Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 11:06 am GMT

PDB ID	:	6TRG
Title	:	Salmonella typhimurium neuraminidase mutant (D100S)
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Deposited on	:	2019-12-18
Resolution	:	1.00 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 (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 (i)) were used in the production of this report:

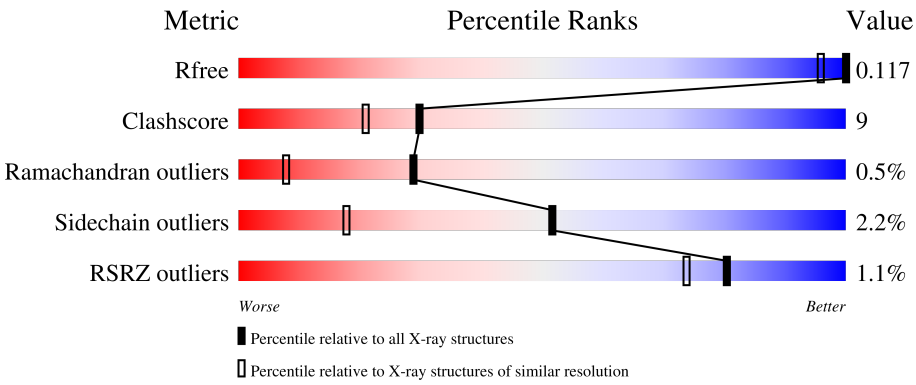
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

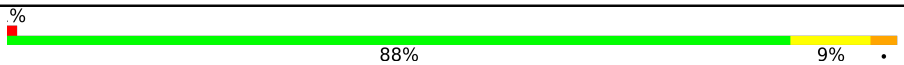
The reported resolution of this entry is 1.00 Å.

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	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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	XXX	379	

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	XXX	404[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	XXX	406	-	-	X	-
2	GOL	XXX	407	-	-	X	-
3	PO4	XXX	408[A]	-	-	X	-
3	PO4	XXX	409	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7070 atoms, of which 3234 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.

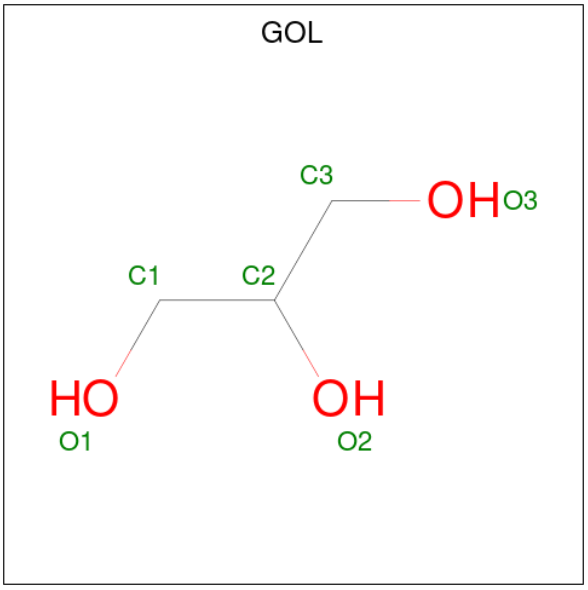
- Molecule 1 is a protein called Sialidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	XXX	379	6345	1984	3162	563	623	13	194	30	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XXX	100	SER	ASP	engineered mutation	UNP P29768

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	XXX	1	14	3	8	3	2	0
2	XXX	1	14	3	8	3	2	0
2	XXX	1	14	3	8	3	2	0

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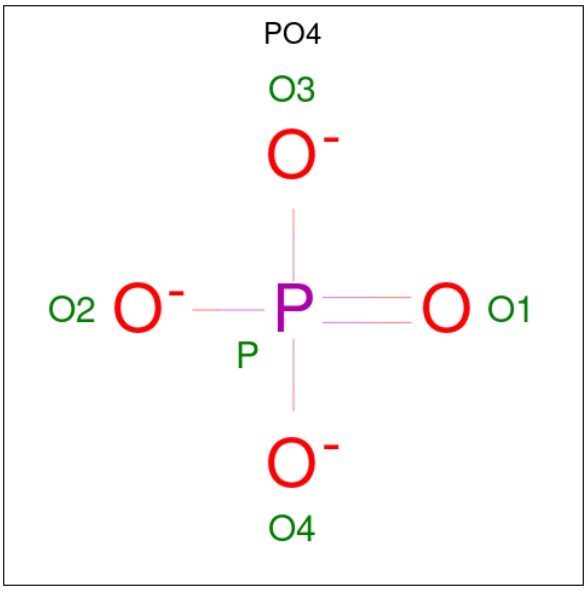
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	XXX	1	28	6	16	6	4	1
			Total	C	H	O		
2	XXX	1	28	6	16	6	4	1
			Total	C	H	O		
2	XXX	1	14	3	8	3	2	0
			Total	C	H	O		
2	XXX	1	14	3	8	3	2	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	XXX	1	10	8	2	0	1
			Total	O	P		
3	XXX	1	5	4	1	0	0

