



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 PM GMT

PDB ID : 4IAN
Title : Crystal Structure of apo Human PRPF4B kinase domain
Authors : Mechin, I.; Haas, K.; Chen, X.; Zhang, Y.; McLean, L.
Deposited on : 2012-12-06
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (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

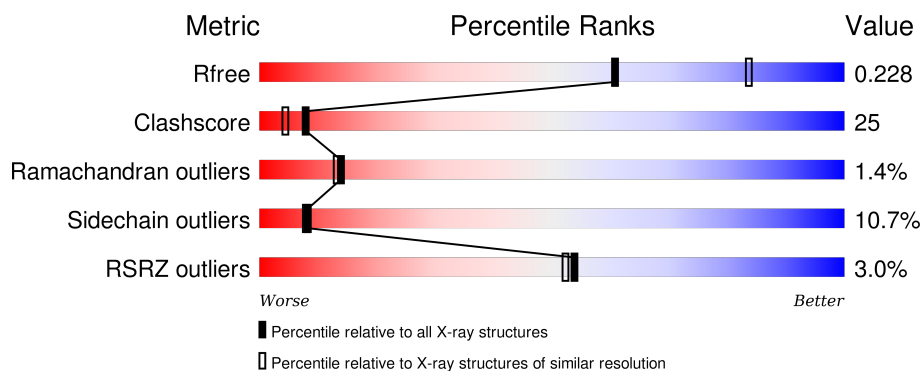
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	<div> <div>51%</div> <div>32%</div> <div>6%</div> <div>10%</div> </div>
1	B	358	<div> <div>4%</div> <div>47%</div> <div>36%</div> <div>6%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1105	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5333 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
1	A	322	Total	C	N	O	P	S	0	0	0
			2630	1682	462	470	1	15			
1	B	320	Total	C	N	O	P	S	0	0	0
			2608	1667	460	464	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

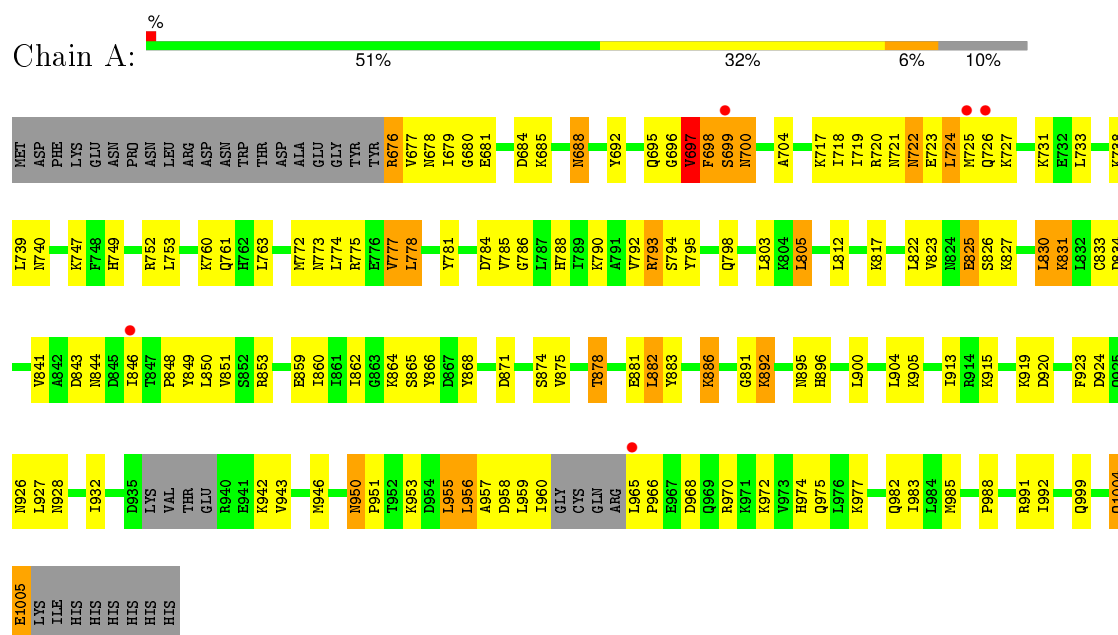
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	29	Total	O	0	0
			29	29		

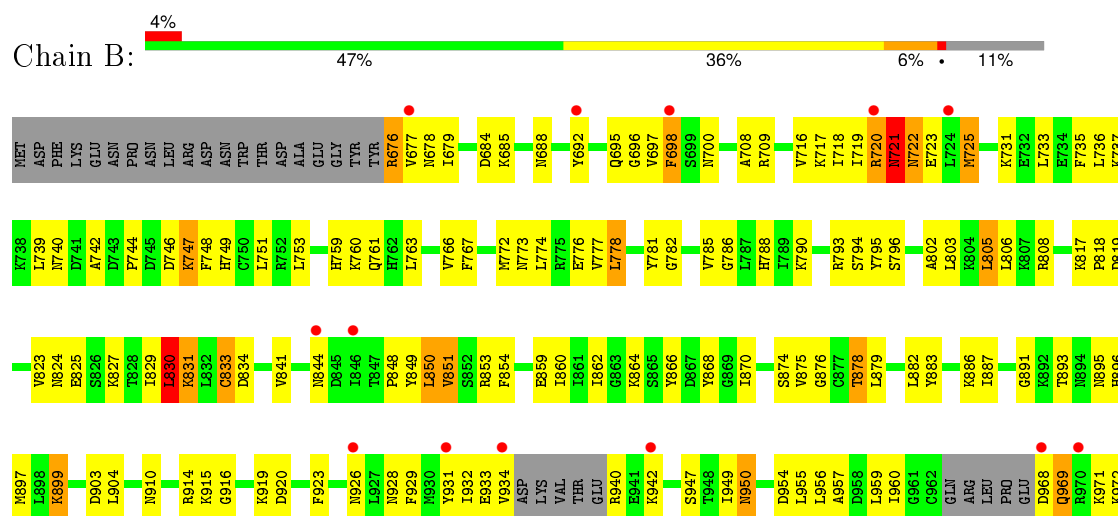
3 Residue-property plots

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: Serine/threonine-protein kinase PRP4 homolog



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.27Å 75.29Å 148.00Å 90.00° 97.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 47.91 – 2.43	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-2.44) 99.5 (47.91-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.288 0.234 , 0.228	Depositor DCC
R_{free} test set	1514 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29964 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 52.31 % 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 4.9547e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.37	0/2659	0.53	0/3572
1	B	0.33	0/2636	0.52	1/3539 (0.0%)
All	All	0.35	0/5295	0.53	1/7111 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	830	LEU	CA-CB-CG	5.85	128.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	721	ASN	Peptide

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	2630	0	2696	137	0
1	B	2608	0	2676	131	0
2	A	25	0	0	0	0
2	B	5	0	0	0	0
3	A	36	0	0	2	0
3	B	29	0	0	1	0
