



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:56 AM GMT

PDB ID : 2JED  
Title : THE CRYSTAL STRUCTURE OF THE KINASE DOMAIN OF THE PROTEIN KINASE C THETA IN COMPLEX WITH NVP-XAA228 AT 2.32Å RESOLUTION.  
Authors : Stark, W.; Bitsch, F.; Berner, A.; Buelens, F.; Graff, P.; Depersin, H.; Geiser, M.; Knecht, R.; Rahuel, J.; Rummel, G.; Schlaeppli, J.M.; Schmitz, R.; Strauss, A.; Wagner, J.  
Deposited on : 2007-01-16  
Resolution : 2.32 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](mailto: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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

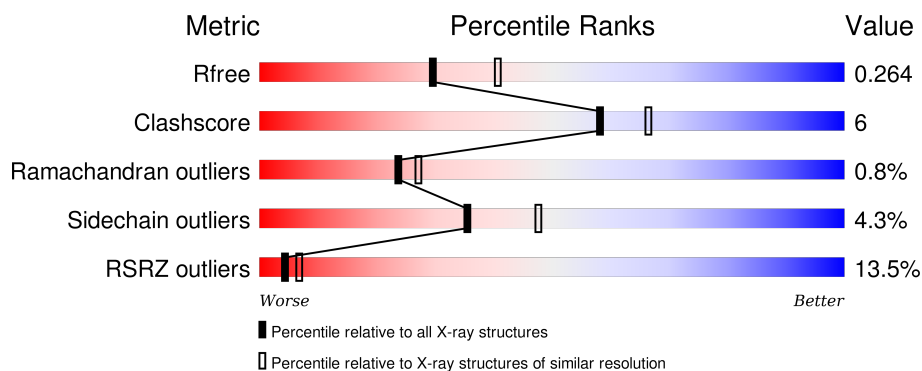
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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  $\geq 3$ , 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	
1	B	352	

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
3	MPD	B	1713	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5884 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.

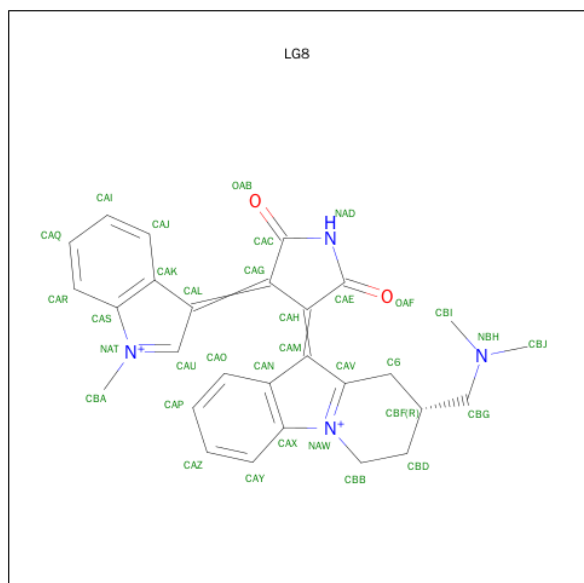
- Molecule 1 is a protein called PROTEIN KINASE C THETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	P	S	0	0	0
			2712	1753	450	488	2	19			
1	B	322	Total	C	N	O	P	S	0	0	0
			2684	1732	455	476	2	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLU	ILE	ENGINEERED MUTATION	UNP Q04759
A	538	GLU	THR	ENGINEERED MUTATION	UNP Q04759
B	381	GLU	ILE	ENGINEERED MUTATION	UNP Q04759
B	538	GLU	THR	ENGINEERED MUTATION	UNP Q04759

- Molecule 2 is 3-(8-DIMETHYLAMINOMETHYL-6,7,8,9-TETRAHYDRO-PYRIDO[1,2-A]INDOL-10-YL)-4-(1-METHYL-1H-INDOL-3-YL)-PYRROLE-2,5-DIONE (three-letter code: LG8) (formula: C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	28	4	2		
2	B	1	Total	C	N	O	0	0
			34	28	4	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

