



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 08:34 AM EST

PDB ID : 4IJP  
Title : Crystal Structure of Human PRPF4B kinase domain in complex with 4-{5-[(2-Chloro-pyridin-4-ylmethyl)-carbamoyl]-thiophen-2-yl}-benzo[b]thiophene-2-carboxylic acid amine  
Authors : Mechin, I.; Haas, K.; Chen, X.; Zhang, Y.; McLean, L.  
Deposited on : unknown  
Resolution : 2.25 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

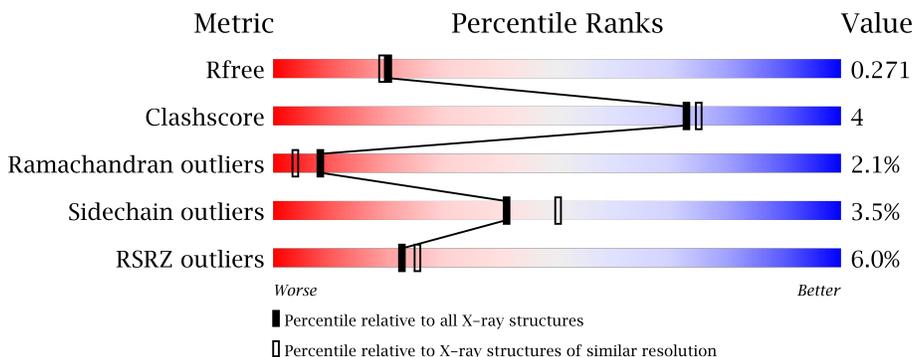
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	358	
1	B	358	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5711 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.

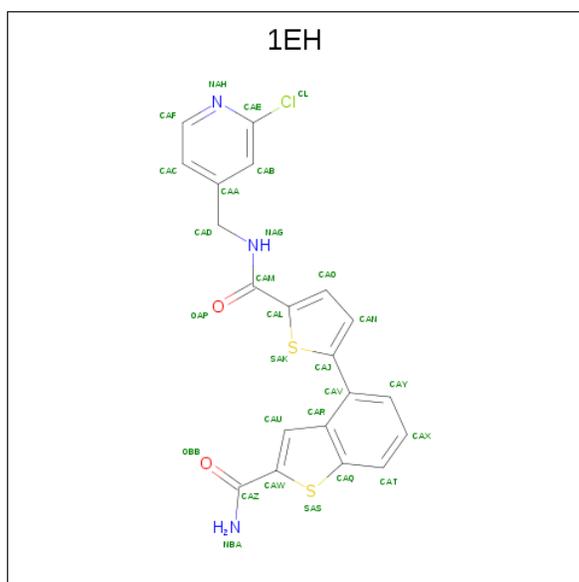
- Molecule 1 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	331	Total	C	N	O	P	S	0	1	0
			2714	1735	475	488	1	15			
1	B	334	Total	C	N	O	P	S	0	1	0
			2738	1750	481	490	1	16			

There are 14 discrepancies between the modelled and reference sequences:

