Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:09 pm BST

PDB ID	:	6D0X
Title	:	Crystal structure of chimeric H.2140 / K.1210 Fab in complex with circumsporozoite protein NANP3
Authors	:	Scally, S.W.; Bosch, A.; Imkeller, K.; Wardemann, H.; Julien, J.P.
Deposited on	:	2018-04-11
Resolution	:	1.85 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 ①) were used in the production of this report:

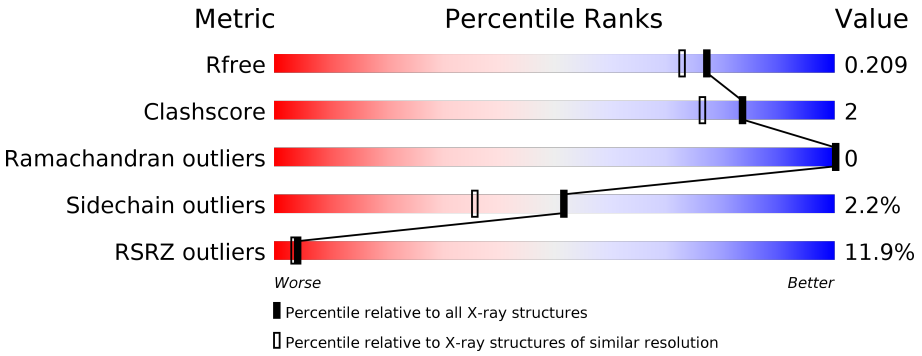
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.85 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	A	227	11% 96%
2	B	213	13% 89% 8%
3	C	12	8% 92% 8%

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	B	302	-	-	-	X
5	PEG	B	303	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3655 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 2140 Antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1665	1049	277	331	8	0	3	0

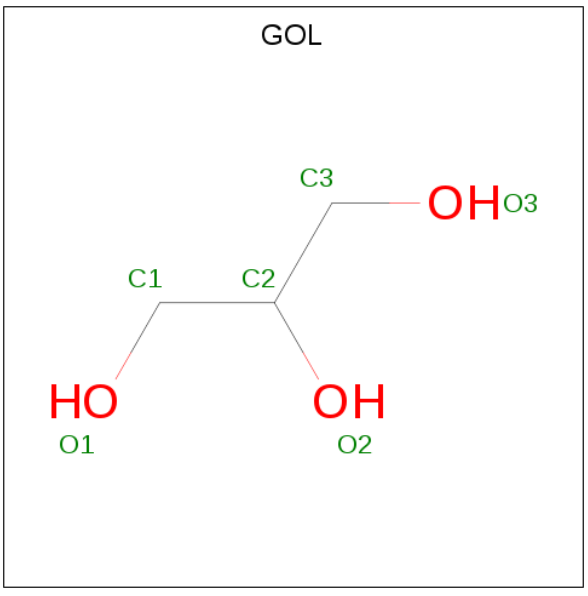
- Molecule 2 is a protein called 1210 Antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	211	1622	1018	268	331	5	0	3	0

- Molecule 3 is a protein called NANP3.

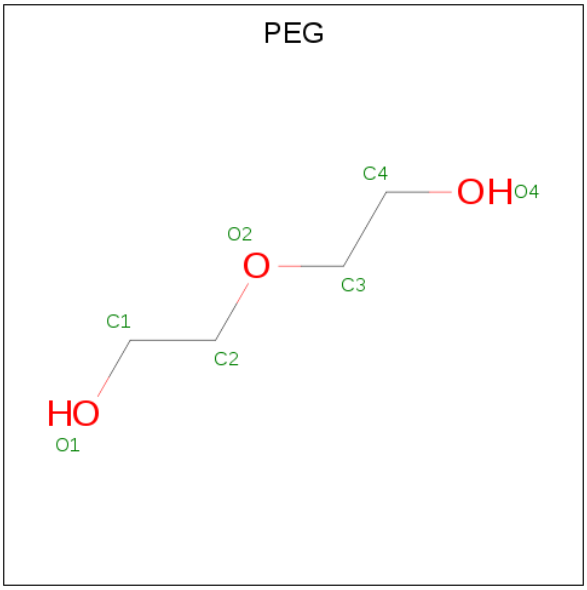
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	74	42	16	16	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

