



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2017 – 06:19 PM EDT

PDB ID : 5W4W
Title : Identification and Profiling of a Selective and Brain Penetrant Radioligand for
In Vivo Target Occupancy Measurement of Casein Kinase 1 (CK1) Inhibitors
Authors : Liu, S.
Deposited on : unknown
Resolution : 1.99 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

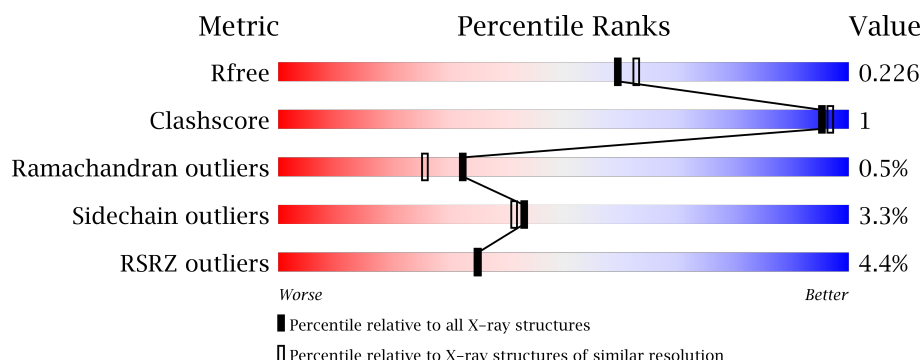
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	331	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	331	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	331	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>5%</div> <div>14%</div> </div> </div>
1	D	331	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10184 atoms, of which 60 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 I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2378	1525	417	422	14			
1	B	291	Total	C	N	O	S	0	0	0
			2378	1525	417	422	14			
1	C	284	Total	C	N	O	S	0	2	0
			2335	1501	406	413	15			
1	D	287	Total	C	N	O	S	0	0	0
			2343	1503	409	417	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P48730
A	-12	HIS	-	expression tag	UNP P48730
A	-11	HIS	-	expression tag	UNP P48730
A	-10	HIS	-	expression tag	UNP P48730
A	-9	HIS	-	expression tag	UNP P48730
A	-8	HIS	-	expression tag	UNP P48730
A	-7	HIS	-	expression tag	UNP P48730
A	-6	SER	-	expression tag	UNP P48730
A	-5	SER	-	expression tag	UNP P48730
A	-4	GLY	-	expression tag	UNP P48730
A	-3	LEU	-	expression tag	UNP P48730
A	-2	VAL	-	expression tag	UNP P48730
A	-1	PRO	-	expression tag	UNP P48730
A	0	ARG	-	expression tag	UNP P48730
A	1	GLY	-	expression tag	UNP P48730
A	2	SER	-	expression tag	UNP P48730
B	-13	MET	-	expression tag	UNP P48730
B	-12	HIS	-	expression tag	UNP P48730
B	-11	HIS	-	expression tag	UNP P48730
B	-10	HIS	-	expression tag	UNP P48730
B	-9	HIS	-	expression tag	UNP P48730