All	All	5333	0	5372	265	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 25.

All (265) 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:876:GLY:HA3	1:B:983:ILE:HD11	1.34	1.06
1:A:676:ARG:HH21	1:A:677:VAL:HG22	1.34	0.92
1:B:740:ASN:HD21	1:B:753:LEU:H	1.16	0.91
1:A:774:LEU:HA	1:A:777:VAL:HG13	1.56	0.87
1:A:950:ASN:HD22	1:A:950:ASN:H	1.22	0.86
1:A:740:ASN:HD21	1:A:753:LEU:H	1.21	0.84
1:B:850:LEU:HD13	1:B:851:VAL:HG23	1.60	0.83
1:B:972:LYS:HZ3	1:B:1005:GLU:HA	1.44	0.82
1:A:823:VAL:HG22	1:A:827:LYS:HA	1.63	0.81
1:B:781:TYR:HB3	1:B:785:VAL:CG2	2.11	0.79
1:A:913:ILE:HG22	1:A:919:LYS:HE2	1.64	0.79
1:A:803:LEU:HD11	1:A:875:VAL:HG21	1.64	0.78
1:B:698:PHE:H	1:B:698:PHE:HD2	1.29	0.78
1:B:933:GLU:HG3	1:B:934:VAL:H	1.49	0.76
1:B:862:ILE:HD11	1:B:923:PHE:HE2	1.49	0.76
1:B:933:GLU:HB3	1:B:942:LYS:HB2	1.69	0.74
1:B:722:ASN:HB3	1:B:725:MET:HB2	1.67	0.74
1:A:781:TYR:HB3	1:A:785:VAL:CG2	2.18	0.74
1:A:950:ASN:H	1:A:950:ASN:ND2	1.86	0.73
1:A:696:GLY:O	1:A:697:VAL:HG13	1.88	0.72
1:A:841:VAL:HG21	1:A:868:TYR:CZ	2.24	0.72
1:A:950:ASN:HD22	1:A:950:ASN:N	1.85	0.71
1:A:695:GLN:NE2	1:A:700:ASN:HB3	2.06	0.71
1:A:722:ASN:ND2	1:A:724:LEU:H	1.89	0.71
1:B:876:GLY:HA3	1:B:983:ILE:CD1	2.18	0.70
1:A:739:LEU:HD22	1:A:805:LEU:HD13	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:ASN:ND2	1:B:753:LEU:H	1.90	0.69
1:A:774:LEU:HA	1:A:777:VAL:CG1	2.22	0.69
1:A:722:ASN:HB3	1:A:725:MET:HG3	1.75	0.69
1:A:740:ASN:ND2	1:A:753:LEU:H	1.91	0.69
1:B:788:HIS:CE1	1:B:790:LYS:HG3	2.27	0.69
1:B:788:HIS:CE1	1:B:790:LYS:HE2	2.28	0.69
1:B:803:LEU:HD11	1:B:875:VAL:HG21	1.75	0.68
1:B:823:VAL:CG2	1:B:827:LYS:HA	2.23	0.68
1:B:926:ASN:HB2	1:B:928:ASN:ND2	2.08	0.68
1:B:679:ILE:H	1:B:679:ILE:HD12	1.57	0.68
1:A:798:GLN:OE1	1:A:830:LEU:HD13	1.93	0.68
1:A:942:LYS:HD3	1:A:943:VAL:H	1.58	0.67
1:B:782:GLY:O	1:B:785:VAL:HG13	1.93	0.67
1:A:895:ASN:ND2	1:A:932:ILE:H	1.93	0.67
1:B:676:ARG:NH2	1:B:677:VAL:HG22	2.10	0.66
1:A:781:TYR:O	1:A:785:VAL:HG21	1.96	0.66
1:B:695:GLN:O	1:B:695:GLN:HG3	1.95	0.66
1:B:748:PHE:HB3	1:B:805:LEU:HB2	1.79	0.65
1:A:722:ASN:ND2	1:A:723:GLU:N	2.44	0.65
1:B:983:ILE:HG22	1:B:992:ILE:HG21	1.79	0.65
1:A:874:SER:O	1:A:878:THR:HG23	1.97	0.64
1:B:968:ASP:O	1:B:971:LYS:HB2	1.96	0.64
1:A:848:PRO:HG2	1:A:849:PTR:CE2	2.27	0.64
