Preliminary Full wwPDB X-ray Structure Validation Report (i)

Jul 29, 2021 – 01:22 PM EDT

Deposition ID : D_1000258589

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

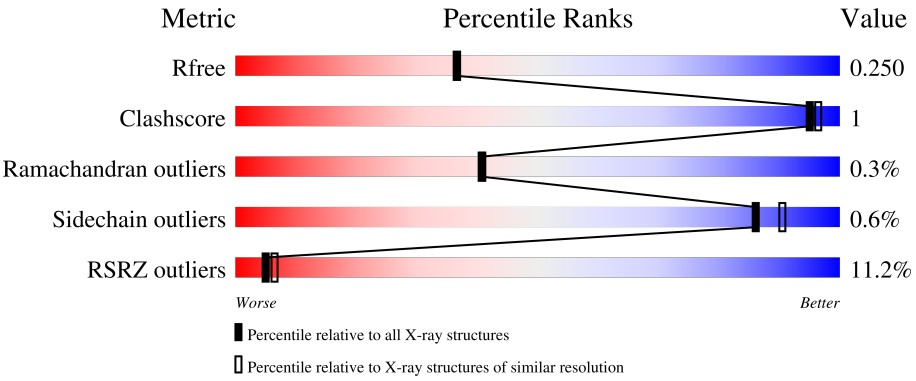
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	AAA	396	12% 95%
1	BBB	396	8% 94% 5%
1	CCC	396	9% 93%
1	DDD	396	14% 91%

2 Entry composition (i)

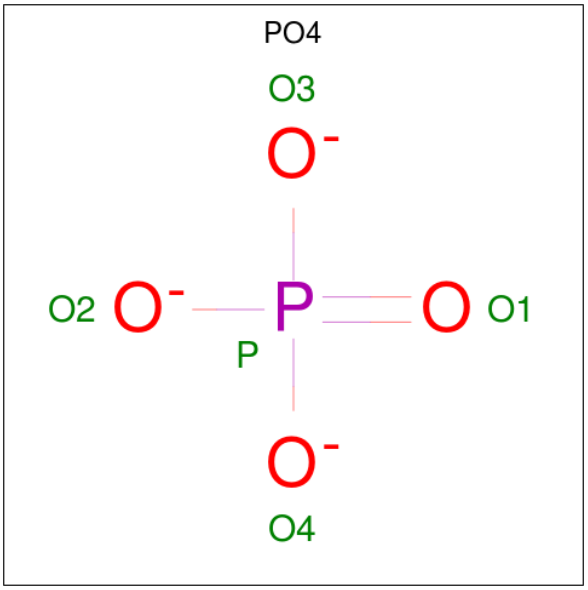
There are 4 unique types of molecules in this entry. The entry contains 11732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PfTrpB2B9-H275E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	385	Total	C	N	O	P	S	0	1	0
			2832	1804	477	538	1	12			
1	BBB	389	Total	C	N	O	P	S	0	3	0
			2927	1866	503	545	1	12			
1	CCC	385	Total	C	N	O	P	S	0	1	0
			2858	1820	488	537	1	12			
1	DDD	379	Total	C	N	O	P	S	0	3	0
			2819	1802	478	526	1	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	EEE	1	Total	O	P		0	0
			5	4	1			
2	EaE	1	Total	O	P		0	0
			5	4	1			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	EbE	1	Total O P 5 4 1	0	0
2	EcE	1	Total O P 5 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	GGG	1	Total Na 1 1	0	0
3	GaG	1	Total Na 1 1	0	0
3	GbG	1	Total Na 1 1	0	0
3	GcG	1	Total Na 1 1	0	0

- Molecule 4 is water.

