



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2016 – 04:01 PM EST

PDB ID : 5CTP
Title : Crystal structure of CK2alpha with N-(3-(3-chloro-4-(phenyl)benzylamino)propyl)acetamide bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.H.; Spring, D.; Hyvonen, M.
Deposited on : 2015-07-24
Resolution : 2.03 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028320

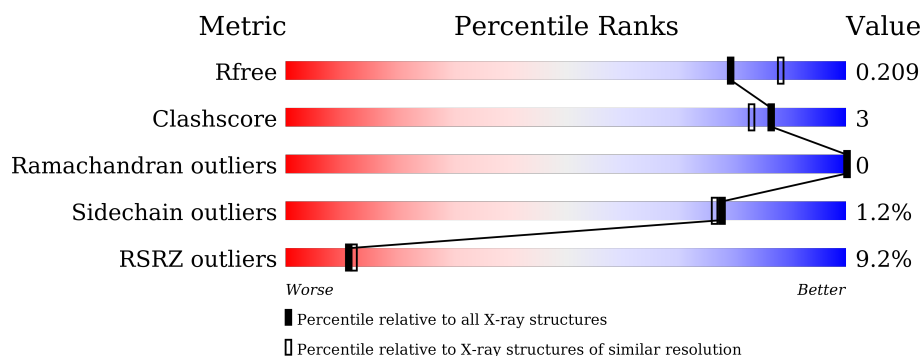
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	352	<div> <div>14%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	352	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>

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
2	ACT	A	401	-	-	-	X
2	ACT	B	401	-	-	-	X
2	ACT	B	403	-	-	-	X
3	54R	A	402	-	-	-	X
3	54R	B	404[A]	-	-	-	X
3	54R	B	404[B]	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5831 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	324	Total	C	N	O	S	0	1	0
			2746	1761	480	494	11			
1	B	327	Total	C	N	O	S	0	3	0
			2786	1786	490	499	11			

There are 50 discrepancies between the modelled and reference sequences:

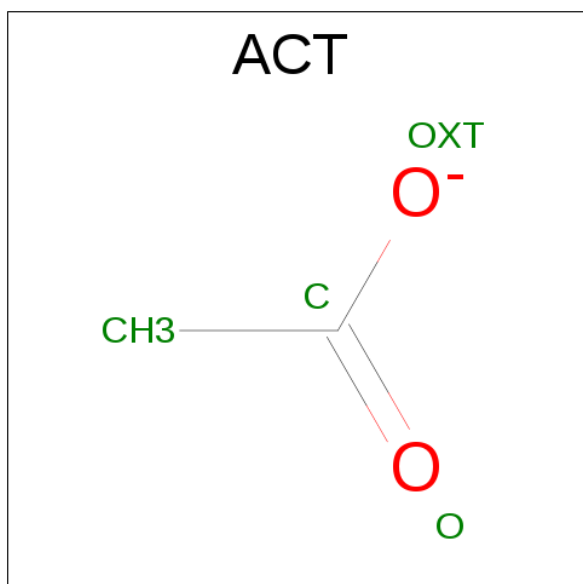
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

Continued on next page...

Continued from previous page...

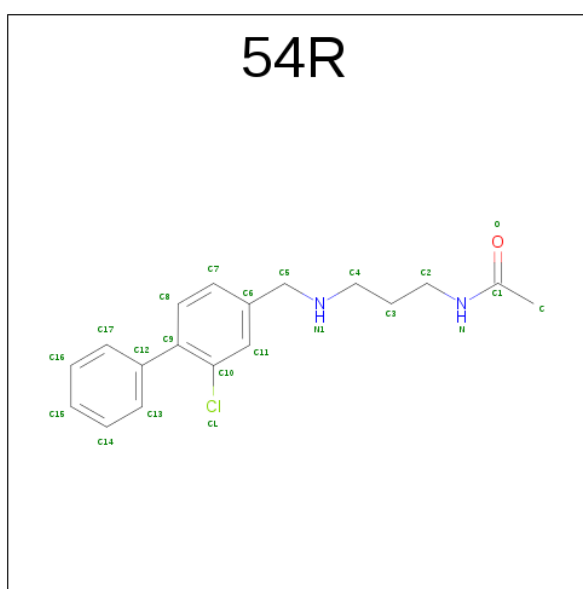
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 3 is N-(3-{[(2-chlorobiphenyl-4-yl)methyl]amino}propyl)acetamide (three-letter code: 54R) (formula: C₁₈H₂₁ClN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			22	18	1	2	1		
3	B	1	Total	C	Cl	N	O	0	1
			44	36	2	4	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