1:A:773:ASN:OD1	1:A:775:ARG:HB3	1.97	0.64
1:B:698:PHE:N	1:B:698:PHE:HD2	1.95	0.64
1:A:740:ASN:HD21	1:A:753:LEU:N	1.96	0.63
1:A:844:ASN:HB3	3:A:1234:HOH:O	1.98	0.63
1:B:721:ASN:N	1:B:721:ASN:OD1	2.27	0.63
1:B:781:TYR:HB3	1:B:785:VAL:HG21	1.79	0.63
1:B:698:PHE:N	1:B:698:PHE:CD2	2.65	0.62
1:B:979:LEU:O	1:B:983:ILE:HG23	1.98	0.62
1:B:823:VAL:HG22	1:B:827:LYS:HA	1.80	0.62
1:B:853:ARG:HD2	1:B:891:GLY:O	1.99	0.62
1:A:774:LEU:HD23	1:A:777:VAL:HG11	1.82	0.61
1:B:773:ASN:OD1	1:B:776:GLU:HG2	2.00	0.61
1:A:846:ILE:O	1:A:846:ILE:HG13	2.00	0.61
1:B:874:SER:O	1:B:878:THR:HG23	2.00	0.60
1:B:844:ASN:HB2	1:B:866:TYR:CZ	2.36	0.60
1:B:972:LYS:HD2	1:B:975:GLN:OE1	2.02	0.60
1:A:823:VAL:CG2	1:A:827:LYS:HA	2.31	0.60
1:B:759:HIS:CD2	1:B:760:LYS:HG3	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:ARG:HB3	1:B:940:ARG:NH1	2.16	0.59
1:A:956:LEU:O	1:A:960:ILE:HG13	2.02	0.59
1:B:772:MET:HB2	1:B:776:GLU:HG3	1.84	0.59
1:A:722:ASN:HD22	1:A:723:GLU:H	1.50	0.59
1:A:677:VAL:HG12	1:A:678:ASN:N	2.17	0.58
1:A:722:ASN:HD22	1:A:723:GLU:N	2.01	0.58
1:A:788:HIS:CE1	1:A:790:LYS:HG3	2.38	0.58
1:B:781:TYR:O	1:B:785:VAL:HG21	2.03	0.58
1:A:892:LYS:HG3	1:A:896:HIS:HD2	1.67	0.58
1:A:1004:GLN:O	1:A:1005:GLU:HB3	2.03	0.58
1:B:972:LYS:NZ	1:B:1005:GLU:HA	2.18	0.58
1:A:793:ARG:HG3	1:A:794:SER:N	2.17	0.58
1:B:722:ASN:HD22	1:B:723:GLU:N	2.01	0.57
1:B:983:ILE:HG22	1:B:992:ILE:CG2	2.34	0.57
1:B:733:LEU:O	1:B:737:LYS:HG2	2.04	0.57
1:A:781:TYR:HB3	1:A:785:VAL:HG21	1.86	0.57
1:A:999:GLN:HA	1:A:1004:GLN:OE1	2.04	0.57
1:B:841:VAL:HG21	1:B:868:TYR:OH	2.05	0.57
1:B:785:VAL:HG23	1:B:786:GLY:N	2.18	0.57
1:A:895:ASN:HD21	1:A:932:ILE:H	1.53	0.57
1:B:895:ASN:ND2	1:B:932:ILE:H	2.02	0.57
1:B:676:ARG:HH21	1:B:677:VAL:HA	1.70	0.56
1:B:859:GLU:OE2	1:B:991:ARG:NH2	2.39	0.56
1:B:785:VAL:CG2	1:B:786:GLY:N	2.69	0.56
1:A:798:GLN:HB2	1:A:830:LEU:HD11	1.87	0.56
1:B:968:ASP:HA	1:B:971:LYS:HG3	1.88	0.56
1:A:966:PRO:HB2	1:A:968:ASP:OD2	2.05	0.56
1:A:739:LEU:CD2	1:A:805:LEU:HD13	2.35	0.55
1:A:830:LEU:O	1:A:831:LYS:HD2	2.05	0.55
1:A:699:SER:HB2	1:A:718:ILE:O	2.06	0.55
1:A:892:LYS:NZ	1:A:892:LYS:HB3	2.22	0.55
1:A:982:GLN:HB3	1:A:992:ILE:HB	1.87	0.55
1:A:965:LEU:HB3	1:A:966:PRO:HD2	1.89	0.55
