Full wwPDB X-ray Structure Validation Report (i)

Nov 26, 2024 – 12:04 am GMT

PDB ID	:	9FBL
Title	:	Structure of human protein kinase CK2 catalytic subunit (CK2alpha) in complex with the cyclic peptidomimetic compound FMP35 discovered by high-throughput screening
Deposited on	:	2024-05-14
Resolution	:	2.18 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:

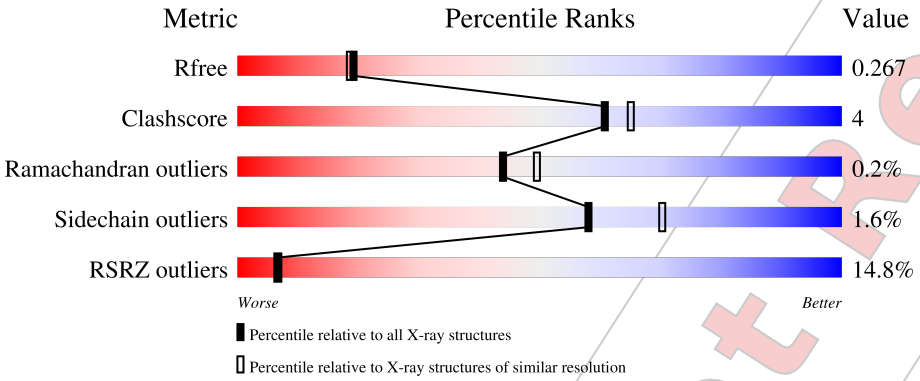
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (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 <=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	13% 83% 12% 5%
1	C	349	15% 82% 12% 6%

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

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Mol	Chain	Length	Quality of chain
2	L	5	60%, 20%, 40%, 40%
2	N	5	20%, 40%, 40%
2	P	5	80%, 20%

2 Entry composition (i)

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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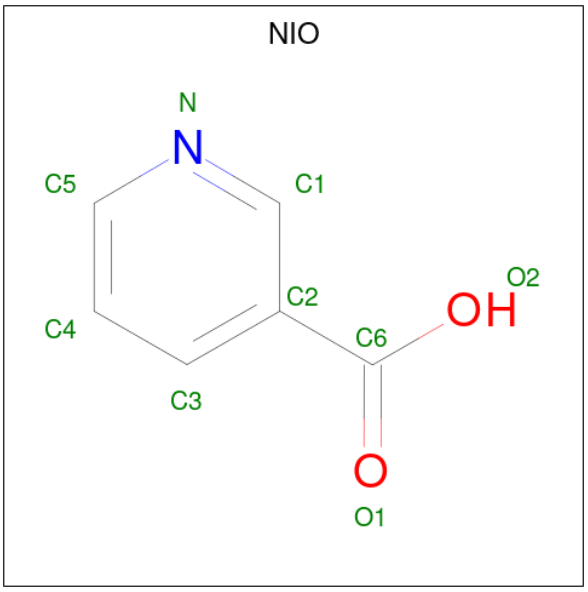
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLN	-	expression tag	UNP P68400
B	-1	ASP	-	expression tag	UNP P68400
B	0	PRO	-	expression tag	UNP P68400
C	-13	MET	-	initiating methionine	UNP P68400
C	-12	GLY	-	expression tag	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.

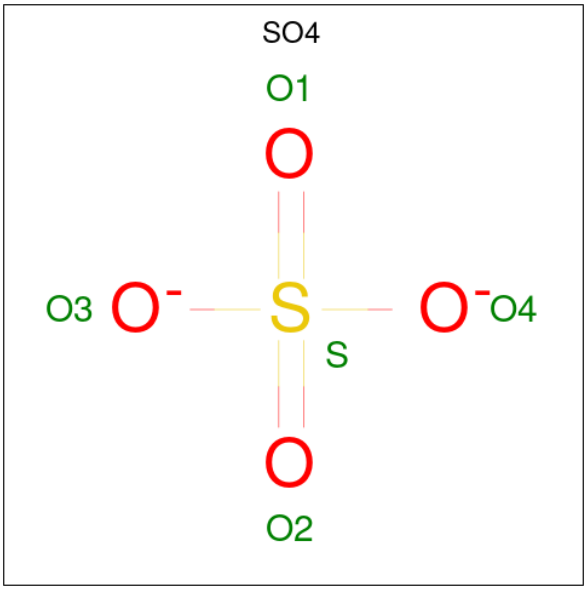
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			
2	N	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			
2	P	5	Total	C	N	O	S	0	0	0
			51	37	7	6	1			

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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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 (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0

- Molecule 6 is water.