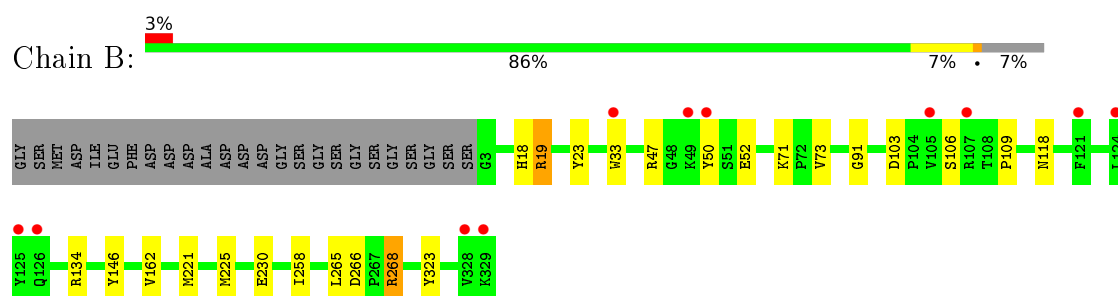
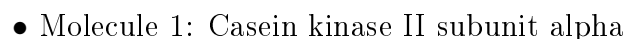


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	159	Total	O	0	0
			159	159		

- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.07Å 68.86Å 333.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.47 – 2.03 83.47 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.7 (83.47-2.03) 99.8 (83.47-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.03Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.185 , 0.199 0.193 , 0.209	Depositor DCC
R_{free} test set	2481 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.4	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	0.96	EDS
Total number of atoms	5831	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: 54R, PO4, ACT

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	0.53	0/2821	0.63	0/3816
1	B	0.74	3/2861 (0.1%)	0.70	8/3869 (0.2%)
All	All	0.64	3/5682 (0.1%)	0.67	8/7685 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19[A]	ARG	C-N	-15.24	1.05	1.34
1	B	19[B]	ARG	C-N	-15.24	1.05	1.34
1	B	18	HIS	C-N	-8.47	1.14	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	HIS	O-C-N	-6.77	111.86	122.70
1	B	19[A]	ARG	O-C-N	-6.45	108.84	121.10
1	B	19[B]	ARG	O-C-N	-6.45	108.84	121.10
1	B	19[A]	ARG	C-N-CD	-6.03	107.34	120.60
1	B	19[B]	ARG	C-N-CD	-6.03	107.34	120.60
1	B	18	HIS	CA-C-N	5.99	130.38	117.20
1	B	19[A]	ARG	CA-C-N	5.25	131.79	117.10
1	B	19[B]	ARG	CA-C-N	5.25	131.79	117.10

There are no chirality outliers.

There are no planarity outliers.