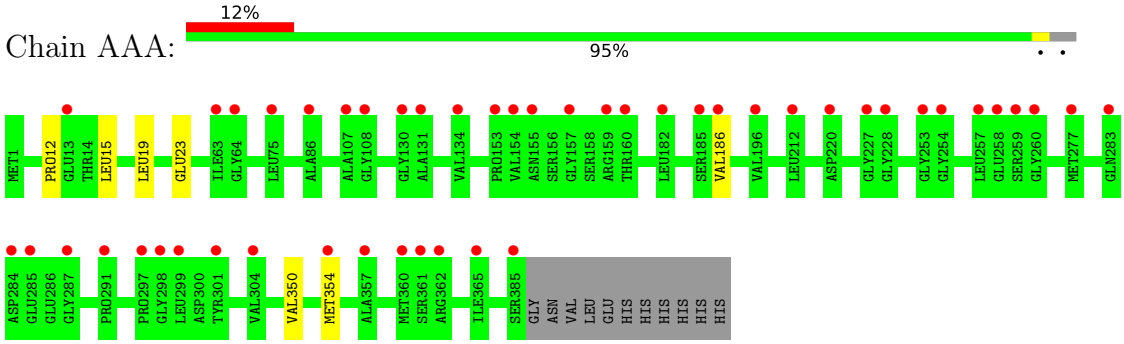
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	FFF	272	Total O 272 272	0	0

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.

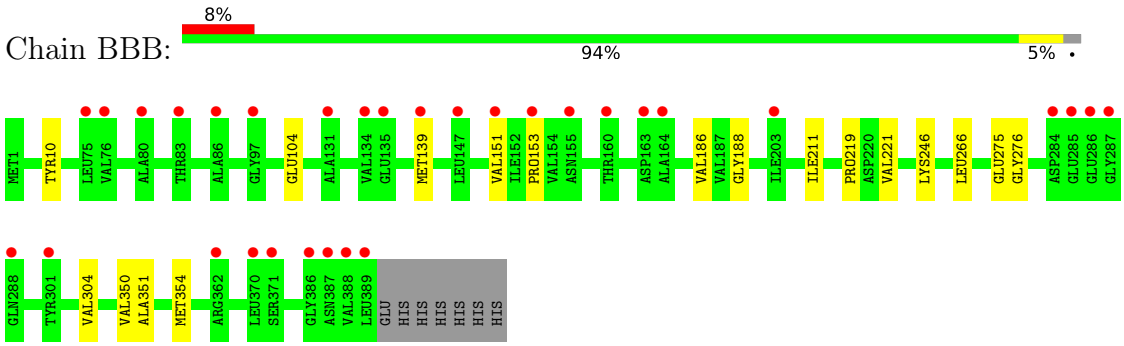
• Molecule 1: PfTrpB2B9-H275E

Chain AAA:



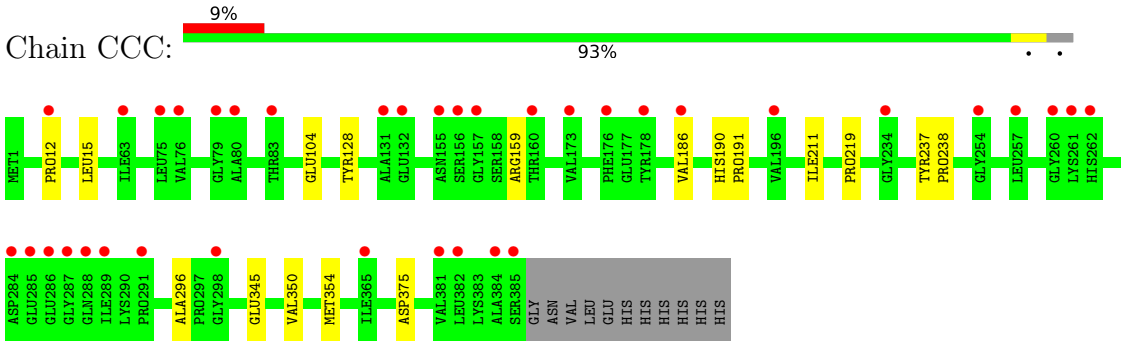
• Molecule 1: PfTrpB2B9-H275E

Chain BBB:



