



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:00 PM GMT

PDB ID : 5B25  
Title : Crystal structure of human PDE1B with inhibitor 3  
Authors : Ida, K.; Lane, W.; Snell, G.; Sogabe, S.  
Deposited on : 2016-01-07  
Resolution : 1.90 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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-20026982

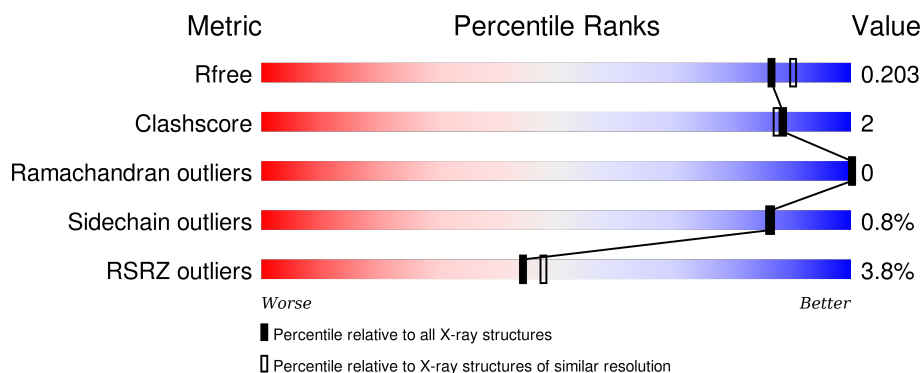
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	338	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	B	338	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>
1	C	338	<div> <div>5%</div> <div>91%</div> <div>7%</div> </div>
1	D	338	<div> <div>4%</div> <div>92%</div> <div>6%</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
5	SO4	C	604	-	-	-	X
5	SO4	D	604	-	-	-	X
6	GOL	A	606	-	-	-	X
6	GOL	A	607	-	-	-	X
6	GOL	B	606	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11932 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 Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2703	1726	460	500	17			
1	B	332	Total	C	N	O	S	0	5	0
			2686	1718	456	495	17			
1	C	332	Total	C	N	O	S	0	4	0
			2684	1715	456	496	17			
1	D	332	Total	C	N	O	S	0	5	0
			2690	1719	459	495	17			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q01064
A	?	-	GLU	deletion	UNP Q01064
A	?	-	ASP	deletion	UNP Q01064
A	?	-	SER	deletion	UNP Q01064
A	?	-	LYS	deletion	UNP Q01064
A	?	-	SER	deletion	UNP Q01064
A	?	-	LYS	deletion	UNP Q01064
A	?	-	ASN	deletion	UNP Q01064
A	?	-	GLN	deletion	UNP Q01064
A	?	-	PRO	deletion	UNP Q01064
A	?	-	SER	deletion	UNP Q01064
A	?	-	PHE	deletion	UNP Q01064
A	?	-	GLN	deletion	UNP Q01064
A	?	-	TRP	deletion	UNP Q01064
A	?	-	ARG	deletion	UNP Q01064
A	?	-	GLN	deletion	UNP Q01064
A	?	-	PRO	deletion	UNP Q01064
A	?	-	SER	deletion	UNP Q01064
A	?	-	LEU	deletion	UNP Q01064
A	?	-	ASP	deletion	UNP Q01064

