



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:24 PM UTC

PDB ID : 9FBL / pdb_00009fbl
Title : Structure of human protein kinase CK2 catalytic subunit (CK2alpha, CSNK2A1 gene product) in complex with the cyclic peptidomimetic compound 15 discovered by high-throughput screening
Authors : Werner, C.; Niefind, K.; Eimermacher, S.; Pietsch, M.; Lindenblatt, D.
Deposited on : 2024-05-14
Resolution : 2.18 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:

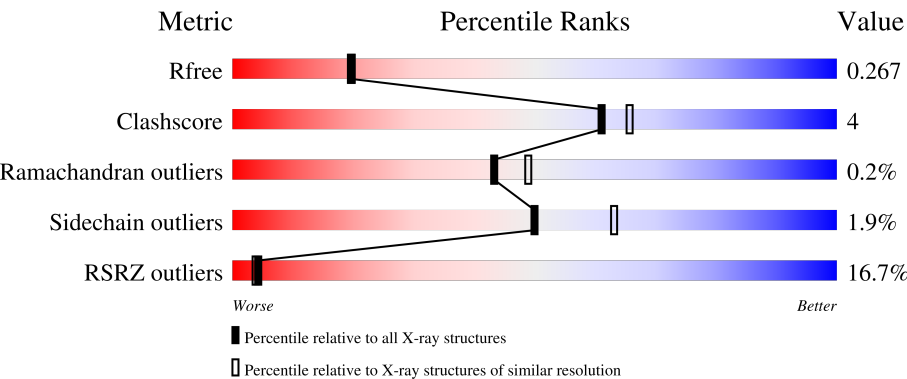
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.18 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.



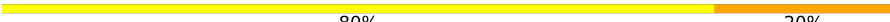
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	13% 83% 11% 5%
1	B	349	17% 82% 13% 5%
1	C	349	17% 81% 13% 6%
2	L	5	60% 60% 40%
2	N	5	20% 20% 40% 40%

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Mol	Chain	Length	Quality of chain
2	P	5	 80% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8840 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	330	Total	C	N	O	S	0	1	0
			2798	1792	493	502	11			
1	B	331	Total	C	N	O	S	0	1	0
			2807	1797	495	503	12			
1	C	329	Total	C	N	O	S	0	1	0
			2792	1789	492	500	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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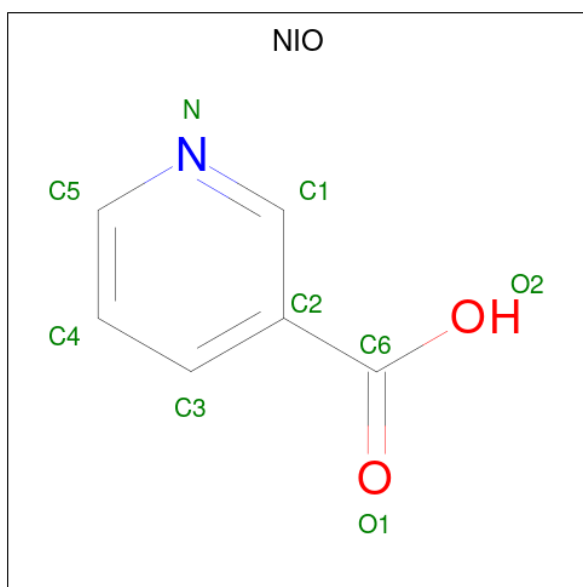
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLN	-	expression tag	UNP P68400
B	-1	ASP	-	expression tag	UNP P68400
B	0	PRO	-	expression tag	UNP P68400
C	-13	MET	-	initiating 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 FMP35.

