



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 01:56 AM EST

PDB ID : 4J1R  
Title : Crystal Structure of GSK3b in complex with inhibitor 15R  
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Deposited on : unknown  
Resolution : 2.70 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.

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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

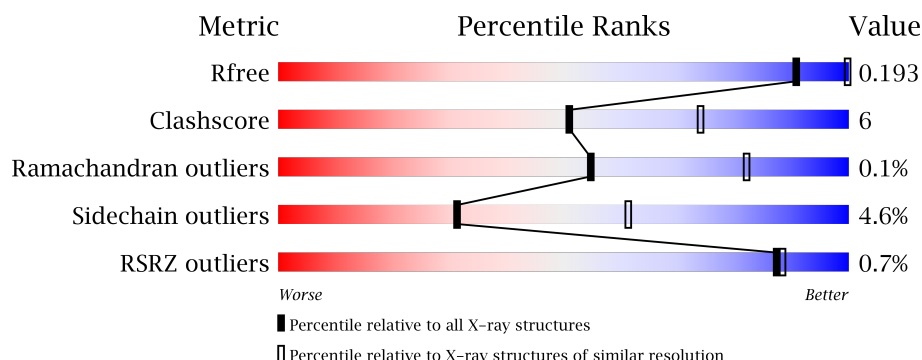
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	424	
1	B	424	
1	C	424	
1	D	424	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	I5R	B	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11248 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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	P	S	0	0	0
			2753	1770	469	502	1	11			
1	B	347	Total	C	N	O	P	S	0	0	0
			2770	1780	475	503	1	11			
1	C	345	Total	C	N	O	P	S	0	0	0
			2754	1770	472	500	1	11			
1	D	346	Total	C	N	O	P	S	0	0	0
			2768	1780	474	502	1	11			

There are 16 discrepancies between the modelled and reference sequences:

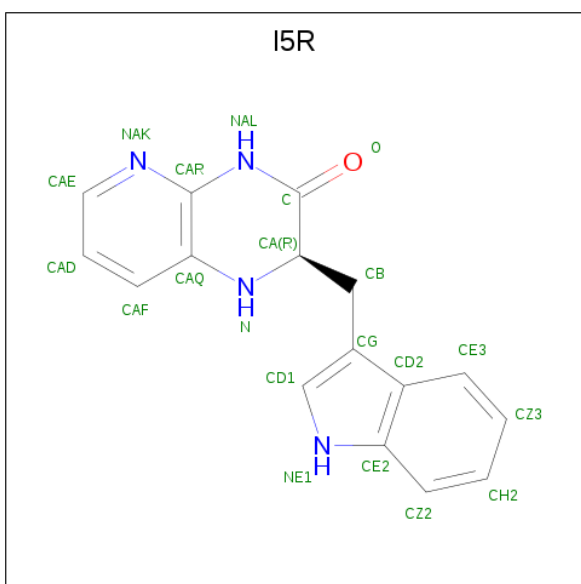
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P49841
A	-2	SER	-	EXPRESSION TAG	UNP P49841
A	-1	PRO	-	EXPRESSION TAG	UNP P49841
A	0	GLY	-	EXPRESSION TAG	UNP P49841
B	-3	GLY	-	EXPRESSION TAG	UNP P49841
B	-2	SER	-	EXPRESSION TAG	UNP P49841
B	-1	PRO	-	EXPRESSION TAG	UNP P49841
B	0	GLY	-	EXPRESSION TAG	UNP P49841
C	-3	GLY	-	EXPRESSION TAG	UNP P49841
C	-2	SER	-	EXPRESSION TAG	UNP P49841
C	-1	PRO	-	EXPRESSION TAG	UNP P49841
C	0	GLY	-	EXPRESSION TAG	UNP P49841
D	-3	GLY	-	EXPRESSION TAG	UNP P49841
D	-2	SER	-	EXPRESSION TAG	UNP P49841
D	-1	PRO	-	EXPRESSION TAG	UNP P49841
D	0	GLY	-	EXPRESSION TAG	UNP P49841