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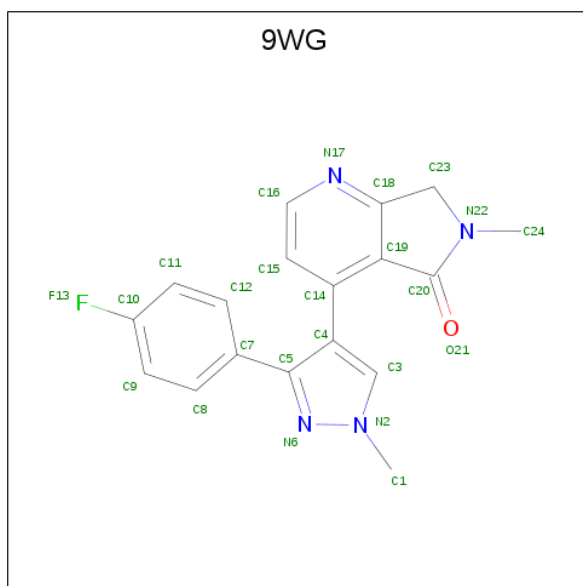
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P48730
B	-7	HIS	-	expression tag	UNP P48730
B	-6	SER	-	expression tag	UNP P48730
B	-5	SER	-	expression tag	UNP P48730
B	-4	GLY	-	expression tag	UNP P48730
B	-3	LEU	-	expression tag	UNP P48730
B	-2	VAL	-	expression tag	UNP P48730
B	-1	PRO	-	expression tag	UNP P48730
B	0	ARG	-	expression tag	UNP P48730
B	1	GLY	-	expression tag	UNP P48730
B	2	SER	-	expression tag	UNP P48730
C	-13	MET	-	expression tag	UNP P48730
C	-12	HIS	-	expression tag	UNP P48730
C	-11	HIS	-	expression tag	UNP P48730
C	-10	HIS	-	expression tag	UNP P48730
C	-9	HIS	-	expression tag	UNP P48730
C	-8	HIS	-	expression tag	UNP P48730
C	-7	HIS	-	expression tag	UNP P48730
C	-6	SER	-	expression tag	UNP P48730
C	-5	SER	-	expression tag	UNP P48730
C	-4	GLY	-	expression tag	UNP P48730
C	-3	LEU	-	expression tag	UNP P48730
C	-2	VAL	-	expression tag	UNP P48730
C	-1	PRO	-	expression tag	UNP P48730
C	0	ARG	-	expression tag	UNP P48730
C	1	GLY	-	expression tag	UNP P48730
C	2	SER	-	expression tag	UNP P48730
D	-13	MET	-	expression tag	UNP P48730
D	-12	HIS	-	expression tag	UNP P48730
D	-11	HIS	-	expression tag	UNP P48730
D	-10	HIS	-	expression tag	UNP P48730
D	-9	HIS	-	expression tag	UNP P48730
D	-8	HIS	-	expression tag	UNP P48730
D	-7	HIS	-	expression tag	UNP P48730
D	-6	SER	-	expression tag	UNP P48730
D	-5	SER	-	expression tag	UNP P48730
D	-4	GLY	-	expression tag	UNP P48730
D	-3	LEU	-	expression tag	UNP P48730
D	-2	VAL	-	expression tag	UNP P48730
D	-1	PRO	-	expression tag	UNP P48730
D	0	ARG	-	expression tag	UNP P48730
D	1	GLY	-	expression tag	UNP P48730

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	SER	-	expression tag	UNP P48730

- Molecule 2 is 4-[3-(4-fluorophenyl)-1-methyl-1H-pyrazol-4-yl]-6-methyl-6,7-dihydro-5H-pyrrolo[3,4-b]pyridin-5-one (three-letter code: 9WG) (formula: C₁₈H₁₅FN₄O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	15	0
			39	18	1	15	4	1		
2	B	1	Total	C	F	H	N	O	15	0
			39	18	1	15	4	1		
2	C	1	Total	C	F	H	N	O	15	0
			39	18	1	15	4	1		
2	D	1	Total	C	F	H	N	O	15	0
			39	18	1	15	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

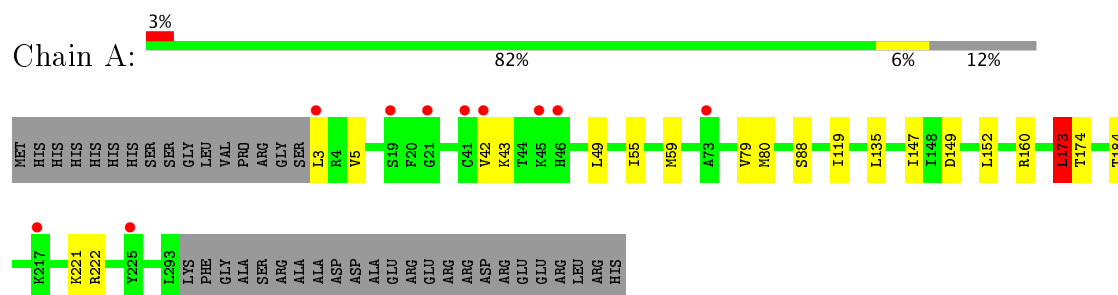
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	139	Total	O		0	0
			139	139			
4	B	135	Total	O		0	0
			135	135			
4	C	121	Total	O		0	0
			121	121			
4	D	124	Total	O		0	0
			124	124			