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q01064
A	?	-	GLU	deletion	UNP Q01064
A	?	-	VAL	deletion	UNP Q01064
B	?	-	ASP	deletion	UNP Q01064
B	?	-	GLU	deletion	UNP Q01064
B	?	-	ASP	deletion	UNP Q01064
B	?	-	SER	deletion	UNP Q01064
B	?	-	LYS	deletion	UNP Q01064
B	?	-	SER	deletion	UNP Q01064
B	?	-	LYS	deletion	UNP Q01064
B	?	-	ASN	deletion	UNP Q01064
B	?	-	GLN	deletion	UNP Q01064
B	?	-	PRO	deletion	UNP Q01064
B	?	-	SER	deletion	UNP Q01064
B	?	-	PHE	deletion	UNP Q01064
B	?	-	GLN	deletion	UNP Q01064
B	?	-	TRP	deletion	UNP Q01064
B	?	-	ARG	deletion	UNP Q01064
B	?	-	GLN	deletion	UNP Q01064
B	?	-	PRO	deletion	UNP Q01064
B	?	-	SER	deletion	UNP Q01064
B	?	-	LEU	deletion	UNP Q01064
B	?	-	ASP	deletion	UNP Q01064
B	?	-	VAL	deletion	UNP Q01064
B	?	-	GLU	deletion	UNP Q01064
B	?	-	VAL	deletion	UNP Q01064
C	?	-	ASP	deletion	UNP Q01064
C	?	-	GLU	deletion	UNP Q01064
C	?	-	ASP	deletion	UNP Q01064
C	?	-	SER	deletion	UNP Q01064
C	?	-	LYS	deletion	UNP Q01064
C	?	-	SER	deletion	UNP Q01064
C	?	-	LYS	deletion	UNP Q01064
C	?	-	ASN	deletion	UNP Q01064
C	?	-	GLN	deletion	UNP Q01064
C	?	-	PRO	deletion	UNP Q01064
C	?	-	SER	deletion	UNP Q01064
C	?	-	PHE	deletion	UNP Q01064
C	?	-	GLN	deletion	UNP Q01064
C	?	-	TRP	deletion	UNP Q01064
C	?	-	ARG	deletion	UNP Q01064
C	?	-	GLN	deletion	UNP Q01064

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP Q01064
C	?	-	SER	deletion	UNP Q01064
C	?	-	LEU	deletion	UNP Q01064
C	?	-	ASP	deletion	UNP Q01064
C	?	-	VAL	deletion	UNP Q01064
C	?	-	GLU	deletion	UNP Q01064
C	?	-	VAL	deletion	UNP Q01064
D	?	-	ASP	deletion	UNP Q01064
D	?	-	GLU	deletion	UNP Q01064
D	?	-	ASP	deletion	UNP Q01064
D	?	-	SER	deletion	UNP Q01064
D	?	-	LYS	deletion	UNP Q01064
D	?	-	SER	deletion	UNP Q01064
D	?	-	LYS	deletion	UNP Q01064
D	?	-	ASN	deletion	UNP Q01064
D	?	-	GLN	deletion	UNP Q01064
D	?	-	PRO	deletion	UNP Q01064
D	?	-	SER	deletion	UNP Q01064
D	?	-	PHE	deletion	UNP Q01064
D	?	-	GLN	deletion	UNP Q01064
D	?	-	TRP	deletion	UNP Q01064
D	?	-	ARG	deletion	UNP Q01064
D	?	-	GLN	deletion	UNP Q01064
D	?	-	PRO	deletion	UNP Q01064
D	?	-	SER	deletion	UNP Q01064
D	?	-	LEU	deletion	UNP Q01064
D	?	-	ASP	deletion	UNP Q01064
D	?	-	VAL	deletion	UNP Q01064
D	?	-	GLU	deletion	UNP Q01064
D	?	-	VAL	deletion	UNP Q01064

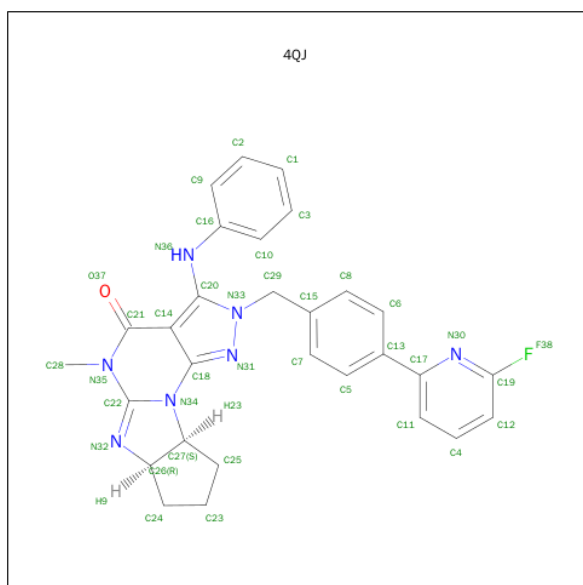
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