- Molecule 4 is water.

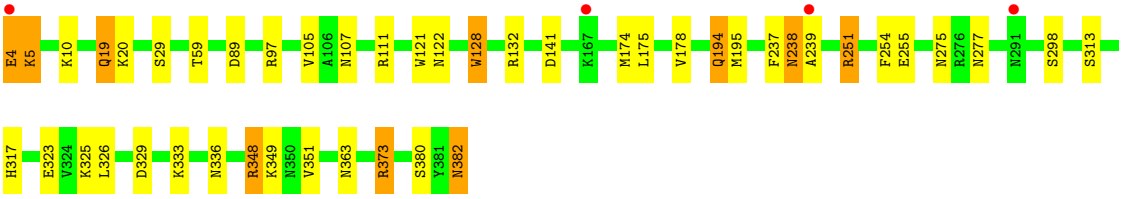
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	XXX	522	584	584	0	60

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: Sialidase

Chain XXX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.17Å 81.64Å 91.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.89 – 1.00 30.87 – 1.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.89-1.00) 98.1 (30.87-1.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.00Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.101 , 0.116 0.102 , 0.117	Depositor DCC
R_{free} test set	9182 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	7.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 62.9	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	0.99	EDS
Total number of atoms	7070	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	XXX	0.87	7/3239 (0.2%)	1.22	22/4367 (0.5%)

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	XXX	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XXX	255	GLU	CD-OE2	-12.96	1.11	1.25
1	XXX	323	GLU	CD-OE2	10.43	1.37	1.25
1	XXX	373	ARG	NE-CZ	7.30	1.42	1.33
1	XXX	195[A]	MET	CG-SD	6.94	1.99	1.81
1	XXX	195[B]	MET	CG-SD	6.94	1.99	1.81
1	XXX	380	SER	CB-OG	6.30	1.50	1.42
1	XXX	194	GLN	CB-CG	-5.71	1.37	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XXX	111[A]	ARG	NE-CZ-NH2	-19.15	110.72	120.30
1	XXX	111[B]	ARG	NE-CZ-NH2	-19.15	110.72	120.30
1	XXX	195[A]	MET	CG-SD-CE	15.78	125.45	100.20
1	XXX	195[B]	MET	CG-SD-CE	15.78	125.45	100.20
1	XXX	111[A]	ARG	NE-CZ-NH1	15.67	128.13	120.30
1	XXX	111[B]	ARG	NE-CZ-NH1	15.67	128.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XXX	111[A]	ARG	CG-CD-NE	-7.45	96.15	111.80
1	XXX	111[B]	ARG	CG-CD-NE	-7.45	96.15	111.80
1	XXX	111[A]	ARG	CD-NE-CZ	7.08	133.51	123.60
1	XXX	111[B]	ARG	CD-NE-CZ	7.08	133.51	123.60
1	XXX	254	PHE	CB-CG-CD1	6.66	125.46	120.80
1	XXX	373	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	XXX	238[A]	ASN	CA-C-O	-6.19	107.09	120.10
1	XXX	238[B]	ASN	CA-C-O	-6.19	107.09	120.10
1	XXX	348[A]	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	XXX	348[B]	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	XXX	329	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	XXX	251	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	XXX	132	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	XXX	239	ALA	O-C-N	5.17	130.97	122.70
1	XXX	194	GLN	CA-CB-CG	5.16	124.76	113.40
1	XXX	97	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	XXX	29[C]	SER	Mainchain

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	XXX	3183	3162	3129	54	2
2	XXX	54	72	72	22	2
3	XXX	15	0	0	4	0
4	XXX	584	0	0	12	0
All	All	3836	3234	3201	60	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 9.

