Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:38 PM EDT

PDB ID	:	6XI1
Title	:	Crystal structure of tetra-tandem repeat in extending RTX adhesin from Aeromonas hydrophila
Authors	:	Ye, Q.; Vance, T.D.R.; Conroy, B.; Davies, P.L.
Deposited on	:	2020-06-19
Resolution	:	1.75 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 ⓘ symbol.

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

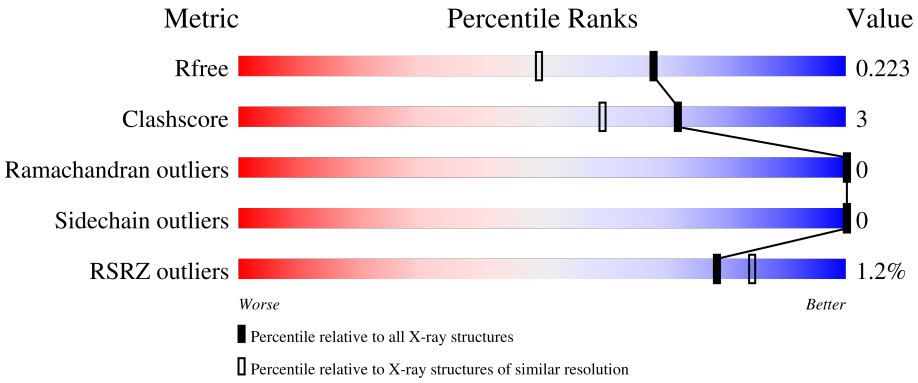
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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

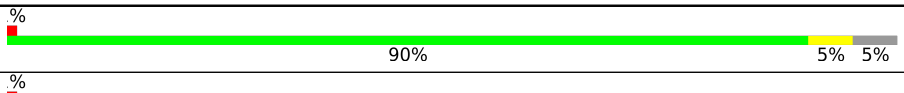
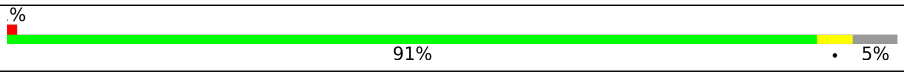
The reported resolution of this entry is 1.75 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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	449	
1	BBB	449	

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	GOL	AAA	505	-	-	X	-
2	GOL	AAA	506	-	-	X	-
2	GOL	BBB	507	-	-	X	-
6	PEG	BBB	508	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7100 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 Flagellin hook IN motif family.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	AAA	425	Total	C	N	O	0	0	0
			3002	1832	474	696			
1	BBB	426	Total	C	N	O	0	0	0
			3010	1836	475	699			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	expression tag	UNP A0KNW4
AAA	2	ALA	-	expression tag	UNP A0KNW4
AAA	3	SER	-	expression tag	UNP A0KNW4
AAA	4	SER	-	expression tag	UNP A0KNW4
AAA	5	HIS	-	expression tag	UNP A0KNW4
AAA	6	HIS	-	expression tag	UNP A0KNW4
AAA	7	HIS	-	expression tag	UNP A0KNW4
AAA	8	HIS	-	expression tag	UNP A0KNW4
AAA	9	HIS	-	expression tag	UNP A0KNW4
AAA	10	HIS	-	expression tag	UNP A0KNW4
AAA	11	SER	-	expression tag	UNP A0KNW4
AAA	12	SER	-	expression tag	UNP A0KNW4
AAA	13	GLY	-	expression tag	UNP A0KNW4
AAA	14	LEU	-	expression tag	UNP A0KNW4
AAA	15	VAL	-	expression tag	UNP A0KNW4
AAA	16	PRO	-	expression tag	UNP A0KNW4
AAA	17	ARG	-	expression tag	UNP A0KNW4
AAA	18	GLY	-	expression tag	UNP A0KNW4
AAA	19	SER	-	expression tag	UNP A0KNW4
AAA	20	HIS	-	expression tag	UNP A0KNW4
AAA	21	MET	-	expression tag	UNP A0KNW4
BBB	1	MET	-	expression tag	UNP A0KNW4
BBB	2	ALA	-	expression tag	UNP A0KNW4
BBB	3	SER	-	expression tag	UNP A0KNW4
BBB	4	SER	-	expression tag	UNP A0KNW4