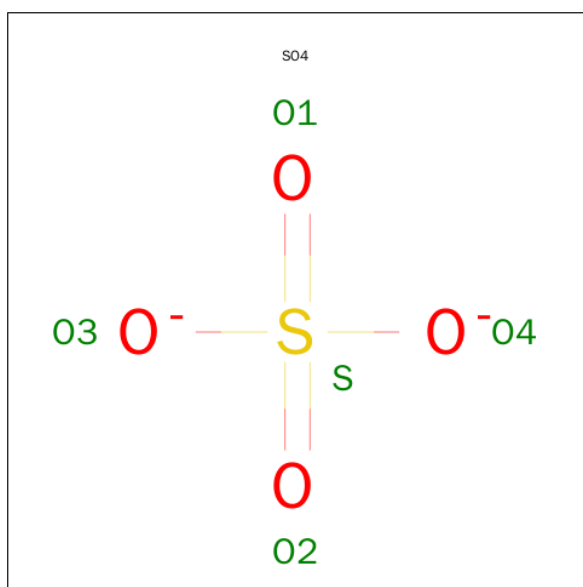
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

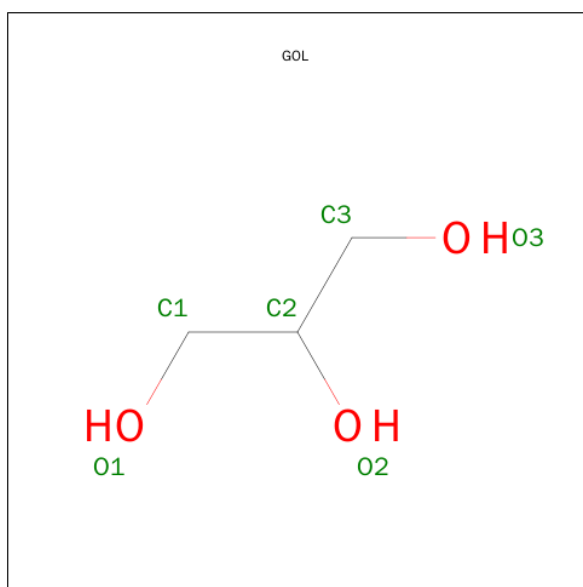
- Molecule 4 is (11R,15S)-4-{[4-(6-fluoropyridin-2-yl)phenyl]methyl}-8-methyl-5-(phenylamino)-1,3,4,8,10-pentazatetracyclo[7.6.0.02,6.011,15]pentadeca-2,5,9-trien-7-one (three-letter code: 4QJ) (formula: C<sub>29</sub>H<sub>26</sub>FN<sub>7</sub>O).





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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

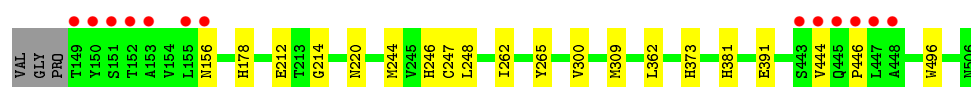
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	235	Total	O	0	0
			235	235		
7	B	213	Total	O	0	0
			213	213		
7	C	246	Total	O	0	0
			246	246		
7	D	217	Total	O	0	0
			217	217		

### 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 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: Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1B

Chain A: 



- Molecule 1: Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1B

Chain B: 



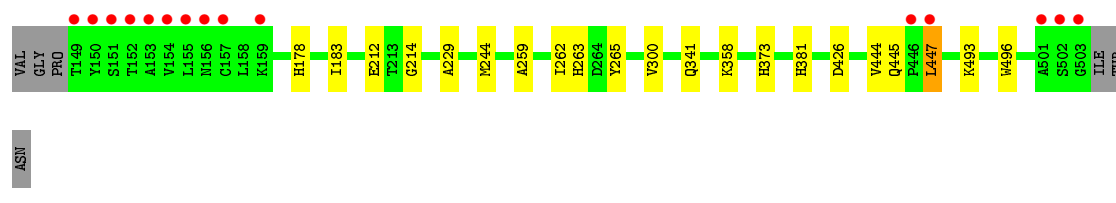
- Molecule 1: Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1B

Chain C: 



- Molecule 1: Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1B

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.88Å 102.88Å 294.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 46.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.90) 99.9 (46.01-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.172 , 0.203 0.172 , 0.203	Depositor DCC
$R_{free}$ test set	6291 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 125023 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.6155e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ZN, 4QJ, 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	0.52	0/2772	0.63	0/3759
1	B	0.53	0/2761	0.63	0/3745
1	C	0.53	0/2756	0.65	0/3738
1	D	0.53	0/2765	0.63	0/3749
All	All	0.53	0/11054	0.64	0/14991

There are no bond length outliers.