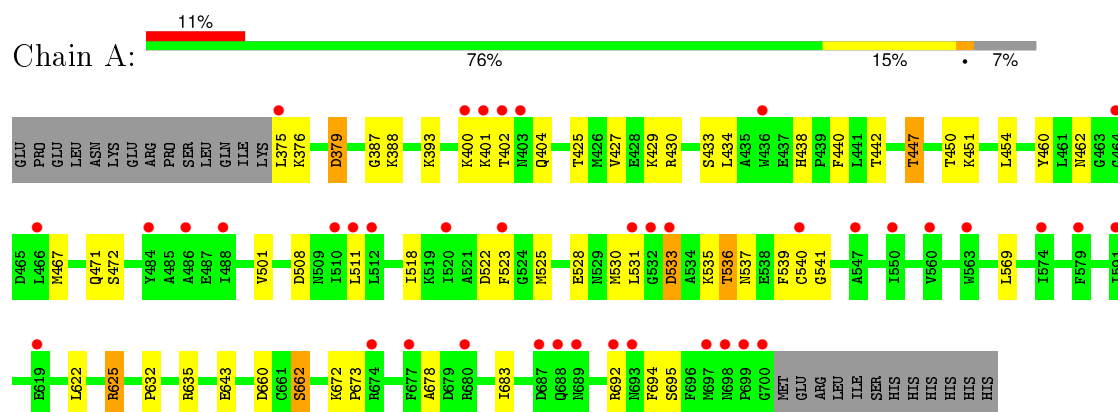
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	217	Total	O	0	0
			217	217		

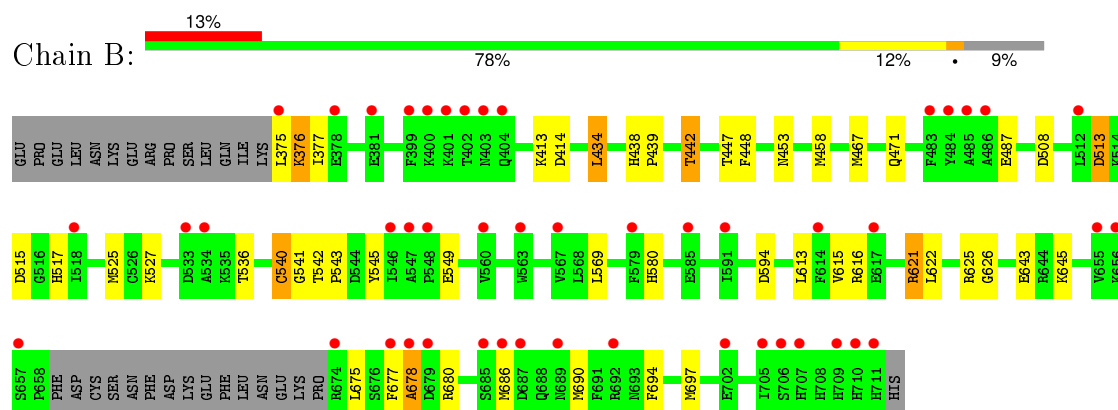
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN KINASE C THETA



#### • Molecule 1: PROTEIN KINASE C THETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.17Å 152.17Å 74.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.32 19.41 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-2.32) 100.0 (19.41-2.32)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.221 0.231 , 0.264	Depositor DCC
$R_{free}$ test set	2131 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.2	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42824 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: LG8, MPD, SEP

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	0.63	1/2762 (0.0%)	0.71	2/3711 (0.1%)
1	B	0.61	1/2734 (0.0%)	0.71	2/3672 (0.1%)
All	All	0.62	2/5496 (0.0%)	0.71	4/7383 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	CYS	C-N	-11.38	1.12	1.33
1	B	540	CYS	CB-SG	-7.83	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	PHE	O-C-N	-7.67	110.43	122.70
1	B	434	LEU	CA-CB-CG	7.28	132.04	115.30
1	A	539	PHE	C-N-CA	6.78	138.65	121.70
1	B	621	ARG	NE-CZ-NH2	-5.65	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	400	LYS	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	2712	0	2653	34	0
1	B	2684	0	2630	30	0
2	A	34	0	28	2	0
2	B	34	0	28	0	0
3	B	8	0	14	3	0
4	A	195	0	0	2	0
4	B	217	0	0	5	0
All	All	5884	0	5353	64	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 6.