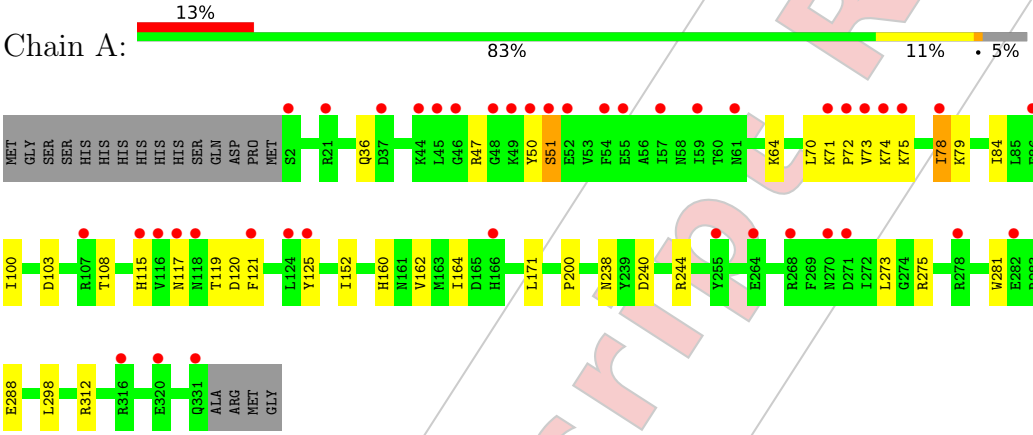
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	60	Total O 61 61	0	1
6	B	82	Total O 84 84	0	2
6	C	51	Total O 51 51	0	0
6	N	1	Total O 1 1	0	0

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.

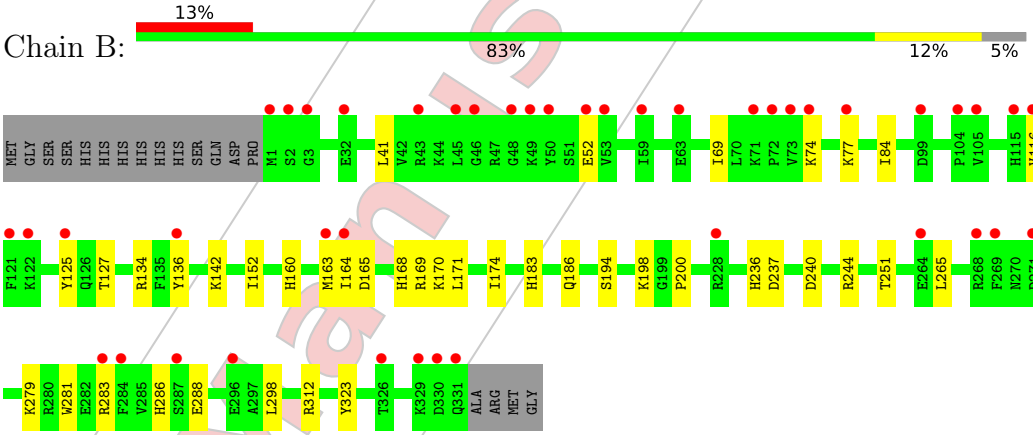
• Molecule 1: Casein kinase II subunit alpha

Chain A:



