Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 08:36 PM EDT

PDB ID	:	3MEL
Title	:	Crystal Structure of Thiamin pyrophosphokinase family protein from Enterococcus faecalis, Northeast Structural Genomics Consortium Target EfR150
Authors	:	Kuzin, A.; Abasidze, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccosanti, C.; Foote, E.L.; Maglaqui, M.; Zhao, L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-03-31
Resolution	:	2.79 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

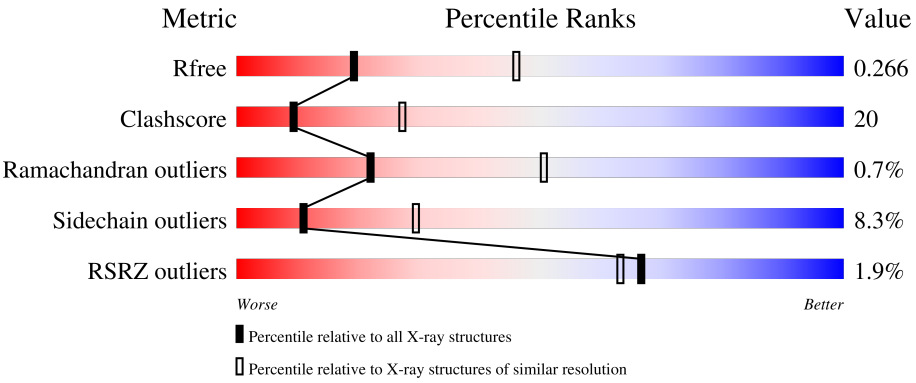
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	222	64% 27%
1	B	222	61% 32%
1	C	222	% 55% 37%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

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Mol	Chain	Length	Quality of chain
1	D	222	6% 60% 32%

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	TPP	A	902	-	X	-	-
2	TPP	D	902	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6859 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 Thiamin pyrophosphokinase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	Se	0	0	0
			1693	1079	279	329	4	2			
1	B	213	Total	C	N	O	S	Se	0	0	0
			1693	1079	279	329	4	2			
1	C	214	Total	C	N	O	S	Se	0	0	0
			1701	1084	280	330	4	3			
1	D	213	Total	C	N	O	S	Se	0	0	0
			1693	1079	279	329	4	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	LEU	-	expression tag	UNP Q82ZE3
A	216	GLU	-	expression tag	UNP Q82ZE3
A	217	HIS	-	expression tag	UNP Q82ZE3
A	218	HIS	-	expression tag	UNP Q82ZE3
A	219	HIS	-	expression tag	UNP Q82ZE3
A	220	HIS	-	expression tag	UNP Q82ZE3
A	221	HIS	-	expression tag	UNP Q82ZE3
A	222	HIS	-	expression tag	UNP Q82ZE3
B	215	LEU	-	expression tag	UNP Q82ZE3
B	216	GLU	-	expression tag	UNP Q82ZE3
B	217	HIS	-	expression tag	UNP Q82ZE3
B	218	HIS	-	expression tag	UNP Q82ZE3
B	219	HIS	-	expression tag	UNP Q82ZE3
B	220	HIS	-	expression tag	UNP Q82ZE3
B	221	HIS	-	expression tag	UNP Q82ZE3
B	222	HIS	-	expression tag	UNP Q82ZE3
C	215	LEU	-	expression tag	UNP Q82ZE3
C	216	GLU	-	expression tag	UNP Q82ZE3
C	217	HIS	-	expression tag	UNP Q82ZE3
C	218	HIS	-	expression tag	UNP Q82ZE3
C	219	HIS	-	expression tag	UNP Q82ZE3

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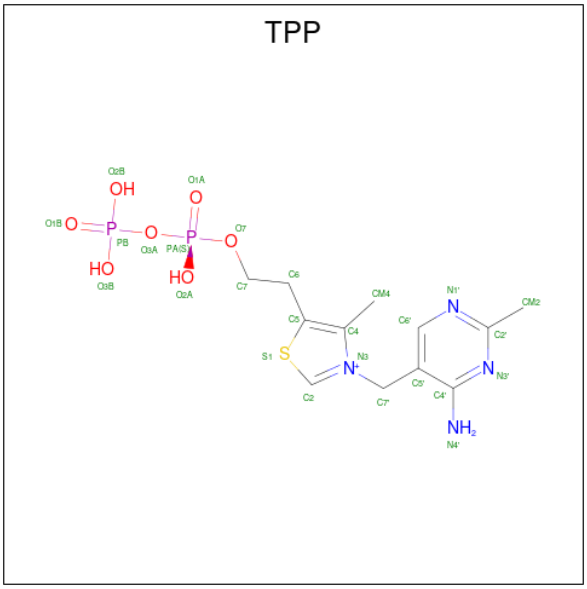
Chain	Residue	Modelled	Actual	Comment	Reference
C	220	HIS	-	expression tag	UNP Q82ZE3
C	221	HIS	-	expression tag	UNP Q82ZE3
C	222	HIS	-	expression tag	UNP Q82ZE3
D	215	LEU	-	expression tag	UNP Q82ZE3
D	216	GLU	-	expression tag	UNP Q82ZE3
D	217	HIS	-	expression tag	UNP Q82ZE3
D	218	HIS	-	expression tag	UNP Q82ZE3
D	219	HIS	-	expression tag	UNP Q82ZE3
D	220	HIS	-	expression tag	UNP Q82ZE3
D	221	HIS	-	expression tag	UNP Q82ZE3
D	222	HIS	-	expression tag	UNP Q82ZE3

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

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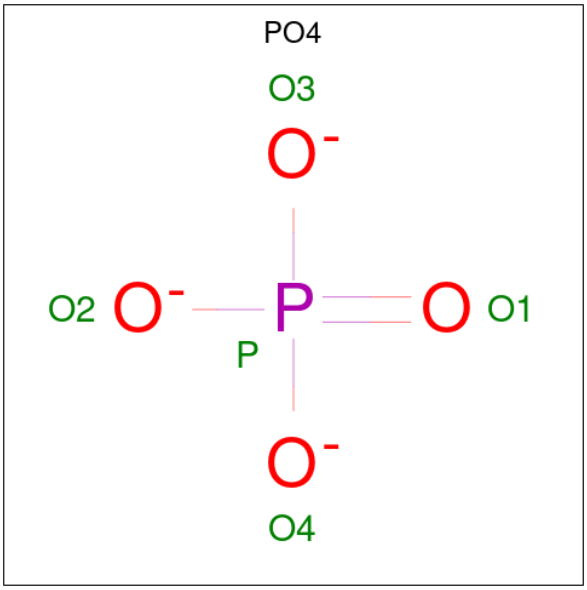
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