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is (2R)-2-(1H-indol-3-ylmethyl)-1,4-dihydropyrido[2,3-b]pyrazin-3(2H)-one (three-letter code: I5R) (formula: C<sub>16</sub>H<sub>14</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	16	4	1		
3	B	1	Total	C	N	O	0	0
			21	16	4	1		
3	C	1	Total	C	N	O	0	0
			21	16	4	1		
3	D	1	Total	C	N	O	0	0
			21	16	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	27	Total	O	0	0
			27	27		
5	C	23	Total	O	0	0
			23	23		
5	D	25	Total	O	0	0
			25	25		



- Molecule 1: Glycogen synthase kinase-3 beta







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.52Å 67.44Å 116.42Å 90.13° 90.08° 81.11°	Depositor
Resolution (Å)	46.96 – 2.70 46.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.96-2.70) 96.8 (46.96-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.173 , 0.193 0.173 , 0.193	Depositor DCC
$R_{free}$ test set	2754 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.440 for -h,-k,l 0.438 for k,h,-l 0.428 for -k,-h,-l	Xtriage
Reported twinning fraction	0.469 for k,h,-l	Depositor
Outliers	0 of 54014 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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, 0.333 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: K, I5R, PO4, PTR

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	0.54	1/2805 (0.0%)	0.59	0/3818
1	B	0.57	2/2821 (0.1%)	0.61	2/3837 (0.1%)
1	C	0.52	0/2805	0.58	1/3817 (0.0%)
1	D	0.55	0/2820	0.61	0/3838
All	All	0.55	3/11251 (0.0%)	0.60	3/15310 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	THR	CB-CG2	-5.99	1.32	1.52
1	B	218	CYS	CB-SG	-5.24	1.73	1.81
1	B	43	THR	CB-OG1	-5.23	1.32	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	180	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	180	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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	2753	0	2757	36	0
1	B	2770	0	2784	41	0
1	C	2754	0	2767	36	0
1	D	2768	0	2777	33	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	21	0	14	0	0
3	B	21	0	14	0	0
3	C	21	0	14	1	0
3	D	21	0	14	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	20	0	0	0	0
5	B	27	0	0	1	0
5	C	23	0	0	4	0
5	D	25	0	0	2	0
All	All	11248	0	11141	144	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 (144) 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:C:297:LYS:HD2	1:C:298:ALA:N	1.46	1.27
1:C:260:ASP:OD2	1:D:144:ARG:NH1	1.84	1.09
1:C:297:LYS:CD	1:C:298:ALA:H	1.64	1.09
1:B:141:ARG:HH21	1:B:141:ARG:HG2	1.16	1.06
1:C:297:LYS:HD2	1:C:298:ALA:H	0.85	0.99
1:C:297:LYS:CD	1:C:298:ALA:N	2.30	0.88
1:B:141:ARG:NH2	1:B:141:ARG:HG2	1.92	0.84
1:D:300:PRO:HB2	1:D:303:LYS:HG2	1.63	0.81
1:A:229:PHE:HB3	1:A:286:PRO:HB3	1.61	0.80
1:A:300:PRO:HB2	1:A:303:LYS:HG2	1.64	0.80
1:B:300:PRO:HB2	1:B:303:LYS:HG2	1.64	0.80
1:C:300:PRO:HB2	1:C:303:LYS:HG2	1.65	0.78
1:D:229:PHE:HB3	1:D:286:PRO:HB3	1.64	0.78
1:B:141:ARG:CG	1:B:141:ARG:HH21	1.96	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:HB2	1:B:284:MET:HE2	1.68	0.75