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	2746	0	2685	13	0
1	B	2786	0	2732	19	0
2	A	4	0	3	0	0
2	B	12	0	9	0	0
3	A	22	0	0	1	0
3	B	44	0	0	6	0
4	B	5	0	0	0	0
5	A	53	0	0	1	0
5	B	159	0	0	1	0
All	All	5831	0	5429	30	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (30) 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:A:119:THR:HG21	1:A:124:LEU:HD21	1.64	0.78
1:B:221:MET:CE	3:B:404[A]:54R:CL	2.71	0.76
1:A:119:THR:CG2	1:A:124:LEU:HD21	2.17	0.75
1:B:221:MET:HE3	3:B:404[A]:54R:CL	2.31	0.67
1:B:225:MET:HG3	3:B:404[A]:54R:C16	2.27	0.64
1:B:266:ASP:OD1	1:B:268:ARG:HD2	1.99	0.62
1:B:221:MET:HE1	3:B:404[A]:54R:CL	2.38	0.59
1:A:43:ARG:HD3	5:A:546:HOH:O	2.03	0.58
1:B:266:ASP:OD1	1:B:268:ARG:CD	2.53	0.57
1:A:119:THR:HG21	1:A:124:LEU:CD2	2.36	0.54
1:A:36:GLN:HG3	1:A:101:VAL:HG21	1.92	0.52
1:A:119:THR:CG2	1:A:124:LEU:CD2	2.87	0.52
1:A:105:VAL:HG12	1:B:23:TYR:HB2	1.92	0.51
1:A:104:PRO:HG2	1:B:19[A]:ARG:HH21	1.76	0.51
1:A:50:TYR:HA	1:A:71:LYS:HD2	1.94	0.50
1:B:225:MET:HG3	3:B:404[B]:54R:C16	2.42	0.49
1:B:50:TYR:HA	1:B:71:LYS:HD2	1.94	0.49
1:B:118:ASN:ND2	5:B:502:HOH:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB2	1:A:230:GLU:HG2	1.93	0.48
1:A:225:MET:HG3	3:A:402:54R:C14	2.44	0.48
1:B:162:VAL:HB	3:B:404[A]:54R:CL	2.52	0.46
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.51	0.45
1:B:103:ASP:HB3	1:B:106:SER:OG	2.17	0.44
1:A:33:TRP:CH2	1:A:109:PRO:HB3	2.53	0.43
1:B:33:TRP:CH2	1:B:109:PRO:HB3	2.53	0.43
1:B:258:ILE:HD13	1:B:265:LEU:HG	2.01	0.41
1:B:134:ARG:HD3	1:B:323:TYR:O	2.20	0.41
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.56	0.41
1:B:47:ARG:HG3	1:B:52:GLU:HG3	2.02	0.41
1:A:165:ASP:HB3	1:A:170:LYS:HB3	2.03	0.41

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	323/352 (92%)	316 (98%)	7 (2%)	0	100	100
1	B	328/352 (93%)	319 (97%)	9 (3%)	0	100	100
All	All	651/704 (92%)	635 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	300/319 (94%)	296 (99%)	4 (1%)	76	74
1	B	304/319 (95%)	301 (99%)	3 (1%)	82	81
All	All	604/638 (95%)	597 (99%)	7 (1%)	78	76

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

Mol	Chain	Res	Type
1	A	21	SER
1	A	73	VAL
1	A	107	ARG
1	A	306	ARG
1	B	73	VAL
1	B	230	GLU
1	B	268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	ASN
1	B	270	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](#)

8 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	ACT	A	401	-	0,3,3	0.00	-	0,3,3	0.00	-
3	54R	A	402	-	23,23,23	0.10	0	28,29,29	0.17	0
2	ACT	B	401	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	B	402	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	B	403	-	0,3,3	0.00	-	0,3,3	0.00	-
3	54R	B	404[A]	-	23,23,23	0.11	0	28,29,29	0.18	0
3	54R	B	404[B]	-	23,23,23	0.08	0	28,29,29	0.18	0
4	PO4	B	405	-	4,4,4	1.95	3 (75%)	6,6,6	0.25	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	ACT	A	401	-	-	0/0/0/0	0/0/0/0
3	54R	A	402	-	-	0/13/13/13	0/2/2/2
2	ACT	B	401	-	-	0/0/0/0	0/0/0/0
2	ACT	B	402	-	-	0/0/0/0	0/0/0/0
2	ACT	B	403	-	-	0/0/0/0	0/0/0/0
3	54R	B	404[A]	-	-	0/13/13/13	0/2/2/2
3	54R	B	404[B]	-	-	0/13/13/13	0/2/2/2
4	PO4	B	405	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	PO4	P-O3	2.17	1.60	1.53
4	B	405	PO4	P-O4	2.19	1.60	1.53
4	B	405	PO4	P-O2	2.20	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	54R	1	0
3	B	404[A]	54R	5	0
3	B	404[B]	54R	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	18:HIS	C	19[A]:ARG	N	1.14
1	B	18:HIS	C	19[B]:ARG	N	1.14
1	B	19[A]:ARG	C	20:PRO	N	1.05
1	B	19[B]:ARG	C	20:PRO	N	1.05