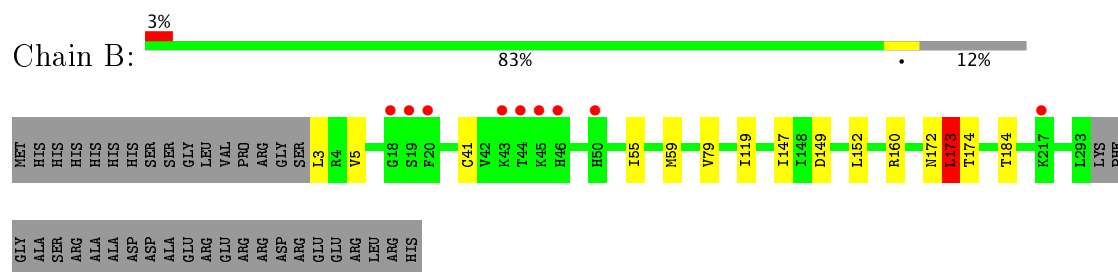
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

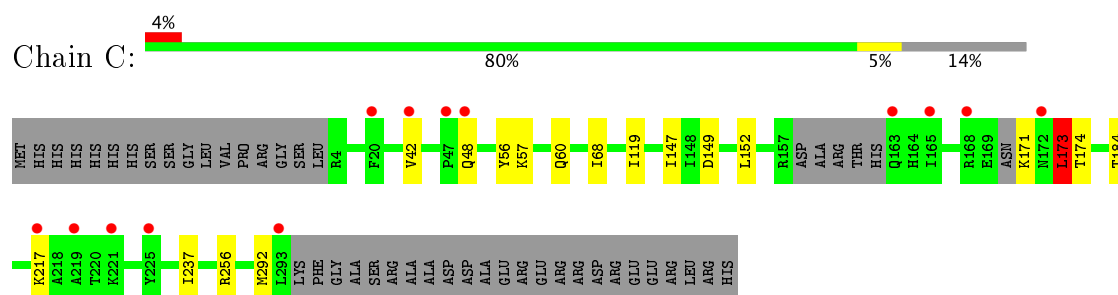
- Molecule 1: Casein kinase I isoform delta



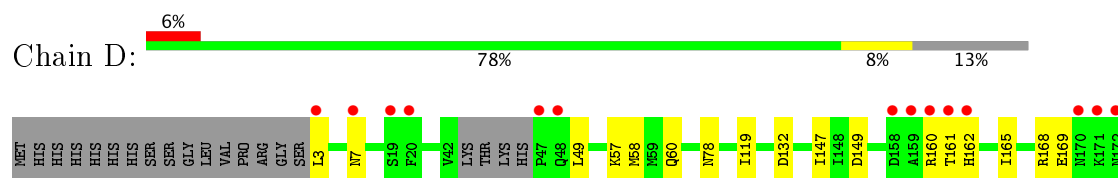
- Molecule 1: Casein kinase I isoform delta

