Supplementary Information (SI) for RSC Chemical Biology.
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Full wwPDB X-ray Structure Validation Report (i)

Nov 26, 2024 – 12:05 am GMT

PDB ID	:	9FBI
Title	:	Structure of human protein kinase CK2 catalytic subunit (CK2alpha) in complex with the cyclic peptidomimetic compound FMP37 discovered by high-throughput screening
Deposited on	:	2024-05-14
Resolution	:	1.16 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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)

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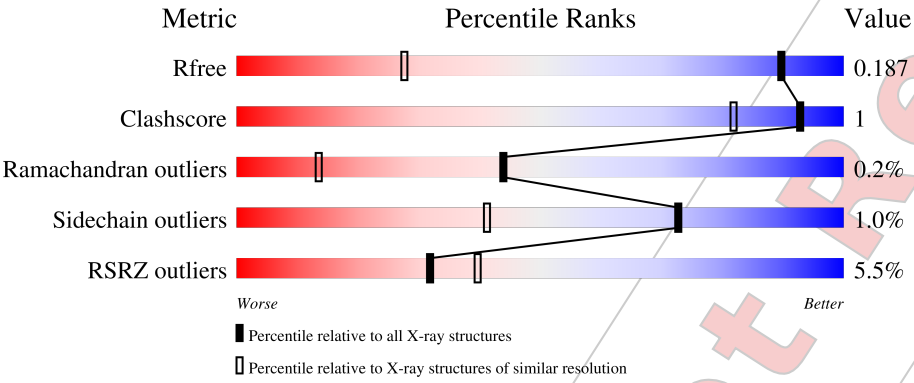
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.16 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	1049 (1.18-1.14)
Clashscore	180529	1146 (1.18-1.14)
Ramachandran outliers	177936	1120 (1.18-1.14)
Sidechain outliers	177891	1120 (1.18-1.14)
RSRZ outliers	164620	1049 (1.18-1.14)

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	364	6% 85% 5% 10%
1	B	364	4% 84% 6% 10%
2	E	5	60% 40%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	407	-	-	X	-

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2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11944 atoms, of which 5708 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	327	Total	C	H	N	O	S	0	3	0
			5540	1791	2754	487	497	11			
1	B	329	Total	C	H	N	O	S	0	11	0
			5677	1832	2829	498	507	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P19784
A	-12	GLY	-	expression tag	UNP P19784
A	-11	SER	-	expression tag	UNP P19784
A	-10	SER	-	expression tag	UNP P19784
A	-9	HIS	-	expression tag	UNP P19784
A	-8	HIS	-	expression tag	UNP P19784
A	-7	HIS	-	expression tag	UNP P19784
A	-6	HIS	-	expression tag	UNP P19784
A	-5	HIS	-	expression tag	UNP P19784
A	-4	HIS	-	expression tag	UNP P19784
A	-3	SER	-	expression tag	UNP P19784
A	-2	GLN	-	expression tag	UNP P19784
A	-1	ASP	-	expression tag	UNP P19784
A	0	PRO	-	expression tag	UNP P19784
A	336	SER	CYS	engineered mutation	UNP P19784
B	-13	MET	-	initiating methionine	UNP P19784
B	-12	GLY	-	expression tag	UNP P19784
B	-11	SER	-	expression tag	UNP P19784
B	-10	SER	-	expression tag	UNP P19784
B	-9	HIS	-	expression tag	UNP P19784
B	-8	HIS	-	expression tag	UNP P19784
B	-7	HIS	-	expression tag	UNP P19784
B	-6	HIS	-	expression tag	UNP P19784
B	-5	HIS	-	expression tag	UNP P19784
B	-4	HIS	-	expression tag	UNP P19784

