Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 07:30 AM BST

PDB ID	:	6SS0
Title	:	Structure of the arginase-2-inhibitory human antigen-binding fragment Fab C0021181
Authors	:	Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; Seewooruthun, C.; Carr, M.
Deposited on	:	2019-09-06
Resolution	:	1.70 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:

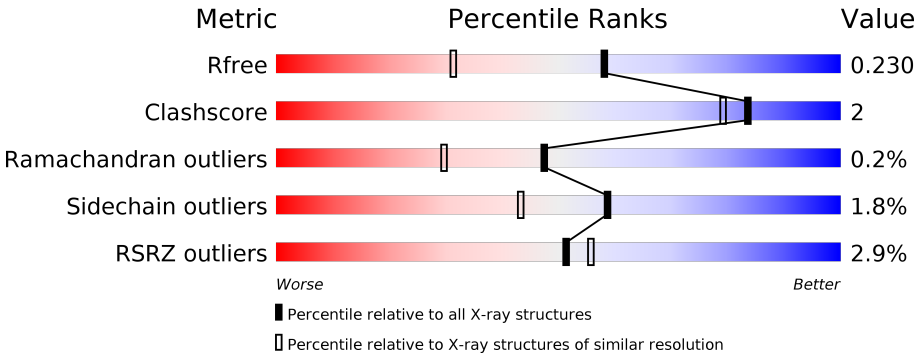
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	HHH	233	3% 87% 6% 7%
1	III	233	5% 87% 8% 5%
2	LLL	220	% 92%
2	MMM	220	% 90% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13546 atoms, of which 6414 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 Fab C0021181 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	216	Total	C	H	N	O	S	89	5	0
			3284	1041	1628	285	320	10			
1	III	221	Total	C	H	N	O	S	92	5	0
			3366	1063	1671	294	328	10			

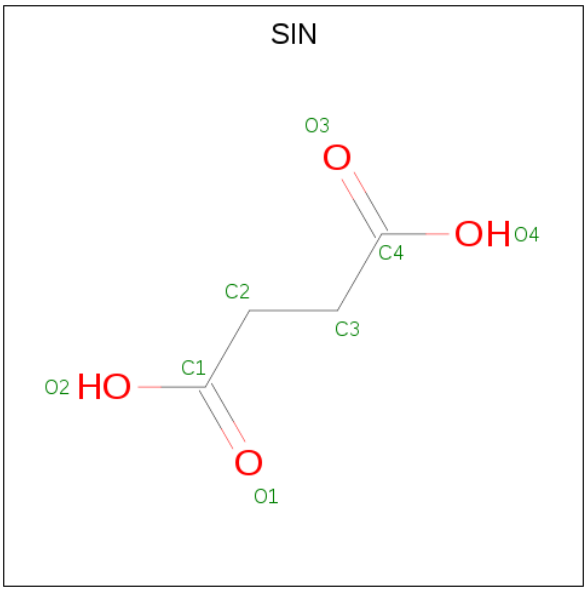
- Molecule 2 is a protein called Fab C0021181 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	LLL	212	Total	C	H	N	O	S	102	1	0
			3102	983	1528	262	325	4			
2	MMM	211	Total	C	H	N	O	S	100	2	0
			3114	987	1535	263	325	4			

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

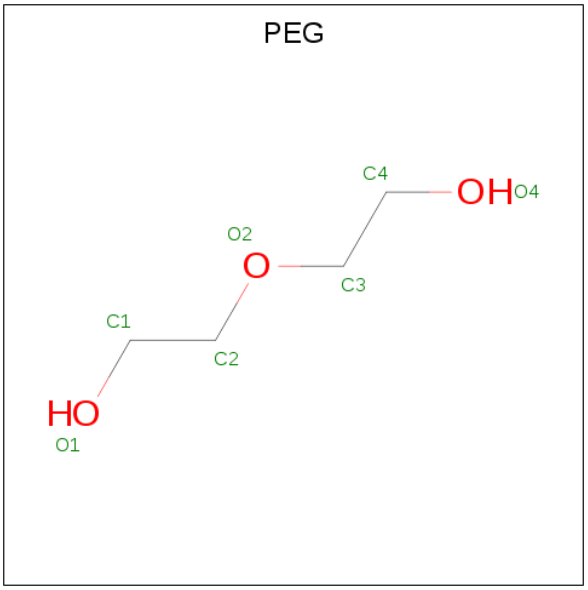
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	HHH	3	Total	Cl	0	0
			3	3		
3	MMM	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	LLL	1	Total	C	H	O	0	0
			12	4	4	4		
4	MMM	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	LLL	1	Total	C	H	O	1	0
			17	4	10	3		
5	MMM	1	Total	C	H	O	1	0
			17	4	10	3		