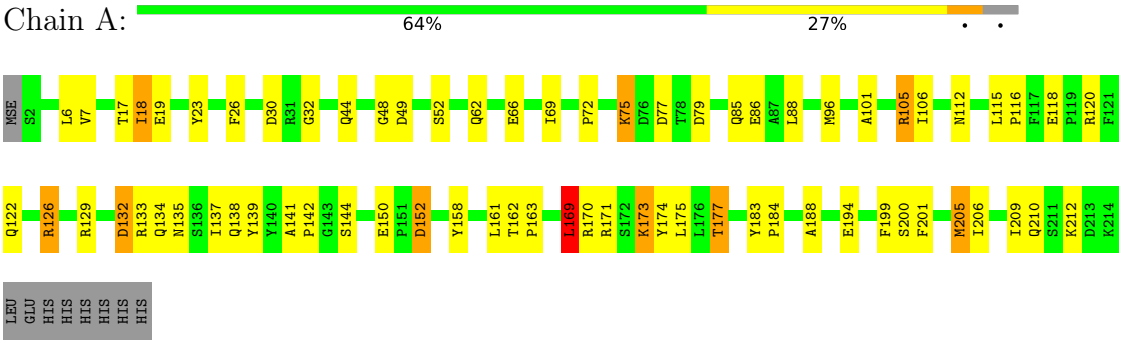
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	1	Total O 1 1	0	0
5	C	2	Total O 2 2	0	0
5	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

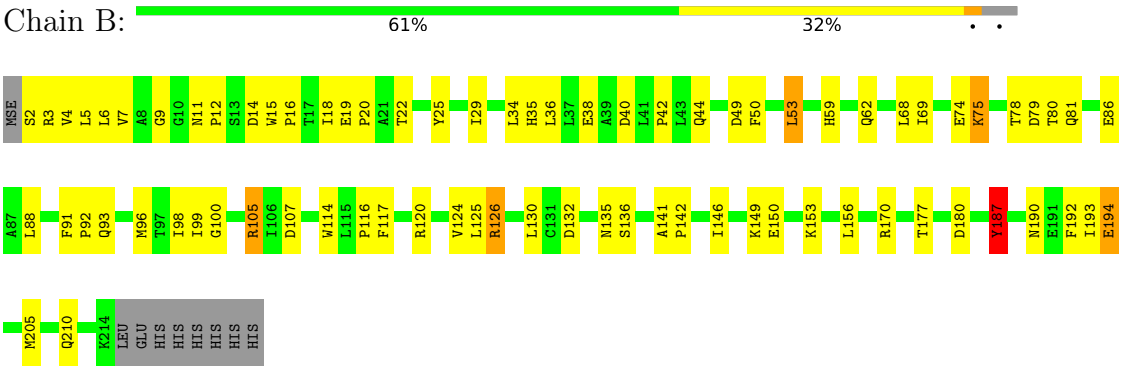
• Molecule 1: Thiamin pyrophosphokinase family protein

Chain A:



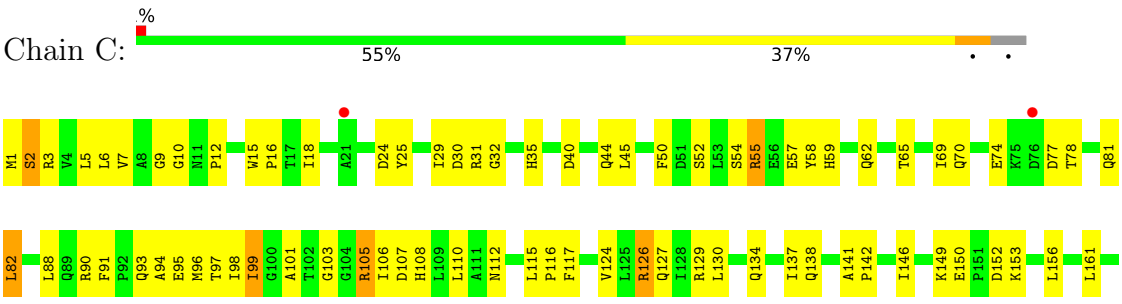
• Molecule 1: Thiamin pyrophosphokinase family protein

Chain B:



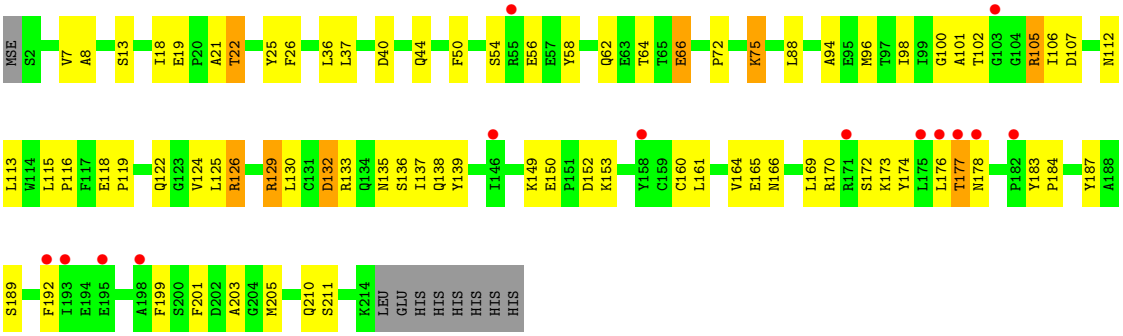
• Molecule 1: Thiamin pyrophosphokinase family protein

Chain C:



• Molecule 1: Thiamin pyrophosphokinase family protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.29Å 102.11Å 94.28Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	48.53 – 2.79 48.53 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.53-2.79) 99.2 (48.53-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.83 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC	Depositor
R, R_{free}	0.207 , 0.275 0.201 , 0.266	Depositor DCC
R_{free} test set	1476 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6859	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, PO4

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	0.48	0/1731	0.64	1/2356 (0.0%)
1	B	0.46	0/1731	0.64	0/2356
1	C	0.42	0/1739	0.60	0/2366
1	D	0.42	0/1731	0.59	0/2356
All	All	0.44	0/6932	0.62	1/9434 (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(^{o})	Ideal(^{o})
1	A	169	LEU	CA-CB-CG	6.99	131.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	187	TYR	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	1693	0	1644	55	0
1	B	1693	0	1644	67	0
1	C	1701	0	1656	90	0
1	D	1693	0	1644	65	0
2	A	26	0	16	1	0
2	D	26	0	16	3	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
All	All	6859	0	6620	266	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 20.