All (64) 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:447:THR:HG21	1:A:694:PHE:O	1.69	0.91
1:A:447:THR:CG2	1:A:694:PHE:O	2.27	0.83
1:B:613:LEU:O	1:B:621:ARG:HD2	1.84	0.76
1:B:442:THR:HG21	4:B:2098:HOH:O	1.84	0.76
1:A:536:THR:HG22	1:A:537:ASN:H	1.51	0.74
1:B:471:GLN:NE2	4:B:2057:HOH:O	2.22	0.71
1:A:442:THR:HG21	4:A:2068:HOH:O	1.93	0.68
1:B:414:ASP:HB2	4:B:2044:HOH:O	1.95	0.65
1:B:467:MET:HE1	3:B:1713:MPD:HM3	1.78	0.65
1:A:402:THR:HG21	1:A:404:GLN:OE1	1.99	0.62
1:B:487:GLU:OE2	1:B:517:HIS:HD2	1.82	0.62
1:A:376:LYS:HB3	1:A:379:ASP:OD1	2.01	0.61
1:A:447:THR:HG22	1:A:695:SEP:HA	1.81	0.61
1:A:442:THR:HG22	1:A:523:PHE:HE1	1.68	0.59
1:A:438:HIS:HD2	1:A:440:PHE:H	1.49	0.59
1:A:678:ALA:HB1	1:A:683:ILE:HD11	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ALA:HB1	1:A:683:ILE:CD1	2.33	0.59
1:A:450:THR:HG22	1:A:451:LYS:N	2.18	0.59
1:B:549:GLU:OE2	1:B:621:ARG:NH2	2.32	0.59
1:A:429:LYS:HE3	1:A:694:PHE:O	2.03	0.58
1:B:375:LEU:O	1:B:376:LYS:HB2	2.04	0.57
1:A:438:HIS:CD2	1:A:440:PHE:H	2.24	0.56
1:B:453:ASN:HD21	1:B:678:ALA:HB2	1.72	0.54
1:A:660:ASP:OD1	1:A:662:SER:HB2	2.08	0.54
1:B:377:ILE:HB	1:B:448:PHE:HE1	1.73	0.52
1:B:375:LEU:O	1:B:376:LYS:CB	2.57	0.52
1:B:545:TYR:OH	4:B:2114:HOH:O	2.18	0.52
1:A:450:THR:CG2	1:A:451:LYS:N	2.74	0.51
1:A:632:PRO:O	1:A:635:ARG:HB2	2.11	0.50
1:A:501:VAL:HG23	1:A:530:MET:HG3	1.93	0.50
1:A:387:GLY:HA3	2:A:1701:LG8:HAQ	1.93	0.50
1:B:442:THR:HG23	1:B:458:MET:CE	2.42	0.50
1:B:594:ASP:O	1:B:616:ARG:NH2	2.45	0.49
1:A:625:ARG:NH2	4:A:2151:HOH:O	2.45	0.49
1:B:467:MET:HE1	3:B:1713:MPD:CM	2.44	0.48
1:A:525:MET:HE1	1:A:541:GLY:N	2.29	0.48
1:B:580:HIS:HD2	4:B:2143:HOH:O	1.97	0.47
1:A:438:HIS:HE1	1:A:643:GLU:OE2	1.98	0.46
1:B:413:LYS:HD3	1:B:686:MET:HE2	1.98	0.46
1:A:522:ASP:HB2	2:A:1701:LG8:HBB1	1.97	0.46
1:A:692:ARG:HA	1:A:692:ARG:HD3	1.44	0.45
1:A:425:THR:HG21	1:A:454:LEU:HD13	1.98	0.45
1:B:615:VAL:O	1:B:621:ARG:HD3	2.15	0.45
1:B:513:ASP:HB3	1:B:515:ASP:H	1.82	0.44
1:A:672:LYS:HA	1:A:673:PRO:HD3	1.76	0.44
1:A:678:ALA:CB	1:A:683:ILE:CD1	2.95	0.44
1:A:533:ASP:OD2	1:A:533:ASP:N	2.46	0.44