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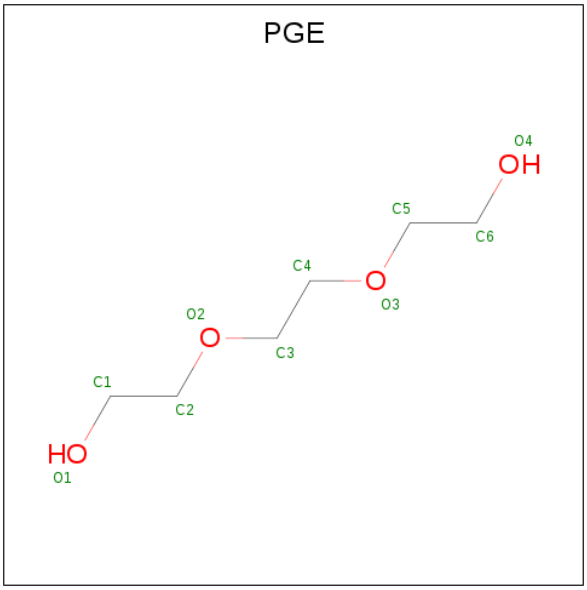
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	MMM	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	MMM	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 7 is water.

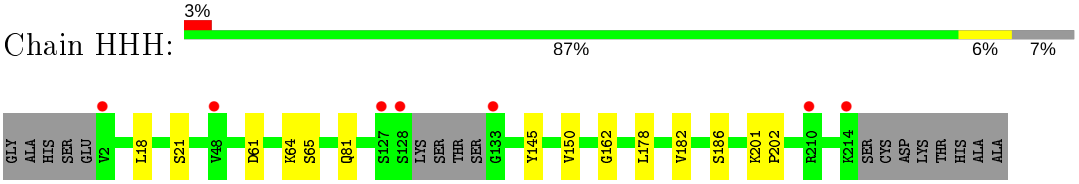
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	HHH	146	Total	O	0	0
			146	146		
7	LLL	156	Total	O	0	1
			157	157		
7	III	140	Total	O	0	0
			140	140		
7	MMM	134	Total	O	0	1
			134	134		

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.

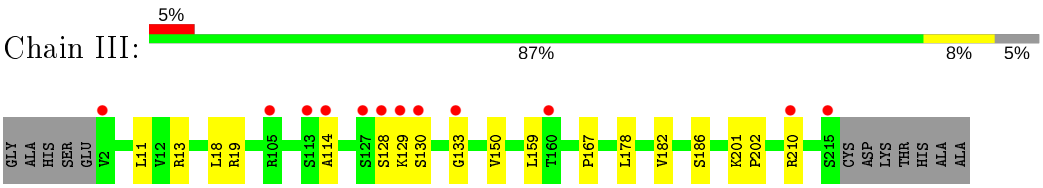
- Molecule 1: Fab C0021181 heavy chain (IgG1)

Chain HHH:



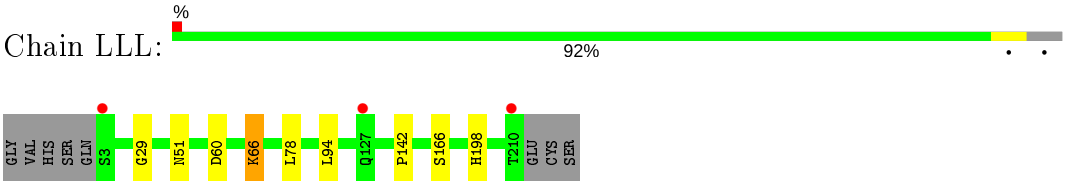
- Molecule 1: Fab C0021181 heavy chain (IgG1)

Chain III:



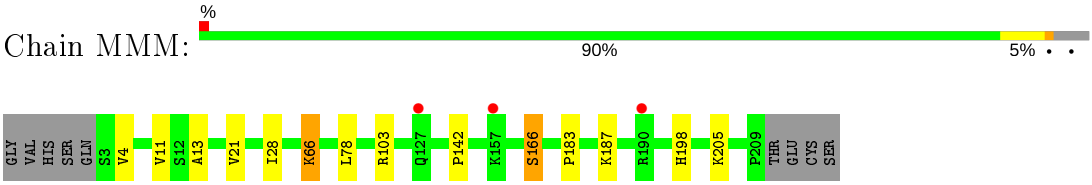
- Molecule 2: Fab C0021181 light chain (IgG1)

Chain LLL:



- Molecule 2: Fab C0021181 light chain (IgG1)