All (266) 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:1:MSE:H2	1:C:2:SER:HA	1.07	1.18
1:B:193:ILE:HG22	1:B:194:GLU:HG3	1.30	1.11
1:C:1:MSE:H2	1:C:2:SER:CA	1.68	1.05
1:D:105:ARG:HH11	1:D:105:ARG:HG2	1.19	1.04
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.21	1.02
1:C:170:ARG:HH12	1:C:177:THR:HG22	1.23	1.01
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.30	0.94
1:B:170:ARG:HH12	1:B:177:THR:HG22	1.30	0.93
1:D:126:ARG:HH12	1:D:138:GLN:NE2	1.64	0.93
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.35	0.91
1:D:150:GLU:H	1:D:210:GLN:HE22	1.14	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLU:H	1:B:210:GLN:HE22	1.05	0.91
1:C:1:MSE:N	1:C:2:SER:HA	1.86	0.90
1:D:88:LEU:HD23	1:D:96:MSE:HE3	1.54	0.87
1:B:78:THR:HG23	1:B:81:GLN:H	1.41	0.86
1:A:126:ARG:HH12	1:A:138:GLN:NE2	1.74	0.84
1:B:105:ARG:HH11	1:B:105:ARG:CG	1.91	0.82
1:D:170:ARG:HH22	1:D:177:THR:HB	1.42	0.82
1:D:132:ASP:HB2	1:D:135:ASN:HB2	1.60	0.81
1:C:150:GLU:H	1:C:210:GLN:NE2	1.80	0.80
1:C:170:ARG:NH1	1:C:177:THR:HG22	1.96	0.80
1:C:187:TYR:CD1	2:D:902:TPP:HM23	2.17	0.79
1:D:7:VAL:HG21	1:D:36:LEU:HD21	1.64	0.79
1:C:101:ALA:HB1	1:C:112:ASN:ND2	1.99	0.77
1:A:150:GLU:H	1:A:210:GLN:HE22	1.31	0.77
1:C:16:PRO:HG2	1:C:99:ILE:HD11	1.68	0.76
1:D:126:ARG:HH21	1:D:126:ARG:HG3	1.50	0.76
1:C:78:THR:HG23	1:C:81:GLN:H	1.50	0.75
1:C:94:ALA:HB3	1:C:96:MSE:HE2	1.68	0.75
1:C:164:VAL:HG12	1:C:181:VAL:HB	1.69	0.74
1:C:164:VAL:HG21	1:C:206:ILE:HD11	1.69	0.74
1:D:126:ARG:HG3	1:D:126:ARG:NH2	2.03	0.74
1:D:126:ARG:NH1	1:D:138:GLN:NE2	2.36	0.74
1:C:1:MSE:N	1:C:24:ASP:OD2	2.17	0.73
1:B:170:ARG:NH1	1:B:177:THR:HG22	2.04	0.73
1:D:161:LEU:HD12	1:D:205:MSE:HE2	1.71	0.72
1:C:9:GLY:O	1:C:35:HIS:HE1	1.74	0.71
1:A:105:ARG:HH11	1:A:105:ARG:CG	2.00	0.70
1:C:1:MSE:N	1:C:3:ARG:H	1.89	0.70
1:B:4:VAL:HB	1:B:96:MSE:CE	2.22	0.69
1:D:105:ARG:HH11	1:D:105:ARG:CG	2.00	0.69
1:C:187:TYR:HD1	2:D:902:TPP:HM23	1.57	0.69
1:C:98:ILE:HB	1:C:130:LEU:HD23	1.75	0.69
1:B:3:ARG:HD3	1:B:22:THR:O	1.93	0.69
1:C:88:LEU:HD11	1:C:124:VAL:HG21	1.73	0.69
1:B:150:GLU:H	1:B:210:GLN:NE2	1.87	0.68
1:C:1:MSE:N	1:C:3:ARG:N	2.41	0.68
1:D:129:ARG:HD2	1:D:138:GLN:HG2	1.74	0.68
1:A:88:LEU:HD23	1:A:96:MSE:HE3	1.75	0.67
1:B:5:LEU:HD11	1:B:99:ILE:HG13	1.75	0.67
1:B:105:ARG:HG2	1:B:105:ARG:NH1	2.06	0.67
1:C:94:ALA:HB3	1:C:96:MSE:CE	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ASP:OD2	1:C:153:LYS:HE3	1.94	0.67
1:B:150:GLU:N	1:B:210:GLN:HE22	1.87	0.67
1:D:125:LEU:HD12	1:D:126:ARG:N	2.09	0.67
1:C:105:ARG:HG2	1:C:105:ARG:NH1	2.05	0.65
1:A:126:ARG:NH1	1:A:138:GLN:NE2	2.45	0.64
1:B:4:VAL:HB	1:B:96:MSE:HE1	1.80	0.64
1:C:129:ARG:NH2	1:C:138:GLN:HG3	2.12	0.64
1:B:69:ILE:HD13	1:B:86:GLU:HG3	1.79	0.64
1:B:141:ALA:HB1	1:B:142:PRO:HD2	1.78	0.64
1:C:1:MSE:H2	1:C:3:ARG:N	1.96	0.64
1:B:170:ARG:HH22	1:B:177:THR:CG2	2.11	0.63
1:C:1:MSE:N	1:C:2:SER:CA	2.50	0.63
1:A:62:GLN:HE22	1:D:62:GLN:HE22	1.47	0.62
1:D:150:GLU:H	1:D:210:GLN:NE2	1.94	0.61
1:D:149:LYS:NZ	1:D:153:LYS:O	2.35	0.60
1:A:137:ILE:HG12	1:A:209:ILE:HG12	1.83	0.60
1:B:116:PRO:HB2	1:B:205:MSE:HE1	1.83	0.60
1:C:12:PRO:O	1:C:15:TRP:HB2	2.00	0.60
1:B:42:PRO:HB3	1:B:44:GLN:HE22	1.67	0.59
1:D:149:LYS:HB2	1:D:192:PHE:CD1	2.37	0.59
1:C:105:ARG:NH2	1:D:189:SER:OG	2.36	0.59
2:A:902:TPP:HM23	1:B:187:TYR:CD1	2.38	0.58
1:D:105:ARG:HG2	1:D:105:ARG:NH1	1.99	0.58
1:A:105:ARG:HG2	1:A:105:ARG:NH1	2.02	0.58
1:C:90:ARG:O	1:C:91:PHE:CD2	2.56	0.57
1:B:98:ILE:HB	1:B:130:LEU:HD23	1.86	0.57
1:A:26:PHE:H	1:A:44:GLN:NE2	2.02	0.57
1:A:170:ARG:HH22	1:A:177:THR:HB	1.68	0.57
1:C:150:GLU:H	1:C:210:GLN:HE22	1.53	0.57
1:D:126:ARG:NH1	1:D:138:GLN:HE21	2.02	0.57
1:C:115:LEU:HB2	1:C:116:PRO:HD3	1.86	0.57
1:D:26:PHE:H	1:D:44:GLN:HE21	1.52	0.56
1:B:125:LEU:HD12	1:B:126:ARG:N	2.20	0.56
1:C:78:THR:CG2	1:C:81:GLN:H	2.19	0.56
1:A:106:ILE:HG13	1:B:135:ASN:CG	2.25	0.56
1:A:129:ARG:HD2	1:A:138:GLN:HG2	1.87	0.55
1:B:141:ALA:HB1	1:B:142:PRO:CD	2.36	0.55
1:C:91:PHE:HB3	1:C:94:ALA:HB2	1.87	0.55