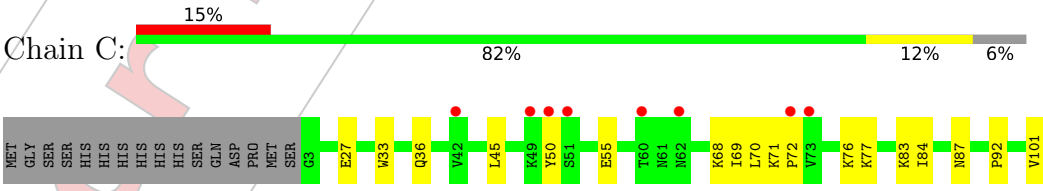
• Molecule 1: Casein kinase II subunit alpha

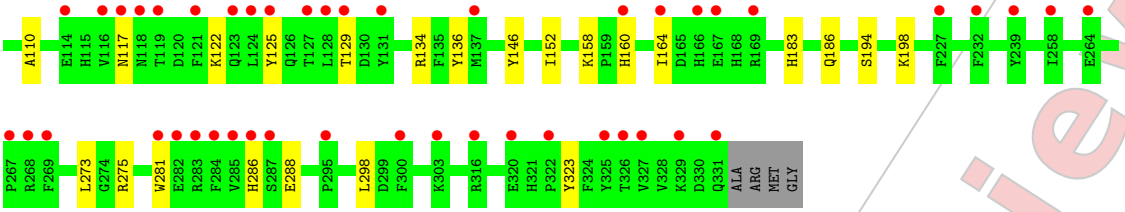
Chain B:



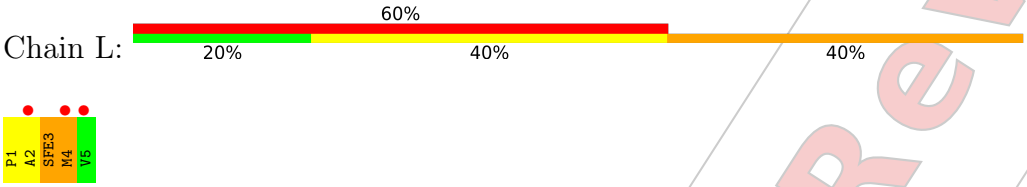
• Molecule 1: Casein kinase II subunit alpha

Chain C:

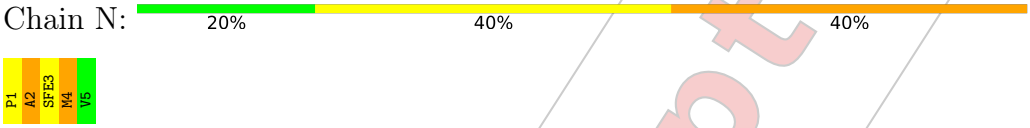




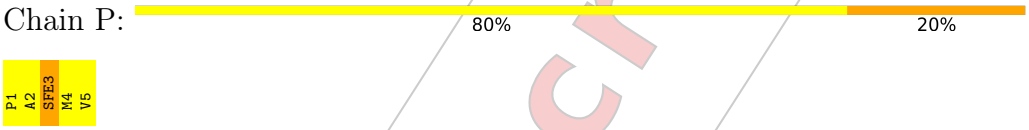
• Molecule 2: Cyclic peptidomimetic compound FMP35



• Molecule 2: Cyclic peptidomimetic compound FMP35



• Molecule 2: Cyclic peptidomimetic compound FMP35



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.84 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.209 , 0.266 0.209 , 0.267	Depositor DCC
R_{free} test set	38474 reflections (2.95%)	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]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[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: NIO, NA, SFE, A1ICC, 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	0.23	0/2874	0.47	0/3887
1	B	0.24	0/2882	0.48	0/3896
1	C	0.23	0/2868	0.47	0/3879
2	L	2.19	1/18 (5.6%)	1.63	1/21 (4.8%)
2	N	2.17	1/18 (5.6%)	1.67	1/21 (4.8%)
2	P	2.11	1/18 (5.6%)	1.46	0/21
All	All	0.29	3/8678 (0.0%)	0.48	2/11725 (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	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	6.30	1.48	1.34
2	N	4	MET	C-N	6.27	1.48	1.34
2	P	4	MET	C-N	6.18	1.48	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	4	MET	CG-SD-CE	6.01	109.81	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	4	MET	CG-SD-CE	5.64	109.22	100.20