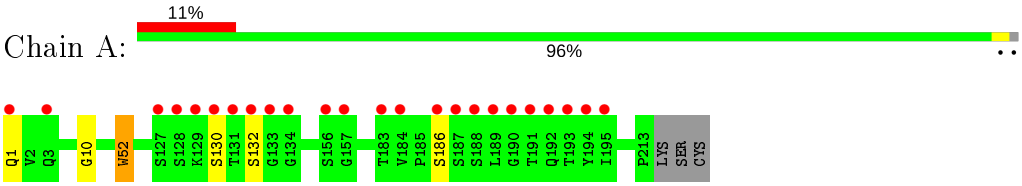
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	B	119	Total O 119 119	0	0
6	C	13	Total O 13 13	0	0

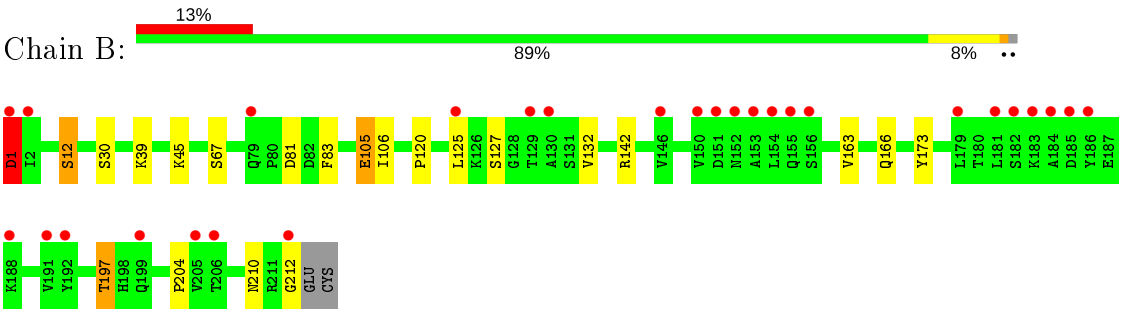
3 Residue-property plots (i)

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

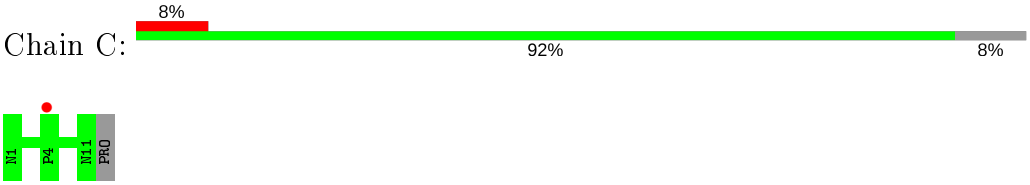
- Molecule 1: 2140 Antibody, heavy chain



- Molecule 2: 1210 Antibody, light chain



- Molecule 3: NANP3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.11Å 83.11Å 157.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 1.85 39.29 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.29-1.85) 94.2 (39.29-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 1.85Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.179 , 0.209 0.179 , 0.209	Depositor DCC
R_{free} test set	2000 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.9	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	0.97	EDS
Total number of atoms	3655	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, PEG

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	0.71	1/1716 (0.1%)	0.70	0/2345
2	B	0.63	0/1665	0.75	2/2271 (0.1%)
3	C	0.70	0/75	0.62	0/104
All	All	0.67	1/3456 (0.0%)	0.72	2/4720 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	TRP	CE3-CZ3	5.52	1.47	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1[A]	ASP	CB-CG-OD1	6.50	124.15	118.30
2	B	1[B]	ASP	CB-CG-OD1	6.50	124.15	118.30

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	A	1665	0	1584	2	0
2	B	1622	0	1531	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	74	0	63	0	0
4	A	6	0	8	1	0
4	B	12	0	16	2	0
5	B	7	0	10	2	0
6	A	137	0	0	0	0
6	B	119	0	0	2	0
6	C	13	0	0	0	0
All	All	3655	0	3212	16	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 2.

