wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2024 – 03:27 pm GMT

PDB ID	:	9FVB
Title	:	Crystal structure of VcSiaP in complex with a VHH antibody (VHH_VcP#2)
Authors	:	Schneberger, N.; Hagelueken, G.
Deposited on	:	2024-06-26
Resolution	:	2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

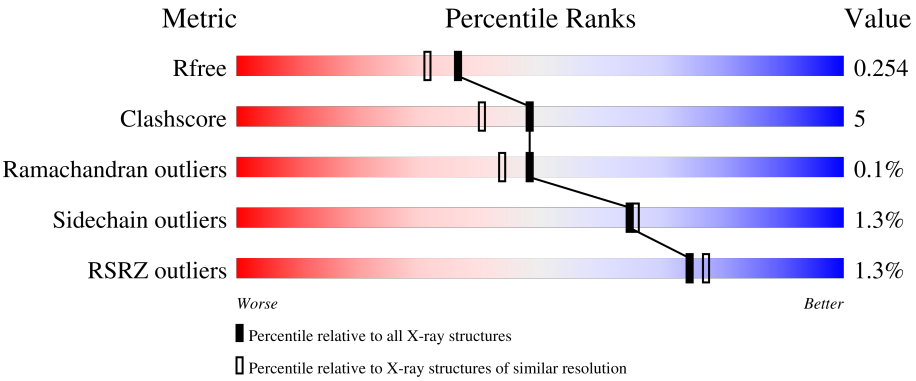
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	303	90% 10%
1	B	303	88% 11%
2	C	139	4% 72% 15% 13%
2	H	139	76% 12% 13%

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
4	GOL	A	302	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13752 atoms, of which 6566 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 Sialic acid-binding periplasmic protein SiaP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	H	N	O	S	0	0	0
			4757	1509	2368	401	463	16			
1	B	301	Total	C	H	N	O	S	0	0	0
			4738	1504	2358	399	461	16			

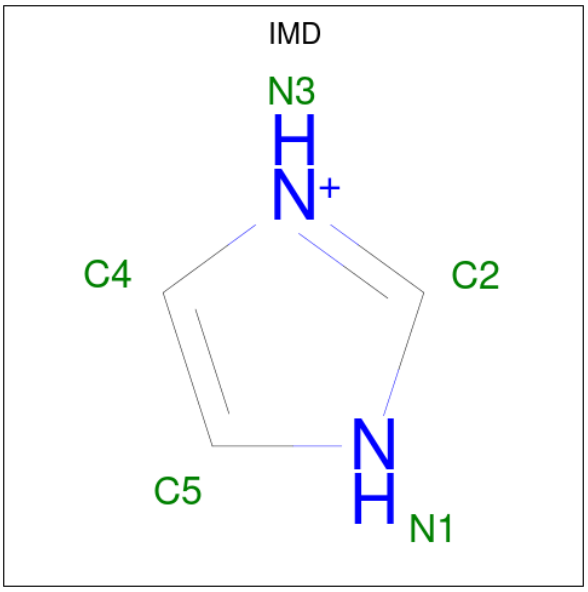
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9KR64
A	-2	ALA	-	expression tag	UNP Q9KR64
A	-1	MET	-	expression tag	UNP Q9KR64
A	0	GLY	-	expression tag	UNP Q9KR64
B	-3	GLY	-	expression tag	UNP Q9KR64
B	-2	ALA	-	expression tag	UNP Q9KR64
B	-1	MET	-	expression tag	UNP Q9KR64
B	0	GLY	-	expression tag	UNP Q9KR64

- Molecule 2 is a protein called VHH_VcP#2.

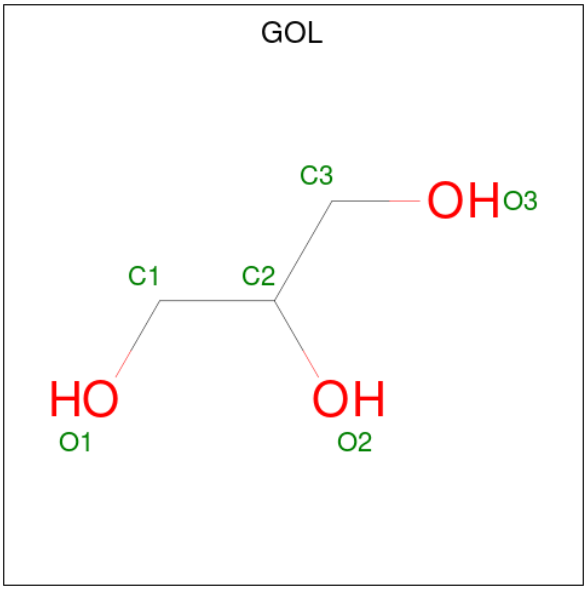
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	121	Total	C	H	N	O	S	0	0	0
			1829	587	890	167	181	4			
2	H	121	Total	C	H	N	O	S	0	0	0
			1829	587	890	167	181	4			