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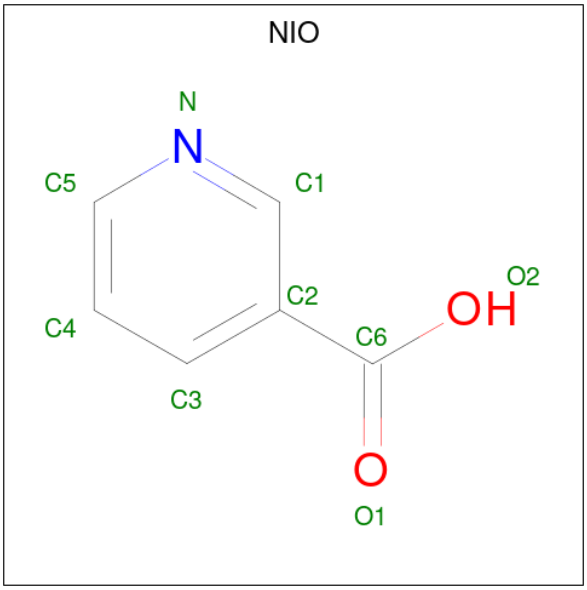
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP P19784
B	-2	GLN	-	expression tag	UNP P19784
B	-1	ASP	-	expression tag	UNP P19784
B	0	PRO	-	expression tag	UNP P19784
B	336	SER	CYS	engineered mutation	UNP P19784

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	Cl	H	N	O	S			
2	E	5	94	35	1	45	6	6	1	0	0	0

- Molecule 3 is NICOTINIC ACID (three-letter code: NIO) (formula: $C_6H_5NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	13	6	4	1	2	0	0
3	B	1	Total	C	H	N	O	0	0
			13	6	4	1	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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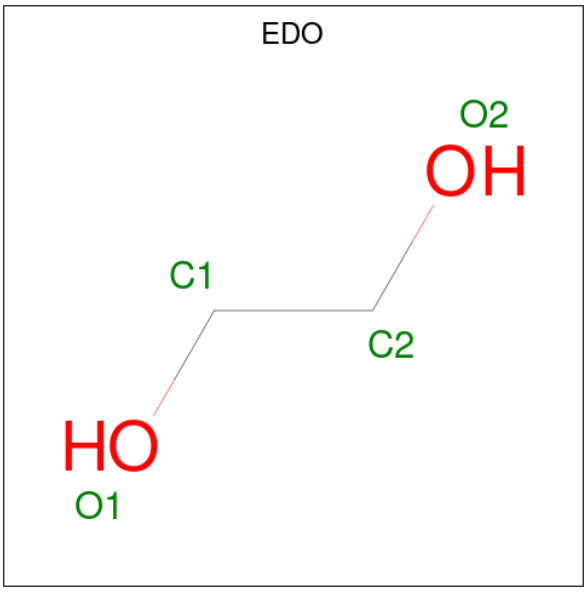

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	211	Total O 218 218	0	7
7	B	254	Total O 263 263	0	9
7	E	4	Total O 4 4	0	0

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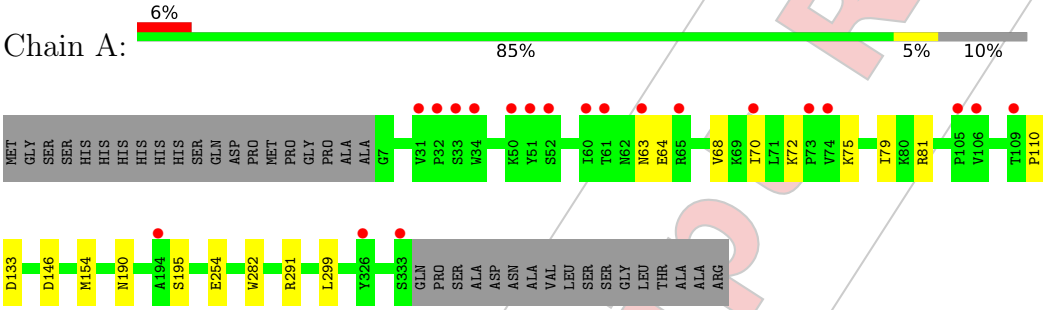
3 Residue-property plots (i)

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.