1:A:290:GLU:HG2	1:A:291:PHE:H	1.50	0.75
3:D:502:I5R:H14	5:D:622:HOH:O	1.88	0.72
1:C:229:PHE:HB3	1:C:286:PRO:HB3	1.72	0.72
1:B:225:PRO:HB2	1:B:284:MET:CE	2.19	0.71
1:D:180:ARG:HD3	1:D:203:SER:O	1.94	0.68
1:D:306:ARG:HB2	1:D:307:PRO:HD2	1.76	0.68
1:D:200:ASP:HA	5:D:622:HOH:O	1.94	0.67
3:C:502:I5R:H14	5:C:620:HOH:O	1.95	0.66
1:D:293:PHE:N	1:D:293:PHE:CD2	2.58	0.66
1:C:39:THR:HG23	1:C:55:SER:OG	1.96	0.65
1:B:285:ASN:N	1:B:286:PRO:CD	2.57	0.65
1:B:285:ASN:O	1:B:286:PRO:C	2.32	0.65
1:A:290:GLU:HG2	1:A:291:PHE:N	2.12	0.65
1:A:39:THR:HG23	1:A:55:SER:OG	1.97	0.64
1:A:88:LEU:HD11	1:A:125:GLU:HB3	1.80	0.62
1:A:100:ILE:HG23	1:A:177:ILE:HD13	1.80	0.62
1:D:180:ARG:NH2	2:D:501:PO4:O4	2.33	0.61
1:B:306:ARG:HB3	1:B:307:PRO:HD2	1.83	0.61
1:C:100:ILE:HG23	1:C:177:ILE:HD13	1.82	0.60
1:B:141:ARG:CG	1:B:141:ARG:NH2	2.58	0.60
1:B:285:ASN:N	1:B:286:PRO:HD2	2.15	0.60
1:D:100:ILE:HG23	1:D:177:ILE:HD13	1.82	0.59
1:B:100:ILE:HG23	1:B:177:ILE:HD13	1.83	0.58
1:B:325:PRO:O	1:B:328:ARG:HG3	2.04	0.58
1:B:180:ARG:NH2	2:B:501:PO4:O4	2.36	0.58
1:C:288:TYR:OH	1:D:64:ASN:OD1	2.20	0.58
1:C:292:LYS:CB	1:D:60:LYS:HD2	2.34	0.57
1:D:190:ASP:OD2	1:D:193:THR:OG1	2.22	0.57
1:A:193:THR:HB	1:A:195:VAL:HG23	1.88	0.56
1:B:106:HIS:NE2	1:B:366:GLU:OE2	2.37	0.55
1:A:324:THR:HG22	1:A:327:ALA:CB	2.37	0.55
1:C:275:THR:HG21	1:C:295:GLN:HA	1.90	0.54
1:C:275:THR:OG1	1:C:295:GLN:HG3	2.08	0.54
1:C:357:PRO:O	1:C:359:LEU:HG	2.08	0.54
1:D:106:HIS:NE2	1:D:366:GLU:OE2	2.37	0.53
1:D:357:PRO:O	1:D:359:LEU:HG	2.08	0.53
1:A:293:PHE:CD2	1:A:293:PHE:N	2.75	0.53
1:B:98:LEU:O	1:B:102:ARG:HG3	2.08	0.53
1:D:98:LEU:O	1:D:102:ARG:HG3	2.09	0.53
1:D:107:CYS:O	1:D:197:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PRO:O	1:B:359:LEU:HG	2.08	0.52
1:D:293:PHE:HD2	1:D:293:PHE:N	2.08	0.52
1:D:280:GLN:O	1:D:284:MET:HG3	2.11	0.51
1:A:357:PRO:O	1:A:359:LEU:HG	2.10	0.51
1:B:88:LEU:HD11	1:B:125:GLU:HB3	1.91	0.51
1:C:98:LEU:O	1:C:102:ARG:HG3	2.11	0.51
1:A:205:LYS:NZ	2:A:501:PO4:O1	2.38	0.51
1:B:138:THR:HG22	1:B:188:LEU:HD23	1.93	0.50
1:C:106:HIS:NE2	1:C:366:GLU:OE2	2.40	0.50
1:A:98:LEU:O	1:A:102:ARG:HG3	2.11	0.50
1:D:144:ARG:O	1:D:148:ARG:HG3	2.12	0.50
1:C:280:GLN:O	1:C:284:MET:HG3	2.11	0.50
1:B:285:ASN:O	1:B:286:PRO:O	2.30	0.49
1:B:265:GLN:NE2	5:B:619:HOH:O	2.40	0.49
1:B:233:ASP:O	1:B:233:ASP:OD1	2.31	0.49
1:C:138:THR:HG22	1:C:188:LEU:HD23	1.95	0.49
1:C:325:PRO:O	1:C:328:ARG:HG3	2.13	0.49
1:B:180:ARG:HD3	1:B:203:SER:O	2.13	0.48
1:A:106:HIS:NE2	1:A:366:GLU:OE2	2.40	0.48
1:A:280:GLN:O	1:A:284:MET:HG3	2.13	0.48
1:B:107:CYS:O	1:B:197:LYS:NZ	2.39	0.48
1:D:138:THR:HG22	1:D:188:LEU:HD23	1.95	0.48
1:A:308:ARG:O	1:A:309:THR:C	2.52	0.47
1:D:95:ASN:O	1:D:99:GLN:HG2	2.14	0.47
1:A:95:ASN:O	1:A:99:GLN:HG2	2.13	0.47
1:B:95:ASN:O	1:B:99:GLN:HG2	2.14	0.47
1:A:138:THR:HG22	1:A:188:LEU:HD23	1.97	0.47
1:B:190:ASP:OD2	1:B:193:THR:OG1	2.23	0.47
1:A:324:THR:HG22	1:A:327:ALA:HB2	1.95	0.47
