Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 02:26 PM EDT

PDB ID	:	4ADG
Title	:	Crystal structure of the Rubella virus envelope Glycoprotein E1 in post-fusion form (crystal form II)
Authors	:	DuBois, R.M.; Vaney, M.C.; Tortorici, M.A.; Al Kurdi, R.; Barba-Spaeth, G.; Rey, F.A.
Deposited on	:	2011-12-26
Resolution	:	2.18 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:

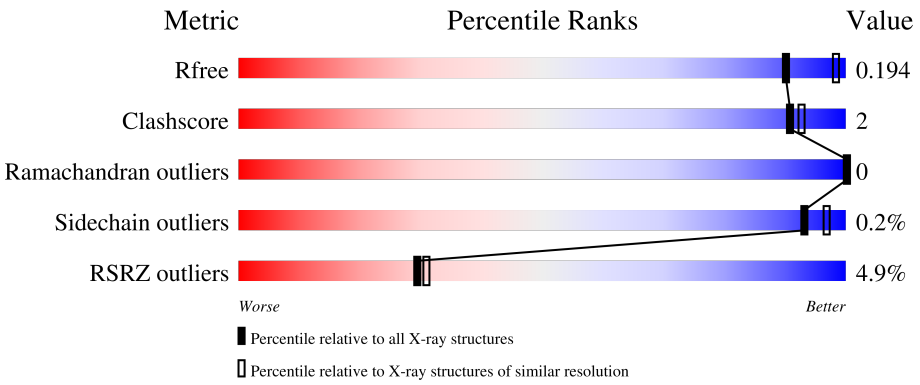
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	473	5% 88% • 9%
1	B	473	4% 87% • 8%
1	C	473	5% 86% 5% 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
2	NAG	C	2001	-	-	-	X
3	GOL	C	1442	-	-	-	X
7	NGA	A	4001	-	-	-	X

2 Entry composition (i)

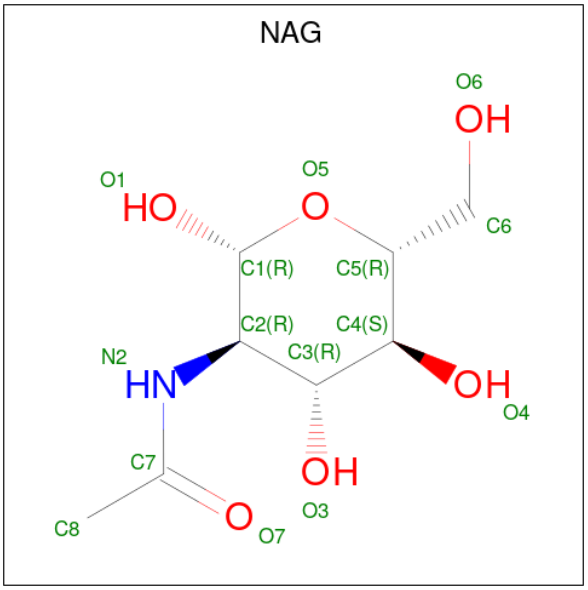
There are 9 unique types of molecules in this entry. The entry contains 11144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 E1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3278	2073	574	608	23	0	6	1
1	B	433	3282	2078	572	609	23	0	7	2
1	C	433	3268	2066	573	606	23	0	4	1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0

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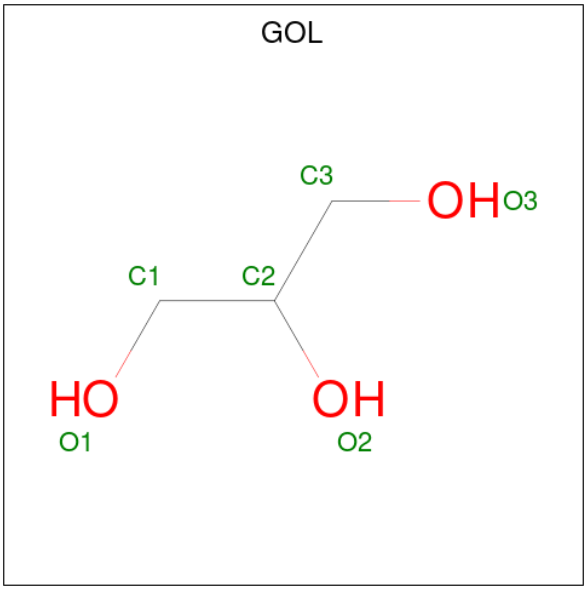
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	14	8	1	5	0	0