There are no bond angle outliers.

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	2703	0	2690	13	0
1	B	2686	0	2680	15	0
1	C	2684	0	2670	15	0
1	D	2690	0	2684	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	38	0	26	0	0
4	B	38	0	26	0	0
4	C	38	0	26	0	0
4	D	38	0	26	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	A	12	0	16	0	0
6	B	18	0	24	0	0
6	C	12	0	16	0	0
6	D	6	0	8	0	0
7	A	235	0	0	0	0
7	B	213	0	0	1	0
7	C	246	0	0	0	0
7	D	217	0	0	0	0
All	All	11932	0	10892	54	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 2.

All (54) 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:381:HIS:HE1	1:A:496:TRP:HE1	1.14	0.95
1:B:381:HIS:HE1	1:B:496:TRP:HE1	1.14	0.95
1:C:381:HIS:HE1	1:C:496:TRP:HE1	1.14	0.95
1:B:244:MET:HG2	1:B:444:VAL:HG21	1.56	0.86
1:B:381:HIS:CE1	1:B:496:TRP:HE1	1.94	0.85
1:D:381:HIS:HE1	1:D:496:TRP:HE1	1.25	0.83
1:A:381:HIS:CE1	1:A:496:TRP:HE1	1.96	0.81
1:C:381:HIS:CE1	1:C:496:TRP:HE1	1.99	0.78
1:A:244:MET:HG2	1:A:444:VAL:HG21	1.69	0.75
1:D:381:HIS:CE1	1:D:496:TRP:HE1	2.07	0.73
1:A:178:HIS:HD2	1:A:212:GLU:OE1	1.78	0.66
1:B:244:MET:HG2	1:B:444:VAL:CG2	2.26	0.65
1:C:244:MET:HG2	1:C:444:VAL:HG21	1.79	0.64
1:C:373:HIS:ND1	1:C:381:HIS:HD2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:HIS:HD2	1:B:212:GLU:OE1	1.81	0.63
1:B:244:MET:CG	1:B:444:VAL:HG21	2.29	0.61
1:C:244:MET:HG2	1:C:444:VAL:HG11	1.84	0.60
1:B:373:HIS:ND1	1:B:381:HIS:HD2	2.00	0.59
1:D:373:HIS:ND1	1:D:381:HIS:HD2	2.01	0.59
1:C:178:HIS:HD2	1:C:212:GLU:OE1	1.86	0.57
1:A:373:HIS:ND1	1:A:381:HIS:HD2	2.04	0.56
1:D:178:HIS:HD2	1:D:212:GLU:OE1	1.89	0.56
1:D:214:GLY:HA3	1:D:265:TYR:CE1	2.41	0.55
1:D:244:MET:HG2	1:D:444:VAL:CG2	2.37	0.55
1:C:214:GLY:HA3	1:C:265:TYR:CE1	2.43	0.54
1:D:244:MET:HG2	1:D:444:VAL:HG21	1.89	0.54
1:A:214:GLY:HA3	1:A:265:TYR:CE1	2.43	0.53
1:A:246:HIS:HB2	1:A:446:PRO:HB3	1.92	0.52
1:C:246:HIS:HB2	1:C:446:PRO:HB3	1.93	0.50
1:A:247:CYS:SG	1:A:444:VAL:HG13	2.52	0.50
1:B:256:ILE:HD13	1:B:365:LEU:HD23	1.93	0.49
1:C:186:GLU:OE2	1:C:190:ARG:HD2	2.13	0.49
1:B:214:GLY:HA3	1:B:265:TYR:CE1	2.48	0.48
1:D:244:MET:CG	1:D:444:VAL:HG21	2.44	0.48
1:C:408:PRO:HG2	1:D:447:LEU:HD11	1.96	0.48
1:C:183:ILE:HD12	1:C:229:ALA:HB1	1.98	0.45
1:A:220:ASN:HB3	1:A:391:GLU:OE1	2.17	0.44
1:B:247:CYS:SG	1:B:444:VAL:HG13	2.57	0.44
1:B:435[A]:VAL:HG23	7:B:802:HOH:O	2.17	0.44
1:D:183:ILE:HD12	1:D:229:ALA:HB1	1.99	0.44
1:B:445:GLN:HB3	1:B:472:GLY:H	1.82	0.44
1:A:248:LEU:HD21	1:A:362:LEU:HD21	2.01	0.43
1:B:183:ILE:HD12	1:B:229:ALA:HB1	2.01	0.43
1:A:156:ASN:HB3	1:C:156:ASN:OD1	2.19	0.43
1:B:256:ILE:CD1	1:B:365:LEU:HD23	2.50	0.42
1:C:358:LYS:HB3	1:C:359:PRO:HD3	2.00	0.42
1:A:262:ILE:HB	1:A:300:VAL:HG21	2.00	0.42
1:C:396:GLY:HA3	1:C:410:CYS:O	2.21	0.41
1:A:244:MET:HG2	1:A:444:VAL:CG2	2.45	0.41
1:D:262:ILE:HB	1:D:300:VAL:HG21	2.01	0.41
1:B:168:VAL:HG11	1:B:230:ASP:HB2	2.02	0.41
1:D:259:ALA:O	1:D:263:HIS:HB3	2.21	0.41
1:C:475:ASN:O	1:C:478:VAL:HG22	2.20	0.40
1:D:426:ASP:OD1	1:D:493:LYS:HD2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	336/338 (99%)	333 (99%)	3 (1%)	0	100	100
1	B	335/338 (99%)	332 (99%)	3 (1%)	0	100	100
1	C	334/338 (99%)	331 (99%)	3 (1%)	0	100	100
1	D	335/338 (99%)	330 (98%)	5 (2%)	0	100	100
All	All	1340/1352 (99%)	1326 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	304/303 (100%)	303 (100%)	1 (0%)	94	95
1	B	303/303 (100%)	302 (100%)	1 (0%)	94	95
1	C	302/303 (100%)	299 (99%)	3 (1%)	82	81
1	D	303/303 (100%)	299 (99%)	4 (1%)	76	73
All	All	1212/1212 (100%)	1203 (99%)	9 (1%)	86	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	MET
1	B	358	LYS