1:B:527:LYS:HG2	1:B:536:THR:HG21	2.00	0.43
1:A:388:LYS:HG3	1:A:393:LYS:HG2	2.00	0.43
1:A:427:VAL:HG13	1:A:528:GLU:HG3	2.01	0.42
1:B:525:MET:HE1	1:B:541:GLY:HA2	2.01	0.42
1:A:460:TYR:CZ	1:A:462:ASN:HB3	2.55	0.42
1:B:677:PHE:HB3	1:B:678:ALA:H	1.57	0.42
1:B:542:THR:HA	1:B:543:PRO:HD3	1.93	0.41
1:B:439:PRO:HB2	1:B:645:LYS:HE3	2.01	0.41
1:B:375:LEU:HD12	1:B:376:LYS:HG3	2.03	0.41
1:B:377:ILE:HB	1:B:448:PHE:CE1	2.54	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:O	1:A:433:SER:HB2	2.19	0.41
1:B:625:ARG:HG2	1:B:626:GLY:N	2.35	0.41
1:B:438:HIS:HE1	1:B:643:GLU:OE2	2.04	0.40
1:B:467:MET:CE	3:B:1713:MPD:HM3	2.50	0.40
1:A:467:MET:O	1:A:471:GLN:HG2	2.21	0.40
1:B:447:THR:HB	1:B:694:PHE:CE2	2.57	0.40
1:A:450:THR:CG2	1:A:451:LYS:H	2.34	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	322/352 (92%)	308 (96%)	13 (4%)	1 (0%)	46	56
1	B	316/352 (90%)	296 (94%)	16 (5%)	4 (1%)	15	14
All	All	638/704 (91%)	604 (95%)	29 (4%)	5 (1%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	LYS
1	B	376	LYS
1	B	678	ALA
1	B	513	ASP
1	B	675	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	293/319 (92%)	277 (94%)	16 (6%)	27	36
1	B	289/319 (91%)	280 (97%)	9 (3%)	47	63
All	All	582/638 (91%)	557 (96%)	25 (4%)	35	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	LEU
1	A	379	ASP
1	A	434	LEU
1	A	447	THR
1	A	472	SER
1	A	508	ASP
1	A	511	LEU
1	A	518	ILE
1	A	531	LEU
1	A	533	ASP
1	A	535	LYS
1	A	536	THR
1	A	569	LEU
1	A	622	LEU
1	A	625	ARG
1	A	662	SER
1	B	434	LEU
1	B	442	THR
1	B	508	ASP
1	B	540	CYS
1	B	569	LEU
1	B	622	LEU
1	B	680	ARG
1	B	690	MET
1	B	697	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	A	558	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	403	ASN
1	B	438	HIS
1	B	453	ASN
1	B	517	HIS
1	B	558	HIS
1	B	580	HIS
1	B	684	ASN
1	B	710	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
1	SEP	A	676	1	8,9,10	1.61	1 (12%)	8,12,14	2.91	1 (12%)
1	SEP	A	695	1	8,9,10	1.80	3 (37%)	8,12,14	1.03	0
1	SEP	B	676	1	8,9,10	1.57	2 (25%)	8,12,14	1.93	2 (25%)
1	SEP	B	695	1	8,9,10	1.64	2 (25%)	8,12,14	1.62	1 (12%)