1:C:134:GLN:NE2	1:C:212:LYS:O	2.37	0.55
1:C:137:ILE:HD11	1:D:106:ILE:HD12	1.87	0.55
1:A:88:LEU:CD2	1:A:96:MSE:HE3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:HD11	1:C:207:ALA:HB2	1.88	0.55
1:B:15:TRP:CD1	1:B:99:ILE:HG22	2.42	0.55
1:B:42:PRO:CB	1:B:44:GLN:HE22	2.20	0.55
1:C:164:VAL:HG12	1:C:181:VAL:CB	2.35	0.55
1:D:94:ALA:HB3	1:D:96:MSE:HE2	1.88	0.55
1:A:72:PRO:O	1:A:75:LYS:HG2	2.07	0.55
1:C:16:PRO:CG	1:C:99:ILE:HD11	2.36	0.55
1:D:149:LYS:HB2	1:D:192:PHE:CE1	2.42	0.54
1:A:173:LYS:HD3	1:A:174:TYR:CE2	2.43	0.54
1:C:164:VAL:CG2	1:C:206:ILE:HD11	2.37	0.54
1:B:98:ILE:O	1:B:99:ILE:HD13	2.08	0.54
1:B:156:LEU:HD13	1:B:192:PHE:CZ	2.43	0.54
1:C:124:VAL:HB	1:C:127:GLN:OE1	2.07	0.54
1:A:72:PRO:HG3	1:D:66:GLU:HB2	1.90	0.53
1:A:129:ARG:CZ	1:A:138:GLN:HE21	2.21	0.53
1:B:96:MSE:HA	1:B:96:MSE:HE2	1.90	0.53
1:C:110:LEU:HD11	1:D:113:LEU:HD21	1.91	0.53
1:A:18:ILE:HG13	1:A:23:TYR:HE2	1.73	0.53
1:B:4:VAL:CG2	1:B:96:MSE:HE1	2.39	0.52
1:B:78:THR:CG2	1:B:81:GLN:HG3	2.38	0.52
1:A:85:GLN:OE1	1:A:120:ARG:HD2	2.10	0.52
1:A:6:LEU:N	1:A:6:LEU:HD12	2.24	0.52
1:A:183:TYR:CD1	1:B:117:PHE:HB3	2.44	0.52
1:C:30:ASP:HB3	4:C:223:PO4:O3	2.09	0.52
1:B:105:ARG:CG	1:B:105:ARG:NH1	2.63	0.51
1:B:99:ILE:HG22	1:B:100:GLY:N	2.26	0.51
1:D:126:ARG:HH21	1:D:126:ARG:CG	2.20	0.51
1:D:26:PHE:H	1:D:44:GLN:NE2	2.07	0.51
1:A:171:ARG:HD2	1:A:194:GLU:OE1	2.11	0.51
1:C:1:MSE:H2	1:C:2:SER:C	2.12	0.51
1:D:7:VAL:HG21	1:D:36:LEU:CD2	2.39	0.51
1:A:126:ARG:O	1:A:129:ARG:NH1	2.44	0.50
1:D:133:ARG:HG3	1:D:133:ARG:HH11	1.76	0.50
1:A:44:GLN:HA	1:A:66:GLU:HG2	1.94	0.50
1:B:4:VAL:HG22	1:B:25:TYR:HB3	1.94	0.50
1:C:117:PHE:HB3	1:D:183:TYR:CD1	2.47	0.50
1:C:129:ARG:HH22	1:C:138:GLN:CD	2.13	0.50
1:C:3:ARG:HG2	1:C:95:GLU:HB3	1.93	0.50
1:A:201:PHE:CE2	1:A:206:ILE:HD12	2.47	0.50
1:A:126:ARG:HA	1:A:126:ARG:NE	2.26	0.49
1:C:1:MSE:H3	1:C:3:ARG:H	1.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:HB3	1:B:120:ARG:NH2	2.26	0.49
1:C:150:GLU:H	1:C:210:GLN:HE21	1.58	0.49
1:D:72:PRO:O	1:D:75:LYS:HG2	2.12	0.49
1:D:199:PHE:HE1	1:D:201:PHE:CE2	2.29	0.49
1:D:173:LYS:HG2	1:D:173:LYS:O	2.11	0.49
1:C:146:ILE:HD12	1:C:146:ILE:C	2.33	0.49
1:A:129:ARG:CZ	1:A:138:GLN:NE2	2.75	0.49
1:C:124:VAL:HG12	1:C:127:GLN:OE1	2.12	0.49
1:D:54:SER:O	1:D:56:GLU:N	2.46	0.49
1:A:132:ASP:HB2	1:A:135:ASN:HB2	1.94	0.49
1:A:161:LEU:HD12	1:A:205:MSE:HE2	1.94	0.49
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.78	0.49
1:D:136:SER:HB2	1:D:153:LYS:HE2	1.94	0.48
1:C:88:LEU:CD1	1:C:124:VAL:HG21	2.40	0.48
1:C:77:ASP:HB2	1:C:82:LEU:HD13	1.96	0.48
1:A:48:GLY:HA2	1:A:79:ASP:OD1	2.13	0.48
1:B:34:LEU:O	1:B:38:GLU:HG2	2.13	0.48
1:B:88:LEU:HD11	1:B:124:VAL:HG21	1.96	0.48
1:A:144:SER:HA	1:A:200:SER:HB3	1.95	0.47
1:A:169:LEU:HD22	1:A:175:LEU:HA	1.96	0.47
1:B:11:ASN:HA	1:B:12:PRO:HD3	1.75	0.47
1:D:133:ARG:HG3	1:D:133:ARG:NH1	2.30	0.47
1:A:162:THR:HB	1:A:163:PRO:HD2	1.96	0.47
1:B:125:LEU:HD12	1:B:125:LEU:C	2.34	0.47
1:B:16:PRO:HG2	1:B:99:ILE:HD12	1.96	0.47
1:C:194:GLU:C	1:C:196:ALA:H	2.18	0.47
1:A:141:ALA:HB1	1:A:142:PRO:HD2	1.97	0.47
1:B:78:THR:HG22	1:B:81:GLN:CD	2.35	0.47
1:C:1:MSE:HB2	1:C:3:ARG:HD3	1.95	0.47
1:C:12:PRO:HA	1:C:15:TRP:CD1	2.49	0.47
1:C:58:TYR:OH	1:C:70:GLN:HG3	2.14	0.47
1:C:101:ALA:HB1	1:C:112:ASN:HD21	1.77	0.47
1:A:62:GLN:HE22	1:D:62:GLN:NE2	2.10	0.47
1:B:14:ASP:O	1:B:132:ASP:HB2	2.15	0.47
1:D:125:LEU:HD12	1:D:125:LEU:C	2.35	0.47
1:B:105:ARG:HH11	1:B:105:ARG:CB	2.28	0.46
1:A:133:ARG:NH1	1:A:133:ARG:HG3	2.30	0.46
1:B:78:THR:HG22	1:B:81:GLN:CG	2.45	0.46
1:B:170:ARG:HH22	1:B:177:THR:HG22	1.79	0.46
1:C:1:MSE:H2	1:C:3:ARG:H	1.58	0.46
1:C:149:LYS:HG2	1:C:150:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:TYR:HA	1:D:44:GLN:HE22	1.81	0.46
1:D:25:TYR:HA	1:D:44:GLN:NE2	2.30	0.46
1:B:25:TYR:CE1	1:B:44:GLN:HB3	2.50	0.46
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.81	0.46
1:D:107:ASP:OD1	1:D:107:ASP:N	2.48	0.46
1:C:153:LYS:HA	1:C:153:LYS:HD3	1.77	0.46