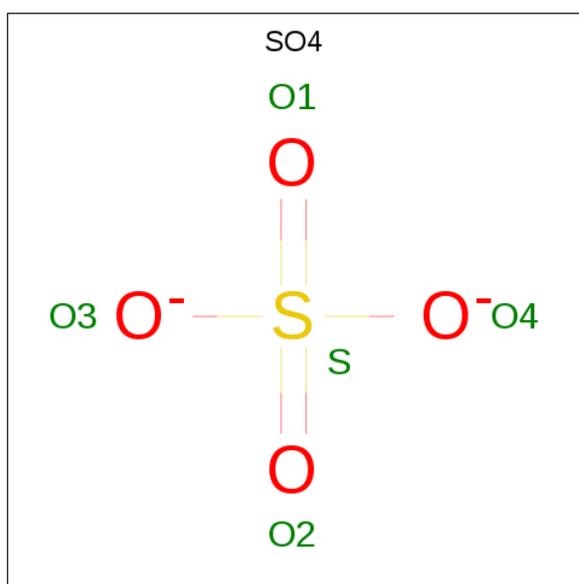
Chain	Residue	Modelled	Actual	Comment	Reference
A	656	MET	-	EXPRESSION TAG	UNP Q13523
A	1008	HIS	-	EXPRESSION TAG	UNP Q13523
A	1009	HIS	-	EXPRESSION TAG	UNP Q13523
A	1010	HIS	-	EXPRESSION TAG	UNP Q13523
A	1011	HIS	-	EXPRESSION TAG	UNP Q13523
A	1012	HIS	-	EXPRESSION TAG	UNP Q13523
A	1013	HIS	-	EXPRESSION TAG	UNP Q13523
B	656	MET	-	EXPRESSION TAG	UNP Q13523
B	1008	HIS	-	EXPRESSION TAG	UNP Q13523
B	1009	HIS	-	EXPRESSION TAG	UNP Q13523
B	1010	HIS	-	EXPRESSION TAG	UNP Q13523
B	1011	HIS	-	EXPRESSION TAG	UNP Q13523
B	1012	HIS	-	EXPRESSION TAG	UNP Q13523
B	1013	HIS	-	EXPRESSION TAG	UNP Q13523

- Molecule 2 is 4-(5-((2-chloropyridin-4-yl)methyl)carbamoyl)thiophen-2-yl)-1-benzothiophene-2-carboxamide (three-letter code: 1EH) (formula: C<sub>20</sub>H<sub>14</sub>ClN<sub>3</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	28	20	1	3	2	2	0	0
2	B	1	28	20	1	3	2	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

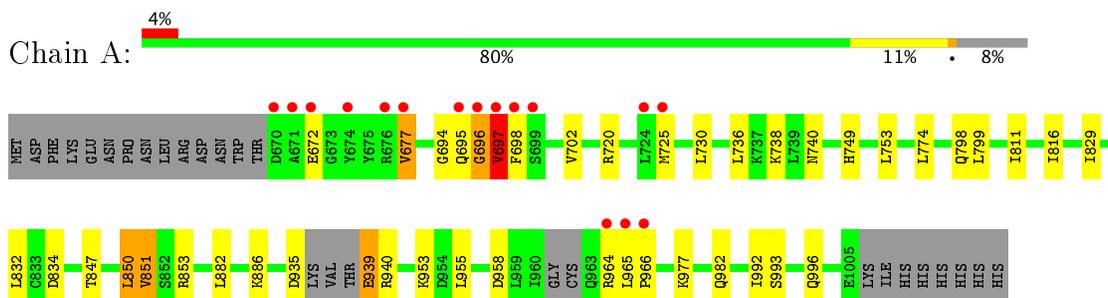
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	92	Total	O	0	0
			92	92		

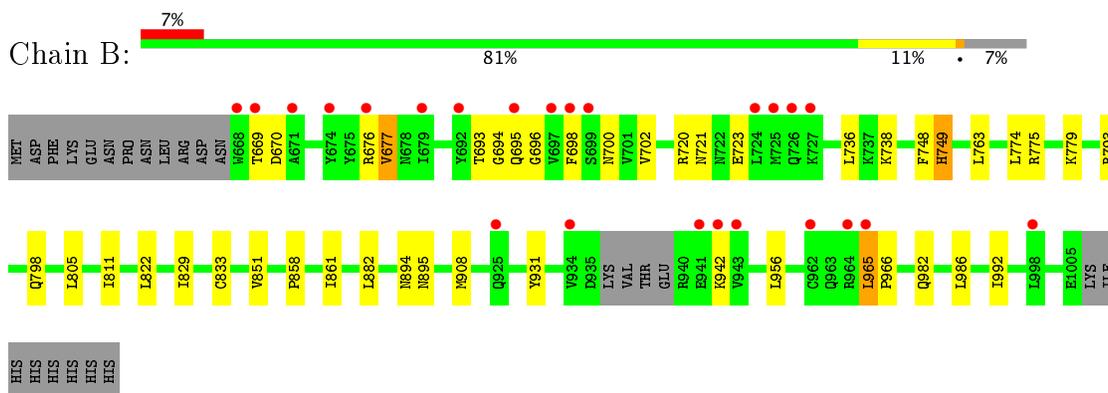
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase PRP4 homolog