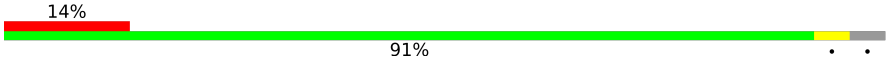
• Molecule 1: PfTrpB2B9-H275E

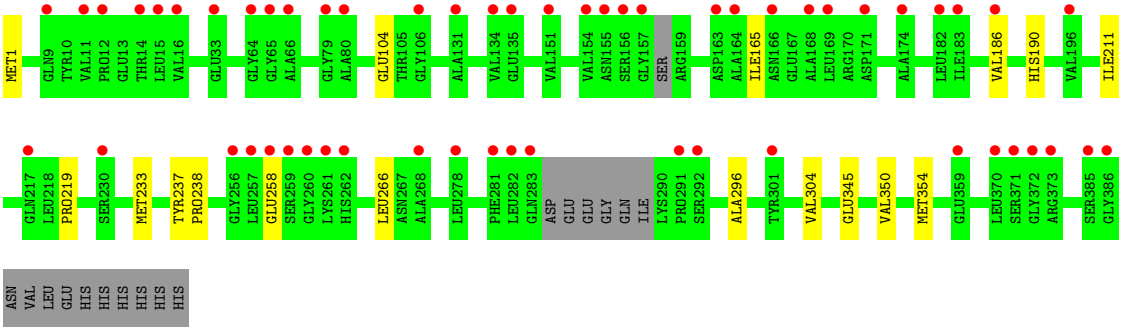
Chain CCC:



• Molecule 1: PfTrpB2B9-H275E

Chain DDD:




MET1
GLN9
TYR10
VAL11
PRO12
GLU13
THR14
LEU15
VAL16
GLU33
GLY64
GLY65
ALA66
GLY79
ALA80
GLU104
THR105
GLY106
ALA131
VAL134
GLU135
VAL151
VAL154
ASN155
SER156
GLY157
SER
ARG159
ASP163
ALA164
ILE165
ASN166
GLU167
ALA168
LEU169
ARG170
ASP171
ALA174
LEU182
ILE183
VAL186
HIS190
VAL196
ILE211
GLN217
LEU218
PRO219
SER230
MET233
TYR237
PRO238
GLY256
LEU257
GLU258
SER259
GLY260
LYS261
HIS262
LEU266
ASN267
ALA268
LEU278
PHE281
LEU282
GLN283
ASP
GLU
GLU
GLY
GLN
ILE
LYS290
PRO291
SER292
ALA296
TYR301
VAL304
GLU345
VAL350
MET354
GLU359
LEU370
SER371
GLY372
ARG373
SER385
GLY386
ASN
VAL
LEU
GLU
HIS
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.01Å 82.68Å 322.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.10) 99.5 (39.11-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.248 0.221 , 0.250	Depositor DCC
R_{free} test set	4501 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11732	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: PO4, NA, LLP

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	AAA	0.67	0/2868	0.70	0/3903
1	BBB	0.65	0/2967	0.70	0/4023
1	CCC	0.67	0/2894	0.70	0/3931
1	DDD	0.67	0/2859	0.70	0/3880
All	All	0.66	0/11588	0.70	0/15737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AAA	2832	0	2687	3	0
1	BBB	2927	0	2859	8	0
1	CCC	2858	0	2757	8	0
1	DDD	2819	0	2717	7	0
2	EEE	5	0	0	0	0
2	EaE	5	0	0	0	0
2	EbE	5	0	0	0	0
2	EcE	5	0	0	0	0
3	GGG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GaG	1	0	0	0	0
3	GbG	1	0	0	0	0
3	GcG	1	0	0	0	0
4	FFF	272	0	0	0	0
All	All	11732	0	11020	26	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 1.