1:B:928:ASN:OD1	1:B:947:SER:HA	2.07	0.54
1:B:862:ILE:HG22	1:B:864:LYS:H	1.72	0.54
1:A:817:LYS:HA	1:A:878:THR:HG21	1.89	0.54
1:B:676:ARG:CZ	1:B:677:VAL:HG22	2.38	0.54
1:B:895:ASN:HD21	1:B:931:TYR:HA	1.72	0.54
1:A:859:GLU:OE2	1:A:991:ARG:NH2	2.41	0.54
1:B:910:ASN:O	1:B:914:ARG:HG3	2.08	0.54
1:A:956:LEU:HD11	1:A:974:HIS:CE1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:ARG:O	1:B:722:ASN:N	2.39	0.53
1:A:784:ASP:OD2	1:A:886:LYS:HD3	2.08	0.53
1:A:772:MET:O	1:A:823:VAL:HG12	2.08	0.53
1:A:955:LEU:HB3	1:A:977:LYS:HD3	1.89	0.53
1:A:795:TYR:CD2	1:A:830:LEU:HD12	2.43	0.53
1:B:1004:GLN:O	1:B:1005:GLU:HB3	2.09	0.53
1:A:983:ILE:O	1:A:991:ARG:HD2	2.09	0.53
1:A:679:ILE:N	1:A:679:ILE:HD12	2.24	0.53
1:B:677:VAL:HG21	1:B:718:ILE:CD1	2.39	0.52
1:B:893:THR:O	1:B:897:MET:HG2	2.09	0.52
1:B:736:LEU:HD13	1:B:767:PHE:HE1	1.75	0.52
1:A:841:VAL:HG21	1:A:868:TYR:CE1	2.45	0.52
1:A:784:ASP:CG	1:A:886:LYS:HD3	2.29	0.52
1:B:698:PHE:HZ	1:B:717:LYS:HZ1	1.58	0.52
1:A:905:LYS:NZ	1:A:985:MET:SD	2.83	0.52
1:B:933:GLU:CG	1:B:934:VAL:H	2.22	0.52
1:B:914:ARG:HA	1:B:919:LYS:HE3	1.91	0.51
1:B:793:ARG:HG3	1:B:794:SER:N	2.24	0.51
1:B:795:TYR:CD2	1:B:830:LEU:HD12	2.46	0.51
1:A:841:VAL:HG21	1:A:868:TYR:OH	2.11	0.51
1:B:793:ARG:NH2	1:B:794:SER:HA	2.26	0.51
1:B:854:PHE:CD2	1:B:887:ILE:HD13	2.46	0.51
1:B:983:ILE:O	1:B:991:ARG:HD2	2.10	0.51
1:B:773:ASN:O	1:B:776:GLU:HG2	2.11	0.51
1:A:788:HIS:O	1:A:792:VAL:HG23	2.12	0.50
1:A:785:VAL:HG22	3:A:1208:HOH:O	2.11	0.50
1:A:956:LEU:O	1:A:958:ASP:O	2.30	0.50
1:A:853:ARG:HD2	1:A:891:GLY:O	2.12	0.50
1:A:676:ARG:NH2	1:A:677:VAL:HG22	2.15	0.50
1:B:864:LYS:HE3	1:B:915:LYS:HE2	1.94	0.50
1:A:862:ILE:HD11	1:A:923:PHE:HE2	1.77	0.50
1:A:999:GLN:HG2	1:B:990:LYS:O	2.12	0.50
1:A:924:ASP:OD1	1:A:928:ASN:HB2	2.11	0.49
1:A:871:ASP:O	1:A:875:VAL:HG23	2.12	0.49
1:B:860:ILE:HD11	1:B:870:ILE:HG21	1.93	0.49
1:B:739:LEU:HD22	1:B:805:LEU:HD13	1.93	0.49
1:B:679:ILE:N	1:B:679:ILE:HD12	2.25	0.49
1:B:679:ILE:HD11	1:B:692:TYR:HE2	1.76	0.49
1:B:748:PHE:HB2	1:B:805:LEU:HG	1.93	0.49
1:B:977:LYS:HG3	1:B:978:ASP:N	2.27	0.49
1:B:904:LEU:HD11	1:B:955:LEU:HG	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:VAL:HG21	1:B:827:LYS:HA	1.92	0.49
1:B:956:LEU:O	1:B:956:LEU:HD23	2.13	0.48