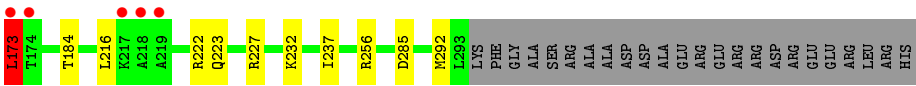


- Molecule 1: Casein kinase I isoform delta



- Molecule 1: Casein kinase I isoform delta





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.88Å 84.58Å 89.04Å 70.37° 74.27° 86.77°	Depositor
Resolution (Å)	20.06 – 1.99 69.47 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.06-1.99) 85.6 (69.47-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.180 , 0.215 0.190 , 0.226	Depositor DCC
R_{free} test set	3758 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10184	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9WG, 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	0.50	0/2433	0.62	0/3270
1	B	0.50	0/2433	0.61	0/3270
1	C	0.51	0/2387	0.62	0/3204
1	D	0.52	0/2396	0.65	2/3219 (0.1%)
All	All	0.51	0/9649	0.63	2/12963 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	ASP	C-N-CA	-5.73	107.37	121.70
1	D	285	ASP	N-CA-C	-5.25	96.81	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2382	8	0
1	B	2378	0	2382	5	0
1	C	2335	0	2341	7	0
1	D	2343	0	2342	6	0
2	A	24	15	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	15	0	0	0
2	C	24	15	0	0	0
2	D	24	15	0	0	0
3	A	15	0	0	0	0
3	B	30	0	0	0	0
3	C	20	0	0	0	0
3	D	10	0	0	0	0
4	A	139	0	0	0	0
4	B	135	0	0	0	0
4	C	121	0	0	0	0
4	D	124	0	0	0	0
All	All	10124	60	9447	26	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 1.

All (26) 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:173:LEU:HD22	1:B:184:THR:HG22	1.85	0.58
1:B:5:VAL:HG11	1:B:79:VAL:HG11	1.85	0.58
1:A:173:LEU:HD22	1:A:184:THR:HG22	1.87	0.56
1:D:173:LEU:HD22	1:D:184:THR:HG22	1.88	0.56
1:C:56:TYR:CB	1:C:68[A]:ILE:HD11	2.36	0.56
1:C:173:LEU:HD22	1:C:184:THR:HG22	1.89	0.55
1:B:119:ILE:HD11	1:B:147:ILE:HG21	1.92	0.51
1:A:49:LEU:HD21	1:A:80:MET:HB2	1.93	0.50
1:A:119:ILE:HD11	1:A:147:ILE:HG21	1.93	0.50
1:C:152:LEU:HD22	1:C:174:THR:HG23	1.93	0.49
1:D:49:LEU:HD22	1:D:78:ASN:HB3	1.94	0.48
1:A:152:LEU:HD22	1:A:174:THR:HG23	1.95	0.48
1:C:119:ILE:HD11	1:C:147:ILE:HG21	1.96	0.48
1:B:152:LEU:HD22	1:B:174:THR:HG23	1.96	0.47
1:D:119:ILE:HD11	1:D:147:ILE:HG21	1.97	0.46
1:A:5:VAL:HG11	1:A:79:VAL:HG11	1.98	0.44
1:C:56:TYR:HB2	1:C:68[A]:ILE:HD11	1.98	0.44
1:A:42:VAL:HG12	1:A:43:LYS:HG3	2.00	0.43
1:C:237:ILE:HD11	1:C:256:ARG:NH2	2.34	0.42
1:C:57:LYS:HA	1:C:60:GLN:HG2	2.02	0.41
1:D:237:ILE:HD11	1:D:256:ARG:NH2	2.35	0.41
1:D:57:LYS:HA	1:D:60:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:HA	1:A:135:LEU:HA	2.03	0.41
1:A:55:ILE:O	1:A:59:MET:HG2	2.21	0.41
1:B:55:ILE:O	1:B:59:MET:HG2	2.21	0.41
1:D:216:LEU:HD13	1:D:227:ARG:HG2	2.02	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	289/331 (87%)	282 (98%)	6 (2%)	1 (0%)	44	40
1	B	289/331 (87%)	282 (98%)	6 (2%)	1 (0%)	44	40
1	C	280/331 (85%)	276 (99%)	3 (1%)	1 (0%)	38	33
1	D	283/331 (86%)	274 (97%)	6 (2%)	3 (1%)	17	9
All	All	1141/1324 (86%)	1114 (98%)	21 (2%)	6 (0%)	32	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	HIS
1	A	173	LEU
1	B	173	LEU
1	C	173	LEU
1	D	7	ASN
1	D	173	LEU