All (26) 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:DDD:211:ILE:HG21	1:DDD:219:PRO:HD3	1.88	0.56
1:BBB:221:VAL:HG22	1:BBB:246:LYS:HE2	1.90	0.54
1:DDD:1:MET:HB3	1:DDD:190:HIS:CG	2.46	0.51
1:CCC:12:PRO:HD2	1:CCC:15:LEU:HD12	1.94	0.49
1:BBB:10:TYR:O	1:BBB:276:GLY:HA2	2.12	0.49
1:DDD:104:GLU:HG3	1:DDD:165:ILE:HG12	1.95	0.48
1:CCC:104:GLU:HA	1:CCC:128:TYR:O	2.14	0.47
1:DDD:266:LEU:HG	1:DDD:304:VAL:HG11	1.96	0.47
1:CCC:211:ILE:HG21	1:CCC:219:PRO:HD3	1.95	0.47
1:BBB:211:ILE:HG21	1:BBB:219:PRO:HD3	1.96	0.46
1:BBB:351:ALA:HA	1:BBB:354:MET:HE2	1.98	0.46
1:CCC:350:VAL:O	1:CCC:354:MET:HG3	2.16	0.45
1:BBB:188:GLY:HA2	1:BBB:275:GLU:O	2.16	0.45
1:BBB:151:VAL:O	1:BBB:153:PRO:HD3	2.17	0.44
1:AAA:12:PRO:HD2	1:AAA:15:LEU:HD12	1.99	0.44
1:CCC:190:HIS:CG	1:CCC:191:PRO:HA	2.53	0.43
1:BBB:266:LEU:HG	1:BBB:304:VAL:HG11	2.00	0.43
1:AAA:350:VAL:O	1:AAA:354:MET:HG3	2.19	0.42
1:AAA:19:LEU:O	1:AAA:23:GLU:HG3	2.20	0.42
1:DDD:237:TYR:HB3	1:DDD:238:PRO:HD3	2.01	0.42
1:CCC:296:ALA:HB1	1:CCC:345:GLU:HG3	2.02	0.41
1:DDD:296:ALA:HB1	1:DDD:345:GLU:HG3	2.02	0.41
1:DDD:350:VAL:O	1:DDD:354:MET:HG3	2.20	0.41
1:CCC:237:TYR:HB3	1:CCC:238:PRO:HD3	2.01	0.41
1:BBB:350:VAL:O	1:BBB:354:MET:HG3	2.20	0.41
1:CCC:190:HIS:ND1	1:CCC:191:PRO:HA	2.36	0.41

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	AAA	383/396 (97%)	372 (97%)	10 (3%)	1 (0%)	41	41
1	BBB	389/396 (98%)	379 (97%)	9 (2%)	1 (0%)	41	41
1	CCC	383/396 (97%)	375 (98%)	7 (2%)	1 (0%)	41	41
1	DDD	375/396 (95%)	367 (98%)	7 (2%)	1 (0%)	41	41
All	All	1530/1584 (97%)	1493 (98%)	33 (2%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	186	VAL
1	AAA	186	VAL
1	BBB	186	VAL
1	CCC	186	VAL

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	AAA	268/312 (86%)	268 (100%)	0	100	100
1	BBB	284/312 (91%)	282 (99%)	2 (1%)	84	88
1	CCC	275/312 (88%)	273 (99%)	2 (1%)	84	88
1	DDD	269/312 (86%)	267 (99%)	2 (1%)	84	88
All	All	1096/1248 (88%)	1090 (100%)	6 (0%)	86	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	104	GLU
1	BBB	139	MET
1	CCC	159	ARG
1	CCC	375	ASP
1	DDD	233	MET
1	DDD	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	AAA	82	1	23,24,25	0.46	0	25,32,34	0.48	0
1	LLP	BBB	82	1	23,24,25	0.45	0	25,32,34	0.63	0
1	LLP	CCC	82	1	23,24,25	0.45	0	25,32,34	0.52	0
1	LLP	DDD	82	1	23,24,25	0.47	0	25,32,34	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	AAA	82	1	-	5/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	BBB	82	1	-	3/16/17/19	0/1/1/1
1	LLP	CCC	82	1	-	3/16/17/19	0/1/1/1
1	LLP	DDD	82	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	82	LLP	C5'-OP4-P-OP1
1	AAA	82	LLP	C5'-OP4-P-OP3
1	BBB	82	LLP	C4-C4'-NZ-CE
1	BBB	82	LLP	O-C-CA-CB
1	CCC	82	LLP	C4-C4'-NZ-CE
1	DDD	82	LLP	C4-C4'-NZ-CE
1	DDD	82	LLP	O-C-CA-CB
1	DDD	82	LLP	CG-CD-CE-NZ
1	AAA	82	LLP	C4-C4'-NZ-CE
1	BBB	82	LLP	CG-CD-CE-NZ
1	CCC	82	LLP	CG-CD-CE-NZ
1	CCC	82	LLP	C5'-OP4-P-OP1
1	AAA	82	LLP	CG-CD-CE-NZ
1	AAA	82	LLP	C5'-OP4-P-OP2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	PO4	EEE	1	-	4,4,4	0.69	0	6,6,6	0.42	0
2	PO4	EaE	2	-	4,4,4	0.68	0	6,6,6	0.42	0
2	PO4	EcE	4	-	4,4,4	0.65	0	6,6,6	0.43	0
2	PO4	EbE	3	-	4,4,4	0.67	0	6,6,6	0.43	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