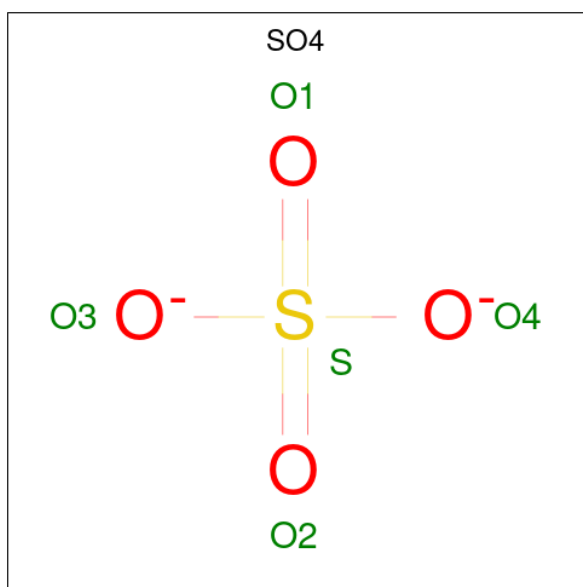
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			
2	N	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			
2	P	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			

- 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	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
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	C	1	Total Na 1 1	0	0

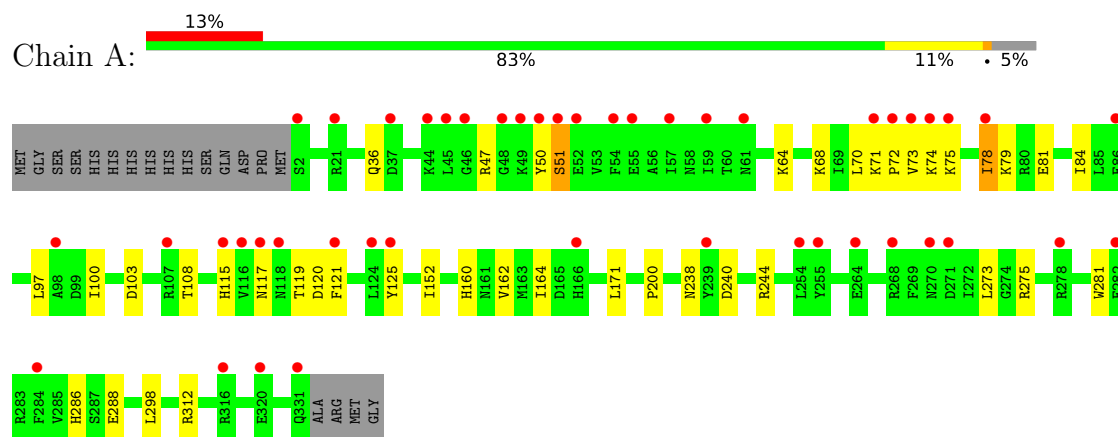
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	60	Total O 61 61	0	1
6	B	82	Total O 84 84	0	2
6	C	51	Total O 51 51	0	0
6	N	1	Total O 1 1	0	0

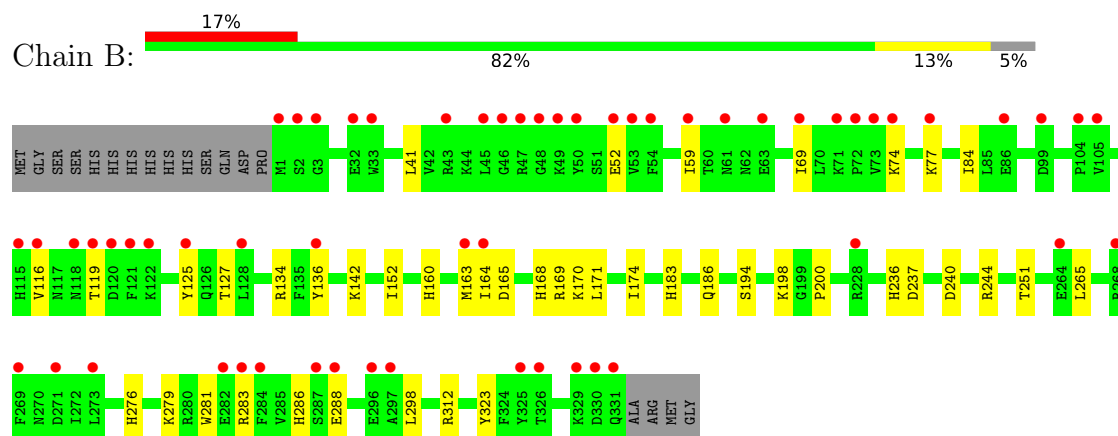
3 Residue-property plots [i](#)

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.