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Mol	Chain	Res	Type
1	C	308	GLU
1	C	365	LEU
1	C	444	VAL
1	D	341	GLN
1	D	358	LYS
1	D	445	GLN
1	D	447	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	178	HIS
1	A	381	HIS
1	A	490	GLN
1	B	178	HIS
1	B	381	HIS
1	B	490	GLN
1	C	178	HIS
1	C	381	HIS
1	C	490	GLN
1	D	178	HIS
1	D	381	HIS
1	D	445	GLN
1	D	490	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	4QJ	A	603	-	40,44,44	0.98	3 (7%)	34,65,65	1.12	3 (8%)
5	SO4	A	604	-	4,4,4	0.31	0	6,6,6	0.08	0
5	SO4	A	605	-	4,4,4	0.31	0	6,6,6	0.10	0
6	GOL	A	606	-	5,5,5	0.17	0	5,5,5	0.47	0
6	GOL	A	607	-	5,5,5	0.16	0	5,5,5	0.52	0
4	4QJ	B	603	-	40,44,44	0.96	3 (7%)	34,65,65	1.19	4 (11%)
5	SO4	B	604	-	4,4,4	0.35	0	6,6,6	0.15	0
5	SO4	B	605	-	4,4,4	0.36	0	6,6,6	0.06	0
6	GOL	B	606	-	5,5,5	0.21	0	5,5,5	0.30	0
6	GOL	B	607	-	5,5,5	0.23	0	5,5,5	0.27	0
6	GOL	B	608	-	5,5,5	0.28	0	5,5,5	0.11	0
4	4QJ	C	603	-	40,44,44	1.01	3 (7%)	34,65,65	1.07	3 (8%)
5	SO4	C	604	-	4,4,4	0.30	0	6,6,6	0.16	0
5	SO4	C	605	-	4,4,4	0.31	0	6,6,6	0.06	0
5	SO4	C	606	-	4,4,4	0.35	0	6,6,6	0.10	0
6	GOL	C	607	-	5,5,5	0.25	0	5,5,5	0.21	0
6	GOL	C	608	-	5,5,5	0.18	0	5,5,5	0.29	0
4	4QJ	D	603	-	40,44,44	1.02	4 (10%)	34,65,65	1.12	3 (8%)
5	SO4	D	604	-	4,4,4	0.50	0	6,6,6	0.11	0
5	SO4	D	605	-	4,4,4	0.32	0	6,6,6	0.06	0
5	SO4	D	606	-	4,4,4	0.34	0	6,6,6	0.06	0
6	GOL	D	607	-	5,5,5	0.14	0	5,5,5	0.63	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
4	4QJ	A	603	-	-	0/10/30/30	0/6/7/7
5	SO4	A	604	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	605	-	-	0/0/0/0	0/0/0/0
6	GOL	A	606	-	-	0/4/4/4	0/0/0/0
6	GOL	A	607	-	-	0/4/4/4	0/0/0/0
4	4QJ	B	603	-	-	0/10/30/30	0/6/7/7
5	SO4	B	604	-	-	0/0/0/0	0/0/0/0
5	SO4	B	605	-	-	0/0/0/0	0/0/0/0
6	GOL	B	606	-	-	0/4/4/4	0/0/0/0
6	GOL	B	607	-	-	0/4/4/4	0/0/0/0
6	GOL	B	608	-	-	0/4/4/4	0/0/0/0
4	4QJ	C	603	-	-	0/10/30/30	0/6/7/7
5	SO4	C	604	-	-	0/0/0/0	0/0/0/0
5	SO4	C	605	-	-	0/0/0/0	0/0/0/0
5	SO4	C	606	-	-	0/0/0/0	0/0/0/0
6	GOL	C	607	-	-	0/4/4/4	0/0/0/0
6	GOL	C	608	-	-	0/4/4/4	0/0/0/0
4	4QJ	D	603	-	-	0/10/30/30	0/6/7/7
5	SO4	D	604	-	-	0/0/0/0	0/0/0/0
5	SO4	D	605	-	-	0/0/0/0	0/0/0/0
5	SO4	D	606	-	-	0/0/0/0	0/0/0/0
6	GOL	D	607	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	4QJ	C18-N34	-3.31	1.35	1.39
4	A	603	4QJ	N31-N33	-3.10	1.34	1.37
4	B	603	4QJ	N31-N33	-3.08	1.34	1.37
4	C	603	4QJ	N31-N33	-3.06	1.34	1.37
4	D	603	4QJ	C18-N34	-2.94	1.35	1.39
4	D	603	4QJ	N31-N33	-2.63	1.34	1.37
4	B	603	4QJ	C18-N34	-2.38	1.36	1.39
4	A	603	4QJ	C18-N34	-2.14	1.36	1.39
4	D	603	4QJ	C20-C14	-2.09	1.38	1.45
4	C	603	4QJ	C21-C14	2.02	1.44	1.41
4	B	603	4QJ	C21-C14	2.05	1.44	1.41
4	A	603	4QJ	C21-C14	2.11	1.45	1.41
4	D	603	4QJ	C21-C14	2.50	1.45	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	4QJ	C15-C29-N33	-3.10	107.71	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	4QJ	C15-C29-N33	-2.92	107.98	112.36
4	B	603	4QJ	C15-C29-N33	-2.68	108.34	112.36
4	C	603	4QJ	C15-C29-N33	-2.62	108.43	112.36
4	B	603	4QJ	C25-C27-N34	-2.40	108.70	114.12
4	C	603	4QJ	C25-C27-N34	-2.35	108.81	114.12
4	A	603	4QJ	C23-C25-C27	2.01	107.64	104.27
4	D	603	4QJ	C23-C25-C27	2.09	107.77	104.27
4	C	603	4QJ	C24-C26-C27	3.03	106.75	102.55
4	B	603	4QJ	C24-C26-C27	3.05	106.78	102.55
4	B	603	4QJ	F38-C19-C12	3.14	120.91	118.79
4	D	603	4QJ	C24-C26-C27	3.83	107.86	102.55
4	A	603	4QJ	C24-C26-C27	3.93	108.00	102.55