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	AAA	384/396 (96%)	0.84	48 (12%) 3 5	27, 54, 83, 96	0
1	BBB	388/396 (97%)	0.56	31 (7%) 12 16	22, 37, 70, 102	0
1	CCC	384/396 (96%)	0.76	37 (9%) 8 10	33, 51, 69, 78	0
1	DDD	378/396 (95%)	0.90	56 (14%) 2 3	34, 58, 80, 95	0
All	All	1534/1584 (96%)	0.76	172 (11%) 5 6	22, 51, 78, 102	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	174	ALA	5.7
1	DDD	291	PRO	5.2
1	DDD	260	GLY	4.9
1	AAA	299	LEU	4.9
1	AAA	298	GLY	4.6
1	AAA	260	GLY	4.4
1	AAA	131	ALA	4.3
1	DDD	259	SER	4.2
1	DDD	164	ALA	4.2
1	DDD	301[A]	TYR	4.2
1	DDD	15	LEU	4.1
1	BBB	287	GLY	4.0
1	CCC	157	GLY	4.0
1	AAA	284	ASP	4.0
1	BBB	131	ALA	4.0
1	CCC	285	GLU	3.9
1	CCC	257	LEU	3.9
1	DDD	257	LEU	3.9
1	CCC	160	THR	3.7
1	AAA	157	GLY	3.7
1	CCC	288	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	AAA	259	SER	3.7
1	DDD	261	LYS	3.7
1	CCC	196	VAL	3.7
1	AAA	155	ASN	3.7
1	DDD	155	ASN	3.7
1	AAA	285	GLU	3.6
1	CCC	382	LEU	3.6
1	CCC	260	GLY	3.6
1	DDD	156	SER	3.5
1	BBB	285	GLU	3.4
1	BBB	288	ALA	3.4
1	BBB	387	ASN	3.4
1	CCC	289	ILE	3.4
1	BBB	388	VAL	3.4
1	AAA	287	GLY	3.4
1	CCC	186	VAL	3.4
1	CCC	286	GLU	3.4
1	AAA	283	GLN	3.3
1	DDD	157	GLY	3.3
1	AAA	360	MET	3.3
1	DDD	385	SER	3.3
1	CCC	63	ILE	3.3
1	AAA	154	VAL	3.3
1	DDD	135	GLU	3.3
1	CCC	156	SER	3.3
1	BBB	75	LEU	3.2
1	AAA	186	VAL	3.2
1	DDD	64	GLY	3.2
1	CCC	384	ALA	3.2
1	DDD	371	SER	3.2
1	AAA	357	ALA	3.1
1	DDD	14	THR	3.1
1	DDD	80	ALA	3.1
1	AAA	361	SER	3.1
1	DDD	256	GLY	3.1
1	BBB	301[A]	TYR	3.1
1	AAA	160	THR	3.1
1	AAA	196	VAL	3.1
1	AAA	63	ILE	3.0
1	CCC	254	GLY	3.0
1	CCC	155	ASN	3.0
1	CCC	176	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	12	PRO	2.9
1	CCC	287	GLY	2.9
1	DDD	281	PHE	2.9
1	AAA	108	GLY	2.9
1	BBB	370	LEU	2.9
1	BBB	134	VAL	2.9
1	AAA	153	PRO	2.9
1	DDD	268	ALA	2.9
1	DDD	282	LEU	2.9
1	DDD	183	ILE	2.9
1	CCC	132	GLU	2.9
1	CCC	178	TYR	2.8
1	BBB	389	LEU	2.8
1	DDD	386	GLY	2.8
1	BBB	155	ASN	2.8
1	DDD	283	GLN	2.8
1	DDD	166	ASN	2.8
1	AAA	75	LEU	2.8
1	DDD	186	VAL	2.7
1	DDD	131	ALA	2.7
1	DDD	262	HIS	2.7
1	DDD	79	GLY	2.7
1	AAA	257	LEU	2.7
1	AAA	365	ILE	2.7
1	DDD	370	LEU	2.7
1	DDD	168	ALA	2.7
1	BBB	386	GLY	2.6
1	CCC	131	ALA	2.6
1	DDD	106	GLY	2.6
1	AAA	253	GLY	2.6
1	BBB	135	GLU	2.6