All (60) 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:XXX:407:GOL:H32	3:XXX:408[A]:PO4:O2	1.12	1.23
2:XXX:407:GOL:C3	3:XXX:408[A]:PO4:O2	1.84	1.23
1:XXX:4[B]:GLU:HG2	1:XXX:5[B]:LYS:N	1.48	1.13
1:XXX:107:ASN:OD1	2:XXX:406:GOL:O2	1.70	1.08
1:XXX:4[B]:GLU:CG	1:XXX:5[B]:LYS:N	2.31	0.93
1:XXX:19:GLN:H	1:XXX:19:GLN:HE21	1.15	0.90
1:XXX:128:TRP:CZ3	1:XXX:175[B]:LEU:HD13	2.09	0.88
1:XXX:107:ASN:CG	2:XXX:406:GOL:O2	2.19	0.81
1:XXX:382[A]:ASN:C	1:XXX:382[A]:ASN:HD22	1.83	0.81
1:XXX:107:ASN:ND2	2:XXX:406:GOL:O2	2.16	0.78
1:XXX:10[B]:LYS:CD	4:XXX:616:HOH:O	2.38	0.72
1:XXX:333:LYS:HE3	4:XXX:748[B]:HOH:O	1.90	0.71
1:XXX:59[B]:THR:CG2	4:XXX:916:HOH:O	2.41	0.68
2:XXX:407:GOL:H32	3:XXX:408[A]:PO4:P	2.32	0.67
1:XXX:20:LYS:HE3	4:XXX:555[B]:HOH:O	1.99	0.63
2:XXX:406:GOL:H11	4:XXX:907:HOH:O	1.97	0.63
1:XXX:59[B]:THR:HG23	4:XXX:916:HOH:O	2.01	0.60
1:XXX:4[B]:GLU:HG2	1:XXX:5[B]:LYS:CB	2.32	0.60
1:XXX:251:ARG:HH11	1:XXX:275:ASN:HD21	1.50	0.59
1:XXX:382[A]:ASN:C	1:XXX:382[A]:ASN:ND2	2.51	0.59
1:XXX:317:HIS:HD2	4:XXX:538:HOH:O	1.85	0.58
1:XXX:4[B]:GLU:HG2	1:XXX:5[B]:LYS:CA	2.31	0.58
1:XXX:174:MET:O	1:XXX:175[B]:LEU:HD12	2.04	0.57
1:XXX:10[B]:LYS:HD3	4:XXX:616:HOH:O	2.00	0.57
1:XXX:348[A]:ARG:HH22	2:XXX:406:GOL:C1	2.17	0.57
1:XXX:107:ASN:ND2	2:XXX:406:GOL:C2	2.70	0.55
2:XXX:406:GOL:O1	2:XXX:406:GOL:O3	2.22	0.55
1:XXX:10[B]:LYS:HD2	4:XXX:616:HOH:O	2.05	0.53
1:XXX:19:GLN:H	1:XXX:19:GLN:NE2	1.95	0.53
1:XXX:107:ASN:ND2	2:XXX:406:GOL:H2	2.24	0.51
1:XXX:121:TRP:HH2	1:XXX:175[B]:LEU:HD11	1.75	0.51
1:XXX:89:ASP:HB2	1:XXX:122:ASN:HD21	1.74	0.51
1:XXX:348[A]:ARG:NH2	2:XXX:406:GOL:O1	2.44	0.51
1:XXX:251:ARG:HH11	1:XXX:275:ASN:ND2	2.09	0.50
1:XXX:107:ASN:CG	2:XXX:406:GOL:C2	2.79	0.49
2:XXX:407:GOL:C2	3:XXX:408[A]:PO4:O2	2.55	0.49
1:XXX:349[A]:LYS:CE	4:XXX:510:HOH:O	2.61	0.48
1:XXX:382[A]:ASN:ND2	1:XXX:382[A]:ASN:O	2.47	0.47
1:XXX:349[A]:LYS:NZ	4:XXX:504:HOH:O	2.44	0.47
1:XXX:348[B]:ARG:HH22	2:XXX:406:GOL:C1	2.27	0.47
1:XXX:107:ASN:CG	2:XXX:406:GOL:H2	2.36	0.46
1:XXX:141:ASP:OD2	2:XXX:404[B]:GOL:C3	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XXX:251:ARG:HD2	1:XXX:275:ASN:HD21	1.81	0.46
1:XXX:348[A]:ARG:HH22	2:XXX:406:GOL:H12	1.81	0.46
1:XXX:317:HIS:HE1	4:XXX:786:HOH:O	1.97	0.46
1:XXX:348[B]:ARG:NH2	2:XXX:406:GOL:O1	2.46	0.46
1:XXX:4[B]:GLU:HG2	1:XXX:5[B]:LYS:H	1.64	0.46
1:XXX:5[A]:LYS:HB3	1:XXX:5[A]:LYS:HE3	1.39	0.45
1:XXX:141:ASP:OD2	2:XXX:404[B]:GOL:H31	2.17	0.45
1:XXX:121:TRP:CH2	1:XXX:175[B]:LEU:HD11	2.51	0.45
1:XXX:175[B]:LEU:CD1	1:XXX:175[B]:LEU:N	2.79	0.45
1:XXX:4[B]:GLU:CG	1:XXX:5[B]:LYS:H	2.20	0.44
1:XXX:237:PHE:C	1:XXX:238[A]:ASN:O	2.50	0.44
1:XXX:105:VAL:HG12	2:XXX:405[A]:GOL:H12	2.00	0.43
1:XXX:336:ASN:HD22	1:XXX:363:ASN:ND2	2.18	0.41
1:XXX:175[B]:LEU:HD12	1:XXX:175[B]:LEU:N	2.34	0.41
1:XXX:298:SER:HA	1:XXX:313:SER:O	2.21	0.41
1:XXX:174:MET:C	1:XXX:175[B]:LEU:HD12	2.41	0.41
1:XXX:325[B]:LYS:HD3	1:XXX:326:LEU:O	2.22	0.40
1:XXX:107:ASN:OD1	2:XXX:406:GOL:C2	2.65	0.40