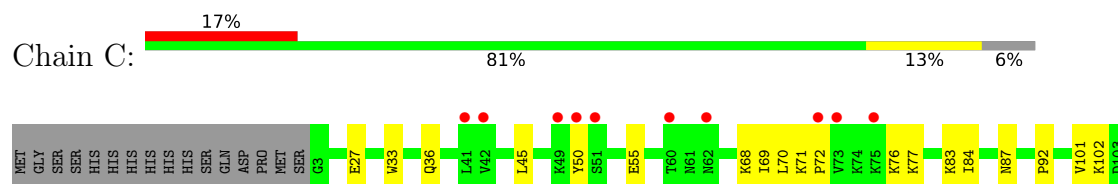
• Molecule 1: Casein kinase II subunit alpha

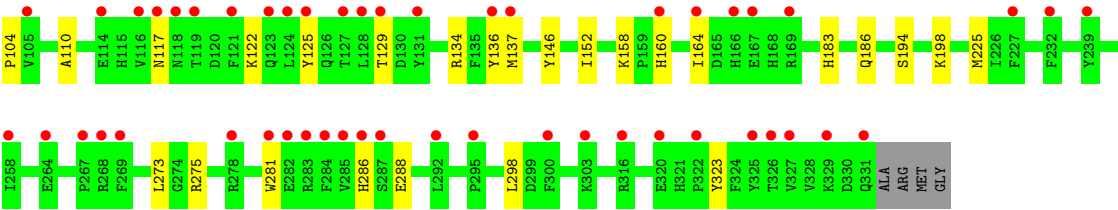


• Molecule 1: Casein kinase II subunit alpha



• Molecule 1: Casein kinase II subunit alpha

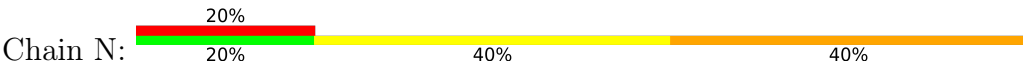




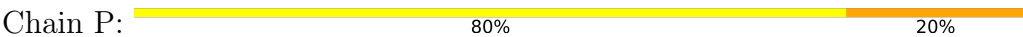
● Molecule 2: Cyclic peptidomimetic compound FMP35



● Molecule 2: Cyclic peptidomimetic compound FMP35



● Molecule 2: Cyclic peptidomimetic compound FMP35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.95Å 206.56Å 76.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 2.18 72.93 – 2.18	Depositor EDS
% Data completeness (in resolution range)	60.1 (72.93-2.18) 56.9 (72.93-2.18)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	0.48	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.209 , 0.266 0.208 , 0.267	Depositor DCC
R_{free} test set	1186 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% 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: A1ICC, SO4, NA, 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	0.07	0/2874	0.25	0/3887
1	B	0.09	0/2882	0.25	0/3896
1	C	0.08	0/2868	0.24	0/3879
2	L	3.04	1/18 (5.6%)	1.35	0/21
2	N	3.02	1/18 (5.6%)	1.42	0/21
2	P	2.95	1/18 (5.6%)	1.27	0/21
All	All	0.25	3/8678 (0.0%)	0.27	0/11725

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	L	0	1
2	N	0	1
2	P	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	L	4	MET	C-N	10.83	1.48	1.33
2	N	4	MET	C-N	10.81	1.48	1.33
2	P	4	MET	C-N	10.63	1.48	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	2	ALA	Peptide
2	N	2	ALA	Peptide
2	P	2	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	2798	0	2736	24	0
1	B	2807	0	2754	21	0
1	C	2792	0	2731	27	0
2	L	51	0	32	1	0
2	N	51	0	32	1	0
2	P	51	0	32	1	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
3	C	9	0	4	0	0
4	A	30	0	0	1	0
4	B	15	0	0	0	0
4	C	20	0	0	0	0
5	C	1	0	0	0	0
6	A	61	0	0	2	0
6	B	84	0	0	0	0
6	C	51	0	0	1	0
6	N	1	0	0	0	0
All	All	8840	0	8329	72	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 4.

