



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 12:13 PM EDT

PDB ID : 4OWK
Title : Crystal Structure of the Vibrio vulnificus Hemolysin/Cytolysin Beta-Trefoil Lectin with N-Acetyl-D-Galactosamine Bound
Authors : Kaus, K.; Olson, R.
Deposited on : 2014-02-02
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

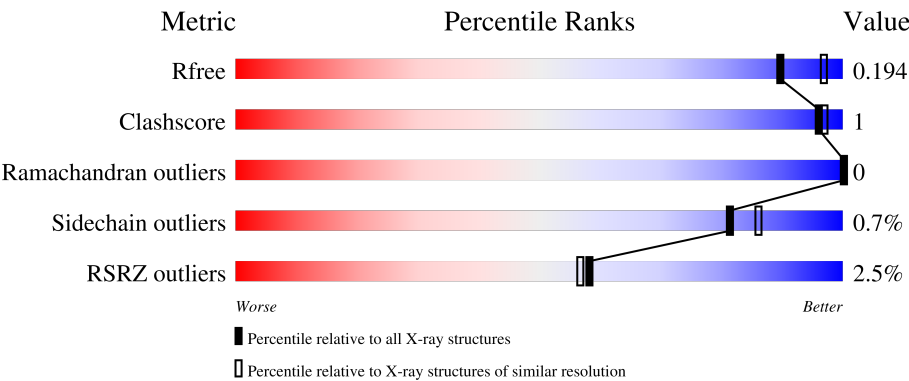
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. 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	138	<div><div>2%</div><div>95%</div><div>5%</div></div>
1	B	138	<div><div>5%</div><div>93%</div><div>5%</div></div>
1	C	138	<div><div>%</div><div>91%</div><div>5%</div></div>
1	D	138	<div><div>2%</div><div>94%</div><div>5%</div></div>
1	E	138	<div><div>3%</div><div>93%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	138	<div><div><div></div><div>2%</div></div><div><div></div><div>93%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
1	G	138	<div><div><div></div><div>%</div></div><div><div></div><div>91%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14600 atoms, of which 6533 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 Cytolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	131	Total	C	H	N	O	S	0	0	0
			1886	617	884	185	195	5			
1	B	131	Total	C	H	N	O	S	0	0	0
			1876	614	883	181	193	5			
1	C	131	Total	C	H	N	O	S	0	0	0
			1914	616	913	186	194	5			
1	D	131	Total	C	H	N	O	S	0	0	0
			1918	617	919	184	193	5			
1	E	136	Total	C	H	N	O	S	0	0	0
			2008	649	957	193	204	5			
1	F	133	Total	C	H	N	O	S	0	0	0
			1979	638	942	192	202	5			
1	G	131	Total	C	H	N	O	S	0	0	0
			1880	615	882	182	196	5			

There are 28 discrepancies between the modelled and reference sequences:

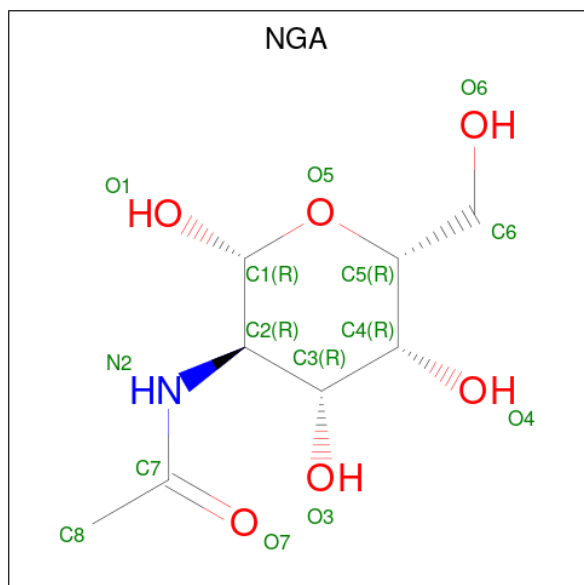
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP P19247
A	335	SER	-	expression tag	UNP P19247
A	336	ALA	-	expression tag	UNP P19247
A	337	MET	-	expression tag	UNP P19247
B	334	GLY	-	expression tag	UNP P19247
B	335	SER	-	expression tag	UNP P19247
B	336	ALA	-	expression tag	UNP P19247
B	337	MET	-	expression tag	UNP P19247
C	334	GLY	-	expression tag	UNP P19247
C	335	SER	-	expression tag	UNP P19247
C	336	ALA	-	expression tag	UNP P19247
C	337	MET	-	expression tag	UNP P19247
D	334	GLY	-	expression tag	UNP P19247
D	335	SER	-	expression tag	UNP P19247
D	336	ALA	-	expression tag	UNP P19247

