	11,11,11	1.08	1 (9%)
4	SO4	B	404	-	4,4,4	0.71	0	6,6,6	0.22	0
4	SO4	A	402	-	4,4,4	0.70	0	6,6,6	0.11	0
4	SO4	C	404	-	4,4,4	0.65	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	402	-	4,4,4	0.59	0	6,6,6	0.26	0
4	SO4	A	405	-	4,4,4	0.72	0	6,6,6	0.17	0
4	SO4	B	403	-	4,4,4	0.71	0	6,6,6	0.26	0
3	NIO	A	401	-	9,9,9	1.08	1 (11%)	11,11,11	1.21	1 (9%)
4	SO4	A	404	-	4,4,4	0.68	0	6,6,6	0.13	0
4	SO4	C	403	-	4,4,4	0.66	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NIO	A	401	-	-	0/4/4/4	0/1/1/1
3	NIO	C	401	-	-	0/4/4/4	0/1/1/1
3	NIO	B	401	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NIO	C2-C6	2.35	1.54	1.49
3	C	401	NIO	C2-C6	2.05	1.53	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NIO	O1-C6-C2	-2.50	114.80	121.45
3	C	401	NIO	O1-C6-C2	-2.33	115.24	121.45
3	B	401	NIO	O1-C6-C2	-2.07	115.94	121.45

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 ⓘ

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(Å ²)	Q<0.9
1	A	331/349 (94%)	0.04	21 (6%) 27 28	12, 27, 56, 99	3 (0%)
1	B	332/349 (95%)	0.16	25 (7%) 22 23	11, 29, 64, 103	1 (0%)
1	C	331/349 (94%)	0.16	25 (7%) 21 23	12, 27, 74, 140	2 (0%)
2	F	3/5 (60%)	-0.12	0 100 100	16, 16, 21, 28	0
2	G	3/5 (60%)	-0.01	0 100 100	18, 18, 22, 30	0
2	H	3/5 (60%)	2.89	2 (66%) 0 0	56, 56, 65, 71	0
All	All	1003/1062 (94%)	0.13	73 (7%) 22 24	11, 27, 65, 140	6 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASN	5.6
1	B	125	TYR	5.6
1	A	125	TYR	5.5
1	C	50	TYR	5.1
1	C	72	PRO	5.0
1	B	270	ASN	5.0
1	A	287[A]	SER	4.6
1	B	121	PHE	4.5
1	B	332	ALA	4.4
1	A	127	THR	4.3
1	B	1	MET	4.3
1	C	2	SER	4.2
1	A	126	GLN	4.2
1	B	118	ASN	4.0
2	H	4	VAL	3.8
1	C	117	ASN	3.5
1	C	73	VAL	3.5
1	B	271	ASP	3.4
2	H	3	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	164	ILE	3.4
1	B	329	LYS	3.2
1	A	316	ARG	3.2
1	B	50	TYR	3.1
1	B	273	LEU	3.1
1	B	280	ARG	3.1
1	C	51	SER	3.1
1	C	118	ASN	3.0
1	A	332	ALA	3.0
1	B	2	SER	3.0
1	B	117	ASN	2.9
1	C	32	GLU	2.9
1	A	329	LYS	2.9
1	A	325	TYR	2.8
1	B	124	LEU	2.8
1	A	117	ASN	2.7
1	B	49	LYS	2.7
1	A	2	SER	2.7
1	C	62	ASN	2.7
1	C	59	ILE	2.7
1	B	268	ARG	2.7
1	C	49	LYS	2.6
1	C	57	ILE	2.6
1	C	75	LYS	2.6
1	A	3	GLY	2.6
1	A	280	ARG	2.6
1	B	160	HIS	2.6
1	C	46	GLY	2.5
1	A	290	GLN	2.5
1	A	116	VAL	2.5
1	B	236[A]	HIS	2.4
1	B	126	GLN	2.4
1	C	60	THR	2.4
1	C	71	LYS	2.4
1	A	114	GLU	2.3
1	B	120	ASP	2.3
1	C	45	LEU	2.3
1	C	74	LYS	2.2
1	B	123	GLN	2.2
1	A	49	LYS	2.2
1	C	107	ARG	2.2
1	A	331	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	119	THR	2.2
1	C	270	ASN	2.2
1	C	37	ASP	2.1
1	A	47	ARG	2.1
1	A	236[A]	HIS	2.1
1	C	329	LYS	2.1
1	C	61	ASN	2.1
1	C	102	LYS	2.1
1	A	32	GLU	2.0
1	B	116	VAL	2.0
1	C	66	VAL	2.0
1	B	331	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	A1ICB	H	5	18/19	0.81	0.16	50,60,64,77	0
2	SFE	H	2	11/12	0.86	0.14	44,48,58,63	0
2	A1ICB	F	5	18/19	0.94	0.08	15,19,24,40	0
2	A1ICB	G	5	18/19	0.94	0.09	17,24,30,38	0
2	SFE	F	2	11/12	0.94	0.07	14,18,22,23	0
2	SFE	G	2	11/12	0.97	0.05	13,16,18,19	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
4	SO4	B	404	5/5	0.72	0.14	50,57,78,87	0
4	SO4	C	404	5/5	0.74	0.11	68,68,77,87	0
4	SO4	A	404	5/5	0.77	0.10	64,64,73,83	0
4	SO4	C	403	5/5	0.86	0.10	50,51,63,68	0
3	NIO	B	401	9/9	0.87	0.10	25,29,37,37	0
4	SO4	A	402	5/5	0.87	0.10	51,58,63,65	0
4	SO4	C	402	5/5	0.90	0.17	37,47,55,62	0
4	SO4	B	403	5/5	0.90	0.11	39,40,53,60	0
4	SO4	A	405	5/5	0.90	0.21	45,46,53,63	0
3	NIO	C	401	9/9	0.91	0.11	30,36,39,44	0
4	SO4	A	403	5/5	0.92	0.13	38,39,47,48	0
3	NIO	A	401	9/9	0.93	0.11	20,22,27,28	0
4	SO4	B	402	5/5	0.96	0.11	34,36,43,49	0
5	NA	A	406	1/1	0.97	0.11	34,34,34,34	0
5	NA	B	405	1/1	0.98	0.05	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.