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 (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	2798	0	2736	23	0
1	B	2807	0	2754	21	0
1	C	2792	0	2731	25	0
2	L	51	0	31	1	0
2	N	51	0	31	1	0
2	P	51	0	31	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	8326	69	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 (69) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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%)	22 21
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%)	44 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 (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	305/320 (95%)	302 (99%)	3 (1%)	73 82
1	B	306/320 (96%)	300 (98%)	6 (2%)	50 62
1	C	304/320 (95%)	301 (99%)	3 (1%)	73 82
2	L	2/2 (100%)	1 (50%)	1 (50%)	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%)	906 (98%)	15 (2%)	58 70

All (15) 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	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	N	4	MET
2	P	5	VAL

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

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	P	3	2	11,11,12	2.22	2 (18%)	10,13,15	0.89	0
2	A1ICC	N	1	2	19,22,23	3.15	8 (42%)	22,30,32	1.60	5 (22%)
2	A1ICC	P	1	2	19,22,23	3.16	9 (47%)	22,30,32	1.62	4 (18%)
2	SFE	L	3	2	11,11,12	2.21	2 (18%)	10,13,15	0.89	0
2	SFE	N	3	2	11,11,12	2.20	2 (18%)	10,13,15	0.89	0
2	A1ICC	L	1	2	19,22,23	3.16	9 (47%)	22,30,32	1.55	4 (18%)

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	P	3	2	-	0/7/7/8	0/1/1/1
2	A1ICC	N	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	L	3	2	-	0/7/7/8	0/1/1/1
2	SFE	N	3	2	-	2/7/7/8	0/1/1/1
2	A1ICC	L	1	2	-	0/8/19/21	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	A1ICC	CB-CA	-8.28	1.36	1.54
2	L	1	A1ICC	CB-CA	-8.27	1.36	1.54
2	P	1	A1ICC	CB-CA	-8.21	1.36	1.54
2	P	3	SFE	CG-CB	6.52	1.60	1.52
2	L	3	SFE	CG-CB	6.48	1.60	1.52
2	N	3	SFE	CG-CB	6.44	1.60	1.52
2	P	1	A1ICC	CB-CG	6.08	1.64	1.53
2	L	1	A1ICC	CB-CG	5.96	1.64	1.53
2	N	1	A1ICC	CB-CG	5.78	1.64	1.53
2	N	1	A1ICC	C30-N29	4.73	1.44	1.34
2	L	1	A1ICC	C30-N29	4.70	1.44	1.34
2	P	1	A1ICC	C30-N29	4.63	1.44	1.34
2	L	1	A1ICC	C32-C30	3.73	1.56	1.50
2	N	1	A1ICC	C32-C30	3.72	1.56	1.50
2	P	1	A1ICC	C32-C30	3.62	1.56	1.50
2	N	1	A1ICC	CD-N	3.29	1.59	1.47
2	L	1	A1ICC	CD-N	3.27	1.58	1.47
2	P	1	A1ICC	CD-N	3.23	1.58	1.47
2	P	1	A1ICC	O31-C30	-3.12	1.17	1.23
2	L	1	A1ICC	O31-C30	-3.12	1.17	1.23
2	N	1	A1ICC	O31-C30	-3.11	1.17	1.23
2	P	1	A1ICC	C41-C36	-2.90	1.37	1.43
2	N	1	A1ICC	C41-C36	-2.86	1.37	1.43
2	L	1	A1ICC	C41-C36	-2.86	1.37	1.43
2	P	3	SFE	CA-C	2.49	1.56	1.49
2	N	3	SFE	CA-C	2.48	1.56	1.49
2	L	3	SFE	CA-C	2.47	1.56	1.49
2	P	1	A1ICC	C32-C41	-2.37	1.40	1.43
2	L	1	A1ICC	C32-N33	2.37	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	A1ICC	C32-N33	2.37	1.35	1.33
2	N	1	A1ICC	C32-N33	2.32	1.35	1.33
2	L	1	A1ICC	C32-C41	-2.03	1.41	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1	A1ICC	C40-C41-C32	-3.77	121.31	124.34
2	L	1	A1ICC	C40-C41-C32	-3.29	121.70	124.34
2	N	1	A1ICC	C40-C41-C32	-3.21	121.76	124.34
2	P	1	A1ICC	C35-C34-N33	-3.09	120.77	123.81
2	L	1	A1ICC	C35-C34-N33	-3.08	120.78	123.81
2	N	1	A1ICC	C35-C34-N33	-2.99	120.86	123.81
2	N	1	A1ICC	C32-C41-C36	2.58	118.35	116.97
2	P	1	A1ICC	C32-C41-C36	2.57	118.34	116.97
2	L	1	A1ICC	C32-C41-C36	2.53	118.32	116.97
2	N	1	A1ICC	CG-N29-C30	-2.41	119.21	122.55
2	P	1	A1ICC	O-C-CA	-2.19	119.03	124.78
2	N	1	A1ICC	CB-CG-N29	-2.16	108.66	112.61
2	L	1	A1ICC	O-C-CA	-2.04	119.43	124.78