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:XXX:373:ARG:HH21	2:XXX:404[B]:GOL:HO2[2_664]	1.24	0.36
1:XXX:373:ARG:HE	2:XXX:404[B]:GOL:O2[2_664]	1.55	0.05

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	XXX	406/379 (107%)	389 (96%)	15 (4%)	2 (0%)	29 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	XXX	178	VAL
1	XXX	351	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	XXX	355/325 (109%)	345 (97%)	10 (3%)	43 12

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

Mol	Chain	Res	Type
1	XXX	4[B]	GLU
1	XXX	5[A]	LYS
1	XXX	5[B]	LYS
1	XXX	19	GLN
1	XXX	128	TRP
1	XXX	194	GLN
1	XXX	277[A]	ASN
1	XXX	277[B]	ASN
1	XXX	382[A]	ASN
1	XXX	382[B]	ASN

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)

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)

12 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	$\#\|Z\| > 2$
2	GOL	XXX	403	-	5,5,5	0.40	0	5,5,5	0.45	0
3	PO4	XXX	408[B]	-	4,4,4	3.92	2 (50%)	6,6,6	1.47	1 (16%)
2	GOL	XXX	404[A]	-	5,5,5	2.15	1 (20%)	5,5,5	2.28	1 (20%)
2	GOL	XXX	405[B]	-	5,5,5	0.49	0	5,5,5	1.40	1 (20%)
2	GOL	XXX	406	-	5,5,5	0.46	0	5,5,5	1.13	1 (20%)
3	PO4	XXX	409	-	4,4,4	3.73	1 (25%)	6,6,6	1.71	3 (50%)
2	GOL	XXX	407	-	5,5,5	0.76	0	5,5,5	1.62	1 (20%)
3	PO4	XXX	408[A]	-	4,4,4	4.42	1 (25%)	6,6,6	2.61	2 (33%)
2	GOL	XXX	405[A]	-	5,5,5	0.61	0	5,5,5	1.09	0
2	GOL	XXX	401	-	5,5,5	1.04	0	5,5,5	1.06	0
2	GOL	XXX	404[B]	-	5,5,5	1.08	1 (20%)	5,5,5	1.85	2 (40%)
2	GOL	XXX	402	-	5,5,5	1.16	1 (20%)	5,5,5	1.36	1 (20%)