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, 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	335/338 (99%)	-0.23	13 (3%) 43 47	14, 24, 45, 114	0
1	B	332/338 (98%)	-0.27	6 (1%) 71 74	14, 23, 45, 98	0
1	C	332/338 (98%)	-0.21	16 (4%) 34 37	14, 24, 49, 84	0
1	D	332/338 (98%)	-0.17	15 (4%) 37 40	13, 24, 48, 93	0
All	All	1331/1352 (98%)	-0.22	50 (3%) 44 48	13, 23, 47, 114	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	THR	8.2
1	A	446	PRO	7.1
1	C	501	ALA	5.4
1	A	447	LEU	5.3
1	C	444	VAL	5.0
1	C	150	TYR	4.9
1	D	150	TYR	4.9
1	A	149	THR	4.7
1	D	149	THR	4.5
1	C	156	ASN	4.0
1	B	446	PRO	4.0
1	A	448	ALA	3.9
1	D	446	PRO	3.9
1	D	503	GLY	3.6
1	B	149	THR	3.6
1	D	153	ALA	3.5
1	A	155	LEU	3.4
1	A	444	VAL	3.4
1	A	150	TYR	3.3
1	D	501	ALA	3.3
1	B	448	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	3.1
1	D	152	THR	3.1
1	A	153	ALA	2.9
1	A	445	GLN	2.8
1	C	159	LYS	2.8
1	C	503	GLY	2.8
1	C	155	LEU	2.8
1	D	157	CYS	2.8
1	A	151	SER	2.7
1	C	500	ALA	2.7
1	C	151	SER	2.7
1	C	154	VAL	2.7
1	D	155	LEU	2.5
1	A	152	THR	2.5
1	D	151	SER	2.5
1	B	444	VAL	2.4
1	D	156	ASN	2.4
1	D	159	LYS	2.4
1	D	447	LEU	2.4
1	A	156	ASN	2.4
1	D	154	VAL	2.4
1	C	446	PRO	2.3
1	A	443	SER	2.3
1	C	153	ALA	2.3
1	C	152	THR	2.3
1	D	502	SER	2.3
1	C	502	SER	2.2
1	B	307	ASP	2.2
1	C	157	CYS	2.1