1:C:164:VAL:HG13	1:C:165:GLU:N	2.30	0.46
1:A:161:LEU:HD12	1:A:205:MSE:CE	2.46	0.46
1:B:49:ASP:O	1:B:50:PHE:HB2	2.17	0.45
1:C:6:LEU:HD12	1:C:6:LEU:N	2.31	0.45
1:C:91:PHE:HB3	1:C:94:ALA:CB	2.46	0.45
1:C:149:LYS:HB2	1:C:192:PHE:CD2	2.51	0.45
1:A:169:LEU:O	1:A:169:LEU:HD23	2.16	0.45
1:A:184:PRO:HG2	1:B:117:PHE:CE2	2.51	0.45
1:B:4:VAL:HB	1:B:96:MSE:HE2	1.94	0.45
1:B:29:ILE:CD1	1:B:80:THR:HG23	2.46	0.45
1:C:124:VAL:CB	1:C:127:GLN:OE1	2.64	0.45
1:D:54:SER:C	1:D:56:GLU:H	2.20	0.45
1:A:115:LEU:N	1:A:116:PRO:HD2	2.32	0.45
1:D:115:LEU:N	1:D:116:PRO:HD2	2.32	0.45
1:B:78:THR:HG22	1:B:81:GLN:OE1	2.17	0.45
1:A:75:LYS:HD2	1:A:77:ASP:O	2.17	0.45
1:C:54:SER:O	1:C:57:GLU:HB2	2.17	0.45
1:B:4:VAL:CB	1:B:96:MSE:HE1	2.46	0.44
1:D:116:PRO:HG3	1:D:139:TYR:CD1	2.52	0.44
1:B:78:THR:HG22	1:B:81:GLN:HG3	1.99	0.44
1:B:136:SER:HB2	1:B:153:LYS:HE2	1.99	0.44
1:D:98:ILE:HB	1:D:130:LEU:HD23	2.00	0.44
1:B:53:LEU:N	1:B:53:LEU:HD23	2.33	0.44
1:A:101:ALA:HB1	1:A:112:ASN:ND2	2.33	0.44
1:C:7:VAL:HA	1:C:99:ILE:HG22	1.99	0.44
1:D:50:PHE:CD2	1:D:58:TYR:HE1	2.35	0.44
1:C:25:TYR:CD1	1:C:44:GLN:OE1	2.70	0.44
1:D:166:ASN:OD1	1:D:178:ASN:HA	2.18	0.44
1:D:169:LEU:HD13	1:D:176:LEU:HD12	2.00	0.43
1:D:172:SER:HB2	1:D:174:TYR:O	2.18	0.43
1:B:19:GLU:HA	1:B:20:PRO:HD3	1.85	0.43
1:B:62:GLN:HG3	1:B:68:LEU:HD22	1.99	0.43
1:C:55:ARG:HD2	1:C:55:ARG:HA	1.66	0.43
1:C:124:VAL:CG1	1:C:127:GLN:OE1	2.66	0.43
1:C:194:GLU:HG3	1:C:196:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:HD3	1:C:194:GLU:OE1	2.18	0.43
1:D:199:PHE:HE1	1:D:201:PHE:HE2	1.65	0.43
1:B:9:GLY:O	1:B:35:HIS:HE1	2.02	0.43
1:A:26:PHE:H	1:A:44:GLN:HE21	1.64	0.43
1:A:132:ASP:HB3	1:A:134:GLN:H	1.84	0.43
1:B:6:LEU:HD12	1:B:6:LEU:N	2.33	0.43
1:C:171:ARG:HD3	1:C:194:GLU:CD	2.38	0.43
1:C:90:ARG:C	1:C:91:PHE:CD2	2.92	0.43
1:C:1:MSE:H3	1:C:3:ARG:N	2.11	0.43
1:D:19:GLU:O	1:D:22:THR:HG23	2.18	0.43
1:D:54:SER:C	1:D:56:GLU:N	2.72	0.43
1:B:75:LYS:NZ	1:B:79:ASP:OD1	2.51	0.42
1:B:91:PHE:N	1:B:92:PRO:HD3	2.33	0.42
1:D:118:GLU:HA	1:D:119:PRO:HD3	1.96	0.42
1:C:29:ILE:O	1:C:32:GLY:N	2.48	0.42
1:C:50:PHE:C	1:C:52:SER:H	2.22	0.42
1:A:48:GLY:HA2	1:A:79:ASP:CG	2.39	0.42
1:A:69:ILE:HD12	1:A:86:GLU:HG3	2.01	0.42
1:B:69:ILE:CD1	1:B:86:GLU:HG3	2.48	0.42
1:B:12:PRO:O	1:B:15:TRP:HB2	2.19	0.42
1:D:37:LEU:HD22	1:D:64:THR:HG21	2.02	0.42
1:A:152:ASP:O	1:A:212:LYS:HD3	2.19	0.42
1:D:88:LEU:HD11	1:D:124:VAL:HG21	2.00	0.42
1:D:164:VAL:CG1	1:D:165:GLU:N	2.82	0.42
1:D:102:THR:HG22	1:D:132:ASP:OD1	2.20	0.42
1:C:150:GLU:N	1:C:210:GLN:HE22	2.17	0.41
1:A:116:PRO:HG3	1:A:139:TYR:CD1	2.54	0.41
1:C:5:LEU:HD12	1:C:97:THR:O	2.20	0.41
1:C:141:ALA:O	1:C:142:PRO:C	2.57	0.41
1:C:45:LEU:HD11	1:C:69:ILE:HD12	2.02	0.41
1:C:164:VAL:HG12	1:C:181:VAL:CG2	2.50	0.41
1:B:7:VAL:HG21	1:B:36:LEU:HG	2.03	0.41
1:D:101:ALA:HB1	1:D:112:ASN:HD22	1.86	0.41
1:D:115:LEU:O	1:D:118:GLU:HG3	2.20	0.41
1:A:115:LEU:O	1:A:118:GLU:HG3	2.21	0.41
1:A:141:ALA:HB1	1:A:142:PRO:CD	2.51	0.41
1:D:8:ALA:HB3	1:D:100:GLY:C	2.41	0.41
1:C:126:ARG:NH2	1:C:138:GLN:OE1	2.53	0.41
1:A:188:ALA:HB1	1:B:107:ASP:OD2	2.20	0.41
1:B:114:TRP:O	1:B:117:PHE:HB2	2.20	0.41
1:A:7:VAL:O	1:A:32:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:THR:HG22	1:C:81:GLN:CG	2.51	0.40
1:A:158:TYR:HE1	1:A:199:PHE:CD2	2.39	0.40
1:C:107:ASP:N	1:C:107:ASP:OD1	2.52	0.40
2:D:902:TPP:N4'	2:D:902:TPP:C2	2.85	0.40
1:C:106:ILE:HD12	1:D:137:ILE:HD11	2.02	0.40
1:D:165:GLU:HB2	1:D:203:ALA:HB3	2.01	0.40
1:C:105:ARG:NH2	1:C:108:HIS:CE1	2.90	0.40
1:C:169:LEU:O	1:C:170:ARG:HD2	2.20	0.40
1:D:160:CYS:O	1:D:184:PRO:HA	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	211/222 (95%)	203 (96%)	8 (4%)	0	100	100
1	B	211/222 (95%)	201 (95%)	9 (4%)	1 (0%)	29	58
1	C	212/222 (96%)	194 (92%)	16 (8%)	2 (1%)	17	44
1	D	211/222 (95%)	198 (94%)	10 (5%)	3 (1%)	11	31
All	All	845/888 (95%)	796 (94%)	43 (5%)	6 (1%)	22	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	ALA
1	C	103	GLY
1	D	13	SER
1	C	10	GLY
1	B	187	TYR
1	D	187	TYR