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Chain	Residue	Modelled	Actual	Comment	Reference
D	337	MET	-	expression tag	UNP P19247
E	334	GLY	-	expression tag	UNP P19247
E	335	SER	-	expression tag	UNP P19247
E	336	ALA	-	expression tag	UNP P19247
E	337	MET	-	expression tag	UNP P19247
F	334	GLY	-	expression tag	UNP P19247
F	335	SER	-	expression tag	UNP P19247
F	336	ALA	-	expression tag	UNP P19247
F	337	MET	-	expression tag	UNP P19247
G	334	GLY	-	expression tag	UNP P19247
G	335	SER	-	expression tag	UNP P19247
G	336	ALA	-	expression tag	UNP P19247
G	337	MET	-	expression tag	UNP P19247

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 8	H 15	N 1	O 6	0	0
2	B	1	Total 30	C 8	H 15	N 1	O 6	0	0
2	C	1	Total 30	C 8	H 15	N 1	O 6	0	0
2	D	1	Total 30	C 8	H 15	N 1	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	
			30	8	15	1	6	
2	F	1	Total	C	H	N	O	
			30	8	15	1	6	
2	G	1	Total	C	H	N	O	
			30	8	15	1	6	

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			14	3	8	3	0	0
3	C	1	Total	C	H	O		
			14	3	8	3	0	0
3	D	1	Total	C	H	O		
			14	3	8	3	0	0
3	E	1	Total	C	H	O		
			14	3	8	3	0	0
3	F	1	Total	C	H	O		
			14	3	8	3	0	0
3	G	1	Total	C	H	O		
			14	3	8	3	0	0

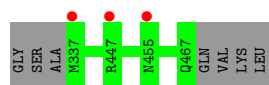
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total 95	O 95	0	0
4	B	79	Total 79	O 79	0	0
4	C	93	Total 93	O 93	0	0
4	D	91	Total 91	O 91	0	0
4	E	171	Total 171	O 171	0	0
4	F	169	Total 169	O 169	0	0
4	G	147	Total 147	O 147	0	0

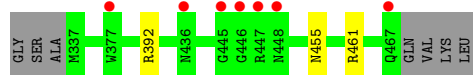
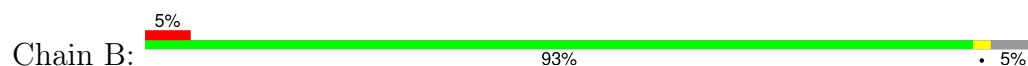
3 Residue-property plots [i](#)

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.

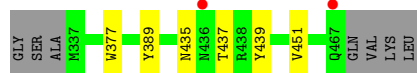
- Molecule 1: Cytolysin



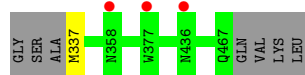
- Molecule 1: Cytolysin



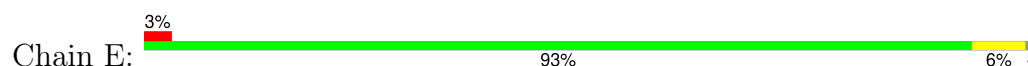
- Molecule 1: Cytolysin



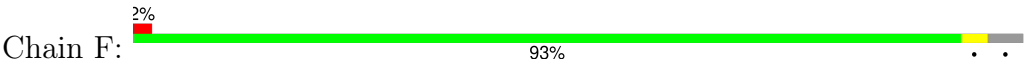
- Molecule 1: Cytolysin



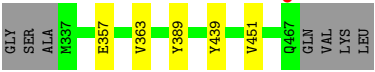
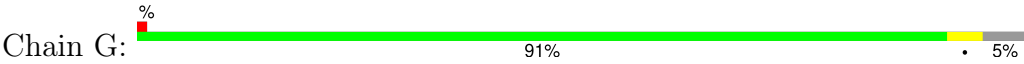
- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



● Molecule 1: Cytolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.39Å 79.83Å 148.69Å 90.00° 89.48° 90.00°	Depositor
Resolution (Å)	37.17 – 2.00 37.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (37.17-2.00) 95.0 (37.17-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.158 , 0.191 0.162 , 0.194	Depositor DCC
R_{free} test set	4166 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14600	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 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, NGA

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	0.49	0/1022	0.58	0/1394
1	B	0.45	0/1013	0.59	0/1382
1	C	0.45	0/1021	0.60	0/1393
1	D	0.45	0/1019	0.53	0/1389
1	E	0.67	0/1071	0.73	1/1457 (0.1%)
1	F	0.68	0/1057	0.74	1/1438 (0.1%)
1	G	0.57	0/1016	0.67	0/1383
All	All	0.55	0/7219	0.64	2/9836 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	390	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	F	398	CYS	CA-CB-SG	-6.46	102.38	114.00

There are no chirality outliers.