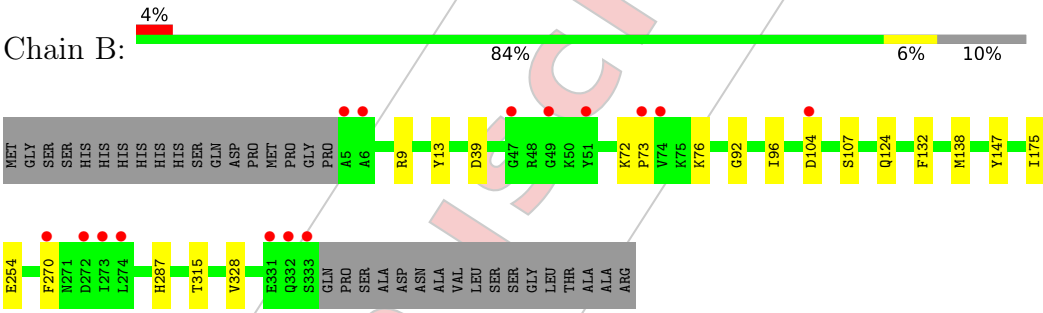
• Molecule 1: Casein kinase II subunit alpha'

Chain A:



• Molecule 1: Casein kinase II subunit alpha'

Chain B:



• Molecule 2: Cyclic peptidomimetic compound FMP37

Chain E:

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.45Å 71.07Å 102.88Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	58.46 – 1.16 58.46 – 1.16	Depositor EDS
% Data completeness (in resolution range)	51.9 (58.46-1.16) 49.2 (58.46-1.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.16Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.145 , 0.185 0.152 , 0.187	Depositor DCC
R_{free} test set	118220 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11944	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 22.86 % 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 5.2323e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

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5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SFE, EDO, A1ICB, NIO, CL, NA

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	0.83	3/2858 (0.1%)	0.83	3/3857 (0.1%)
1	B	0.89	4/2939 (0.1%)	0.87	2/3966 (0.1%)
2	E	1.69	0/18	1.92	0/21
All	All	0.87	7/5815 (0.1%)	0.86	5/7844 (0.1%)

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	E	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	GLU	CG-CD	8.94	1.65	1.51
1	B	253	GLU	CG-CD	7.89	1.63	1.51
1	B	13	TYR	CE1-CZ	-5.92	1.30	1.38
1	A	64	GLU	CG-CD	5.65	1.60	1.51
1	B	254	GLU	CG-CD	5.58	1.60	1.51
1	B	253	GLU	CB-CG	5.13	1.61	1.52
1	A	195	SER	CB-OG	5.11	1.48	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	MET	CG-SD-CE	-7.45	88.29	100.20
1	A	121	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	39	ASP	CB-CG-OD2	-5.15	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	MET	CG-SD-CE	5.05	108.28	100.20
1	A	146	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	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	2786	2754	2752	8	1
1	B	2848	2829	2804	8	0
2	E	49	45	32	0	0
3	A	9	4	4	0	0
3	B	9	4	4	0	0
4	A	24	36	35	5	0
4	B	24	36	34	1	0
5	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	218	0	0	0	0
7	B	263	0	0	2	0
7	E	4	0	0	0	0
All	All	6236	5708	5665	16	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 1.

All (16) 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:287:HIS:HD2	7:B:600[A]:HOH:O	1.85	0.58
1:A:68:VAL:HG12	1:A:70:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASP:HB3	1:B:107:SER:OG	2.14	0.47
1:A:190:ASN:HD22	4:A:407:EDO:C2	2.27	0.46
1:A:81:ARG:HH22	4:A:407:EDO:C1	2.29	0.45
1:A:81:ARG:HH22	4:A:407:EDO:H11	1.83	0.44
1:A:133:ASP:HA	4:A:405:EDO:H11	2.00	0.44
1:B:92:GLY:HA3	1:B:147:TYR:CE2	2.54	0.42
1:B:72:LYS:O	1:B:73:PRO:C	2.57	0.42
1:B:315:THR:HB	4:B:406:EDO:H21	2.01	0.42
1:B:76:LYS:HE2	7:B:668:HOH:O	2.20	0.42
1:A:282:TRP:HB3	1:A:299:LEU:HD22	2.00	0.41
1:B:132:PHE:CE1	1:B:328[A]:VAL:HG12	2.56	0.41
1:A:190:ASN:HD22	4:A:407:EDO:H21	1.86	0.41
1:B:96:ILE:HB	1:B:175:ILE:HG22	2.02	0.41
1:A:79:ILE:HD13	1:A:110:PRO:HG2	2.01	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:63:ASN:OD1	1:A:291:ARG:HH22[2_555]	1.60	0.00