1:C:190:ASP:OD2	1:C:193:THR:OG1	2.24	0.47
1:C:95:ASN:O	1:C:99:GLN:HG2	2.15	0.47
1:A:324:THR:CG2	1:A:327:ALA:HB2	2.44	0.47
1:D:289:THR:HG23	1:D:290:GLU:N	2.31	0.46
1:B:89:GLN:NE2	1:B:93:PHE:O	2.48	0.46
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.77	0.46
1:C:239:ASP:OD1	5:C:619:HOH:O	2.21	0.46
1:A:291:PHE:CD2	1:A:291:PHE:N	2.83	0.46
1:B:180:ARG:NH2	1:B:214:VAL:HG12	2.32	0.45
1:C:107:CYS:O	1:C:197:LYS:NZ	2.38	0.45
1:C:180:ARG:NH1	5:C:615:HOH:O	2.49	0.45
1:A:124:ASP:O	1:A:125:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLN:NE2	1:C:93:PHE:O	2.50	0.45
1:D:306:ARG:CB	1:D:307:PRO:HD2	2.44	0.44
1:B:121:GLU:OE2	1:B:121:GLU:N	2.38	0.44
1:C:233:ASP:OD1	1:C:233:ASP:O	2.36	0.44
1:B:157:TYR:CZ	1:B:351:PRO:HG2	2.53	0.44
1:B:225:PRO:HB2	1:B:284:MET:HE1	1.97	0.44
1:C:180:ARG:HD3	1:C:203:SER:O	2.17	0.44
1:A:124:ASP:C	1:A:125:GLU:HG3	2.38	0.44
1:B:65:GLY:HA3	1:B:67:PHE:CE2	2.53	0.44
1:C:297:LYS:HA	1:C:297:LYS:HD3	1.64	0.44
1:C:310:PRO:HA	1:C:311:PRO:HD3	1.77	0.43
1:C:261:SER:H	1:C:264:ASP:HB3	1.83	0.43
1:C:157:TYR:CZ	1:C:351:PRO:HG2	2.54	0.43
1:A:324:THR:HG22	1:A:327:ALA:HB3	2.00	0.43
1:D:65:GLY:HA3	1:D:67:PHE:CE2	2.52	0.43
1:A:308:ARG:HA	1:A:308:ARG:HD2	1.63	0.43
1:B:193:THR:HB	1:B:195:VAL:HG23	2.01	0.43
1:B:229:PHE:HB3	1:B:286:PRO:HA	1.99	0.43
1:D:233:ASP:OD1	1:D:233:ASP:O	2.37	0.43
1:B:137:GLU:OE2	1:B:141:ARG:HD3	2.18	0.42
1:A:144:ARG:O	1:A:148:ARG:HG3	2.19	0.42
1:C:180:ARG:NH2	2:C:501:PO4:O1	2.50	0.42
1:C:180:ARG:NH2	1:C:214:VAL:HG12	2.34	0.42
1:A:233:ASP:OD1	1:A:233:ASP:O	2.38	0.42
1:D:141:ARG:HG2	1:D:141:ARG:HH21	1.84	0.42
1:B:91:LYS:O	1:B:92:ARG:C	2.57	0.42
1:D:157:TYR:CZ	1:D:351:PRO:HG2	2.55	0.42
1:D:70:VAL:HG11	3:D:502:I5R:CE3	2.49	0.42
1:D:289:THR:CG2	1:D:290:GLU:N	2.83	0.42
1:A:157:TYR:CZ	1:A:351:PRO:HG2	2.55	0.42
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.89	0.42
1:A:78:SER:HB2	1:A:80:GLU:HG3	2.01	0.41
1:D:63:GLY:HA3	1:D:70:VAL:HB	2.02	0.41
1:B:306:ARG:CB	1:B:307:PRO:HD2	2.49	0.41
1:A:89:GLN:NE2	1:A:93:PHE:O	2.49	0.41
1:C:78:SER:HB2	1:C:80:GLU:HG3	2.02	0.41
1:D:297:LYS:HD2	1:D:297:LYS:HA	1.89	0.41
1:B:144:ARG:O	1:B:148:ARG:HG3	2.20	0.41
1:C:116:PHE:HB2	5:C:621:HOH:O	2.21	0.41
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.89	0.41
1:A:155:VAL:HG12	1:A:159:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:HIS:CE1	1:A:236:SER:HB2	2.55	0.41
1:C:173:HIS:CE1	1:C:236:SER:HB2	2.56	0.41
1:A:61:VAL:HB	1:B:291:PHE:CD1	2.56	0.41
1:D:193:THR:HB	1:D:195:VAL:HG23	2.03	0.40
1:B:182:ILE:HB	1:B:242:SER:CB	2.52	0.40
1:A:228:ILE:HG21	1:A:266:LEU:HB2	2.03	0.40
1:A:246:VAL:O	1:A:250:LEU:HG	2.22	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	339/424 (80%)	325 (96%)	14 (4%)	0	100	100
1	B	342/424 (81%)	328 (96%)	13 (4%)	1 (0%)	44	73
1	C	340/424 (80%)	327 (96%)	13 (4%)	0	100	100
1	D	341/424 (80%)	327 (96%)	14 (4%)	0	100	100
All	All	1362/1696 (80%)	1307 (96%)	54 (4%)	1 (0%)	55	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	ASN