There are no planarity outliers.

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	1002	884	919	0	0
1	B	993	883	909	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1001	913	919	2	0
1	D	999	919	920	1	0
1	E	1051	957	987	4	0
1	F	1037	942	975	2	0
1	G	998	882	929	2	0
2	A	15	15	15	0	0
2	B	15	15	15	1	0
2	C	15	15	15	0	0
2	D	15	15	15	0	0
2	E	15	15	15	0	0
2	F	15	15	15	0	0
2	G	15	15	15	0	0
3	A	6	8	8	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	6	8	8	0	0
3	F	6	8	8	0	0
3	G	6	8	8	0	0
4	A	95	0	0	0	0
4	B	79	0	0	2	0
4	C	93	0	0	0	0
4	D	91	0	0	1	0
4	E	171	0	0	2	1
4	F	169	0	0	1	0
4	G	147	0	0	0	1
All	All	8067	6533	6711	14	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 1.

All (14) 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:D:337:MET:N	4:D:690:HOH:O	2.17	0.78
1:G:357:GLU:HB3	1:G:363:VAL:HG21	1.69	0.74
1:E:458:ASN:OD1	4:E:601:HOH:O	2.10	0.70
2:B:501:NGA:O7	4:B:654:HOH:O	2.14	0.66
1:F:336:ALA:N	4:F:747:HOH:O	2.33	0.60
1:E:433:ASP:OD2	4:E:676:HOH:O	2.20	0.48
1:B:461:ARG:NH1	4:B:675:HOH:O	2.35	0.46
1:E:439:TYR:HB3	1:E:451:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASN:HB2	1:C:437:THR:HG22	1.99	0.44
1:E:378:ASN:HA	1:E:393:VAL:CG1	2.48	0.43
1:C:439:TYR:HB3	1:C:451:VAL:HB	2.01	0.42
1:B:392:ARG:O	1:B:392:ARG:HG3	2.20	0.41
1:F:439:TYR:HB3	1:F:451:VAL:HB	2.02	0.40
1:G:439:TYR:HB3	1:G:451:VAL:HB	2.04	0.40

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)
4:E:624:HOH:O	4:G:604:HOH:O[1_655]	2.08	0.12

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	129/138 (94%)	125 (97%)	4 (3%)	0	100	100
1	B	129/138 (94%)	123 (95%)	6 (5%)	0	100	100
1	C	129/138 (94%)	125 (97%)	4 (3%)	0	100	100
1	D	129/138 (94%)	125 (97%)	4 (3%)	0	100	100
1	E	134/138 (97%)	130 (97%)	4 (3%)	0	100	100
1	F	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
1	G	129/138 (94%)	126 (98%)	3 (2%)	0	100	100
All	All	910/966 (94%)	882 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	102/116 (88%)	102 (100%)	0	100	100
1	B	100/116 (86%)	99 (99%)	1 (1%)	73	78
1	C	102/116 (88%)	100 (98%)	2 (2%)	50	55
1	D	101/116 (87%)	101 (100%)	0	100	100
1	E	109/116 (94%)	108 (99%)	1 (1%)	75	81
1	F	109/116 (94%)	109 (100%)	0	100	100
1	G	103/116 (89%)	102 (99%)	1 (1%)	73	78
All	All	726/812 (89%)	721 (99%)	5 (1%)	81	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	455	ASN
1	C	377	TRP
1	C	389	TYR
1	E	389	TYR
1	G	389	TYR

Sometimes 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	NGA	G	501	-	15,15,15	0.63	0	21,21,21	1.14	2 (9%)
2	NGA	C	501	-	15,15,15	0.46	0	21,21,21	0.74	0
3	GOL	C	502	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	F	502	-	5,5,5	0.42	0	5,5,5	0.39	0
2	NGA	D	501	-	15,15,15	0.39	0	21,21,21	0.76	0
2	NGA	E	501	-	15,15,15	0.55	0	21,21,21	0.81	0
2	NGA	B	501	-	15,15,15	0.54	0	21,21,21	1.52	4 (19%)
3	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.30	0
2	NGA	F	501	-	15,15,15	0.73	0	21,21,21	1.18	4 (19%)
3	GOL	D	502	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	E	502	-	5,5,5	0.33	0	5,5,5	0.38	0
3	GOL	G	502	-	5,5,5	0.37	0	5,5,5	0.32	0
2	NGA	A	501	-	15,15,15	0.49	0	21,21,21	1.07	2 (9%)