All (72) 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:84:ILE:HG23	1:B:152:ILE:HD13	1.75	0.68
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.78	0.65
1:C:36:GLN:HG3	1:C:104:PRO:HG3	1.83	0.61
1:B:279:LYS:HG3	1:B:283:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HB3	1:C:77:LYS:HE3	1.83	0.60
1:C:84:ILE:HG23	1:C:152:ILE:HD13	1.84	0.59
1:A:275:ARG:NH2	6:A:504:HOH:O	2.38	0.57
1:C:71:LYS:N	1:C:72:PRO:HD3	2.20	0.57
1:A:70:LEU:HD13	1:A:78:ILE:HG12	1.87	0.56
1:A:75:LYS:HG3	1:A:79:LYS:HE2	1.86	0.55
1:B:116:VAL:HG11	1:B:163:MET:HB3	1.87	0.55
1:A:71:LYS:O	1:A:73:VAL:N	2.39	0.54
1:A:73:VAL:HG22	1:A:74:LYS:H	1.72	0.54
1:C:275:ARG:NH1	6:C:505:HOH:O	2.41	0.53
1:C:286:HIS:CE1	1:C:288:GLU:HB2	2.44	0.53
1:B:52:GLU:HB2	1:B:69:ILE:HB	1.91	0.53
1:A:164:ILE:HD13	1:A:171:LEU:HD12	1.89	0.52
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.45	0.52
1:B:136:TYR:CZ	1:B:164:ILE:HD11	2.45	0.52
1:C:136:TYR:CZ	1:C:164:ILE:HD11	2.45	0.52
1:C:281:TRP:HB3	1:C:298:LEU:HD22	1.92	0.51
1:A:121:PHE:N	1:A:162:VAL:O	2.42	0.51
1:B:286:HIS:CE1	1:B:288:GLU:HB2	2.46	0.50
1:C:27:GLU:OE2	1:C:76:LYS:HE3	2.11	0.50
1:A:275:ARG:NH1	6:A:507:HOH:O	2.46	0.49
1:B:163:MET:HG2	1:B:174:ILE:HD13	1.96	0.47
1:B:164:ILE:HD13	1:B:171:LEU:HD12	1.96	0.47
1:A:68:LYS:NZ	1:A:81:GLU:OE2	2.44	0.47
1:A:103:ASP:HB3	1:A:108:THR:H	1.79	0.47
1:B:136:TYR:OH	1:B:169:ARG:HA	2.15	0.47
1:B:183:HIS:HB2	1:B:186:GLN:HG3	1.97	0.47
1:C:134:ARG:HG2	1:C:323:TYR:CZ	2.49	0.46
1:A:97:LEU:HD21	1:A:100:ILE:HD11	1.98	0.46
1:A:281:TRP:HB3	1:A:298:LEU:HD22	1.98	0.46
1:C:50:TYR:O	1:C:71:LYS:N	2.44	0.46
1:B:236:HIS:CE1	1:B:237:ASP:OD2	2.69	0.46
1:A:240:ASP:O	1:A:244:ARG:HG2	2.17	0.45
1:B:194:SER:O	1:B:198:LYS:HG3	2.17	0.45
1:B:240:ASP:O	1:B:244:ARG:HG2	2.17	0.45
1:C:194:SER:O	1:C:198:LYS:HG3	2.16	0.44
1:B:200:PRO:HD2	1:B:312:ARG:NH2	2.33	0.44
1:A:64:LYS:O	1:A:115:HIS:HB2	2.18	0.44
1:C:69:ILE:HD13	1:C:110:ALA:HB2	2.00	0.43
1:C:36:GLN:O	2:P:3:SFE:HA2C	2.19	0.43