1:B:723:GLU:CD	1:B:723:GLU:H	2.16	0.48
1:B:739:LEU:CD2	1:B:805:LEU:HD13	2.43	0.48
1:B:933:GLU:HG3	1:B:934:VAL:N	2.25	0.48
1:A:698:PHE:CD2	1:A:698:PHE:N	2.74	0.48
1:B:823:VAL:HG23	1:B:829:ILE:O	2.14	0.48
1:A:773:ASN:O	1:A:777:VAL:HG12	2.13	0.48
1:B:676:ARG:C	1:B:676:ARG:HE	2.17	0.48
1:B:722:ASN:ND2	1:B:723:GLU:N	2.61	0.48
1:B:983:ILE:HG13	1:B:984:LEU:N	2.29	0.48
1:A:892:LYS:H	1:A:896:HIS:HD2	1.62	0.47
1:B:747:LYS:HB2	1:B:747:LYS:HE3	1.57	0.47
1:B:785:VAL:HG22	3:B:1216:HOH:O	2.15	0.47
1:A:723:GLU:H	1:A:723:GLU:CD	2.17	0.47
1:A:942:LYS:HD3	1:A:943:VAL:N	2.29	0.47
1:B:817:LYS:HA	1:B:878:THR:HG21	1.96	0.47
1:B:954:ASP:OD2	1:B:957:ALA:HB2	2.14	0.47
1:A:862:ILE:HD11	1:A:923:PHE:CE2	2.50	0.47
1:A:822:LEU:HG	1:A:833:CYS:SG	2.55	0.47
1:A:698:PHE:HB2	1:A:725:MET:CE	2.45	0.47
1:A:988:PRO:HA	1:A:991:ARG:HB2	1.96	0.47
1:B:875:VAL:O	1:B:879:LEU:HG	2.15	0.46
1:B:716:VAL:HG22	1:B:766:VAL:HG22	1.96	0.46
1:A:830:LEU:HD22	1:A:830:LEU:O	2.16	0.46
1:A:862:ILE:HD12	1:A:862:ILE:HA	1.75	0.46
1:B:742:ALA:C	1:B:744:PRO:HD3	2.35	0.46
1:B:679:ILE:HD11	1:B:692:TYR:CE2	2.50	0.46
1:B:883:TYR:HE1	1:B:959:LEU:O	1.99	0.46
1:B:934:VAL:HB	1:B:942:LYS:NZ	2.31	0.46
1:A:679:ILE:N	1:A:679:ILE:CD1	2.79	0.46
1:B:796:SER:OG	1:B:879:LEU:HD22	2.16	0.46
1:A:957:ALA:C	1:A:958:ASP:O	2.50	0.46
1:A:677:VAL:CG1	1:A:678:ASN:N	2.78	0.45
1:A:722:ASN:OD1	1:A:725:MET:HG3	2.16	0.45
1:B:677:VAL:HG12	1:B:678:ASN:N	2.32	0.45
1:A:679:ILE:H	1:A:679:ILE:CD1	2.30	0.45
1:B:949:ILE:O	1:B:950:ASN:HB2	2.16	0.45
1:A:774:LEU:HD23	1:A:777:VAL:CG1	2.45	0.45
1:B:751:LEU:HD22	1:B:833:CYS:HB2	1.98	0.45
1:A:679:ILE:HD11	1:A:692:TYR:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:HIS:HA	1:A:831:LYS:HE2	1.99	0.45
1:A:747:LYS:HB2	1:A:747:LYS:HE3	1.71	0.45
1:A:695:GLN:O	1:A:696:GLY:C	2.55	0.44
1:A:698:PHE:HB2	1:A:725:MET:HE2	1.99	0.44
1:A:724:LEU:O	1:A:727:LYS:HB3	2.16	0.44
1:B:862:ILE:HG23	1:B:916:GLY:HA3	1.99	0.44
1:A:785:VAL:CG2	1:A:786:GLY:N	2.80	0.44
1:A:680:GLY:O	1:A:681:GLU:C	2.56	0.44
1:A:970:ARG:NH1	1:A:974:HIS:NE2	2.66	0.44
1:B:929:PHE:CE2	1:B:931:TYR:HB2	2.52	0.44
1:B:793:ARG:HA	1:B:1002:PHE:CE2	2.52	0.44
1:A:926:ASN:O	1:A:927:LEU:HB2	2.18	0.44
1:B:899:LYS:HE2	1:B:903:ASP:OD1	2.18	0.44
1:A:982:GLN:NE2	1:B:999:GLN:HG2	2.32	0.43