### 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	304/365 (83%)	288 (95%)	16 (5%)	26	54
1	B	305/365 (84%)	292 (96%)	13 (4%)	33	64
1	C	303/365 (83%)	289 (95%)	14 (5%)	31	61
1	D	305/365 (84%)	292 (96%)	13 (4%)	33	64
All	All	1217/1460 (83%)	1161 (95%)	56 (5%)	31	61

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	144	ARG
1	A	147	SER
1	A	152	THR
1	A	169	LEU
1	A	193	THR
1	A	233	ASP
1	A	288	TYR
1	A	289	THR
1	A	291	PHE
1	A	299	HIS
1	A	302	THR
1	A	306	ARG
1	A	308	ARG
1	A	324	THR
1	A	329	LEU
1	B	39	THR
1	B	90	ASP
1	B	118	SER
1	B	141	ARG
1	B	144	ARG
1	B	152	THR
1	B	169	LEU
1	B	233	ASP
1	B	275	THR
1	B	299	HIS
1	B	302	THR
1	B	328	ARG
1	B	369	SER
1	C	39	THR

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Mol	Chain	Res	Type
1	C	90	ASP
1	C	141	ARG
1	C	144	ARG
1	C	152	THR
1	C	169	LEU
1	C	233	ASP
1	C	288	TYR
1	C	289	THR
1	C	290	GLU
1	C	297	LYS
1	C	299	HIS
1	C	302	THR
1	C	328	ARG
1	D	39	THR
1	D	90	ASP
1	D	152	THR
1	D	169	LEU
1	D	180	ARG
1	D	219	SER
1	D	233	ASP
1	D	288	TYR
1	D	290	GLU
1	D	299	HIS
1	D	302	THR
1	D	306	ARG
1	D	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	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](#)