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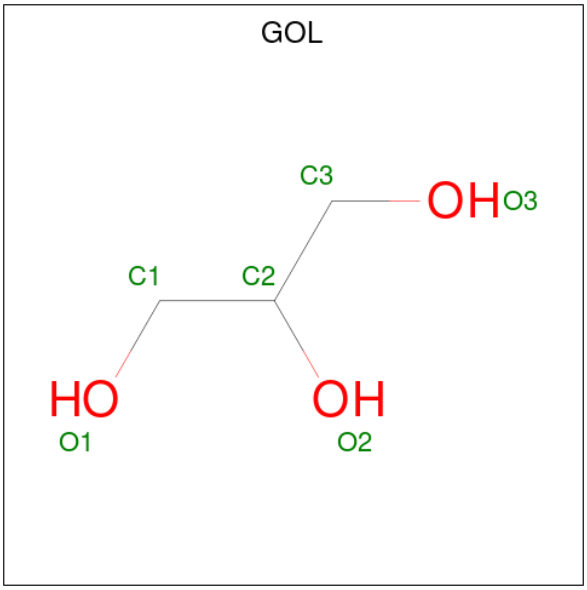
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	5	HIS	-	expression tag	UNP A0KNW4
BBB	6	HIS	-	expression tag	UNP A0KNW4
BBB	7	HIS	-	expression tag	UNP A0KNW4
BBB	8	HIS	-	expression tag	UNP A0KNW4
BBB	9	HIS	-	expression tag	UNP A0KNW4
BBB	10	HIS	-	expression tag	UNP A0KNW4
BBB	11	SER	-	expression tag	UNP A0KNW4
BBB	12	SER	-	expression tag	UNP A0KNW4
BBB	13	GLY	-	expression tag	UNP A0KNW4
BBB	14	LEU	-	expression tag	UNP A0KNW4
BBB	15	VAL	-	expression tag	UNP A0KNW4
BBB	16	PRO	-	expression tag	UNP A0KNW4
BBB	17	ARG	-	expression tag	UNP A0KNW4
BBB	18	GLY	-	expression tag	UNP A0KNW4
BBB	19	SER	-	expression tag	UNP A0KNW4
BBB	20	HIS	-	expression tag	UNP A0KNW4
BBB	21	MET	-	expression tag	UNP A0KNW4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 6 3 3	0	0
2	AAA	1	Total C O 6 3 3	0	0
2	AAA	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 6 3 3	0	0
2	AAA	1	Total C O 6 3 3	0	0
2	AAA	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Cl 1 1	0	0

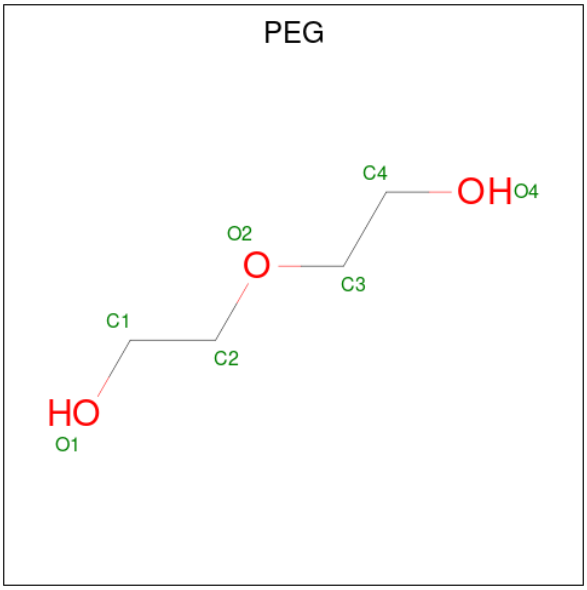
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total Na 1 1	0	0
4	AAA	1	Total Na 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	13	Total Ca 13 13	0	0
5	AAA	13	Total Ca 13 13	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