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	183/189 (97%)	167 (91%)	16 (9%)	10 27
1	B	183/189 (97%)	168 (92%)	15 (8%)	11 30
1	C	184/189 (97%)	167 (91%)	17 (9%)	9 24
1	D	183/189 (97%)	170 (93%)	13 (7%)	14 36
All	All	733/756 (97%)	672 (92%)	61 (8%)	11 29

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	18	ILE
1	A	19	GLU
1	A	30	ASP
1	A	49	ASP
1	A	52	SER
1	A	75	LYS
1	A	105	ARG
1	A	122	GLN
1	A	126	ARG
1	A	132	ASP
1	A	152	ASP
1	A	169	LEU
1	A	173	LYS
1	A	177	THR
1	A	205	MSE
1	B	2	SER
1	B	18	ILE
1	B	40	ASP
1	B	53	LEU
1	B	59	HIS
1	B	74	GLU
1	B	75	LYS
1	B	93	GLN

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Mol	Chain	Res	Type
1	B	105	ARG
1	B	126	ARG
1	B	146	ILE
1	B	149	LYS
1	B	180	ASP
1	B	190	ASN
1	B	194	GLU
1	C	2	SER
1	C	18	ILE
1	C	31	ARG
1	C	40	ASP
1	C	55	ARG
1	C	59	HIS
1	C	62	GLN
1	C	65	THR
1	C	74	GLU
1	C	82	LEU
1	C	93	GLN
1	C	99	ILE
1	C	105	ARG
1	C	126	ARG
1	C	156	LEU
1	C	164	VAL
1	C	170	ARG
1	D	18	ILE
1	D	22	THR
1	D	40	ASP
1	D	66	GLU
1	D	75	LYS
1	D	105	ARG
1	D	122	GLN
1	D	126	ARG
1	D	129	ARG
1	D	132	ASP
1	D	152	ASP
1	D	177	THR
1	D	211	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN

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Mol	Chain	Res	Type
1	A	134	GLN
1	A	138	GLN
1	A	178	ASN
1	A	210	GLN
1	B	35	HIS
1	B	127	GLN
1	B	210	GLN
1	C	35	HIS
1	C	93	GLN
1	C	108	HIS
1	C	178	ASN
1	C	210	GLN
1	D	44	GLN
1	D	62	GLN
1	D	70	GLN
1	D	127	GLN
1	D	134	GLN
1	D	138	GLN
1	D	178	ASN
1	D	179	GLN
1	D	210	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	TPP	D	902	3	22,27,27	5.62	13 (59%)	29,40,40	5.02	19 (65%)
2	TPP	A	902	3	22,27,27	5.73	13 (59%)	29,40,40	4.95	19 (65%)
4	PO4	B	223	-	4,4,4	0.73	0	6,6,6	0.74	0
4	PO4	C	223	-	4,4,4	0.70	0	6,6,6	0.51	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	TPP	D	902	3	-	6/16/17/17	0/2/2/2
2	TPP	A	902	3	-	5/16/17/17	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	TPP	C4-N3	14.50	1.52	1.39
2	D	902	TPP	C4-N3	13.67	1.51	1.39
2	A	902	TPP	C4'-N3'	9.60	1.48	1.35
2	D	902	TPP	C4'-N3'	9.13	1.48	1.35
2	A	902	TPP	C2'-N1'	8.77	1.48	1.34
2	A	902	TPP	C5'-C4'	8.74	1.57	1.42
2	D	902	TPP	C2'-N1'	8.74	1.48	1.34
2	D	902	TPP	C5'-C4'	8.36	1.57	1.42
2	D	902	TPP	C6'-C5'	8.27	1.55	1.37
2	A	902	TPP	C6'-C5'	7.87	1.54	1.37
2	A	902	TPP	C2'-N3'	7.36	1.47	1.34
2	D	902	TPP	C2'-N3'	6.78	1.46	1.34
2	D	902	TPP	C6-C5	6.53	1.53	1.50
2	D	902	TPP	C6'-N1'	5.98	1.47	1.34
2	A	902	TPP	C6'-N1'	5.81	1.46	1.34
2	D	902	TPP	C2-N3	5.65	1.47	1.36
2	A	902	TPP	C6-C5	5.55	1.53	1.50
2	A	902	TPP	C2-N3	5.43	1.47	1.36
2	A	902	TPP	C4'-N4'	5.24	1.47	1.34
2	D	902	TPP	C4'-N4'	5.04	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	TPP	C7'-C5'	2.74	1.56	1.51
2	A	902	TPP	C7'-C5'	2.29	1.56	1.51
2	A	902	TPP	PB-O1B	2.13	1.57	1.50
2	A	902	TPP	PA-O1A	2.09	1.58	1.50
2	D	902	TPP	PB-O1B	2.04	1.57	1.50
2	D	902	TPP	PA-O1A	2.02	1.58	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	TPP	C6-C5-C4	-13.60	116.52	127.43
2	D	902	TPP	C6-C5-C4	-12.94	117.05	127.43
2	D	902	TPP	C5'-C4'-N3'	-9.01	107.08	121.24
2	D	902	TPP	C5'-C4'-N4'	-8.36	110.33	122.19
2	A	902	TPP	C5'-C4'-N3'	-8.12	108.48	121.24
2	D	902	TPP	CM4-C4-N3	-8.02	112.31	122.53
2	A	902	TPP	N1'-C2'-N3'	-7.40	112.81	125.54
2	A	902	TPP	CM4-C4-N3	-7.33	113.19	122.53
2	A	902	TPP	CM4-C4-C5	-7.31	111.61	127.60
2	D	902	TPP	N1'-C2'-N3'	-7.07	113.36	125.54
2	D	902	TPP	C6'-C5'-C4'	-7.01	106.17	115.72
2	A	902	TPP	C5'-C4'-N4'	-6.89	112.42	122.19
2	A	902	TPP	C6'-C5'-C4'	-6.68	106.63	115.72
2	A	902	TPP	C5'-C6'-N1'	-6.56	112.89	123.82
2	D	902	TPP	C5'-C6'-N1'	-6.36	113.22	123.82
2	D	902	TPP	C7'-N3-C2	-6.09	114.35	125.35
2	D	902	TPP	N4'-C4'-N3'	-5.73	108.93	117.03
2	D	902	TPP	CM4-C4-C5	-5.62	115.31	127.60
2	A	902	TPP	N4'-C4'-N3'	-5.01	109.95	117.03
2	A	902	TPP	C7'-N3-C2	-4.89	116.52	125.35
2	A	902	TPP	CM2-C2'-N1'	-4.46	112.23	117.14
2	A	902	TPP	C7'-C5'-C6'	-4.32	112.43	120.69
2	D	902	TPP	C7'-C5'-C4'	-4.06	109.90	121.83
2	D	902	TPP	CM2-C2'-N1'	-4.01	112.72	117.14
2	A	902	TPP	O3B-PB-O3A	4.00	118.06	104.64
2	D	902	TPP	O3B-PB-O3A	3.91	117.74	104.64
2	A	902	TPP	C7'-C5'-C4'	-3.60	111.23	121.83
2	A	902	TPP	O2B-PB-O1B	-3.54	96.81	110.68
2	D	902	TPP	O2B-PB-O1B	-3.45	97.17	110.68
2	D	902	TPP	C7'-C5'-C6'	-3.36	114.27	120.69
2	D	902	TPP	O7-PA-O1A	-3.20	96.58	109.07
2	A	902	TPP	O7-PA-O1A	-2.92	97.67	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	902	TPP	O2A-PA-O7	2.85	121.00	107.75
2	A	902	TPP	O3B-PB-O1B	2.77	121.54	110.68
2	A	902	TPP	O2A-PA-O7	2.72	120.38	107.75
2	D	902	TPP	O3B-PB-O1B	2.64	121.02	110.68
2	A	902	TPP	O2A-PA-O1A	2.12	122.71	112.24
2	D	902	TPP	O2A-PA-O1A	2.09	122.59	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	TPP	C6'-C5'-C7'-N3
2	A	902	TPP	C4-C5-C6-C7
2	A	902	TPP	C5-C6-C7-O7
2	A	902	TPP	C7-O7-PA-O2A
2	D	902	TPP	C6'-C5'-C7'-N3
2	D	902	TPP	C4-C5-C6-C7
2	D	902	TPP	C5-C6-C7-O7
2	D	902	TPP	C7-O7-PA-O1A
2	D	902	TPP	C7-O7-PA-O2A
2	A	902	TPP	C7-O7-PA-O3A
2	D	902	TPP	C7-O7-PA-O3A