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
1	SEP	A	676	1	-	0/6/8/10	0/0/0/0
1	SEP	A	695	1	-	0/6/8/10	0/0/0/0
1	SEP	B	676	1	-	0/6/8/10	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	695	1	-	0/6/8/10	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	676	SEP	P-O3P	2.01	1.61	1.54
1	B	695	SEP	P-O2P	2.08	1.62	1.54
1	A	695	SEP	P-O2P	2.16	1.62	1.54
1	A	695	SEP	P-O3P	2.67	1.64	1.54
1	B	676	SEP	P-O1P	3.17	1.61	1.51
1	A	676	SEP	P-O1P	3.28	1.61	1.51
1	A	695	SEP	P-O1P	3.45	1.62	1.51
1	B	695	SEP	P-O1P	3.46	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	SEP	O2P-P-OG	-2.30	99.95	106.56
1	B	676	SEP	O-C-CA	-2.06	120.13	125.49
1	B	676	SEP	OG-CB-CA	4.70	112.28	108.27
1	A	676	SEP	OG-CB-CA	7.53	114.70	108.27

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
1	A	695	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	LG8	A	1701	-	37,39,39	1.79	9 (24%)	39,59,59	1.92	10 (25%)
2	LG8	B	1712	-	37,39,39	1.73	8 (21%)	39,59,59	1.63	7 (17%)
3	MPD	B	1713	-	6,7,7	0.34	0	7,10,10	0.57	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	LG8	A	1701	-	-	0/12/65/65	0/6/6/6
2	LG8	B	1712	-	-	0/12/65/65	0/6/6/6
3	MPD	B	1713	-	-	0/5/5/5	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	LG8	CAU-NAT	-5.51	1.31	1.38
2	B	1712	LG8	CAU-NAT	-4.95	1.32	1.38
2	B	1712	LG8	CAX-NAW	-3.21	1.34	1.40
2	A	1701	LG8	CAX-NAW	-2.83	1.35	1.40
2	A	1701	LG8	CAS-NAT	-2.74	1.36	1.39
2	B	1712	LG8	CAG-CAH	-2.51	1.36	1.45
2	A	1701	LG8	CAG-CAH	-2.41	1.36	1.45
2	A	1701	LG8	C6-CBF	2.18	1.56	1.53
2	A	1701	LG8	CAN-CAM	2.24	1.51	1.46
2	B	1712	LG8	CAN-CAM	2.39	1.51	1.46
2	B	1712	LG8	C6-CBF	2.73	1.57	1.53
2	A	1701	LG8	CAM-CAH	2.83	1.49	1.36
2	B	1712	LG8	CAM-CAH	2.95	1.49	1.36
2	B	1712	LG8	CAK-CAL	2.98	1.51	1.45
2	A	1701	LG8	CAK-CAL	2.99	1.51	1.45
2	B	1712	LG8	CAL-CAG	3.26	1.48	1.39
2	A	1701	LG8	CAL-CAG	3.32	1.48	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	LG8	CAS-CAK-CAL	-5.05	102.45	107.00
2	B	1712	LG8	CAS-CAK-CAL	-4.78	102.69	107.00
2	A	1701	LG8	CAX-CAN-CAM	-4.61	103.58	107.53
2	B	1712	LG8	CAX-CAN-CAM	-4.25	103.89	107.53
2	A	1701	LG8	CAC-NAD-CAE	-3.59	107.70	111.29
2	A	1701	LG8	CBA-NAT-CAS	-3.50	123.19	125.78
2	B	1712	LG8	CAC-NAD-CAE	-3.40	107.89	111.29
2	A	1701	LG8	CAR-CAS-NAT	-2.37	128.44	131.45
2	A	1701	LG8	CAN-CAM-CAH	-2.28	122.22	128.80
2	B	1712	LG8	CAN-CAM-CAH	-2.11	122.70	128.80
2	A	1701	LG8	CAK-CAS-NAT	2.03	109.97	108.09
2	A	1701	LG8	CAH-CAE-NAD	2.10	110.02	106.16
2	B	1712	LG8	CAK-CAS-NAT	2.19	110.12	108.09
2	B	1712	LG8	CAH-CAE-NAD	2.31	110.41	106.16