1:C:183:HIS:HB2	1:C:186:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TRP:HB3	1:B:298:LEU:HD22	1.99	0.43
1:C:45:LEU:HD11	1:C:55:GLU:HB2	2.01	0.43
1:A:64:LYS:HE2	1:A:115:HIS:CE1	2.54	0.43
1:B:165:ASP:HB3	1:B:170:LYS:HB2	2.01	0.43
1:C:33:TRP:CE2	1:C:102:LYS:HE2	2.54	0.43
1:C:122:LYS:HD3	1:C:160[B]:HIS:CE1	2.54	0.43
1:A:200:PRO:HD2	1:A:312:ARG:NH2	2.34	0.42
1:C:71:LYS:N	1:C:72:PRO:CD	2.83	0.42
1:C:273:LEU:HD12	1:C:273:LEU:HA	1.88	0.42
1:A:238:ASN:ND2	4:A:403:SO4:O2	2.51	0.41
1:B:251:THR:HG23	1:B:276:HIS:HB2	2.02	0.41
1:C:36:GLN:HB3	1:C:101:VAL:HB	2.02	0.41
1:C:83:LYS:NZ	1:C:87:ASN:OD1	2.53	0.41
1:A:117:ASN:O	1:A:119:THR:N	2.48	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.91	0.41
1:B:168:HIS:HB3	1:B:170:LYS:HE2	2.02	0.41
1:C:158:LYS:NZ	1:C:160[A]:HIS:HB3	2.36	0.41
1:B:74:LYS:HB2	1:B:77:LYS:HE2	2.01	0.41
1:A:120:ASP:OD2	1:A:160[B]:HIS:HD2	2.03	0.41
1:B:41:LEU:HD12	2:N:2:ALA:HB1	2.01	0.41
1:C:92:PRO:HD2	1:C:146:TYR:CG	2.56	0.41
1:C:137:MET:HE3	1:C:225:MET:HE1	2.03	0.41
1:A:286:HIS:CE1	1:A:288:GLU:HB2	2.56	0.41
1:C:68:LYS:HE3	1:C:70:LEU:HD21	2.02	0.41
1:C:137:MET:HE2	1:C:137:MET:HA	2.04	0.40
1:A:36:GLN:O	2:L:3:SFE:HA2C	2.21	0.40
1:A:50:TYR:O	1:A:51:SER:HB3	2.20	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	329/349 (94%)	313 (95%)	14 (4%)	2 (1%)	21	20
1	B	330/349 (95%)	318 (96%)	12 (4%)	0	100	100
1	C	328/349 (94%)	316 (96%)	12 (4%)	0	100	100
2	L	2/5 (40%)	2 (100%)	0	0	100	100
2	N	2/5 (40%)	2 (100%)	0	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	993/1062 (94%)	953 (96%)	38 (4%)	2 (0%)	43	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	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	305/320 (95%)	302 (99%)	3 (1%)	68	79
1	B	306/320 (96%)	299 (98%)	7 (2%)	44	56
1	C	304/320 (95%)	301 (99%)	3 (1%)	68	79
2	L	2/2 (100%)	0	2 (100%)	0	0
2	N	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	921/966 (95%)	904 (98%)	17 (2%)	50	65