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	328/364 (90%)	319 (97%)	8 (2%)	1 (0%)	37 12
1	B	338/364 (93%)	327 (97%)	11 (3%)	0	100 100
2	E	2/5 (40%)	2 (100%)	0	0	100 100
All	All	668/733 (91%)	648 (97%)	19 (3%)	1 (0%)	44 14

All (1) Ramachandran outliers are listed below:

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Mol	Chain	Res	Type
1	A	72	LYS

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	302/327 (92%)	301 (100%)	1 (0%)	91	75
1	B	309/327 (94%)	303 (98%)	6 (2%)	52	13
2	E	2/2 (100%)	2 (100%)	0	100	100
All	All	613/656 (93%)	606 (99%)	7 (1%)	73	37

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	B	9[A]	ARG
1	B	9[B]	ARG
1	B	124	GLN
1	B	181	GLU
1	B	253	GLU
1	B	270	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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

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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	E	2	2	11,11,12	1.05	0	10,13,15	1.07	0
2	A1ICB	E	5	2	16,19,20	3.11	7 (43%)	20,26,28	2.08	6 (30%)

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	E	2	2	-	1/7/7/8	0/1/1/1
2	A1ICB	E	5	2	-	0/8/19/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	A1ICB	CB-CA	-8.23	1.36	1.54
2	E	5	A1ICB	CB-CG	5.91	1.64	1.53
2	E	5	A1ICB	C09-N11	4.05	1.43	1.34
2	E	5	A1ICB	C05-CL06	3.47	1.81	1.73
2	E	5	A1ICB	C04-C09	2.87	1.56	1.50
2	E	5	A1ICB	CD-N	2.57	1.56	1.47
2	E	5	A1ICB	O10-C09	-2.23	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	A1ICB	CG-N11-C09	-3.61	117.54	122.55
2	E	5	A1ICB	C01-C02-C03	-3.55	115.68	120.94
2	E	5	A1ICB	CD-CG-N11	-3.48	105.36	112.68
2	E	5	A1ICB	C07-C05-C04	-3.31	117.54	121.36
2	E	5	A1ICB	C03-C04-C05	3.21	121.58	117.92
2	E	5	A1ICB	C05-C04-C09	-2.57	118.48	122.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
2	E	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	NIO	A	401	-	9,9,9	1.06	1 (11%)	11,11,11	0.98	1 (9%)
4	EDO	A	405	-	3,3,3	0.30	0	2,2,2	0.61	0
4	EDO	A	406	-	3,3,3	0.35	0	2,2,2	0.13	0
4	EDO	B	406	-	3,3,3	1.22	0	2,2,2	1.24	0
4	EDO	B	402	-	3,3,3	0.17	0	2,2,2	0.58	0
4	EDO	B	407	-	3,3,3	0.26	0	2,2,2	0.48	0
3	NIO	B	401	-	9,9,9	1.47	2 (22%)	11,11,11	1.82	4 (36%)
4	EDO	A	403	-	3,3,3	0.49	0	2,2,2	0.11	0
4	EDO	A	404	-	3,3,3	0.79	0	2,2,2	1.20	0
4	EDO	A	407	-	3,3,3	0.38	0	2,2,2	0.42	0
4	EDO	B	405	-	3,3,3	0.26	0	2,2,2	0.36	0
4	EDO	A	402	-	3,3,3	0.36	0	2,2,2	0.31	0
4	EDO	B	403	-	3,3,3	0.36	0	2,2,2	0.37	0
4	EDO	B	404	-	3,3,3	0.34	0	2,2,2	0.46	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.