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	PTR	A	216	1	15,16,17	1.18	1 (6%)	19,22,24	1.19	2 (10%)
1	PTR	B	216	1	15,16,17	1.12	0	19,22,24	1.03	1 (5%)
1	PTR	C	216	1	15,16,17	1.05	2 (13%)	19,22,24	0.80	0
1	PTR	D	216	1	15,16,17	1.06	1 (6%)	19,22,24	0.91	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
1	PTR	A	216	1	-	0/9/11/13	0/1/1/1
1	PTR	B	216	1	-	0/9/11/13	0/1/1/1
1	PTR	C	216	1	-	0/9/11/13	0/1/1/1
1	PTR	D	216	1	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	PTR	OH-CZ	-2.86	1.34	1.40
1	D	216	PTR	OH-CZ	-2.85	1.34	1.40
1	C	216	PTR	CA-C	2.11	1.53	1.50
1	A	216	PTR	CA-C	2.20	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PTR	CB-CA-C	-2.33	106.92	111.41
1	B	216	PTR	CE2-CZ-CE1	2.23	123.69	120.19
1	A	216	PTR	CE2-CZ-CE1	2.26	123.74	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
2	PO4	A	501	-	4,4,4	0.95	0	6,6,6	0.25	0
3	I5R	A	502	-	23,24,24	3.20	7 (30%)	27,34,34	3.80	12 (44%)
2	PO4	B	501	-	4,4,4	0.78	0	6,6,6	0.46	0
3	I5R	B	502	-	23,24,24	3.21	9 (39%)	27,34,34	3.94	13 (48%)
2	PO4	C	501	-	4,4,4	0.70	0	6,6,6	0.83	0
3	I5R	C	502	-	23,24,24	3.59	12 (52%)	27,34,34	4.22	15 (55%)
2	PO4	D	501	-	4,4,4	0.63	0	6,6,6	0.63	0
3	I5R	D	502	-	23,24,24	3.21	9 (39%)	27,34,34	3.90	13 (48%)