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	P	3	SFE	1	0
2	L	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	406	-	4,4,4	0.59	0	6,6,6	0.04	0
3	NIO	C	401	-	9,9,9	0.86	0	11,11,11	0.92	0
4	SO4	B	404	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	A	402	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	B	402	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	C	402	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	C	405	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	C	403	-	4,4,4	0.59	0	6,6,6	0.05	0
3	NIO	A	401	-	9,9,9	0.87	0	11,11,11	0.92	0
4	SO4	A	407	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	A	403	-	4,4,4	0.59	0	6,6,6	0.05	0
3	NIO	B	401	-	9,9,9	0.88	0	11,11,11	0.90	0
4	SO4	B	403	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	C	404	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	A	404	-	4,4,4	0.59	0	6,6,6	0.05	0
4	SO4	A	405	-	4,4,4	0.59	0	6,6,6	0.04	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	C	401	-	-	0/4/4/4	0/1/1/1
3	NIO	B	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.

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
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, 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	330/349 (94%)	0.92	44 (13%) 8 8	21, 45, 85, 134	1 (0%)
1	B	331/349 (94%)	0.92	47 (14%) 7 7	24, 46, 86, 133	1 (0%)
1	C	329/349 (94%)	1.00	54 (16%) 5 5	25, 48, 87, 167	1 (0%)
2	L	3/5 (60%)	2.50	3 (100%) 0 0	57, 57, 67, 71	0
2	N	3/5 (60%)	1.65	0 100 100	55, 55, 56, 64	0
2	P	3/5 (60%)	0.75	0 100 100	44, 44, 47, 55	0
All	All	999/1062 (94%)	0.96	148 (14%) 7 6	21, 47, 87, 167	3 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	VAL	6.6
1	C	73	VAL	5.8
1	A	116	VAL	5.6
1	B	45	LEU	5.5
1	C	125	TYR	4.9
1	C	118	ASN	4.6
1	C	114	GLU	4.2
1	B	164	ILE	4.1
1	A	121	PHE	4.0
1	A	50	TYR	4.0
1	B	121	PHE	3.8
1	A	72	PRO	3.8
1	C	281	TRP	3.8
1	B	50	TYR	3.7
1	C	284	PHE	3.7
1	A	54	PHE	3.6
1	B	104	PRO	3.6
1	B	72	PRO	3.5
1	B	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	131	TYR	3.5
1	B	49	LYS	3.4
1	B	120	ASP	3.4
1	A	115	HIS	3.4
1	B	116	VAL	3.3
1	A	166	HIS	3.3
1	C	329	LYS	3.3
1	B	163	MET	3.3
1	A	57	ILE	3.2
1	B	264	GLU	3.2
1	A	75	LYS	3.1
1	B	271	ASP	3.1
1	C	327	VAL	3.1
1	C	320	GLU	3.1