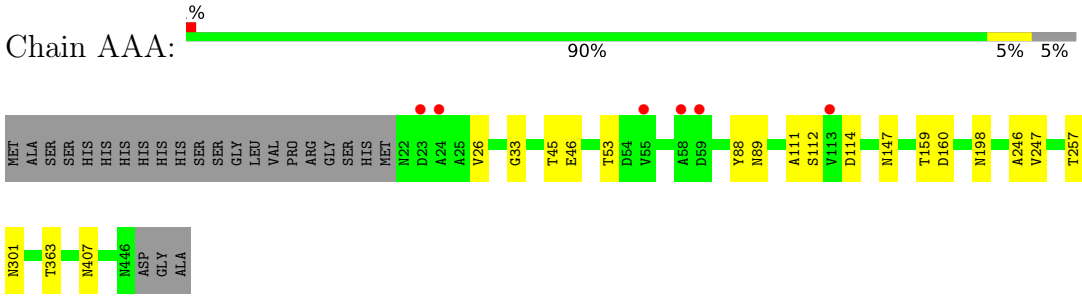
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	505	Total O 505 505	0	0
7	BBB	469	Total O 469 469	0	0

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.

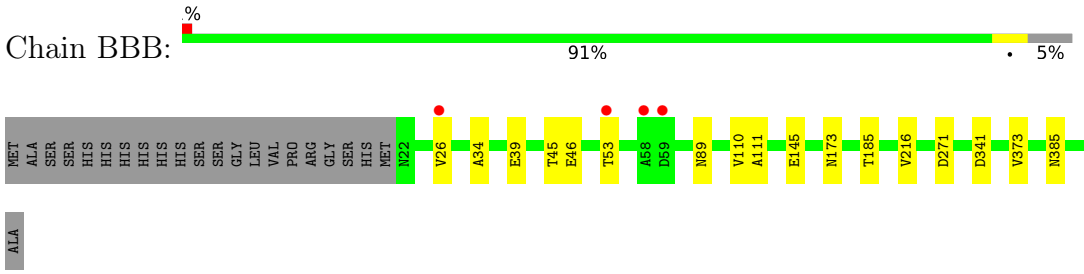
• Molecule 1: Flagellin hook IN motif family

Chain AAA:



• Molecule 1: Flagellin hook IN motif family

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.67Å 50.37Å 124.60Å 97.56° 98.24° 101.72°	Depositor
Resolution (Å)	48.64 – 1.75 48.64 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.64-1.75) 97.3 (48.64-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.181 , 0.210 0.196 , 0.223	Depositor DCC
R_{free} test set	5436 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7100	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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: GOL, CA, PEG, NA, CL

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	0.82	0/3036	0.86	0/4167
1	BBB	0.80	0/3044	0.83	0/4178
All	All	0.81	0/6080	0.85	0/8345

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	3002	0	2843	23	0
1	BBB	3010	0	2847	18	0
2	AAA	36	0	48	13	0
2	BBB	42	0	56	7	0
3	AAA	1	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	13	0	0	0	0
5	BBB	13	0	0	0	0
6	BBB	7	0	9	4	0
7	AAA	505	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	469	0	0	1	0
All	All	7100	0	5803	41	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 3.