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	78	ILE
1	A	125	TYR

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Mol	Chain	Res	Type
1	B	59	ILE
1	B	119	THR
1	B	125	TYR
1	B	127	THR
1	B	142	LYS
1	B	160	HIS
1	B	265	LEU
1	C	117	ASN
1	C	125	TYR
1	C	129	THR
2	L	4	MET
2	L	5	VAL
2	N	4	MET
2	P	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	115	HIS
1	A	207	GLN
1	A	276	HIS
1	B	29	HIS
1	B	160	HIS
1	C	276	HIS

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	A1ICC	N	1	2	19,22,23	3.26	8 (42%)	19,30,32	1.56	3 (15%)
2	SFE	N	3	2	10,11,12	1.11	1 (10%)	10,13,15	0.90	0
2	SFE	L	3	2	10,11,12	1.10	1 (10%)	10,13,15	0.90	0
2	A1ICC	L	1	2	19,22,23	3.29	9 (47%)	19,30,32	1.50	3 (15%)
2	A1ICC	P	1	2	19,22,23	3.29	9 (47%)	19,30,32	1.55	4 (21%)
2	SFE	P	3	2	10,11,12	1.12	1 (10%)	10,13,15	0.90	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
2	A1ICC	N	1	2	-	0/8/19/21	0/3/3/3
2	SFE	N	3	2	-	2/7/7/8	0/1/1/1
2	SFE	L	3	2	-	0/7/7/8	0/1/1/1
2	A1ICC	L	1	2	-	0/8/19/21	0/3/3/3
2	A1ICC	P	1	2	-	0/8/19/21	0/3/3/3
2	SFE	P	3	2	-	0/7/7/8	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	A1ICC	CB-CA	-8.29	1.36	1.54
2	L	1	A1ICC	CB-CA	-8.28	1.36	1.54
2	P	1	A1ICC	CB-CA	-8.22	1.36	1.54
2	P	1	A1ICC	CB-CG	6.10	1.64	1.53
2	L	1	A1ICC	CB-CG	5.99	1.64	1.53
2	N	1	A1ICC	CB-CG	5.81	1.64	1.53
2	L	1	A1ICC	CA-N	5.68	1.58	1.48
2	P	1	A1ICC	CA-N	5.64	1.58	1.48
2	N	1	A1ICC	CA-N	5.54	1.58	1.48
2	N	1	A1ICC	C30-N29	4.43	1.44	1.34
2	L	1	A1ICC	C30-N29	4.40	1.44	1.34
2	P	1	A1ICC	C30-N29	4.33	1.44	1.34
2	N	1	A1ICC	CD-N	3.44	1.59	1.47
2	L	1	A1ICC	CD-N	3.42	1.58	1.47
2	P	1	A1ICC	CD-N	3.38	1.58	1.47
2	P	1	A1ICC	C41-C36	-2.84	1.37	1.43
2	N	1	A1ICC	C41-C36	-2.81	1.37	1.43
2	L	1	A1ICC	C41-C36	-2.80	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	A1ICC	O31-C30	-2.74	1.17	1.23
2	L	1	A1ICC	O31-C30	-2.74	1.17	1.23
2	N	1	A1ICC	O31-C30	-2.73	1.17	1.23
2	P	1	A1ICC	C32-C41	-2.39	1.40	1.43
2	P	3	SFE	CA-C	2.38	1.56	1.50
2	L	3	SFE	CA-C	2.38	1.56	1.50
2	N	3	SFE	CA-C	2.37	1.56	1.50
2	P	1	A1ICC	C32-N33	2.37	1.35	1.33
2	L	1	A1ICC	C32-N33	2.37	1.35	1.33
2	N	1	A1ICC	C32-N33	2.31	1.35	1.33
2	L	1	A1ICC	C32-C41	-2.04	1.41	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	A1ICC	C40-C41-C32	-3.51	121.32	124.39
2	P	1	A1ICC	C35-C34-N33	-3.13	120.77	123.83
2	L	1	A1ICC	C35-C34-N33	-3.12	120.78	123.83
2	L	1	A1ICC	C40-C41-C32	-3.06	121.70	124.39
2	N	1	A1ICC	C35-C34-N33	-3.03	120.86	123.83
2	N	1	A1ICC	C40-C41-C32	-3.00	121.76	124.39
2	P	1	A1ICC	O-C-CA	-2.23	119.03	124.77
2	N	1	A1ICC	CB-CG-N29	-2.21	108.66	112.67
2	L	1	A1ICC	O-C-CA	-2.08	119.43	124.77
2	P	1	A1ICC	CA-CB-CG	2.05	106.58	103.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	3	SFE	N-CB-CG-CD2
2	N	3	SFE	N-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	SFE	1	0
2	P	3	SFE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	A	404	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	A	407	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	B	402	-	4,4,4	0.67	0	6,6,6	0.07	0
4	SO4	C	405	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	C	402	-	4,4,4	0.67	0	6,6,6	0.08	0
3	NIO	B	401	-	9,9,9	0.88	0	11,11,11	0.93	0
4	SO4	A	403	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	C	403	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	C	404	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	A	406	-	4,4,4	0.67	0	6,6,6	0.05	0
4	SO4	A	402	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	B	403	-	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	B	404	-	4,4,4	0.67	0	6,6,6	0.08	0
3	NIO	C	401	-	9,9,9	0.87	0	11,11,11	0.95	1 (9%)
3	NIO	A	401	-	9,9,9	0.88	0	11,11,11	0.94	0
4	SO4	A	405	-	4,4,4	0.67	0	6,6,6	0.06	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	B	401	-	-	0/4/4/4	0/1/1/1
3	NIO	C	401	-	-	0/4/4/4	0/1/1/1
3	NIO	A	401	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	401	NIO	O1-C6-C2	-2.00	116.21	121.46

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
4	A	403	SO4	1	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.