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



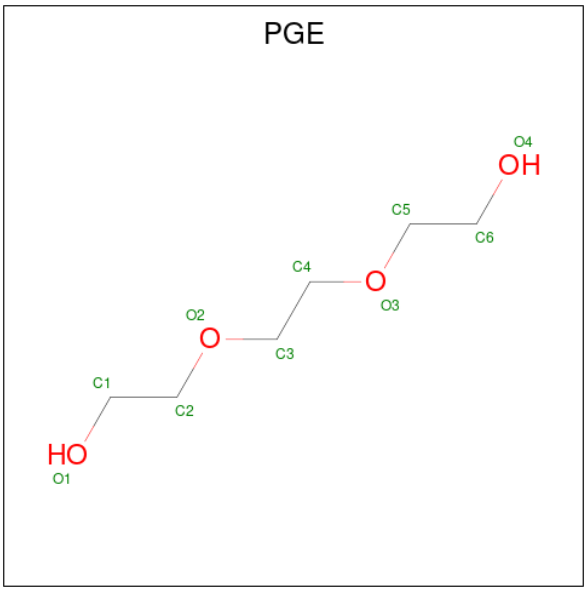
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N 10 3 5 2	0	0
3	B	1	Total C H N 10 3 5 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

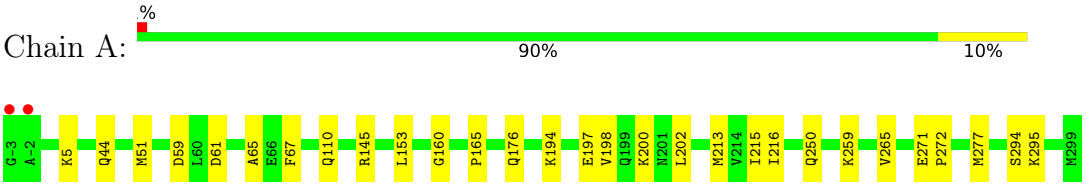
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	201	Total O 201 201	0	0
6	B	182	Total O 182 182	0	0
6	C	45	Total O 45 45	0	0
6	H	65	Total O 65 65	0	0

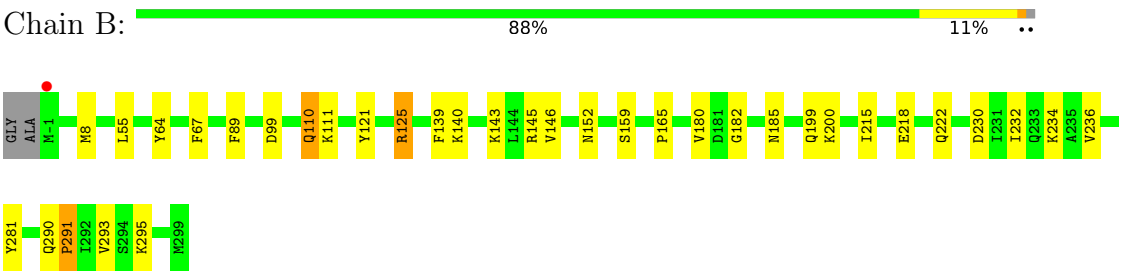
3 Residue-property plots (i)

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.

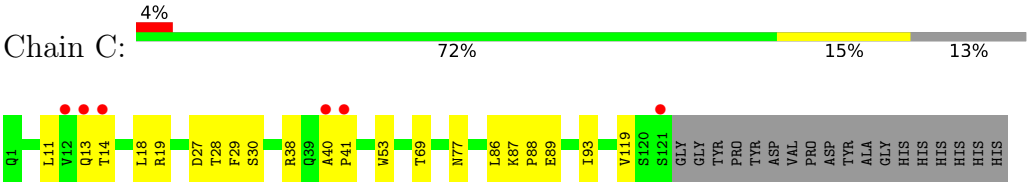
• Molecule 1: Sialic acid-binding periplasmic protein SiaP



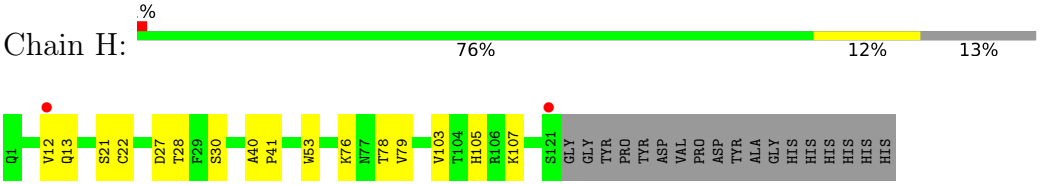
• Molecule 1: Sialic acid-binding periplasmic protein SiaP



• Molecule 2: VHH_VcP#2



• Molecule 2: VHH_VcP#2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.30Å 50.34Å 133.99Å 90.00° 114.88° 90.00°	Depositor
Resolution (Å)	46.38 – 2.05 46.38 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.38-2.05) 99.5 (46.38-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.257 0.194 , 0.254	Depositor DCC
R_{free} test set	55790 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 37.6	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	0.95	EDS
Total number of atoms	13752	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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: IMD, PGE, GOL