All (16) 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:B:67:SER:HB2	5:B:303:PEG:H42	1.52	0.91
2:B:12:SER:HB3	2:B:105[A]:GLU:OE2	2.00	0.62
2:B:30:SER:HA	5:B:303:PEG:H41	1.86	0.58
1:A:1:GLN:N	1:A:1:GLN:OE1	2.37	0.55
1:A:10:GLY:HA3	4:A:301:GOL:H32	1.88	0.54
2:B:197:THR:HG23	2:B:204:PRO:HB3	1.90	0.53
2:B:106:ILE:HD11	4:B:302:GOL:H11	1.91	0.52
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.90	0.52
2:B:210:ASN:O	2:B:212:GLY:N	2.43	0.52
2:B:125:LEU:C	2:B:127:SER:H	2.18	0.47
2:B:39:LYS:NZ	2:B:81:ASP:OD1	2.49	0.46
2:B:83:PHE:HB2	4:B:302:GOL:H12	1.98	0.46
2:B:45:LYS:NZ	6:B:405:HOH:O	2.46	0.45
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.53	0.44
2:B:1[A]:ASP:N	6:B:401:HOH:O	2.29	0.42
2:B:142:ARG:NH2	2:B:163:VAL:HG11	2.34	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	A	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
2	B	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
3	C	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
All	All	445/452 (98%)	429 (96%)	16 (4%)	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	A	183/189 (97%)	179 (98%)	4 (2%)	52	36
2	B	180/188 (96%)	174 (97%)	6 (3%)	38	20
3	C	7/9 (78%)	7 (100%)	0	100	100
All	All	370/386 (96%)	360 (97%)	10 (3%)	52	28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TRP
1	A	130	SER
1	A	132	SER
1	A	186	SER
2	B	1[A]	ASP
2	B	1[B]	ASP
2	B	12	SER
2	B	105[A]	GLU
2	B	105[B]	GLU
2	B	197	THR

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

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 carbohydrates in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
4	GOL	A	301	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
4	GOL	B	301	-	5,5,5	1.01	0	5,5,5	0.78	0
5	PEG	B	303	-	6,6,6	0.46	0	5,5,5	0.22	0
4	GOL	B	302	-	5,5,5	1.11	0	5,5,5	0.75	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
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	B	301	-	-	2/4/4/4	-
5	PEG	B	303	-	-	2/4/4/4	-
4	GOL	B	302	-	-	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})
4	A	301	GOL	C3-C2-C1	-2.10	103.53	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GOL	O1-C1-C2-C3
4	B	301	GOL	O1-C1-C2-O2
5	B	303	PEG	O1-C1-C2-O2
5	B	303	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	1	0
5	B	303	PEG	2	0
4	B	302	GOL	2	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	224/227 (98%)	0.52	24 (10%) 6 4	28, 44, 105, 141	0
2	B	211/213 (99%)	0.75	28 (13%) 3 2	29, 57, 97, 112	0
3	C	11/12 (91%)	0.91	1 (9%) 9 8	30, 34, 49, 73	0
All	All	446/452 (98%)	0.64	53 (11%) 4 3	28, 48, 100, 141	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	154	LEU	8.2
1	A	131	THR	7.9
1	A	130	SER	7.7
1	A	191	THR	6.1
2	B	182	SER	5.9
2	B	153	ALA	5.6
2	B	181	LEU	5.6
1	A	189	LEU	4.7
2	B	184	ALA	4.7
1	A	190	GLY	4.6
1	A	194	TYR	4.4
1	A	132	SER	4.3
2	B	150	VAL	4.3
1	A	127	SER	4.3
1	A	188	SER	4.0
1	A	128	SER	3.9
2	B	206	THR	3.8
2	B	129	THR	3.5
1	A	133	GLY	3.4
1	A	129	LYS	3.3
2	B	191	VAL	3.3
2	B	151	ASP	3.3
2	B	146	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	185	ASP	3.2
2	B	183	LYS	3.2
2	B	192	TYR	3.2
2	B	152	ASN	3.1
1	A	187	SER	3.1
2	B	188	LYS	3.1
2	B	130	ALA	3.0
2	B	205	VAL	3.0
2	B	2	ILE	2.9
2	B	156	SER	2.8
1	A	195	ILE	2.8
1	A	193	THR	2.8
2	B	1[A]	ASP	2.8
1	A	156	SER	2.7
1	A	1	GLN	2.7
1	A	184	VAL	2.7
2	B	125	LEU	2.7
1	A	157	GLY	2.7
2	B	212	GLY	2.7
2	B	199	GLN	2.6
1	A	186	SER	2.5
2	B	155	GLN	2.4
1	A	183	THR	2.4
2	B	179	LEU	2.3
1	A	192	GLN	2.3
2	B	79	GLN	2.3
2	B	186	TYR	2.2
3	C	4	PRO	2.1
1	A	134	GLY	2.1
1	A	3	GLN	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 carbohydrates 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
5	PEG	B	303	7/7	0.49	0.82	151,151,151,151	7
4	GOL	B	302	6/6	0.69	0.43	92,94,95,95	0
4	GOL	B	301	6/6	0.80	0.29	103,104,106,106	0
4	GOL	A	301	6/6	0.85	0.14	73,75,75,76	0

6.5 Other polymers

There are no such residues in this entry.