1	A	331	GLN	3.1
1	C	264	GLU	3.1
1	B	52	GLU	3.0
1	C	167	GLU	3.0
1	C	121	PHE	3.0
1	C	325	TYR	3.0
1	B	136	TYR	3.0
1	B	119	THR	3.0
1	A	59	ILE	2.9
1	A	51	SER	2.9
2	L	4	MET	2.9
1	A	255	TYR	2.9
1	C	164	ILE	2.9
1	B	74	LYS	2.9
1	A	124	LEU	2.8
1	B	105	VAL	2.8
1	A	107	ARG	2.8
1	C	287	SER	2.8
1	A	74	LYS	2.8
1	C	124	LEU	2.8
1	C	316	ARG	2.8
1	A	117	ASN	2.8
1	B	283	ARG	2.8
1	A	320	GLU	2.8
1	A	118	ASN	2.7
1	C	129	THR	2.7
1	C	283	ARG	2.7
1	C	137	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	331	GLN	2.7
1	A	125	TYR	2.7
1	C	49	LYS	2.6
1	C	51	SER	2.6
1	B	273	LEU	2.6
1	C	160[A]	HIS	2.6
1	B	296	GLU	2.6
1	B	118	ASN	2.6
1	C	117	ASN	2.6
1	A	48	GLY	2.6
1	B	115	HIS	2.6
1	B	77	LYS	2.6
1	B	63	GLU	2.6
1	B	125	TYR	2.5
1	A	21	ARG	2.5
1	A	316	ARG	2.5
1	C	72	PRO	2.5
1	C	267	PRO	2.5
1	A	55	GLU	2.5
1	C	285	VAL	2.5
1	A	268	ARG	2.5
1	A	2	SER	2.5
1	B	73	VAL	2.5
2	L	5	VAL	2.5
1	C	239	TYR	2.5
1	A	49	LYS	2.5
1	B	71	LYS	2.5
1	B	326	THR	2.5
1	C	326	THR	2.5
1	C	295	PRO	2.4
1	C	322	PRO	2.4
1	C	232	PHE	2.4
1	B	46	GLY	2.4
1	A	71	LYS	2.4
1	B	2	SER	2.4
1	C	258	ILE	2.4
1	B	268	ARG	2.4
1	C	268	ARG	2.4
1	A	270	ASN	2.4
1	C	269	PHE	2.4
1	C	127	THR	2.4
1	A	78	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	300	PHE	2.3
1	C	119	THR	2.3
1	A	86	GLU	2.3
1	C	50	TYR	2.3
1	C	166	HIS	2.3
1	C	128	LEU	2.3
1	B	59	ILE	2.3
1	B	43	ARG	2.3
1	C	60	THR	2.2
1	A	98	ALA	2.2
1	A	37	ASP	2.2
1	A	44	LYS	2.2
1	A	284	PHE	2.2
1	C	123	GLN	2.2
1	A	282	GLU	2.2
1	B	329	LYS	2.2
1	C	169	ARG	2.2
1	C	62	ASN	2.2
1	A	45	LEU	2.2
1	A	73	VAL	2.2
1	A	52	GLU	2.1
1	A	271	ASP	2.1
1	C	286	HIS	2.1
1	B	32	GLU	2.1
1	B	228[A]	ARG	2.1
2	L	2	ALA	2.1
1	C	282	GLU	2.1
1	C	303	LYS	2.1
1	B	53	VAL	2.1
1	C	105	VAL	2.1
1	B	122	LYS	2.1
1	B	99	ASP	2.1
1	B	330	ASP	2.1
1	B	287	SER	2.1
1	A	46	GLY	2.0
1	B	3	GLY	2.0
1	B	48	GLY	2.0
1	C	42	VAL	2.0
1	B	331	GLN	2.0
1	B	269	PHE	2.0
1	B	284	PHE	2.0
1	C	227	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLU	2.0
1	A	61	ASN	2.0
1	A	278	ARG	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	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 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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	0.87	0.11	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.