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	255/288 (88%)	249 (98%)	6 (2%)	54	56
1	B	255/288 (88%)	249 (98%)	6 (2%)	54	56
1	C	251/288 (87%)	244 (97%)	7 (3%)	49	49
1	D	251/288 (87%)	237 (94%)	14 (6%)	25	19
All	All	1012/1152 (88%)	979 (97%)	33 (3%)	43	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	149	ASP
1	A	160	ARG
1	A	173	LEU
1	A	221	LYS
1	A	222	ARG
1	B	3	LEU
1	B	41	CYS
1	B	149	ASP
1	B	160	ARG
1	B	172	ASN
1	B	173	LEU
1	C	42	VAL
1	C	48	GLN
1	C	149	ASP
1	C	171	LYS
1	C	173	LEU
1	C	217	LYS
1	C	292	MET
1	D	3	LEU
1	D	58	MET
1	D	132	ASP
1	D	149	ASP
1	D	160	ARG
1	D	161	THR
1	D	165	ILE
1	D	168	ARG
1	D	169	GLU

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Mol	Chain	Res	Type
1	D	173	LEU
1	D	222	ARG
1	D	223	GLN
1	D	232	LYS
1	D	292	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	275	ASN
1	B	78	ASN
1	C	271	GLN
1	C	275	ASN
1	D	223	GLN
1	D	271	GLN
1	D	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9WG	A	4001	-	23,27,27	0.78	1 (4%)	27,40,40	1.44	1 (3%)
3	SO4	A	4002	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	A	4003	-	4,4,4	0.26	0	6,6,6	0.42	0
3	SO4	A	4004	-	4,4,4	0.33	0	6,6,6	0.13	0
2	9WG	B	4001	-	23,27,27	0.77	1 (4%)	27,40,40	1.37	1 (3%)
3	SO4	B	4002	-	4,4,4	0.10	0	6,6,6	0.24	0
3	SO4	B	4003	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	B	4004	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	B	4005	-	4,4,4	0.11	0	6,6,6	0.08	0
3	SO4	B	4006	-	4,4,4	0.39	0	6,6,6	0.23	0
3	SO4	B	4007	-	4,4,4	0.22	0	6,6,6	0.29	0
2	9WG	C	401	-	23,27,27	0.92	2 (8%)	27,40,40	1.14	1 (3%)
3	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	C	403	-	4,4,4	0.42	0	6,6,6	0.39	0
3	SO4	C	404	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	C	405	-	4,4,4	0.19	0	6,6,6	0.13	0
2	9WG	D	401	-	23,27,27	0.83	2 (8%)	27,40,40	1.16	1 (3%)
3	SO4	D	402	-	4,4,4	0.25	0	6,6,6	0.23	0
3	SO4	D	403	-	4,4,4	0.37	0	6,6,6	0.31	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	9WG	A	4001	-	-	0/7/20/20	0/4/4/4
3	SO4	A	4002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4004	-	-	0/0/0/0	0/0/0/0
2	9WG	B	4001	-	-	0/7/20/20	0/4/4/4
3	SO4	B	4002	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4003	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4004	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4005	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4006	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4007	-	-	0/0/0/0	0/0/0/0
2	9WG	C	401	-	-	0/7/20/20	0/4/4/4
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	403	-	-	0/0/0/0	0/0/0/0
3	SO4	C	404	-	-	0/0/0/0	0/0/0/0
3	SO4	C	405	-	-	0/0/0/0	0/0/0/0
2	9WG	D	401	-	-	0/7/20/20	0/4/4/4
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	SO4	D	403	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	9WG	C5-N6	-2.71	1.33	1.35
2	D	401	9WG	C5-N6	-2.44	1.33	1.35
2	A	4001	9WG	C5-N6	-2.29	1.33	1.35
2	B	4001	9WG	C5-N6	-2.14	1.33	1.35
2	D	401	9WG	C4-C5	2.13	1.43	1.40
2	C	401	9WG	C4-C5	2.70	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	9WG	C18-C23-N22	4.96	104.13	102.21
2	D	401	9WG	C18-C23-N22	5.03	104.16	102.21
2	B	4001	9WG	C18-C23-N22	6.35	104.67	102.21
2	A	4001	9WG	C18-C23-N22	6.71	104.80	102.21