- Molecule 1: Serine/threonine-protein kinase PRP4 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.14Å 52.54Å 79.13Å 102.56° 105.25° 92.29°	Depositor
Resolution (Å)	47.61 – 2.25 47.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.61-2.25) 90.7 (47.62-2.25)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.24Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.9.1, BUSTER 2.9.1	Depositor
R, $R_{free}$	0.250 , 0.265 0.257 , 0.271	Depositor DCC
$R_{free}$ test set	1832 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 24.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.094 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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: 1EH, SO4, 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	0.39	0/2748	0.60	1/3692 (0.0%)
1	B	0.39	0/2776	0.59	0/3733
All	All	0.39	0/5524	0.60	1/7425 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	GLY	C-N-CA	6.24	137.30	121.70

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	2714	0	2770	22	0
1	B	2738	0	2786	17	0
2	A	28	0	14	2	0
2	B	28	0	14	2	0
3	A	20	0	0	0	0
3	B	10	0	0	0	0
4	A	81	0	0	0	0
4	B	92	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5711	0	5584	43	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 4.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:LEU:HB3	1:B:966:PRO:HD3	1.32	1.12
1:B:965:LEU:HB3	1:B:966:PRO:CD	2.09	0.81
1:A:965:LEU:HB3	1:A:966:PRO:HD2	1.64	0.79
1:B:677:VAL:HG11	1:B:702:VAL:HG11	1.77	0.66
1:B:798:GLN:HE22	1:B:829:ILE:HA	1.63	0.62
2:B:1101:1EH:H8	2:B:1101:1EH:H12	1.86	0.56
1:A:798:GLN:HE22	1:A:829:ILE:HA	1.69	0.56
1:B:698:PHE:HA	1:B:720:ARG:HD2	1.87	0.55
1:A:696:GLY:H	1:A:697:VAL:HB	1.73	0.53
1:A:720:ARG:HD3	1:A:725:MET:HG3	1.90	0.53
1:A:677:VAL:HG21	1:A:695:GLN:HE22	1.73	0.53
1:A:740:ASN:HD21	1:A:753:LEU:H	1.57	0.52
1:A:677:VAL:HG11	1:A:702:VAL:HG11	1.91	0.52
1:B:908:MET:HG3	1:B:986:LEU:HD23	1.92	0.52
1:A:697:VAL:HG13	1:A:698:PHE:N	2.27	0.49
1:A:850:LEU:HD13	1:A:851:VAL:HG23	1.94	0.49
1:A:697:VAL:HG13	1:A:698:PHE:H	1.77	0.48
1:A:695:GLN:NE2	1:A:702:VAL:HG13	2.29	0.48
1:B:669:THR:HG21	1:B:721:ASN:HD22	1.80	0.47
1:A:965:LEU:HB3	1:A:966:PRO:CD	2.42	0.46
1:A:935:ASP:HB2	1:A:939:GLU:HB3	1.97	0.46
1:B:858:PRO:HA	1:B:861:ILE:HD12	1.98	0.46
1:B:695:GLN:HA	1:B:696:GLY:HA2	1.80	0.46
1:B:774:LEU:HD13	1:B:882:LEU:HD21	1.98	0.45
2:B:1101:1EH:CAN	2:B:1101:1EH:H12	2.47	0.45
1:A:749:HIS:CD2	1:A:798:GLN:HE21	2.34	0.44
1:B:895:ASN:HD21	1:B:931:TYR:HA	1.82	0.44
1:B:738:LYS:HD3	1:B:811:ILE:HD11	1.98	0.44
1:A:993:SER:H	1:A:996:GLN:HE21	1.64	0.44
1:A:955:LEU:HD23	1:A:977:LYS:HD2	2.01	0.43
1:B:749:HIS:CD2	1:B:798:GLN:HE21	2.35	0.43
1:A:738:LYS:HE3	1:A:811:ILE:HD11	2.01	0.42
1:B:695:GLN:HB2	1:B:700:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:GLN:HB3	1:A:992:ILE:HB	2.01	0.42
1:B:982:GLN:HB3	1:B:992:ILE:HB	2.02	0.42
2:A:1101:1EH:H12	2:A:1101:1EH:H8	2.01	0.42
1:B:748:PHE:HB3	1:B:805:LEU:HB2	2.01	0.42
1:B:822:LEU:HD23	1:B:833:CYS:SG	2.60	0.42
1:A:816:ILE:HG12	1:A:832[A]:LEU:HD11	2.02	0.41
1:A:774:LEU:HD13	1:A:882:LEU:HD11	2.02	0.41
2:A:1101:1EH:CAN	2:A:1101:1EH:H12	2.50	0.41
1:A:847:THR:HG23	1:A:850:LEU:HB2	2.03	0.40
1:A:697:VAL:CG1	1:A:698:PHE:N	2.84	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	325/358 (91%)	304 (94%)	15 (5%)	6 (2%)	10	5
1	B	330/358 (92%)	305 (92%)	17 (5%)	8 (2%)	7	3
All	All	655/716 (92%)	609 (93%)	32 (5%)	14 (2%)	8	4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	965	LEU
1	A	694	GLY
1	A	697	VAL
1	A	851	VAL
1	B	677	VAL
1	B	851	VAL
1	A	964	ARG
1	B	723	GLU