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	PO4	A	501	-	-	0/0/0/0	0/0/0/0
3	I5R	A	502	-	-	0/3/16/16	0/4/4/4
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
3	I5R	B	502	-	-	0/3/16/16	0/4/4/4
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
3	I5R	C	502	-	-	0/3/16/16	0/4/4/4
2	PO4	D	501	-	-	0/0/0/0	0/0/0/0
3	I5R	D	502	-	-	0/3/16/16	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	I5R	CAR-NAK	-7.94	1.22	1.35
3	A	502	I5R	CAR-NAK	-7.15	1.23	1.35
3	B	502	I5R	CAR-NAK	-6.62	1.24	1.35
3	D	502	I5R	CAR-NAK	-6.46	1.24	1.35
3	C	502	I5R	CA-C	-5.51	1.39	1.52
3	B	502	I5R	CA-C	-4.35	1.42	1.52
3	D	502	I5R	CA-C	-4.28	1.42	1.52
3	A	502	I5R	CZ2-CE2	-4.18	1.34	1.41
3	D	502	I5R	CZ2-CE2	-4.03	1.34	1.41
3	B	502	I5R	CZ2-CE2	-3.98	1.34	1.41
3	A	502	I5R	CA-C	-3.95	1.42	1.52
3	C	502	I5R	CZ2-CE2	-3.74	1.35	1.41
3	C	502	I5R	C-NAL	-3.61	1.30	1.35
3	B	502	I5R	CE3-CD2	-3.09	1.35	1.42
3	D	502	I5R	CE3-CD2	-2.92	1.36	1.42
3	A	502	I5R	CE3-CD2	-2.74	1.36	1.42
3	C	502	I5R	CD2-CE2	-2.72	1.35	1.42
3	C	502	I5R	CE3-CD2	-2.70	1.36	1.42
3	A	502	I5R	CD2-CE2	-2.52	1.35	1.42
3	C	502	I5R	CAQ-N	-2.38	1.34	1.39
3	D	502	I5R	CD2-CE2	-2.31	1.36	1.42
3	B	502	I5R	CD2-CE2	-2.27	1.36	1.42
3	B	502	I5R	CAR-NAL	2.39	1.41	1.38
3	D	502	I5R	CAR-NAL	2.73	1.41	1.38
3	C	502	I5R	CA-N	3.17	1.51	1.46
3	D	502	I5R	CAE-NAK	3.39	1.41	1.34
3	B	502	I5R	O-C	3.57	1.30	1.23
3	A	502	I5R	CAE-NAK	3.64	1.42	1.34
3	B	502	I5R	CAE-NAK	3.90	1.43	1.34
3	D	502	I5R	O-C	3.91	1.31	1.23
3	C	502	I5R	CAR-NAL	3.99	1.43	1.38
3	C	502	I5R	CAE-NAK	4.09	1.43	1.34
3	C	502	I5R	O-C	5.51	1.34	1.23
3	C	502	I5R	CAQ-CAR	7.83	1.49	1.41
3	B	502	I5R	CAQ-CAR	9.34	1.51	1.41
3	D	502	I5R	CAQ-CAR	9.34	1.51	1.41
3	A	502	I5R	CAQ-CAR	9.96	1.52	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	I5R	CB-CA-N	-10.73	98.24	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	I5R	CB-CA-N	-10.50	98.52	111.17
3	B	502	I5R	CB-CA-N	-10.47	98.56	111.17
3	C	502	I5R	CB-CA-N	-9.81	99.36	111.17
3	D	502	I5R	CB-CG-CD1	-8.09	117.98	127.97
3	C	502	I5R	CAQ-CAR-NAL	-7.83	111.71	118.11
3	B	502	I5R	CB-CG-CD1	-7.68	118.48	127.97
3	C	502	I5R	CB-CG-CD1	-7.41	118.82	127.97
3	A	502	I5R	CB-CG-CD1	-7.10	119.20	127.97
3	A	502	I5R	CAQ-CAR-NAL	-6.81	112.55	118.11
3	A	502	I5R	CB-CA-C	-5.56	103.22	111.19
3	D	502	I5R	CAQ-CAR-NAL	-5.54	113.58	118.11
3	B	502	I5R	O-C-NAL	-5.25	115.59	122.09
3	C	502	I5R	O-C-NAL	-5.20	115.65	122.09
3	B	502	I5R	CAQ-CAR-NAL	-4.85	114.14	118.11
3	D	502	I5R	O-C-NAL	-4.56	116.44	122.09
3	C	502	I5R	CB-CA-C	-4.24	105.11	111.19
3	A	502	I5R	O-C-NAL	-4.14	116.97	122.09
3	B	502	I5R	CB-CA-C	-4.00	105.45	111.19
3	C	502	I5R	CAF-CAQ-CAR	-3.91	114.11	117.95
3	D	502	I5R	CB-CA-C	-3.78	105.78	111.19
3	B	502	I5R	CAD-CAE-NAK	-3.77	117.18	123.43
3	C	502	I5R	O-C-CA	-3.66	112.50	119.09
3	A	502	I5R	CAF-CAQ-CAR	-3.38	114.62	117.95
3	B	502	I5R	CAF-CAQ-CAR	-3.36	114.65	117.95
3	A	502	I5R	CAD-CAE-NAK	-3.05	118.37	123.43
3	D	502	I5R	CAD-CAE-NAK	-2.95	118.53	123.43
3	D	502	I5R	CAF-CAQ-CAR	-2.84	115.16	117.95
3	C	502	I5R	CAD-CAE-NAK	-2.82	118.76	123.43
3	C	502	I5R	C-CA-N	-2.58	107.91	112.15
3	B	502	I5R	O-C-CA	-2.19	115.13	119.09
3	D	502	I5R	O-C-CA	-2.18	115.15	119.09
3	D	502	I5R	CAD-CAF-CAQ	2.01	122.83	118.61
3	A	502	I5R	CAD-CAF-CAQ	2.21	123.24	118.61
3	B	502	I5R	CAD-CAF-CAQ	2.33	123.50	118.61
3	A	502	I5R	CB-CG-CD2	2.56	130.23	126.25
3	C	502	I5R	CAE-NAK-CAR	2.56	122.06	116.74
3	C	502	I5R	CAR-CAQ-N	2.80	122.63	118.91
3	C	502	I5R	CAQ-CAR-NAK	2.84	123.16	118.18
3	D	502	I5R	CAE-NAK-CAR	3.16	123.30	116.74
3	A	502	I5R	CAE-NAK-CAR	3.27	123.52	116.74
3	C	502	I5R	CB-CG-CD2	3.34	131.44	126.25
3	A	502	I5R	CA-C-NAL	3.46	121.10	116.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	I5R	CB-CG-CD2	3.65	131.93	126.25
3	B	502	I5R	CAE-NAK-CAR	3.67	124.37	116.74
3	D	502	I5R	CB-CG-CD2	4.17	132.73	126.25
3	D	502	I5R	CA-C-NAL	6.51	125.27	116.36
3	B	502	I5R	NAL-CAR-NAK	6.98	124.79	116.89
3	C	502	I5R	NAL-CAR-NAK	7.00	124.81	116.89
3	D	502	I5R	NAL-CAR-NAK	7.24	125.08	116.89
3	B	502	I5R	CA-C-NAL	7.49	126.61	116.36
3	A	502	I5R	NAL-CAR-NAK	7.95	125.88	116.89
3	C	502	I5R	CA-C-NAL	9.07	128.77	116.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PO4	1	0
2	B	501	PO4	1	0
2	C	501	PO4	1	0
3	C	502	I5R	1	0
2	D	501	PO4	1	0
3	D	502	I5R	2	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	343/424 (80%)	0.00	1 (0%) 93 94	25, 59, 99, 128	0
1	B	346/424 (81%)	0.07	3 (0%) 84 85	26, 59, 101, 142	0
1	C	344/424 (81%)	0.02	3 (0%) 84 85	37, 59, 99, 132	0
1	D	345/424 (81%)	0.07	2 (0%) 89 90	38, 59, 100, 137	0
All	All	1378/1696 (81%)	0.04	9 (0%) 87 88	25, 59, 101, 142	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ILE	6.6
1	D	92	ARG	3.8
1	C	104	LEU	2.7
1	B	123	LYS	2.7
1	C	384	ILE	2.7
1	A	297	LYS	2.4
1	B	36	LYS	2.4
1	C	91	LYS	2.1
1	B	104	LEU	2.0