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 [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	291/331 (87%)	-0.16	10 (3%) 46 46	19, 35, 80, 121	0
1	B	291/331 (87%)	-0.21	9 (3%) 49 49	20, 35, 79, 114	0
1	C	284/331 (85%)	-0.16	13 (4%) 33 33	19, 33, 75, 94	0
1	D	287/331 (86%)	-0.05	19 (6%) 19 19	19, 36, 80, 106	0
All	All	1153/1324 (87%)	-0.14	51 (4%) 35 35	19, 35, 79, 121	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	HIS	5.9
1	D	160	ARG	5.5
1	D	159	ALA	5.5
1	D	170	ASN	5.5
1	D	217	LYS	4.9
1	D	172	ASN	4.8
1	A	45	LYS	4.6
1	D	161	THR	4.5
1	B	18	GLY	3.9
1	B	19	SER	3.9
1	B	20	PHE	3.8
1	B	46	HIS	3.7
1	B	44	THR	3.6
1	A	3	LEU	3.5
1	D	218	ALA	3.4
1	C	293	LEU	3.4
1	A	42	VAL	3.3
1	C	42	VAL	3.3
1	D	20	PHE	3.1
1	A	41	CYS	2.9
1	C	172	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	43	LYS	2.8
1	C	219	ALA	2.7
1	D	158	ASP	2.7
1	A	19	SER	2.7
1	D	19	SER	2.7
1	A	73	ALA	2.6
1	C	47	PRO	2.6
1	D	47	PRO	2.6
1	D	162	HIS	2.5
1	D	7	ASN	2.5
1	C	20	PHE	2.5
1	B	50	HIS	2.5
1	D	171	LYS	2.5
1	D	3	LEU	2.4
1	B	217	LYS	2.3
1	C	163	GLN	2.3
1	A	21	GLY	2.3
1	C	165	ILE	2.3
1	C	217	LYS	2.3
1	C	225	TYR	2.2
1	A	217	LYS	2.2
1	D	173	LEU	2.2
1	D	219	ALA	2.2
1	D	48	GLN	2.1
1	B	45	LYS	2.1
1	C	48	GLN	2.1
1	C	168	ARG	2.0
1	D	174	THR	2.0
1	C	221	LYS	2.0
1	A	225	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	D	402	5/5	0.98	0.10	0.48	49,51,53,54	0
3	SO4	D	403	5/5	1.00	0.09	0.39	41,43,45,45	0
3	SO4	B	4006	5/5	0.93	0.15	0.31	63,69,71,72	0
3	SO4	B	4003	5/5	0.99	0.07	-0.09	41,42,43,46	0
2	9WG	A	4001	24/24	0.96	0.09	-0.38	30,39,46,47	15
2	9WG	B	4001	24/24	0.96	0.08	-0.51	33,41,45,46	15
3	SO4	B	4007	5/5	0.96	0.08	-0.52	69,71,72,73	0
3	SO4	A	4003	5/5	0.99	0.08	-0.53	43,43,46,48	0
2	9WG	D	401	24/24	0.96	0.08	-0.57	30,36,42,43	15
3	SO4	C	403	5/5	0.99	0.08	-0.59	41,41,44,45	0
3	SO4	B	4004	5/5	0.96	0.07	-0.73	92,93,93,94	0
3	SO4	C	402	5/5	0.99	0.08	-0.81	42,44,46,46	0
2	9WG	C	401	24/24	0.97	0.07	-0.86	28,35,39,41	15
3	SO4	C	404	5/5	0.95	0.12	-1.02	104,104,104,105	0
3	SO4	B	4005	5/5	0.98	0.07	-1.75	53,55,56,58	0
3	SO4	B	4002	5/5	0.98	0.07	-	60,63,63,66	0
3	SO4	A	4004	5/5	0.98	0.06	-	55,58,59,62	0
3	SO4	C	405	5/5	0.94	0.08	-	97,98,98,98	0
3	SO4	A	4002	5/5	0.98	0.08	-	57,60,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.