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Mol	Chain	Res	Type
1	B	749	HIS
1	B	942	LYS
1	A	853	ARG
1	A	834	ASP
1	B	676	ARG
1	B	694	GLY

### 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	298/323 (92%)	286 (96%)	12 (4%)	36	43
1	B	300/323 (93%)	291 (97%)	9 (3%)	46	56
All	All	598/646 (93%)	577 (96%)	21 (4%)	41	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	GLU
1	A	677	VAL
1	A	697	VAL
1	A	730	LEU
1	A	736	LEU
1	A	799	LEU
1	A	850	LEU
1	A	886	LYS
1	A	939	GLU
1	A	940	ARG
1	A	953	LYS
1	A	958	ASP
1	B	670	ASP
1	B	693	THR
1	B	736	LEU
1	B	763	LEU
1	B	775	ARG

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Mol	Chain	Res	Type
1	B	779	LYS
1	B	793	ARG
1	B	894	ASN
1	B	956	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	695	GLN
1	A	740	ASN
1	A	749	HIS
1	A	798	GLN
1	A	810	ASN
1	A	928	ASN
1	A	996	GLN
1	B	700	ASN
1	B	721	ASN
1	B	722	ASN
1	B	740	ASN
1	B	749	HIS
1	B	798	GLN
1	B	894	ASN
1	B	895	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](#)

2 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	849	1	15,16,17	1.24	1 (6%)	19,22,24	0.94	0
1	PTR	B	849	1	15,16,17	1.28	2 (13%)	19,22,24	1.20	3 (15%)

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	849	1	-	0/9/11/13	0/1/1/1
1	PTR	B	849	1	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	849	PTR	CE2-CZ	2.25	1.43	1.38
1	A	849	PTR	CA-C	2.89	1.54	1.50
1	B	849	PTR	CA-C	2.98	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	849	PTR	O-C-CA	-2.12	119.16	125.02
1	B	849	PTR	CG-CB-CA	-2.01	110.25	114.29
1	B	849	PTR	OH-CZ-CE2	2.36	126.33	119.23