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	0.61	0/2435	0.75	3/3291 (0.1%)
1	B	0.65	2/2426 (0.1%)	0.72	0/3279
2	C	0.58	0/961	0.73	0/1303
2	H	0.63	0/961	0.77	0/1303
All	All	0.63	2/6783 (0.0%)	0.74	3/9176 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	PRO	N-CD	-10.32	1.33	1.47
1	B	290	GLN	C-N	5.58	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	MET	CG-SD-CE	6.91	111.25	100.20
1	A	44	GLN	N-CA-CB	-5.54	100.62	110.60
1	A	51	MET	CG-SD-CE	5.34	108.74	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	ARG	Sidechain

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	2389	2368	2367	23	0
1	B	2380	2358	2359	22	0
2	C	939	890	888	14	0
2	H	939	890	888	11	0
3	A	5	5	5	2	0
3	B	5	5	5	3	0
4	A	6	8	8	7	0
5	B	10	14	14	0	0
5	C	10	14	14	0	0
5	H	10	14	14	0	0
6	A	201	0	0	6	0
6	B	182	0	0	1	1
6	C	45	0	0	1	0
6	H	65	0	0	2	0
All	All	7186	6566	6562	71	1

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 5.

The worst 5 of 71 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:A:59:ASP:O	4:A:302:GOL:H2	1.78	0.84
1:B:200:LYS:O	1:B:200:LYS:HD3	1.82	0.78
2:C:27:ASP:OD1	2:C:28:THR:N	2.22	0.72
2:H:13:GLN:NE2	6:H:301:HOH:O	2.21	0.71
1:A:250:GLN:OE1	6:A:401:HOH:O	2.09	0.69

All (1) 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)
6:B:487:HOH:O	6:B:564:HOH:O[2_556]	2.13	0.07

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	301/303 (99%)	296 (98%)	5 (2%)	0	100 100
1	B	299/303 (99%)	293 (98%)	5 (2%)	1 (0%)	37 30
2	C	119/139 (86%)	114 (96%)	5 (4%)	0	100 100
2	H	119/139 (86%)	117 (98%)	2 (2%)	0	100 100
All	All	838/884 (95%)	820 (98%)	17 (2%)	1 (0%)	48 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	291	PRO

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	260/260 (100%)	257 (99%)	3 (1%)	67 68
1	B	260/260 (100%)	256 (98%)	4 (2%)	60 60
2	C	97/111 (87%)	96 (99%)	1 (1%)	73 74
2	H	97/111 (87%)	96 (99%)	1 (1%)	73 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	714/742 (96%)	705 (99%)	9 (1%)	65 66

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	11	LEU
2	H	21	SER
1	B	67	PHE
1	B	99	ASP
1	B	110	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	B	134	ASN
2	C	1	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PGE	H	201	-	9,9,9	0.44	0	8,8,8	0.37	0
3	IMD	B	301	-	3,5,5	0.63	0	4,5,5	0.60	0
5	PGE	C	201	-	9,9,9	0.41	0	8,8,8	0.51	0
3	IMD	A	301	-	3,5,5	0.47	0	4,5,5	0.85	0
4	GOL	A	302	-	5,5,5	1.65	1 (20%)	5,5,5	0.64	0
5	PGE	B	302	-	9,9,9	0.51	0	8,8,8	0.67	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	PGE	H	201	-	-	3/7/7/7	-
3	IMD	B	301	-	-	-	0/1/1/1
5	PGE	C	201	-	-	4/7/7/7	-
3	IMD	A	301	-	-	-	0/1/1/1
4	GOL	A	302	-	-	0/4/4/4	-
5	PGE	B	302	-	-	5/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	GOL	C3-C2	2.96	1.63	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	201	PGE	O2-C3-C4-O3
5	B	302	PGE	O2-C3-C4-O3
5	H	201	PGE	O3-C5-C6-O4
5	B	302	PGE	O1-C1-C2-O2
5	C	201	PGE	O3-C5-C6-O4

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	IMD	3	0
3	A	301	IMD	2	0
4	A	302	GOL	7	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	A	303/303 (100%)	-0.52	2 (0%)	84	86	22, 32, 51, 91	0
1	B	301/303 (99%)	-0.47	1 (0%)	90	92	20, 33, 53, 98	0
2	C	121/139 (87%)	0.27	6 (4%)	35	38	28, 46, 85, 119	0
2	H	121/139 (87%)	0.02	2 (1%)	69	71	27, 39, 66, 91	0
All	All	846/884 (95%)	-0.31	11 (1%)	74	77	20, 35, 63, 119	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	12	VAL	3.6
2	C	121	SER	2.8
1	A	-3	GLY	2.5
2	C	41	PRO	2.4
2	C	14	THR	2.3

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

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
4	GOL	A	302	6/6	0.64	0.20	51,74,126,126	0
5	PGE	H	201	10/10	0.79	0.14	50,71,93,95	0
5	PGE	B	302	10/10	0.86	0.10	28,43,52,59	0
5	PGE	C	201	10/10	0.87	0.10	33,47,59,65	0
3	IMD	A	301	5/5	0.90	0.12	25,35,46,56	0
3	IMD	B	301	5/5	0.95	0.10	22,30,38,41	0

6.5 Other polymers (i)

There are no such residues in this entry.