Chain MMM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.40Å 67.37Å 94.33Å 90.00° 100.24° 90.00°	Depositor
Resolution (Å)	46.54 – 1.70 46.54 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.54-1.70) 99.9 (46.54-1.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.189 , 0.224 0.198 , 0.230	Depositor DCC
R_{free} test set	4494 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13546	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 21.77 % 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 6.5471e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, PEG, PGE, SIN

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	HHH	0.64	0/1693	0.76	0/2302
1	III	0.65	0/1733	0.76	0/2357
2	LLL	0.64	0/1612	0.75	0/2204
2	MMM	0.65	0/1617	0.75	0/2209
All	All	0.64	0/6655	0.75	0/9072

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	HHH	1656	1628	1618	9	2
1	III	1695	1671	1663	10	2
2	LLL	1574	1528	1523	4	0
2	MMM	1579	1535	1529	9	0
3	HHH	3	0	0	0	0
3	MMM	1	0	0	0	0
4	LLL	8	4	4	0	0
4	MMM	8	4	4	0	0
5	LLL	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	MMM	14	20	20	0	0
6	MMM	10	14	14	0	0
7	HHH	146	0	0	1	0
7	III	140	0	0	2	0
7	LLL	157	0	0	2	0
7	MMM	134	0	0	2	0
All	All	7132	6414	6385	31	2

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 2.

All (31) 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)
2:MMM:183:PRO:O	2:MMM:187:LYS:HG2	1.94	0.67
1:III:150:VAL:CG2	1:III:178:LEU:HD21	2.29	0.63
2:MMM:103:ARG:NH1	7:MMM:401:HOH:O	2.32	0.62
1:III:150:VAL:HG22	1:III:178:LEU:HD21	1.81	0.61
2:MMM:28:ILE:O	2:MMM:66[A]:LYS:HE3	2.01	0.60
1:HHH:150:VAL:CG2	1:HHH:178:LEU:HD21	2.33	0.58
1:III:159:LEU:HD23	1:III:182:VAL:HG21	1.89	0.55
1:HHH:178:LEU:HD12	1:HHH:178:LEU:C	2.29	0.53
2:MMM:28:ILE:O	2:MMM:66[A]:LYS:CE	2.57	0.53
1:III:178:LEU:HD12	1:III:178:LEU:C	2.31	0.51
1:HHH:150:VAL:HG22	1:HHH:178:LEU:HD21	1.93	0.50
2:MMM:198:HIS:HD2	7:MMM:501:HOH:O	1.93	0.50
2:MMM:13:ALA:HB3	2:MMM:78:LEU:HD12	1.93	0.50
1:III:210:ARG:HG3	7:III:409:HOH:O	2.11	0.50
2:LLL:29:GLY:O	7:LLL:401:HOH:O	2.19	0.49
1:III:19:ARG:HD2	7:III:425:HOH:O	2.13	0.49
1:III:167:PRO:HG2	2:MMM:166:SER:OG	2.13	0.48
2:MMM:11:VAL:HG21	2:MMM:21:VAL:HG22	1.95	0.47
2:LLL:198:HIS:HD2	7:LLL:525:HOH:O	1.98	0.45
2:LLL:51:ASN:HD21	2:LLL:66:LYS:HE3	1.81	0.45
2:LLL:142:PRO:O	2:LLL:198:HIS:HE1	1.99	0.45
1:HHH:61:ASP:OD2	7:HHH:401:HOH:O	2.21	0.44
2:MMM:142:PRO:O	2:MMM:198:HIS:HE1	2.01	0.44
1:III:13[A]:ARG:HG3	1:III:13[A]:ARG:O	2.16	0.43
1:HHH:64:LYS:O	1:HHH:65:SER:OG	2.34	0.43
1:HHH:201:LYS:N	1:HHH:202:PRO:CD	2.82	0.42
1:HHH:18:LEU:HA	1:HHH:18:LEU:HD23	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:145:TYR:CE1	1:HHH:150:VAL:HG13	2.55	0.42
1:III:13[B]:ARG:NH1	1:III:114:ALA:HB3	2.35	0.41
1:HHH:162:GLY:O	1:HHH:182:VAL:HA	2.20	0.41
1:III:201:LYS:N	1:III:202:PRO:CD	2.83	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:21:SER:HG	1:III:133:GLY:H[2_656]	1.33	0.27
1:HHH:81:GLN:HE21	1:III:129:LYS:HG2[2_656]	1.34	0.26

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	HHH	217/233 (93%)	213 (98%)	4 (2%)	0	100 100
1	III	224/233 (96%)	217 (97%)	5 (2%)	2 (1%)	17 5
2	LLL	211/220 (96%)	205 (97%)	6 (3%)	0	100 100
2	MMM	211/220 (96%)	207 (98%)	4 (2%)	0	100 100
All	All	863/906 (95%)	842 (98%)	19 (2%)	2 (0%)	47 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	III	130	SER
1	III	128	SER