There are no ring outliers.

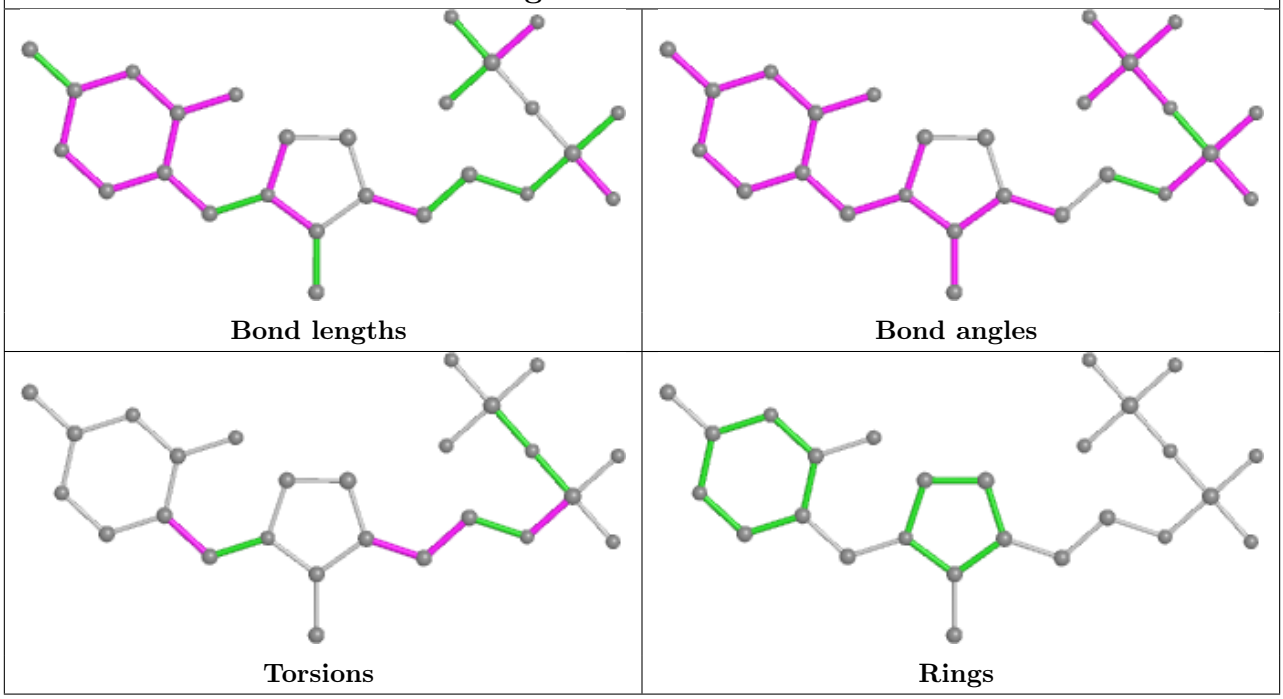
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	TPP	3	0
2	A	902	TPP	1	0
4	C	223	PO4	1	0

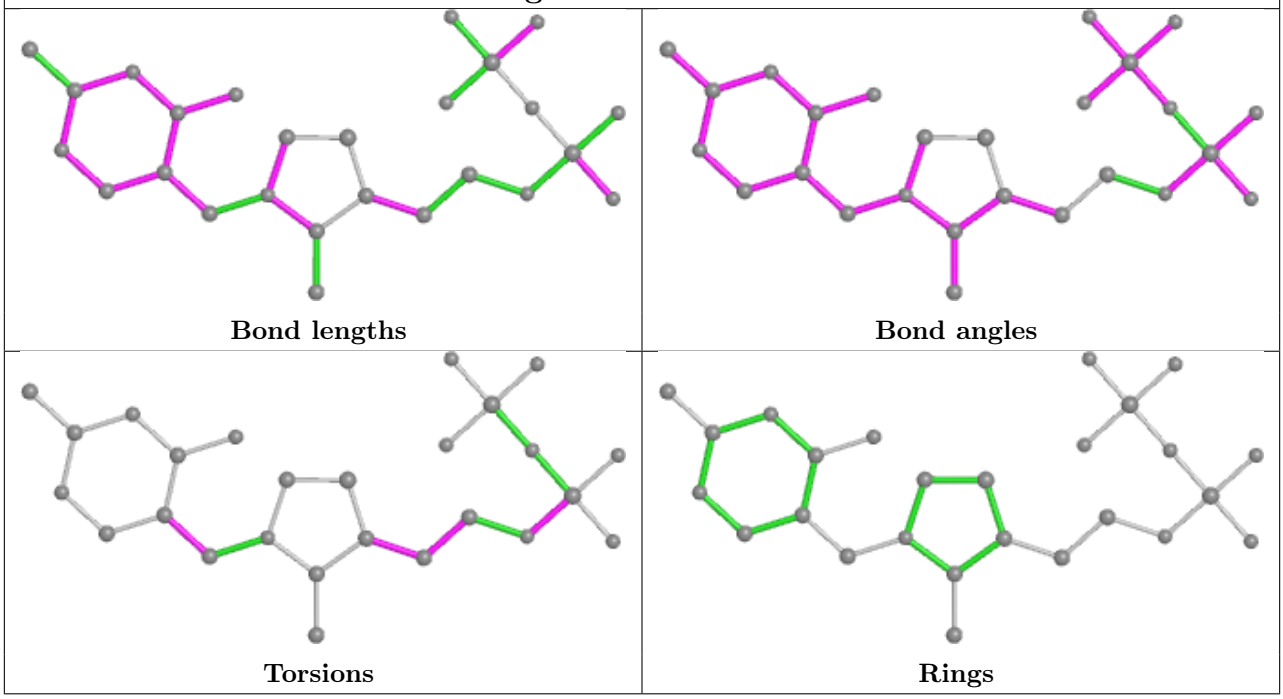
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand TPP D 902