1	CCC	261	LYS	2.6
1	CCC	284	ASP	2.5
1	AAA	301	TYR	2.5
1	AAA	258	GLU	2.5
1	AAA	277	MET	2.5
1	DDD	359	GLU	2.5
1	AAA	227	GLY	2.5
1	CCC	291	PRO	2.5
1	AAA	185	SER	2.5
1	BBB	76	VAL	2.5
1	BBB	153	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	362	ARG	2.5
1	DDD	196	VAL	2.4
1	DDD	171	ASP	2.4
1	AAA	64	GLY	2.4
1	AAA	304	VAL	2.4
1	BBB	160	THR	2.4
1	DDD	278	LEU	2.4
1	BBB	151	VAL	2.4
1	CCC	365	ILE	2.4
1	DDD	163	ASP	2.4
1	AAA	86	ALA	2.4
1	AAA	254	GLY	2.4
1	CCC	173	VAL	2.4
1	CCC	80	ALA	2.4
1	AAA	362	ARG	2.4
1	AAA	130	GLY	2.4
1	DDD	258	GLU	2.3
1	BBB	80	ALA	2.3
1	BBB	163	ASP	2.3
1	BBB	203	ILE	2.3
1	BBB	371	SER	2.3
1	CCC	385	SER	2.3
1	AAA	13	GLU	2.3
1	AAA	228	GLY	2.3
1	AAA	212	LEU	2.3
1	DDD	66	ALA	2.3
1	DDD	9	GLN	2.3
1	CCC	83	THR	2.2
1	CCC	262	HIS	2.2
1	AAA	159	ARG	2.2
1	BBB	286	GLU	2.2
1	BBB	97	GLY	2.2
1	DDD	11	VAL	2.2
1	DDD	134	VAL	2.2
1	CCC	12	PRO	2.2
1	AAA	220	ASP	2.2
1	DDD	373[A]	ARG	2.2
1	DDD	169	LEU	2.2
1	AAA	385	SER	2.2
1	BBB	147	LEU	2.2
1	AAA	134	VAL	2.2
1	CCC	381	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	86	ALA	2.1
1	AAA	291	PRO	2.1
1	BBB	139	MET	2.1
1	CCC	298	GLY	2.1
1	DDD	217	GLN	2.1
1	AAA	297	PRO	2.1
1	CCC	75	LEU	2.1
1	DDD	292	SER	2.1
1	CCC	76	VAL	2.1
1	DDD	65	GLY	2.1
1	DDD	372	GLY	2.1
1	DDD	230	SER	2.0
1	BBB	83	THR	2.0
1	BBB	164	ALA	2.0
1	DDD	154	VAL	2.0
1	AAA	354	MET	2.0
1	AAA	182	LEU	2.0
1	AAA	107	ALA	2.0
1	DDD	151	VAL	2.0
1	CCC	79	GLY	2.0
1	DDD	33	GLU	2.0
1	DDD	182	LEU	2.0
1	BBB	284	ASP	2.0
1	CCC	234	GLY	2.0
1	DDD	16	VAL	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. 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
1	LLP	BBB	82	24/?	0.94	0.21	26,29,32,32	0
1	LLP	CCC	82	24/?	0.94	0.21	34,40,42,43	0
1	LLP	DDD	82	24/?	0.94	0.23	39,44,47,48	0
1	LLP	AAA	82	24/?	0.95	0.21	33,43,47,50	0

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	NA	GcG	4	1/?	0.79	0.16	52,52,52,52	0
2	PO4	EbE	3	5/?	0.87	0.22	82,83,84,84	0
2	PO4	EEE	1	5/?	0.90	0.16	63,64,65,66	0
2	PO4	EaE	2	5/?	0.92	0.14	76,76,77,77	0
3	NA	GGG	1	1/?	0.95	0.31	57,57,57,57	0
2	PO4	EcE	4	5/?	0.96	0.10	72,72,73,73	0
3	NA	GbG	3	1/?	0.97	0.14	47,47,47,47	0
3	NA	GaG	2	1/?	0.97	0.13	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.