1:A:697:VAL:HG23	1:A:698:PHE:H	1.83	0.43
1:A:953:LYS:HE3	1:A:958:ASP:OD2	2.19	0.43
1:B:802:ALA:O	1:B:806:LEU:HD13	2.18	0.43
1:A:825:GLU:HG2	1:A:826:SER:N	2.32	0.43
1:B:697:VAL:HG12	1:B:697:VAL:O	2.18	0.43
1:B:731:LYS:HG2	1:B:735:PHE:CE2	2.54	0.43
1:B:954:ASP:CG	1:B:957:ALA:HB2	2.38	0.43
1:A:698:PHE:HZ	1:A:717:LYS:HZ2	1.63	0.43
1:B:772:MET:O	1:B:823:VAL:HG12	2.19	0.43
1:A:950:ASN:HA	1:A:951:PRO:HD3	1.82	0.43
1:A:864:LYS:CG	1:A:865:SER:N	2.82	0.43
1:A:773:ASN:HB3	1:A:822:LEU:CD2	2.49	0.43
1:B:782:GLY:C	1:B:785:VAL:HG13	2.38	0.43
1:B:788:HIS:HE1	1:B:790:LYS:HG3	1.77	0.43
1:A:982:GLN:CD	1:B:999:GLN:HG2	2.39	0.43
1:A:825:GLU:CG	1:A:826:SER:N	2.81	0.42
1:A:740:ASN:HD21	1:A:752:ARG:HA	1.85	0.42
1:A:985:MET:O	1:A:991:ARG:HD3	2.19	0.42
1:B:933:GLU:O	1:B:934:VAL:C	2.57	0.42
1:B:731:LYS:HG2	1:B:735:PHE:HE2	1.83	0.42
1:A:864:LYS:HE3	1:A:915:LYS:HE2	2.01	0.42
1:B:848:PRO:HG2	1:B:849:PTR:CE2	2.50	0.42
1:B:749:HIS:HA	1:B:831:LYS:HE2	2.00	0.42
1:B:719:ILE:HG22	1:B:720:ARG:N	2.35	0.42
1:A:882:LEU:HD12	1:A:882:LEU:HA	1.80	0.42
1:B:708:ALA:O	1:B:709:ARG:NH2	2.51	0.42
1:A:695:GLN:HA	1:A:700:ASN:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:PHE:CZ	1:A:834:ASP:OD1	2.73	0.42
1:A:896:HIS:O	1:A:900:LEU:HG	2.20	0.42
1:B:684:ASP:O	1:B:685:LYS:HB2	2.19	0.42
1:A:792:VAL:HG21	1:A:883:TYR:HD2	1.85	0.42
1:B:823:VAL:HG22	1:B:824:ASN:N	2.35	0.41
1:A:676:ARG:HE	1:A:677:VAL:HG23	1.86	0.41
1:B:854:PHE:CE2	1:B:887:ILE:HD13	2.55	0.41
1:A:688:ASN:O	1:A:704:ALA:HA	2.20	0.41
1:B:969:GLN:HE21	1:B:969:GLN:HA	1.85	0.41
1:A:817:LYS:HA	1:A:878:THR:CG2	2.49	0.41
1:B:760:LYS:O	1:B:761:GLN:HB2	2.20	0.41
1:A:860:ILE:HD13	1:A:866:TYR:CD2	2.56	0.41
1:A:760:LYS:O	1:A:761:GLN:HB2	2.21	0.41
1:A:859:GLU:CD	1:A:991:ARG:HH22	2.23	0.41
1:A:719:ILE:HG22	1:A:720:ARG:N	2.36	0.41
1:B:774:LEU:O	1:B:777:VAL:HG22	2.20	0.41
1:A:774:LEU:O	1:A:778:LEU:HB2	2.21	0.41
1:A:722:ASN:CB	1:A:725:MET:HG3	2.47	0.41
1:A:684:ASP:O	1:A:685:LYS:HB2	2.21	0.41
1:A:738:LYS:O	1:A:738:LYS:HD2	2.21	0.41
1:A:904:LEU:HA	1:A:953:LYS:HB3	2.03	0.41
1:B:957:ALA:O	1:B:960:ILE:O	2.39	0.41
1:B:777:VAL:CG2	1:B:778:LEU:N	2.84	0.41
1:A:972:LYS:O	1:A:975:GLN:HB2	2.22	0.40
1:A:958:ASP:O	1:A:959:LEU:HB3	2.19	0.40