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	330/349 (94%)	1.03	46 (13%)	6 5	21, 45, 85, 134	1 (0%)
1	B	331/349 (94%)	1.03	58 (17%)	4 3	24, 46, 86, 133	1 (0%)
1	C	329/349 (94%)	1.11	59 (17%)	3 3	25, 48, 87, 167	1 (0%)
2	L	3/5 (60%)	2.63	3 (100%)	0 0	57, 57, 67, 71	0
2	N	3/5 (60%)	1.78	1 (33%)	1 1	55, 55, 56, 64	0
2	P	3/5 (60%)	0.86	0 100	100	44, 44, 47, 55	0
All	All	999/1062 (94%)	1.07	167 (16%)	4 4	21, 47, 87, 167	3 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	VAL	6.8
1	C	73	VAL	6.0
1	A	116	VAL	5.9
1	B	45	LEU	5.7
1	C	125	TYR	5.1
1	C	118	ASN	4.7
1	A	121	PHE	4.2
1	B	164	ILE	4.2
1	A	50	TYR	4.2
1	C	114	GLU	4.2
1	C	281	TRP	4.0
1	B	121	PHE	4.0
1	A	72	PRO	4.0
1	B	50	TYR	3.9
1	C	284	PHE	3.8
1	A	54	PHE	3.8
1	B	104	PRO	3.7
1	B	72	PRO	3.7
1	C	131	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.6
1	B	120	ASP	3.5
1	A	115	HIS	3.5
1	B	49	LYS	3.5
1	B	116	VAL	3.5
1	A	166	HIS	3.4
1	A	57	ILE	3.4
1	B	163	MET	3.4
1	C	329	LYS	3.3
1	B	264	GLU	3.3
1	C	327	VAL	3.2
1	C	121	PHE	3.2
1	C	325	TYR	3.2
1	B	271	ASP	3.2
1	A	75	LYS	3.2
1	A	331	GLN	3.2
1	B	136	TYR	3.1
1	C	320	GLU	3.1
1	C	264	GLU	3.1
1	B	119	THR	3.1
1	B	52	GLU	3.1
1	C	167	GLU	3.1
1	A	59	ILE	3.1
1	A	255	TYR	3.0
1	A	51	SER	3.0
2	L	4	MET	3.0
1	A	124	LEU	3.0
1	B	105	VAL	3.0
1	C	164	ILE	3.0
1	C	124	LEU	2.9
1	C	287	SER	2.9
1	B	74	LYS	2.9
1	A	107	ARG	2.9
1	A	117	ASN	2.9
1	C	129	THR	2.9
1	A	74	LYS	2.9
1	A	118	ASN	2.9
1	A	125	TYR	2.9
1	C	316	ARG	2.8
1	B	283	ARG	2.8
1	C	137	MET	2.8
1	A	320	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	283	ARG	2.8
1	C	331	GLN	2.8
1	B	273	LEU	2.8
1	C	51	SER	2.7
1	A	48	GLY	2.7
1	C	160[A]	HIS	2.7
1	C	49	LYS	2.7
1	B	125	TYR	2.7
1	B	118	ASN	2.7
1	C	117	ASN	2.7
1	B	115	HIS	2.7
1	B	296	GLU	2.7
1	C	72	PRO	2.7
1	C	267	PRO	2.7
1	C	285	VAL	2.7
1	C	239	TYR	2.6
1	B	73	VAL	2.6
1	B	77	LYS	2.6
2	L	5	VAL	2.6
1	B	63	GLU	2.6
1	C	232	PHE	2.6
1	A	2	SER	2.6
1	A	21	ARG	2.6
1	A	316	ARG	2.6
1	B	46	GLY	2.6
1	A	55	GLU	2.6
1	B	326	THR	2.6
1	C	326	THR	2.6
1	C	295	PRO	2.6
1	C	322	PRO	2.6
1	A	268	ARG	2.6
1	C	269	PHE	2.5
1	C	258	ILE	2.5
1	A	49	LYS	2.5
1	B	71	LYS	2.5
1	B	2	SER	2.5
1	A	270	ASN	2.5
1	C	127	THR	2.5
1	C	300	PHE	2.5
1	A	71	LYS	2.5
1	A	78	ILE	2.5