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



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

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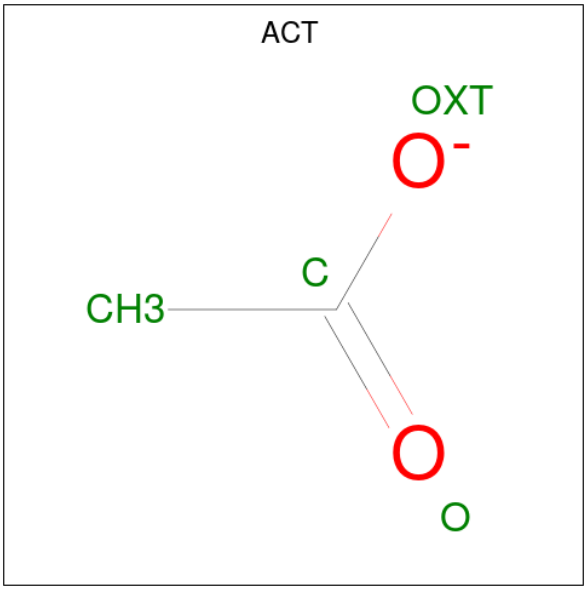
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

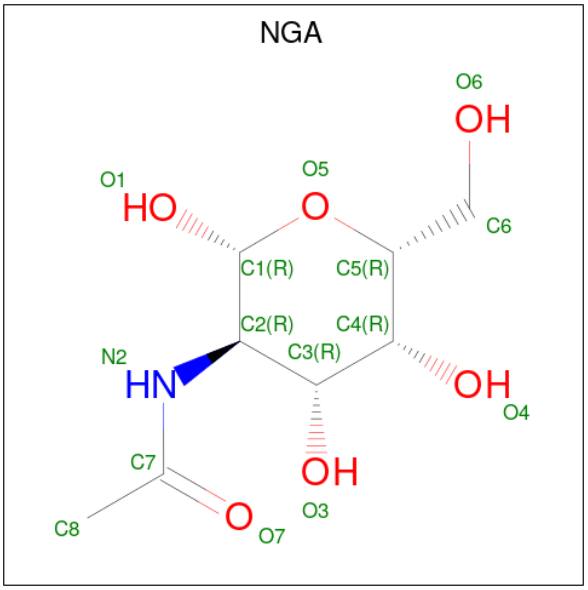


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

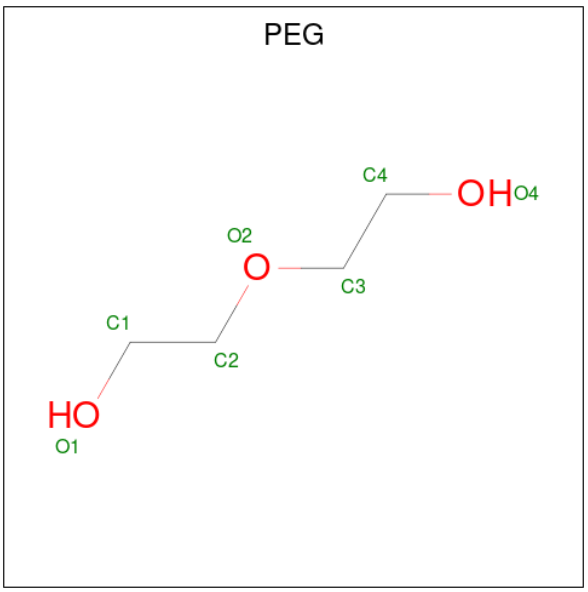
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	1	1	1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is water.