1:A:881:GLU:HA	1:A:886:LYS:O	2.21	0.40
1:B:696:GLY:HA2	1:B:697:VAL:HA	1.76	0.40
1:A:676:ARG:HE	1:A:677:VAL:CG2	2.35	0.40
1:B:899:LYS:HG2	1:B:931:TYR:CE1	2.56	0.40
1:A:785:VAL:HG23	1:A:786:GLY:N	2.36	0.40
1:A:878:THR:O	1:A:882:LEU:N	2.54	0.40
1:A:1004:GLN:O	1:A:1005:GLU:CB	2.67	0.40
1:B:817:LYS:HB2	1:B:818:PRO:CD	2.52	0.40
1:A:959:LEU:O	1:A:960:ILE:HG12	2.21	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	315/358 (88%)	293 (93%)	18 (6%)	4 (1%)	15	15
1	B	313/358 (87%)	290 (93%)	18 (6%)	5 (2%)	12	11
All	All	628/716 (88%)	583 (93%)	36 (6%)	9 (1%)	14	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	697	VAL
1	B	851	VAL
1	A	851	VAL
1	B	721	ASN
1	A	699	SER
1	B	746	ASP
1	B	950	ASN
1	A	722	ASN
1	B	834	ASP

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	290/323 (90%)	258 (89%)	32 (11%)	8	7
1	B	287/323 (89%)	257 (90%)	30 (10%)	8	9
All	All	577/646 (89%)	515 (89%)	62 (11%)	8	8

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	ARG
1	A	688	ASN
1	A	697	VAL
1	A	698	PHE
1	A	700	ASN
1	A	721	ASN
1	A	724	LEU
1	A	726	GLN
1	A	731	LYS
1	A	733	LEU
1	A	763	LEU
1	A	777	VAL
1	A	778	LEU
1	A	793	ARG
1	A	805	LEU
1	A	812	LEU
1	A	825	GLU
1	A	830	LEU
1	A	831	LYS
1	A	843	ASP
1	A	850	LEU
1	A	878	THR
1	A	882	LEU
1	A	886	LYS
1	A	892	LYS
1	A	920	ASP
1	A	946	MET
1	A	950	ASN
1	A	955	LEU
1	A	956	LEU
1	A	1004	GLN
1	A	1005	GLU
1	B	676	ARG
1	B	688	ASN
1	B	698	PHE
1	B	700	ASN
1	B	720	ARG
1	B	721	ASN
1	B	722	ASN
1	B	725	MET
1	B	747	LYS
1	B	763	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	778	LEU
1	B	805	LEU
1	B	808	ARG
1	B	819	ASP
1	B	825	GLU
1	B	830	LEU
1	B	831	LYS
1	B	833	CYS
1	B	850	LEU
1	B	878	THR
1	B	882	LEU
1	B	886	LYS
1	B	896	HIS
1	B	899	LYS
1	B	920	ASP
1	B	969	GLN
1	B	977	LYS
1	B	983	ILE
1	B	991	ARG
1	B	1005	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	695	GLN
1	A	707	ASN
1	A	722	ASN
1	A	740	ASN
1	A	840	HIS
1	A	895	ASN
1	A	896	HIS
1	A	921	GLN
1	A	950	ASN
1	B	688	ASN
1	B	700	ASN
1	B	707	ASN
1	B	722	ASN
1	B	740	ASN
1	B	895	ASN
1	B	896	HIS
1	B	921	GLN
1	B	969	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	974	HIS
1	B	995	ASN
1	B	1004	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	14,16,17	0.66	0	18,22,24	1.27	3 (16%)