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	324/352 (92%)	0.89	49 (15%) 3 3	32, 66, 114, 154	0
1	B	327/352 (92%)	0.35	11 (3%) 49 55	20, 35, 72, 108	0
All	All	651/704 (92%)	0.62	60 (9%) 11 12	20, 50, 103, 154	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	9.6
1	B	50	TYR	7.9
1	B	124	LEU	6.7
1	A	49	LYS	6.4
1	A	125	TYR	5.7
1	B	125	TYR	5.4
1	A	47	ARG	5.3
1	B	329	LYS	5.0
1	A	270	ASN	4.7
1	A	288	GLU	4.6
1	A	48	GLY	4.5
1	B	121	PHE	4.5
1	A	126	GLN	4.3
1	A	284	PHE	4.2
1	A	33	TRP	4.0
1	A	301	LEU	3.9
1	A	282	GLU	3.7
1	B	105	VAL	3.7
1	A	307	TYR	3.5
1	A	281	TRP	3.5
1	B	49	LYS	3.4
1	A	272	ILE	3.3
1	A	255	TYR	3.2
1	A	121	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	126	GLN	3.2
1	A	46	GLY	3.1
1	B	33	TRP	3.1
1	A	269	PHE	3.1
1	A	271	ASP	3.1
1	A	5	VAL	2.9
1	A	124	LEU	2.8
1	A	107	ARG	2.8
1	A	316	ARG	2.8
1	A	326	THR	2.7
1	B	107	ARG	2.7
1	A	300	PHE	2.6
1	A	72	PRO	2.5
1	A	123	GLN	2.5
1	A	105	VAL	2.4
1	A	325	TYR	2.4
1	A	52	GLU	2.4
1	A	290	GLN	2.4
1	A	227	PHE	2.3
1	A	292	LEU	2.3
1	A	291	HIS	2.3
1	A	122	LYS	2.3
1	A	233	PHE	2.3
1	A	130	ASP	2.3
1	A	249	LEU	2.2
1	A	257	TYR	2.2
1	A	305	LEU	2.2
1	B	328	VAL	2.2
1	A	104	PRO	2.2
1	A	204	VAL	2.2
1	A	109	PRO	2.1
1	A	252	GLU	2.1
1	A	324	PHE	2.1
1	A	278	ARG	2.0
1	A	280	ARG	2.0
1	A	242	LEU	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 [i](#)

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
2	ACT	B	403	4/4	0.86	0.25	12.46	50,51,52,52	0
2	ACT	B	401	4/4	0.81	0.26	6.35	45,46,47,48	0
2	ACT	A	401	4/4	0.81	0.28	6.20	46,54,56,57	0
3	54R	A	402	22/22	0.68	0.40	3.24	90,105,123,124	0
3	54R	B	404[A]	22/22	0.83	0.27	2.10	86,93,99,100	22
3	54R	B	404[B]	22/22	0.83	0.27	2.03	19,31,38,40	22
2	ACT	B	402	4/4	0.95	0.17	1.29	46,46,49,50	0
4	PO4	B	405	5/5	0.91	0.14	-	65,70,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.