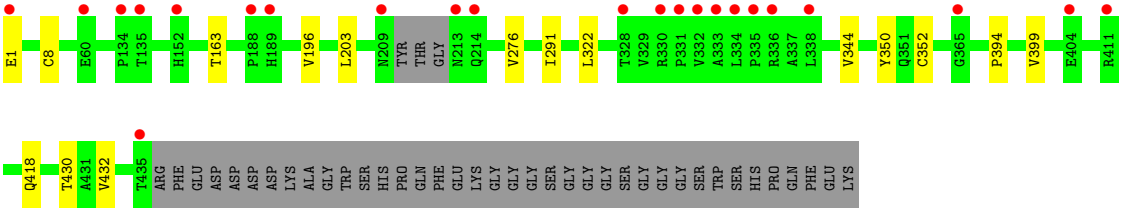
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	421	421	421	0	0
			Total	O		
9	B	386	386	386	0	0
			Total	O		
9	C	344	344	344	0	0

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.

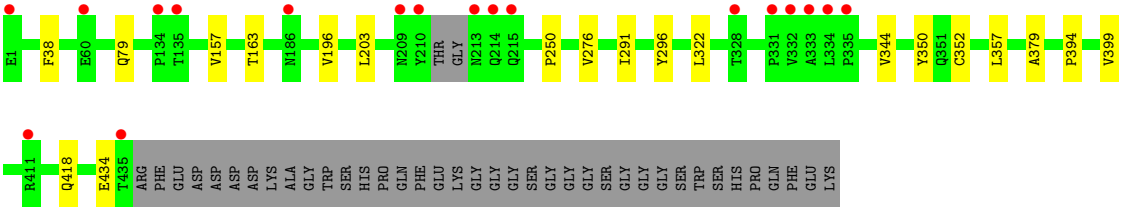
• Molecule 1: E1 ENVELOPE GLYCOPROTEIN

Chain A:



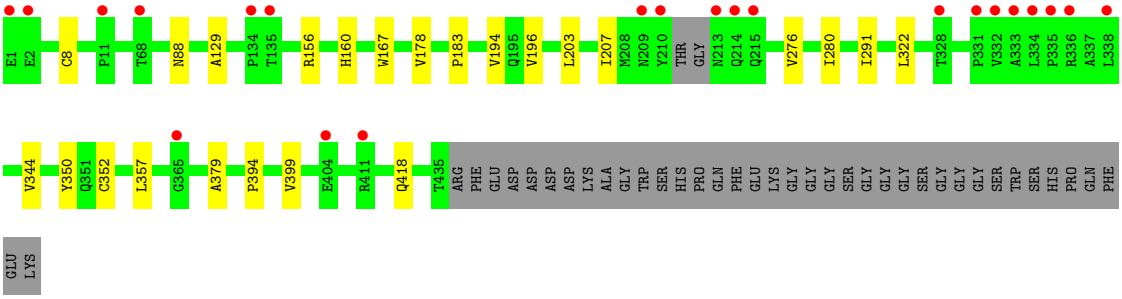
• Molecule 1: E1 ENVELOPE GLYCOPROTEIN

Chain B:



• Molecule 1: E1 ENVELOPE GLYCOPROTEIN

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.68Å 126.55Å 130.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.18 19.97 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.18) 98.9 (19.97-2.18)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.19Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.178 , 0.193 0.177 , 0.194	Depositor DCC
R_{free} test set	5179 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: GOL, CL, ACT, CA, NAG, NGA, 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	0.36	0/3396	0.60	0/4665
1	B	0.36	0/3402	0.58	0/4677
1	C	0.35	0/3383	0.59	0/4650
All	All	0.36	0/10181	0.59	0/13992