All (41) 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:AAA:159:THR:HB	2:AAA:505:GOL:O3	1.75	0.86
1:AAA:114:ASP:HB3	7:AAA:624:HOH:O	1.75	0.84
1:AAA:363:THR:HG22	1:AAA:407:ASN:OD1	1.79	0.83
1:AAA:258:GLU:OE2	2:AAA:506:GOL:H11	1.84	0.78
1:AAA:160:ASP:H	2:AAA:505:GOL:H32	1.54	0.72
1:BBB:46:GLU:OE1	6:BBB:508:PEG:H12	1.90	0.72
1:AAA:45:THR:HG22	1:AAA:89:ASN:OD1	1.90	0.72
1:AAA:112:SER:HB3	7:AAA:624:HOH:O	1.90	0.70
1:BBB:45:THR:HG22	1:BBB:89:ASN:OD1	1.92	0.69
1:AAA:257:THR:HG22	1:AAA:301:ASN:OD1	1.94	0.67
1:BBB:34:ALA:O	6:BBB:508:PEG:H21	1.94	0.67
1:BBB:173:ASN:O	2:BBB:503:GOL:H32	1.94	0.66
1:AAA:246:ALA:O	2:AAA:506:GOL:H32	1.97	0.65
1:AAA:160:ASP:H	2:AAA:505:GOL:C3	2.11	0.62
1:BBB:110:VAL:HA	2:BBB:507:GOL:H11	1.81	0.62
1:BBB:111:ALA:H	2:BBB:507:GOL:H12	1.66	0.60
1:AAA:246:ALA:O	2:AAA:506:GOL:C3	2.54	0.56
1:BBB:385:ASN:O	2:BBB:502:GOL:O3	2.23	0.55
1:AAA:159:THR:CB	2:AAA:505:GOL:O3	2.54	0.54
1:BBB:34:ALA:O	6:BBB:508:PEG:C2	2.56	0.53
1:AAA:258:GLU:OE2	2:AAA:506:GOL:C1	2.54	0.53
1:BBB:39:GLU:OE2	6:BBB:508:PEG:O1	2.26	0.53
1:BBB:111:ALA:N	2:BBB:507:GOL:H12	2.24	0.53
1:AAA:26:VAL:CG1	1:AAA:53:THR:OG1	2.57	0.53
1:AAA:147:ASN:ND2	1:AAA:198:ASN:HD22	2.08	0.52
1:BBB:26:VAL:CG1	1:BBB:53:THR:OG1	2.57	0.52
1:AAA:247:VAL:HA	2:AAA:506:GOL:H32	1.93	0.51
1:AAA:246:ALA:O	2:AAA:506:GOL:H11	2.12	0.50
1:AAA:147:ASN:HD22	1:AAA:198:ASN:HD22	1.60	0.50
1:BBB:216:VAL:HA	2:BBB:503:GOL:H12	1.93	0.49
1:BBB:341:ASP:HB2	1:BBB:373:VAL:HG22	1.94	0.48
1:BBB:111:ALA:H	2:BBB:507:GOL:C1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:173:ASN:OD1	1:BBB:185:THR:HG22	2.18	0.44
1:BBB:341:ASP:CB	1:BBB:373:VAL:HG22	2.48	0.43
1:BBB:271:ASP:OD1	1:BBB:271:ASP:N	2.53	0.42
1:AAA:159:THR:HB	2:AAA:505:GOL:HO3	1.80	0.41
1:AAA:111:ALA:H	2:AAA:504:GOL:C1	2.33	0.41