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	XXX	403	-	-	2/4/4/4	-
2	GOL	XXX	404[A]	-	-	0/4/4/4	-
2	GOL	XXX	405[B]	-	-	4/4/4/4	-
2	GOL	XXX	406	-	-	2/4/4/4	-
2	GOL	XXX	407	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	XXX	405[A]	-	-	0/4/4/4	-
2	GOL	XXX	401	-	-	0/4/4/4	-
2	GOL	XXX	404[B]	-	-	2/4/4/4	-
2	GOL	XXX	402	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	XXX	408[A]	PO4	P-O1	-8.55	1.30	1.50
3	XXX	408[B]	PO4	P-O2	-7.55	1.31	1.54
3	XXX	409	PO4	P-O1	7.41	1.68	1.50
2	XXX	404[A]	GOL	O2-C2	4.66	1.57	1.43
2	XXX	404[B]	GOL	O1-C1	2.13	1.51	1.42
2	XXX	402	GOL	O2-C2	2.12	1.49	1.43
3	XXX	408[B]	PO4	P-O1	2.08	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	XXX	404[A]	GOL	O3-C3-C2	4.87	133.54	110.20
3	XXX	408[A]	PO4	O2-P-O1	-4.58	94.15	110.89
3	XXX	408[A]	PO4	O4-P-O1	3.97	125.44	110.89
2	XXX	405[B]	GOL	O1-C1-C2	2.83	123.76	110.20
2	XXX	404[B]	GOL	O1-C1-C2	2.77	123.48	110.20
2	XXX	404[B]	GOL	C3-C2-C1	2.71	122.22	111.70
3	XXX	408[B]	PO4	O2-P-O1	-2.60	101.38	110.89
3	XXX	409	PO4	O4-P-O2	2.22	115.09	107.97
2	XXX	407	GOL	O3-C3-C2	-2.19	99.71	110.20
2	XXX	402	GOL	O2-C2-C1	2.18	118.74	109.12
3	XXX	409	PO4	O4-P-O3	-2.17	101.00	107.97
3	XXX	409	PO4	O2-P-O1	2.09	118.55	110.89
2	XXX	406	GOL	C3-C2-C1	-2.04	103.78	111.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	XXX	405[B]	GOL	O1-C1-C2-C3
2	XXX	405[B]	GOL	C1-C2-C3-O3
2	XXX	406	GOL	O1-C1-C2-C3
2	XXX	405[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	XXX	402	GOL	O1-C1-C2-C3
2	XXX	402	GOL	C1-C2-C3-O3
2	XXX	403	GOL	O1-C1-C2-C3
2	XXX	403	GOL	O1-C1-C2-O2
2	XXX	406	GOL	O1-C1-C2-O2
2	XXX	405[B]	GOL	O1-C1-C2-O2
2	XXX	404[B]	GOL	O1-C1-C2-O2
2	XXX	404[B]	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	XXX	406	GOL	15	0
2	XXX	407	GOL	4	0
3	XXX	408[A]	PO4	4	0
2	XXX	405[A]	GOL	1	0
2	XXX	404[B]	GOL	2	2

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	XXX	379/379 (100%)	-0.38	4 (1%) 80 74	5, 8, 17, 31	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	XXX	239	ALA	4.4
1	XXX	291	ASN	2.3
1	XXX	4[B]	GLU	2.2
1	XXX	167	LYS	2.1

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, 95th 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	PO4	XXX	409	5/5	0.80	0.24	15,22,25,36	5
2	GOL	XXX	404[B]	6/6	0.86	0.25	6,7,13,13	14
2	GOL	XXX	404[A]	6/6	0.86	0.25	11,12,20,21	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	XXX	402	6/6	0.88	0.14	14,17,26,28	2
3	PO4	XXX	408[A]	5/5	0.93	0.15	6,10,10,13	5
3	PO4	XXX	408[B]	5/5	0.93	0.15	8,10,15,16	5
2	GOL	XXX	406	6/6	0.93	0.19	6,7,32,34	14
2	GOL	XXX	407	6/6	0.95	0.12	10,17,20,21	2
2	GOL	XXX	405[B]	6/6	0.96	0.23	5,6,9,11	14
2	GOL	XXX	403	6/6	0.96	0.15	13,23,64,66	2
2	GOL	XXX	405[A]	6/6	0.96	0.23	6,9,13,15	14
2	GOL	XXX	401	6/6	0.98	0.07	11,13,14,16	2

6.5 Other polymers (i)

There are no such residues in this entry.