1	B	268	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	268	ARG	2.5
1	C	50	TYR	2.4
1	C	119	THR	2.4
1	C	128	LEU	2.4
1	C	166	HIS	2.4
1	B	59	ILE	2.4
1	A	98	ALA	2.4
1	A	86	GLU	2.4
1	A	284	PHE	2.4
1	C	60	THR	2.4
1	B	43	ARG	2.3
1	A	45	LEU	2.3
1	A	37	ASP	2.3
1	A	73	VAL	2.3
1	C	123	GLN	2.3
1	C	62	ASN	2.3
1	A	44	LYS	2.3
1	A	282	GLU	2.3
1	C	169	ARG	2.3
1	B	329	LYS	2.3
2	L	2	ALA	2.3
1	C	286	HIS	2.2
1	A	271	ASP	2.2
1	A	52	GLU	2.2
1	B	53	VAL	2.2
1	C	105	VAL	2.2
1	A	46	GLY	2.2
1	B	3	GLY	2.2
1	B	48	GLY	2.2
1	B	32	GLU	2.2
1	B	228[A]	ARG	2.2
1	B	269	PHE	2.2
1	B	284	PHE	2.2
1	C	227	PHE	2.2
1	C	42	VAL	2.2
1	C	282	GLU	2.2
1	B	287	SER	2.2
1	C	303	LYS	2.2
1	B	99	ASP	2.2
1	B	330	ASP	2.2
1	B	122	LYS	2.1
1	A	61	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLN	2.1
1	B	54	PHE	2.1
1	B	297	ALA	2.1
1	C	292	LEU	2.1
1	A	264	GLU	2.1
1	B	61	ASN	2.1
1	A	239	TYR	2.1
1	C	136	TYR	2.1
1	A	278	ARG	2.1
1	B	69	ILE	2.1
1	B	128	LEU	2.1
1	B	86	GLU	2.1
1	B	325	TYR	2.1
1	B	282	GLU	2.0
1	B	288	GLU	2.0
1	A	254	LEU	2.0
1	C	41	LEU	2.0
1	C	278	ARG	2.0
1	B	33	TRP	2.0
2	N	2	ALA	2.0
1	B	47	ARG	2.0
1	C	75	LYS	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	A1ICC	L	1	20/21	0.86	0.15	49,68,76,79	0
2	A1ICC	N	1	20/21	0.89	0.14	41,63,75,85	0
2	SFE	L	3	11/12	0.89	0.15	43,49,61,62	0
2	SFE	N	3	11/12	0.89	0.17	37,52,59,66	0
2	A1ICC	P	1	20/21	0.92	0.10	35,46,58,61	0
2	SFE	P	3	11/12	0.93	0.10	35,45,52,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
4	SO4	C	405	5/5	0.57	0.15	94,101,107,124	0
4	SO4	A	403	5/5	0.59	0.16	86,88,108,121	0
4	SO4	A	406	5/5	0.65	0.17	74,83,91,120	0
4	SO4	C	403	5/5	0.69	0.15	75,80,102,108	0
4	SO4	A	407	5/5	0.69	0.11	85,100,111,122	0
4	SO4	B	404	5/5	0.76	0.14	77,78,103,115	0
4	SO4	C	404	5/5	0.78	0.12	79,101,106,113	0
4	SO4	A	405	5/5	0.79	0.17	68,88,96,108	0
4	SO4	B	402	5/5	0.79	0.15	73,92,117,120	0
4	SO4	A	402	5/5	0.79	0.14	70,78,87,97	0
4	SO4	B	403	5/5	0.81	0.12	61,81,91,113	0
4	SO4	C	402	5/5	0.83	0.14	55,73,82,91	0
4	SO4	A	404	5/5	0.84	0.11	61,68,88,95	0
5	NA	C	406	1/1	0.84	0.12	51,51,51,51	0
3	NIO	A	401	9/9	0.90	0.11	46,48,56,59	0
3	NIO	C	401	9/9	0.90	0.13	36,51,58,64	0
3	NIO	B	401	9/9	0.94	0.09	42,46,57,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.