2	B	1712	LG8	CAS-NAT-CAU	2.38	109.81	108.45
2	A	1701	LG8	CAG-CAC-NAD	2.40	110.57	106.16
2	A	1701	LG8	CAS-NAT-CAU	4.29	110.90	108.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	LG8	2	0
3	B	1713	MPD	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/352 (92%)	0.74	40 (12%) 5 9	26, 47, 59, 71	0
1	B	320/352 (90%)	0.87	47 (14%) 3 5	37, 47, 66, 92	0
All	All	644/704 (91%)	0.81	87 (13%) 4 7	26, 47, 62, 92	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	ALA	7.8
1	B	711	HIS	6.7
1	B	674	ARG	6.5
1	B	710	HIS	6.0
1	B	533	ASP	5.5
1	A	677	PHE	5.4
1	B	709	HIS	5.2
1	B	375	LEU	5.1
1	B	656	LYS	5.1
1	B	679	ASP	5.1
1	A	692	ARG	4.7
1	B	692	ARG	4.2
1	B	657	SER	4.0
1	A	693	ASN	3.9
1	B	685	SER	3.7
1	A	532	GLY	3.7
1	A	698	ASN	3.7
1	A	401	LYS	3.6
1	B	401	LYS	3.6
1	A	547	ALA	3.4
1	A	540	CYS	3.4
1	A	533	ASP	3.3
1	B	705	ILE	3.2
1	A	689	ASN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	483	PHE	3.1
1	B	378	GLU	3.0
1	A	699	PRO	3.0
1	A	511	LEU	2.9
1	A	560	VAL	2.9
1	A	563	TRP	2.9
1	B	400	LYS	2.8
1	A	375	LEU	2.8
1	A	484	TYR	2.8
1	B	579	PHE	2.7
1	B	689	ASN	2.7
1	A	520	ILE	2.7
1	B	686	MET	2.7
1	B	687	ASP	2.7
1	B	707	HIS	2.6
1	B	486	ALA	2.6
1	B	402	THR	2.6
1	A	680	ARG	2.6
1	B	399	PHE	2.6
1	B	403	ASN	2.6
1	B	404	GLN	2.6
1	B	655	VAL	2.6
1	A	512	LEU	2.5
1	B	702	GLU	2.5
1	A	579	PHE	2.5
1	A	688	GLN	2.5
1	B	560	VAL	2.5
1	B	567	VAL	2.5
1	A	591	ILE	2.4
1	A	574	ILE	2.4
1	B	617	GLU	2.4
1	A	488	ILE	2.4
1	B	706	SER	2.4
1	A	510	ILE	2.4
1	B	547	ALA	2.4
1	A	486	ALA	2.4
1	B	534	ALA	2.3
1	A	687	ASP	2.3
1	A	400	LYS	2.3
1	B	563	TRP	2.3
1	B	512	LEU	2.3
1	A	464	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	485	ALA	2.2
1	B	585	GLU	2.2
1	A	697	MET	2.2
1	B	518	ILE	2.2
1	A	466	LEU	2.2
1	A	531	LEU	2.2
1	A	674	ARG	2.2
1	A	700	GLY	2.2
1	A	403	ASN	2.2
1	B	548	PRO	2.2
1	A	436	TRP	2.1
1	A	550	ILE	2.1
1	A	523	PHE	2.1
1	B	614	PHE	2.1
1	A	402	THR	2.1
1	B	546	ILE	2.1
1	B	677	PHE	2.0
1	A	619	GLU	2.0
1	B	381	GLU	2.0
1	B	484	TYR	2.0
1	B	591	ILE	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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	676	10/11	0.92	0.14	-	55,57,64,64	0
1	SEP	B	695	10/11	0.87	0.15	-	43,44,49,51	0
1	SEP	A	695	10/11	0.87	0.13	-	50,55,57,57	0
1	SEP	B	676	10/11	0.69	0.44	-	86,87,87,87	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MPD	B	1713	8/8	0.85	0.29	3.89	59,61,62,65	0
2	LG8	A	1701	34/34	0.96	0.20	0.36	35,39,42,45	0
2	LG8	B	1712	34/34	0.96	0.15	-0.40	38,41,46,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.