For Manuscript Review

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NIO	A	401	-	-	0/4/4/4	0/1/1/1
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
3	NIO	B	401	-	-	0/4/4/4	0/1/1/1
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	B	404	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NIO	C2-C6	3.28	1.56	1.49
3	B	401	NIO	O2-C6	-2.25	1.23	1.30
3	A	401	NIO	C2-C6	2.07	1.53	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	NIO	O2-C6-C2	3.32	123.45	114.85
3	B	401	NIO	O1-C6-C2	-3.17	113.01	121.45
3	B	401	NIO	C1-C2-C6	2.07	125.25	120.62
3	A	401	NIO	O1-C6-C2	-2.04	116.02	121.45
3	B	401	NIO	C5-N-C1	2.00	120.31	116.85

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
4	B	405	EDO	O1-C1-C2-O2
4	A	407	EDO	O1-C1-C2-O2
4	B	404	EDO	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2

For Manuscript Review

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0
4	B	406	EDO	1	0
4	A	407	EDO	4	0

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.

For Manuscript Review

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^{th} 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	327/364 (89%)	0.53	21 (6%) 27 34	8, 20, 48, 76	3 (0%)
1	B	329/364 (90%)	0.28	15 (4%) 38 45	6, 15, 43, 69	9 (2%)
2	E	3/5 (60%)	0.79	0 100 100	19, 19, 29, 33	0
All	All	659/733 (89%)	0.41	36 (5%) 32 40	6, 18, 45, 76	12 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	PRO	8.4
1	B	5	ALA	6.0
1	A	74	VAL	5.3
1	B	73	PRO	4.8
1	A	61	THR	4.5
1	A	33	SER	3.8
1	B	74	VAL	3.7
1	A	51	TYR	3.6
1	B	49	GLY	3.5
1	B	6	ALA	3.5
1	A	60	ILE	3.4
1	B	51	TYR	3.3
1	B	333	SER	3.3
1	A	106	VAL	3.1
1	A	105	PRO	3.1
1	B	47	GLY	3.0
1	B	274	LEU	3.0
1	B	331[A]	GLU	2.8
1	A	31	VAL	2.8
1	A	34	TRP	2.7
1	A	333	SER	2.7
1	B	270	PHE	2.7
1	A	52	SER	2.6

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For Manuscript Review

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Mol	Chain	Res	Type	RSRZ
1	A	326	TYR	2.5
1	B	272	ASP	2.5
1	B	273	ILE	2.5
1	A	63	ASN	2.4
1	A	65	ARG	2.4
1	A	50	LYS	2.4
1	A	70	ILE	2.3
1	B	332	GLN	2.3
1	A	109	THR	2.1
1	A	32	PRO	2.1
1	A	194	ALA	2.1
1	A	120	THR	2.1
1	B	104	ASP	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, 95^{th} 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	E	5	18/19	0.94	0.07	17,20,24,27	0
2	SFE	E	2	11/12	0.97	0.05	18,20,24,24	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, 95^{th} 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
4	EDO	B	404	4/4	0.82	0.13	33,39,42,43	0
4	EDO	A	406	4/4	0.83	0.15	56,68,70,70	0
4	EDO	B	403	4/4	0.85	0.15	45,54,55,55	0

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For Manuscript Review

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	405	4/4	0.85	0.13	43,53,54,55	0
4	EDO	B	407	4/4	0.85	0.14	48,58,61,64	0
4	EDO	B	405	4/4	0.86	0.14	47,57,59,59	0
4	EDO	A	402	4/4	0.91	0.10	42,51,52,53	0
6	NA	B	408	1/1	0.92	0.15	65,65,65,65	0
4	EDO	A	403	4/4	0.93	0.08	31,38,41,42	0
3	NIO	A	401	9/9	0.93	0.11	22,33,40,41	0
4	EDO	A	407	4/4	0.94	0.09	25,35,40,42	0
3	NIO	B	401	9/9	0.94	0.09	17,25,31,33	0
4	EDO	B	406	4/4	0.95	0.09	9,15,18,18	0
4	EDO	A	404	4/4	0.96	0.08	14,21,25,26	0
4	EDO	B	402	4/4	0.97	0.06	19,23,25,27	0
5	CL	A	408	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.

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