Ligand TPP A 902



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^{th} 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	211/222 (95%)	-0.06	0 100 100	25, 36, 49, 59	0
1	B	211/222 (95%)	-0.18	0 100 100	24, 40, 56, 81	0
1	C	211/222 (95%)	0.05	2 (0%) 84 82	35, 48, 66, 86	0
1	D	211/222 (95%)	0.38	14 (6%) 18 13	31, 50, 74, 80	0
All	All	844/888 (95%)	0.05	16 (1%) 66 63	24, 43, 68, 86	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	ILE	4.0
1	D	103	GLY	3.9
1	D	55	ARG	3.1
1	D	182	PRO	2.7
1	D	178	ASN	2.6
1	D	177	THR	2.5
1	D	146	ILE	2.4
1	C	76	ASP	2.4
1	D	171	ARG	2.4
1	D	176	LEU	2.3
1	D	192	PHE	2.3
1	D	158	TYR	2.3
1	D	195	GLU	2.2
1	D	198	ALA	2.2
1	D	175	LEU	2.2
1	C	21	ALA	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

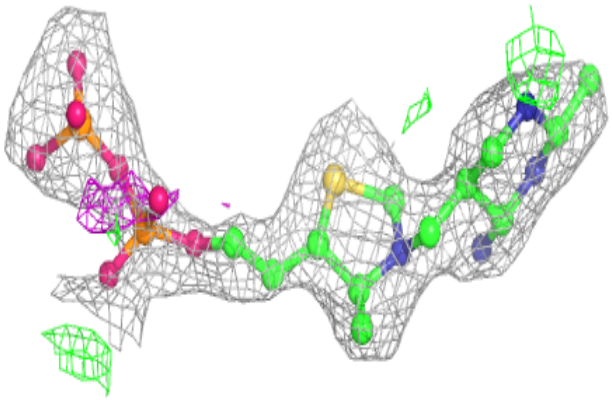
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

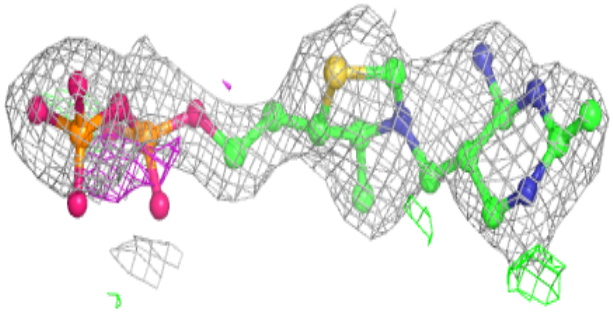
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	223	1/1	0.69	0.18	61,61,61,61	0
3	MG	B	224	1/1	0.74	0.30	50,50,50,50	0
3	MG	A	225	1/1	0.83	0.25	63,63,63,63	0
3	MG	D	223	1/1	0.87	0.33	61,61,61,61	0
4	PO4	B	223	5/5	0.89	0.28	51,52,63,69	0
2	TPP	D	902	26/26	0.90	0.22	38,52,129,185	0
3	MG	B	225	1/1	0.91	0.17	47,47,47,47	0
2	TPP	A	902	26/26	0.92	0.20	32,48,129,185	0
3	MG	A	226	1/1	0.92	0.35	40,40,40,40	0
3	MG	D	224	1/1	0.93	0.32	62,62,62,62	0
4	PO4	C	223	5/5	0.93	0.17	53,53,63,68	0
3	MG	B	226	1/1	0.95	0.30	48,48,48,48	0
3	MG	C	225	1/1	0.95	0.22	25,25,25,25	0
3	MG	C	224	1/1	0.96	0.37	43,43,43,43	0
3	MG	A	224	1/1	0.98	0.18	33,33,33,33	0

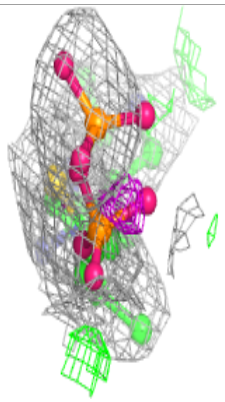
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TPP D 902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

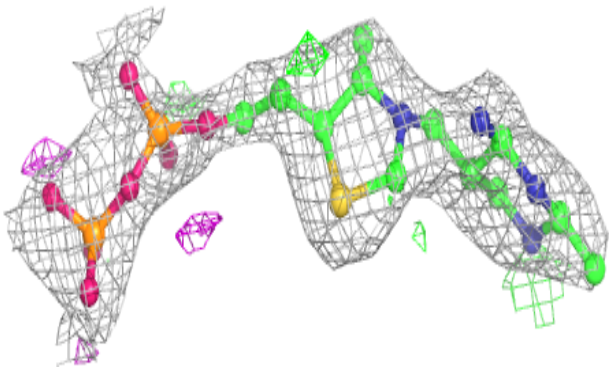


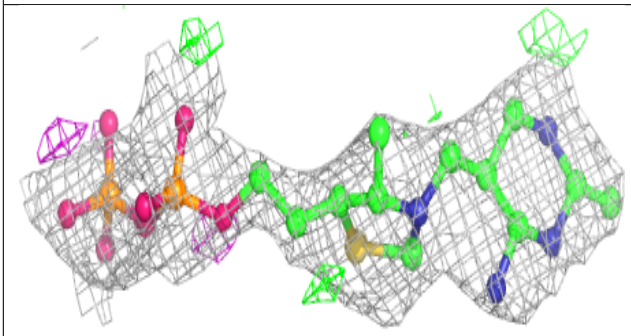


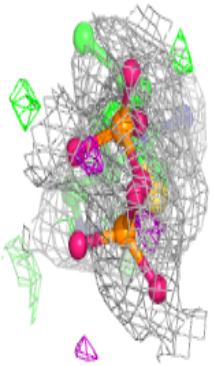


Electron density around TPP A 902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.