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 [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	1EH	A	1101	-	23,31,31	1.97	2 (8%)	23,44,44	1.65	3 (13%)
3	SO4	A	1102	-	4,4,4	0.20	0	6,6,6	0.06	0
3	SO4	A	1103	-	4,4,4	0.22	0	6,6,6	0.06	0
3	SO4	A	1104	-	4,4,4	0.19	0	6,6,6	0.05	0
3	SO4	A	1105	-	4,4,4	0.20	0	6,6,6	0.05	0
2	1EH	B	1101	-	23,31,31	1.89	2 (8%)	23,44,44	1.70	3 (13%)
3	SO4	B	1102	-	4,4,4	0.19	0	6,6,6	0.05	0
3	SO4	B	1103	-	4,4,4	0.20	0	6,6,6	0.06	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	1EH	A	1101	-	-	0/10/17/17	0/4/4/4
3	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1103	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1104	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1105	-	-	0/0/0/0	0/0/0/0
2	1EH	B	1101	-	-	0/10/17/17	0/4/4/4
3	SO4	B	1102	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1103	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	1EH	CAV-CAJ	-7.80	1.40	1.48
2	B	1101	1EH	CAV-CAJ	-7.43	1.41	1.48
2	A	1101	1EH	CAW-SAS	-4.02	1.67	1.72
2	B	1101	1EH	CAW-SAS	-3.82	1.67	1.72

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1101	1EH	CAB-CAE-NAH	-5.51	120.13	125.54
2	A	1101	1EH	CAB-CAE-NAH	-5.27	120.36	125.54
2	A	1101	1EH	CAC-CAF-NAH	-2.77	120.73	123.92
2	B	1101	1EH	CAC-CAF-NAH	-2.64	120.88	123.92
2	A	1101	1EH	CAF-NAH-CAE	4.12	121.50	115.48
2	B	1101	1EH	CAF-NAH-CAE	4.12	121.52	115.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	1EH	2	0
2	B	1101	1EH	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	330/358 (92%)	0.19	16 (4%) 31 35	29, 45, 75, 102	0
1	B	333/358 (93%)	0.31	24 (7%) 16 18	27, 47, 79, 104	0
All	All	663/716 (92%)	0.25	40 (6%) 23 25	27, 46, 78, 104	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	698	PHE	14.0
1	A	698	PHE	10.8
1	B	697	VAL	7.8
1	A	695	GLN	6.1
1	B	724	LEU	5.9
1	A	964	ARG	5.3
1	A	671	ALA	5.1
1	A	965	LEU	5.0
1	B	934	VAL	4.7
1	B	671	ALA	4.5
1	B	965	LEU	4.4
1	B	669	THR	4.0
1	B	676	ARG	4.0
1	A	699	SER	3.9
1	B	668	TRP	3.9
1	A	697	VAL	3.8
1	B	695	GLN	3.7
1	A	724	LEU	3.6
1	B	674	TYR	3.3
1	A	696	GLY	3.2
1	B	692	TYR	3.2
1	B	943	VAL	3.0
1	B	925	GLN	3.0
1	A	966	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	677	VAL	2.7
1	B	964	ARG	2.7
1	B	941	GLU	2.6
1	A	672	GLU	2.6
1	B	998	LEU	2.5
1	A	670	ASP	2.4
1	B	942	LYS	2.4
1	A	674	TYR	2.2
1	B	725	MET	2.2
1	B	727	LYS	2.1
1	B	962	CYS	2.1
1	B	699	SER	2.1
1	B	679	ILE	2.0
1	B	726	GLN	2.0
1	A	676	ARG	2.0
1	A	725	MET	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	PTR	A	849	16/17	0.73	0.17	-	53,57,61,61	0
1	PTR	B	849	16/17	0.86	0.10	-	45,50,54,54	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
2	1EH	B	1101	28/28	0.87	0.20	1.13	42,93,135,207	0
3	SO4	A	1102	5/5	0.96	0.14	1.08	74,78,79,79	0
2	1EH	A	1101	28/28	0.93	0.18	0.08	39,88,139,213	0
3	SO4	B	1103	5/5	0.68	0.20	-	119,124,125,125	0
3	SO4	A	1105	5/5	0.77	0.18	-	116,120,121,122	0
3	SO4	B	1102	5/5	0.94	0.15	-	86,90,91,92	0
3	SO4	A	1103	5/5	0.92	0.12	-	77,82,82,83	0
3	SO4	A	1104	5/5	0.94	0.12	-	108,112,113,114	0

## 6.5 Other polymers

There are no such residues in this entry.