## 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 ⓘ

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
5	SO4	C	604	5/5	0.96	0.18	5.24	40,43,45,47	0
5	SO4	D	604	5/5	0.95	0.17	4.57	30,31,37,38	0
6	GOL	A	606	6/6	0.89	0.16	4.36	37,42,47,49	0
6	GOL	A	607	6/6	0.89	0.19	2.88	38,39,43,53	0
6	GOL	B	606	6/6	0.91	0.12	2.17	37,40,46,46	0
6	GOL	C	608	6/6	0.72	0.20	1.60	53,60,68,69	0
6	GOL	D	607	6/6	0.88	0.17	1.18	30,35,38,39	0
6	GOL	B	607	6/6	0.95	0.12	0.20	29,30,32,38	0
4	4QJ	B	603	38/38	0.97	0.08	0.09	16,19,23,28	0
6	GOL	C	607	6/6	0.95	0.10	0.02	27,28,32,42	0
4	4QJ	A	603	38/38	0.97	0.08	-0.20	17,19,23,28	0
4	4QJ	D	603	38/38	0.97	0.08	-0.26	15,19,24,32	0
4	4QJ	C	603	38/38	0.97	0.08	-0.42	15,20,26,31	0
5	SO4	A	605	5/5	0.98	0.08	-1.11	35,36,41,46	0
3	MG	D	602	1/1	0.97	0.05	-2.62	28,28,28,28	0
3	MG	C	602	1/1	0.98	0.03	-4.19	26,26,26,26	0
3	MG	B	602	1/1	0.99	0.03	-6.34	26,26,26,26	0
2	ZN	A	601	1/1	1.00	0.03	-6.53	31,31,31,31	0
2	ZN	B	601	1/1	1.00	0.03	-6.65	29,29,29,29	0
2	ZN	C	601	1/1	1.00	0.03	-7.73	29,29,29,29	0
3	MG	A	602	1/1	0.99	0.03	-8.42	26,26,26,26	0
2	ZN	D	601	1/1	1.00	0.02	-19.21	29,29,29,29	0
5	SO4	B	604	5/5	0.98	0.12	-	38,38,40,41	0
5	SO4	A	604	5/5	0.99	0.10	-	34,39,40,46	0
5	SO4	D	606	5/5	0.98	0.15	-	44,46,49,52	0
6	GOL	B	608	6/6	0.74	0.29	-	37,46,48,68	0
5	SO4	D	605	5/5	0.89	0.15	-	64,66,72,81	0
5	SO4	B	605	5/5	0.86	0.23	-	68,75,83,93	0
5	SO4	C	605	5/5	0.95	0.18	-	64,65,73,78	0
5	SO4	C	606	5/5	0.98	0.14	-	44,46,51,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.