1:AAA:258:GLU:CD	2:AAA:506:GOL:H11	2.40	0.41
1:BBB:145:GLU:OE2	7:BBB:601:HOH:O	2.22	0.41
1:AAA:45:THR:HA	1:AAA:88:TYR:O	2.21	0.40
1:AAA:33:GLY:HA3	1:AAA:46:GLU:HG2	2.03	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	AAA	423/449 (94%)	421 (100%)	2 (0%)	0	100	100
1	BBB	424/449 (94%)	421 (99%)	3 (1%)	0	100	100
All	All	847/898 (94%)	842 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	329/348 (94%)	329 (100%)	0	100	100
1	BBB	330/348 (95%)	330 (100%)	0	100	100
All	All	659/696 (95%)	659 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 29 are monoatomic - leaving 14 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	GOL	BBB	506	4	5,5,5	0.10	0	5,5,5	0.24	0
2	GOL	AAA	504	-	5,5,5	0.13	0	5,5,5	0.21	0
2	GOL	AAA	502	-	5,5,5	0.24	0	5,5,5	0.80	0
2	GOL	BBB	507	-	5,5,5	0.18	0	5,5,5	0.30	0
6	PEG	BBB	508	-	6,6,6	0.72	0	5,5,5	0.49	0
2	GOL	AAA	506	-	5,5,5	0.16	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	AAA	501	-	5,5,5	0.56	0	5,5,5	1.51	1 (20%)
2	GOL	BBB	504	-	5,5,5	0.27	0	5,5,5	0.45	0
2	GOL	AAA	503	-	5,5,5	0.15	0	5,5,5	0.78	0
2	GOL	BBB	503	-	5,5,5	0.17	0	5,5,5	0.34	0
2	GOL	AAA	505	-	5,5,5	0.19	0	5,5,5	0.49	0
2	GOL	BBB	501	-	5,5,5	0.19	0	5,5,5	0.31	0
2	GOL	BBB	502	-	5,5,5	0.19	0	5,5,5	0.38	0
2	GOL	BBB	505	-	5,5,5	0.13	0	5,5,5	0.43	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	GOL	BBB	506	4	-	3/4/4/4	-
2	GOL	AAA	504	-	-	2/4/4/4	-
2	GOL	AAA	502	-	-	4/4/4/4	-
2	GOL	BBB	507	-	-	0/4/4/4	-
6	PEG	BBB	508	-	-	3/4/4/4	-
2	GOL	AAA	506	-	-	2/4/4/4	-
2	GOL	AAA	501	-	-	4/4/4/4	-
2	GOL	BBB	504	-	-	2/4/4/4	-
2	GOL	AAA	503	-	-	3/4/4/4	-
2	GOL	BBB	503	-	-	3/4/4/4	-
2	GOL	AAA	505	-	-	0/4/4/4	-
2	GOL	BBB	501	-	-	0/4/4/4	-
2	GOL	BBB	502	-	-	2/4/4/4	-
2	GOL	BBB	505	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	501	GOL	O2-C2-C3	2.77	121.31	109.12