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	HHH	185/193 (96%)	184 (100%)	1 (0%)	88 83
1	III	190/193 (98%)	187 (98%)	3 (2%)	62 48
2	LLL	178/184 (97%)	173 (97%)	5 (3%)	43 25
2	MMM	178/184 (97%)	173 (97%)	5 (3%)	43 25
All	All	731/754 (97%)	717 (98%)	14 (2%)	59 41

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	186	SER
2	LLL	60	ASP
2	LLL	66	LYS
2	LLL	78	LEU
2	LLL	94	LEU
2	LLL	166	SER
1	III	11	LEU
1	III	18	LEU
1	III	186	SER
2	MMM	4	VAL
2	MMM	66[A]	LYS
2	MMM	66[B]	LYS
2	MMM	166	SER
2	MMM	205	LYS

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	PEG	LLL	302	-	6,6,6	0.17	0	5,5,5	0.10	0
4	SIN	LLL	301	-	1,7,7	0.14	0	2,8,8	1.54	0
6	PGE	MMM	305	-	9,9,9	0.18	0	8,8,8	0.14	0
4	SIN	MMM	301	-	1,7,7	0.25	0	2,8,8	1.07	0
5	PEG	MMM	302	-	6,6,6	0.15	0	5,5,5	0.06	0
5	PEG	MMM	303	-	6,6,6	0.17	0	5,5,5	0.10	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
5	PEG	LLL	302	-	-	2/4/4/4	-
4	SIN	LLL	301	-	-	1/1/5/5	-
6	PGE	MMM	305	-	-	4/7/7/7	-
4	SIN	MMM	301	-	-	0/1/5/5	-
5	PEG	MMM	302	-	-	3/4/4/4	-
5	PEG	MMM	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	LLL	301	SIN	C1-C2-C3-C4
5	MMM	303	PEG	O1-C1-C2-O2
5	LLL	302	PEG	O2-C3-C4-O4
5	MMM	302	PEG	O2-C3-C4-O4
5	MMM	303	PEG	O2-C3-C4-O4
6	MMM	305	PGE	O1-C1-C2-O2
5	LLL	302	PEG	O1-C1-C2-O2
5	MMM	302	PEG	C1-C2-O2-C3
6	MMM	305	PGE	C4-C3-O2-C2
5	MMM	302	PEG	O1-C1-C2-O2
6	MMM	305	PGE	C1-C2-O2-C3
6	MMM	305	PGE	O2-C3-C4-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	HHH	216/233 (92%)	0.15	7 (3%) 47 52	19, 27, 41, 74	0
1	III	221/233 (94%)	0.21	12 (5%) 25 28	18, 26, 44, 82	0
2	LLL	212/220 (96%)	-0.13	3 (1%) 75 79	18, 25, 37, 54	0
2	MMM	211/220 (95%)	0.00	3 (1%) 75 79	18, 25, 45, 53	0
All	All	860/906 (94%)	0.06	25 (2%) 51 56	18, 26, 43, 82	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	128	SER	6.5
1	III	215	SER	6.1
1	HHH	128	SER	4.7
1	HHH	2	VAL	4.7
1	III	114	ALA	3.5
1	HHH	127	SER	3.4
2	MMM	157	LYS	3.1
1	III	130	SER	3.0
2	MMM	190	ARG	2.9
2	LLL	127	GLN	2.9
2	MMM	127	GLN	2.8
1	III	129	LYS	2.8
2	LLL	3	SER	2.6
1	III	127	SER	2.6
1	III	2	VAL	2.5
1	III	105	ARG	2.5
2	LLL	210	THR	2.5
1	HHH	133	GLY	2.3
1	III	210	ARG	2.3
1	III	133	GLY	2.2
1	III	160	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	HHH	210	ARG	2.2
1	III	113	SER	2.1
1	HHH	214	LYS	2.0
1	HHH	48	VAL	2.0

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

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
5	PEG	MMM	303	7/7	0.58	0.19	65,66,68,68	1
4	SIN	LLL	301	8/8	0.59	0.27	63,68,73,76	0
4	SIN	MMM	301	8/8	0.62	0.23	62,64,65,66	0
6	PGE	MMM	305	10/10	0.62	0.19	62,65,66,67	1
5	PEG	LLL	302	7/7	0.72	0.18	48,50,51,51	1
5	PEG	MMM	302	7/7	0.73	0.21	60,61,65,66	1
3	CL	MMM	304	1/1	0.98	0.09	28,28,28,28	0
3	CL	HHH	303	1/1	0.99	0.12	31,31,31,31	0
3	CL	HHH	302	1/1	0.99	0.14	22,22,22,22	0
3	CL	HHH	301	1/1	1.00	0.12	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.