1	PTR	B	849	1	14,16,17	0.68	0	18,22,24	1.62	5 (27%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	849	PTR	O3P-P-OH	-4.03	90.78	105.22
1	B	849	PTR	O2P-P-OH	-2.83	95.07	105.22
1	B	849	PTR	O3P-P-O1P	2.26	117.86	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	849	PTR	O2P-P-O1P	2.34	118.12	110.58
1	A	849	PTR	O3P-P-O1P	2.45	118.46	110.58
1	A	849	PTR	O2P-P-O1P	2.48	118.55	110.58
1	B	849	PTR	O3P-P-O2P	2.85	118.23	107.38
1	A	849	PTR	O3P-P-O2P	2.88	118.35	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	849	PTR	1	0
1	B	849	PTR	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	SO4	A	1101	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	A	1102	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	A	1103	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	1104	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	A	1105	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	B	1101	-	4,4,4	0.21	0	6,6,6	0.08	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	SO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1103	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1104	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1105	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/358 (89%)	0.18	5 (1%) 74 74	19, 37, 72, 95	0
1	B	319/358 (89%)	0.26	14 (4%) 38 37	22, 44, 77, 99	0
All	All	640/716 (89%)	0.22	19 (2%) 54 52	19, 41, 76, 99	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	LEU	4.4
1	B	934	VAL	3.5
1	A	726	GLN	3.4
1	B	844	ASN	3.1
1	B	968	ASP	3.1
1	B	926	ASN	3.1
1	A	846	ILE	3.0
1	A	965	LEU	2.9
1	B	677	VAL	2.9
1	A	725	MET	2.8
1	B	942	LYS	2.8
1	A	699	SER	2.6
1	B	846	ILE	2.5
1	B	698	PHE	2.4
1	B	970	ARG	2.3
1	B	720	ARG	2.3
1	B	983	ILE	2.2
1	B	931	TYR	2.1
1	B	692	TYR	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	A	849	16/17	0.88	0.15	-	39,58,77,77	0
1	PTR	B	849	16/17	0.90	0.15	-	49,59,75,75	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1105	5/5	0.91	0.26	4.86	88,89,90,90	0
2	SO4	B	1101	5/5	0.95	0.13	-	62,63,63,64	0
2	SO4	A	1102	5/5	0.92	0.15	-	86,86,87,88	0
2	SO4	A	1101	5/5	0.90	0.26	-	98,98,99,99	0
2	SO4	A	1103	5/5	0.94	0.20	-	85,86,86,86	0
2	SO4	A	1104	5/5	0.86	0.21	-	89,90,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.