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	502	GOL	O1-C1-C2-C3
2	AAA	502	GOL	C1-C2-C3-O3
2	AAA	502	GOL	O2-C2-C3-O3
2	AAA	503	GOL	O1-C1-C2-O2
2	AAA	503	GOL	O1-C1-C2-C3
2	BBB	503	GOL	O1-C1-C2-O2
2	BBB	503	GOL	O1-C1-C2-C3
2	AAA	506	GOL	C1-C2-C3-O3
2	BBB	502	GOL	O1-C1-C2-C3
6	BBB	508	PEG	C4-C3-O2-C2
2	AAA	502	GOL	O1-C1-C2-O2
2	BBB	506	GOL	O1-C1-C2-C3
2	AAA	504	GOL	O1-C1-C2-C3
2	AAA	501	GOL	O1-C1-C2-C3
2	AAA	501	GOL	C1-C2-C3-O3
6	BBB	508	PEG	O2-C3-C4-O4
2	BBB	506	GOL	O1-C1-C2-O2
2	BBB	502	GOL	O1-C1-C2-O2
2	AAA	501	GOL	O1-C1-C2-O2
2	BBB	503	GOL	O2-C2-C3-O3
6	BBB	508	PEG	O1-C1-C2-O2
2	AAA	506	GOL	O2-C2-C3-O3
2	AAA	501	GOL	O2-C2-C3-O3
2	AAA	504	GOL	O1-C1-C2-O2
2	BBB	506	GOL	C1-C2-C3-O3
2	AAA	503	GOL	C1-C2-C3-O3
2	BBB	504	GOL	O1-C1-C2-C3
2	BBB	504	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	504	GOL	1	0
2	BBB	507	GOL	4	0
6	BBB	508	PEG	4	0
2	AAA	506	GOL	7	0
2	BBB	503	GOL	2	0
2	AAA	505	GOL	5	0
2	BBB	502	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	425/449 (94%)	-0.12	6 (1%)	75	82	12, 23, 47, 76	0
1	BBB	426/449 (94%)	-0.15	4 (0%)	84	89	14, 26, 42, 68	0
All	All	851/898 (94%)	-0.14	10 (1%)	79	84	12, 24, 45, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	55	VAL	3.7
1	AAA	58	ALA	3.6
1	AAA	113	VAL	3.1
1	AAA	24	ALA	2.4
1	BBB	59	ASP	2.3
1	BBB	26	VAL	2.3
1	BBB	53	THR	2.2
1	AAA	23	ASP	2.2
1	BBB	58	ALA	2.0
1	AAA	59	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no 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
5	CA	AAA	509	1/1	0.79	0.06	55,55,55,55	0
2	GOL	BBB	506	6/6	0.81	0.17	49,64,68,71	0
2	GOL	AAA	506	6/6	0.81	0.18	39,44,46,53	0
2	GOL	BBB	505	6/6	0.82	0.18	43,47,51,52	0
2	GOL	BBB	507	6/6	0.84	0.20	48,51,52,52	0
2	GOL	AAA	504	6/6	0.85	0.19	51,57,58,61	0
2	GOL	BBB	503	6/6	0.85	0.15	30,39,42,56	0
3	CL	AAA	507	1/1	0.88	0.16	63,63,63,63	0
6	PEG	BBB	508	7/7	0.88	0.13	28,34,41,51	0
2	GOL	AAA	501	6/6	0.88	0.15	21,28,33,34	0
2	GOL	AAA	503	6/6	0.89	0.09	26,37,41,47	0
2	GOL	AAA	505	6/6	0.90	0.24	37,43,48,51	0
2	GOL	BBB	502	6/6	0.92	0.13	19,31,37,40	0
2	GOL	BBB	504	6/6	0.92	0.12	22,26,27,38	0
5	CA	BBB	510	1/1	0.94	0.05	33,33,33,33	0
2	GOL	AAA	502	6/6	0.94	0.11	22,33,35,36	0
4	NA	BBB	509	1/1	0.94	0.09	31,31,31,31	0
2	GOL	BBB	501	6/6	0.95	0.08	25,28,35,36	0
5	CA	AAA	521	1/1	0.96	0.05	38,38,38,38	0
5	CA	BBB	514	1/1	0.96	0.07	31,31,31,31	0
5	CA	BBB	511	1/1	0.98	0.05	34,34,34,34	0
5	CA	BBB	522	1/1	0.98	0.09	22,22,22,22	0
5	CA	BBB	512	1/1	0.98	0.04	30,30,30,30	0
5	CA	BBB	521	1/1	0.99	0.04	24,24,24,24	0
5	CA	AAA	518	1/1	0.99	0.13	17,17,17,17	0
5	CA	AAA	510	1/1	0.99	0.09	19,19,19,19	0
5	CA	BBB	517	1/1	0.99	0.06	22,22,22,22	0
5	CA	BBB	515	1/1	0.99	0.05	25,25,25,25	0
5	CA	BBB	513	1/1	0.99	0.04	33,33,33,33	0
5	CA	BBB	516	1/1	0.99	0.07	21,21,21,21	0
4	NA	AAA	508	1/1	0.99	0.05	20,20,20,20	0
5	CA	AAA	512	1/1	0.99	0.04	23,23,23,23	0
5	CA	AAA	511	1/1	0.99	0.09	26,26,26,26	0
5	CA	AAA	514	1/1	1.00	0.07	15,15,15,15	0
5	CA	AAA	517	1/1	1.00	0.10	21,21,21,21	0
5	CA	BBB	518	1/1	1.00	0.10	15,15,15,15	0
5	CA	BBB	520	1/1	1.00	0.10	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	AAA	520	1/1	1.00	0.08	17,17,17,17	0
5	CA	AAA	516	1/1	1.00	0.11	14,14,14,14	0
5	CA	BBB	519	1/1	1.00	0.10	16,16,16,16	0
5	CA	AAA	513	1/1	1.00	0.11	14,14,14,14	0
5	CA	AAA	515	1/1	1.00	0.08	18,18,18,18	0
5	CA	AAA	519	1/1	1.00	0.03	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.