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

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	PTR	C	216	16/17	0.97	0.16	-	20,43,61,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PTR	D	216	16/17	0.99	0.15	-	21,44,58,60	0
1	PTR	A	216	16/17	0.97	0.16	-	33,48,56,73	0
1	PTR	B	216	16/17	0.98	0.14	-	41,53,67,70	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( $\text{\AA}^2$ )	Q<0.9
3	I5R	B	502	21/21	0.98	0.24	2.37	43,65,78,87	0
3	I5R	C	502	21/21	0.98	0.21	1.23	41,56,64,75	0
3	I5R	D	502	21/21	0.98	0.20	1.17	39,62,79,84	0
4	K	D	503	1/1	0.97	0.19	0.87	79,79,79,79	0
3	I5R	A	502	21/21	0.98	0.20	0.85	44,59,67,77	0
2	PO4	D	501	5/5	0.99	0.16	-0.40	41,46,55,85	0
2	PO4	B	501	5/5	0.99	0.14	-1.13	50,51,62,67	0
4	K	A	503	1/1	0.99	0.14	-1.38	68,68,68,68	0
2	PO4	A	501	5/5	0.99	0.15	-1.42	46,59,74,88	0
2	PO4	C	501	5/5	0.98	0.12	-2.55	39,52,71,88	0
4	K	B	503	1/1	0.98	0.10	-2.99	84,84,84,84	0
4	K	C	503	1/1	0.98	0.07	-4.17	77,77,77,77	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.