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	NGA	G	501	-	-	0/6/26/26	0/1/1/1
2	NGA	C	501	-	-	0/6/26/26	0/1/1/1
3	GOL	C	502	-	-	3/4/4/4	-
3	GOL	F	502	-	-	0/4/4/4	-
2	NGA	D	501	-	-	0/6/26/26	0/1/1/1
2	NGA	E	501	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NGA	B	501	-	-	0/6/26/26	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
2	NGA	F	501	-	-	0/6/26/26	0/1/1/1
3	GOL	D	502	-	-	1/4/4/4	-
3	GOL	E	502	-	-	2/4/4/4	-
3	GOL	G	502	-	-	2/4/4/4	-
2	NGA	A	501	-	-	1/6/26/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NGA	O5-C1-C2	3.88	113.42	109.52
2	B	501	NGA	C1-C2-N2	-3.85	106.27	110.73
2	F	501	NGA	C1-C2-N2	3.00	114.21	110.73
2	A	501	NGA	O5-C1-C2	2.71	112.24	109.52
2	G	501	NGA	O7-C7-N2	2.56	126.50	121.98
2	G	501	NGA	O7-C7-C8	-2.47	117.66	122.05
2	F	501	NGA	O5-C1-C2	2.33	111.86	109.52
2	B	501	NGA	C3-C2-N2	-2.29	106.40	110.62
2	F	501	NGA	C3-C2-N2	-2.28	106.41	110.62
2	B	501	NGA	C1-C2-C3	2.15	113.48	110.54
2	F	501	NGA	C1-C2-C3	2.08	113.39	110.54
2	A	501	NGA	O5-C5-C6	2.05	111.52	106.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	E	502	GOL	O1-C1-C2-C3
3	G	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	E	502	GOL	O1-C1-C2-O2
3	G	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-O2
2	A	501	NGA	C4-C5-C6-O6
3	C	502	GOL	O2-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NGA	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, 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	A	131/138 (94%)	-0.12	3 (2%) 61 59	32, 42, 63, 98	0
1	B	131/138 (94%)	-0.08	7 (5%) 33 31	29, 43, 72, 110	0
1	C	131/138 (94%)	-0.25	2 (1%) 71 70	28, 41, 65, 82	0
1	D	131/138 (94%)	-0.06	3 (2%) 61 59	26, 46, 79, 98	0
1	E	136/138 (98%)	-0.58	4 (2%) 54 52	16, 26, 51, 72	0
1	F	133/138 (96%)	-0.72	3 (2%) 61 59	14, 23, 52, 68	0
1	G	131/138 (94%)	-0.59	1 (0%) 82 82	16, 31, 54, 80	0
All	All	924/966 (95%)	-0.35	23 (2%) 58 57	14, 38, 64, 110	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	ARG	5.1
1	B	446	GLY	4.5
1	E	468	GLN	4.5
1	B	448	ASN	3.9
1	B	377	TRP	3.8
1	F	386	GLU	3.7
1	B	445	GLY	3.5
1	E	336	ALA	3.4
1	B	467	GLN	3.3
1	C	436	ASN	3.1
1	B	436	ASN	2.8
1	A	337	MET	2.7
1	D	436	ASN	2.5
1	E	471	LEU	2.4
1	G	467	GLN	2.4
1	D	358	ASN	2.3
1	A	447	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	467	GLN	2.2
1	D	377	TRP	2.2
1	F	358	ASN	2.1
1	A	455	ASN	2.1
1	F	363	VAL	2.1
1	E	463	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	GOL	F	502	6/6	0.83	0.14	60,72,77,79	0
3	GOL	G	502	6/6	0.84	0.14	59,72,80,87	0
3	GOL	A	502	6/6	0.85	0.17	73,88,90,90	0
3	GOL	E	502	6/6	0.87	0.12	51,64,74,81	0
3	GOL	C	502	6/6	0.87	0.13	74,89,91,91	0
3	GOL	D	502	6/6	0.87	0.13	63,76,80,82	0
2	NGA	A	501	15/15	0.91	0.10	39,53,67,69	0
2	NGA	C	501	15/15	0.91	0.11	40,63,78,88	0
2	NGA	B	501	15/15	0.92	0.10	38,59,78,78	0
2	NGA	F	501	15/15	0.92	0.10	23,46,64,75	0
2	NGA	G	501	15/15	0.92	0.10	31,49,74,74	0
2	NGA	E	501	15/15	0.94	0.08	24,35,52,53	0
2	NGA	D	501	15/15	0.95	0.08	45,62,77,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.