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 (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	3278	0	3110	8	0
1	B	3282	0	3103	12	0
1	C	3268	0	3097	15	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	28	0	26	0	0
3	A	6	0	8	0	0
3	B	18	0	24	2	0
3	C	48	0	64	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	1	0
6	A	1	0	0	0	0
7	A	14	0	13	1	0
8	C	7	0	10	0	0
9	A	421	0	0	0	0
9	B	386	0	0	0	0
9	C	344	0	0	0	0
All	All	11144	0	9490	33	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 (33) 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:C:357:LEU:HB2	3:C:1439:GOL:H12	1.75	0.67
1:B:357:LEU:HB2	3:B:1436:GOL:H31	1.80	0.62
1:C:178[A]:VAL:HG13	1:C:183:PRO:HA	1.84	0.59
1:A:432:VAL:HG22	7:A:4001:NGA:H62	1.93	0.51
1:B:276:VAL:HG12	1:B:291:ILE:HG12	1.93	0.51
1:C:88:ASN:HD21	5:C:1446:ACT:H2	1.76	0.50
1:A:276:VAL:HG12	1:A:291:ILE:HG12	1.94	0.50
1:C:178[A]:VAL:HG11	1:C:194:VAL:HB	1.94	0.50
1:C:167:TRP:HB2	1:C:178[B]:VAL:HG23	1.94	0.49
1:C:276:VAL:HG12	1:C:291:ILE:HG12	1.94	0.49
1:B:379:ALA:HB3	1:C:8:CYS:HB3	1.96	0.48
1:A:163[B]:THR:HG21	1:A:203:LEU:HG	1.96	0.48
1:C:160:HIS:HB2	1:C:203:LEU:HB2	1.97	0.46
1:A:344:VAL:HG11	1:A:399:VAL:HG11	1.98	0.46
1:B:344:VAL:HG11	1:B:399:VAL:HG11	1.98	0.45
1:B:163[B]:THR:HG21	1:B:203:LEU:HG	1.99	0.45
1:B:350:TYR:CZ	1:B:394:PRO:HB3	2.53	0.44
1:A:350:TYR:CZ	1:A:394:PRO:HB3	2.53	0.43
1:A:352:CYS:HB2	1:A:418:GLN:HG2	2.00	0.43
1:C:352:CYS:HB2	1:C:418:GLN:HG2	2.00	0.43
1:C:350:TYR:CZ	1:C:394:PRO:HB3	2.53	0.43
1:C:196:VAL:HG12	1:C:322:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG12	1:A:322:LEU:HD22	2.01	0.42
1:B:352:CYS:HB2	1:B:418:GLN:HG2	2.01	0.42
1:B:79:GLN:H	3:B:1437:GOL:H2	1.83	0.42
1:B:196:VAL:HG12	1:B:322:LEU:HD22	2.01	0.42
1:B:38:PHE:CD1	1:B:157:VAL:HB	2.56	0.41
1:C:344:VAL:HG11	1:C:399:VAL:HG11	2.03	0.40
1:A:8:CYS:HB3	1:C:379:ALA:HB3	2.03	0.40
1:C:156:ARG:HB2	1:C:207:ILE:HB	2.03	0.40
1:B:250:PRO:HB3	1:B:296[B]:TYR:CE1	2.56	0.40
1:B:434:GLU:H	1:B:434:GLU:HG3	1.77	0.40
1:C:129:ALA:HA	1:C:280:ILE:HA	2.03	0.40

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	434/473 (92%)	424 (98%)	10 (2%)	0	100	100
1	B	436/473 (92%)	428 (98%)	8 (2%)	0	100	100
1	C	433/473 (92%)	425 (98%)	8 (2%)	0	100	100
All	All	1303/1419 (92%)	1277 (98%)	26 (2%)	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	350/376 (93%)	348 (99%)	2 (1%)	86 92
1	B	350/376 (93%)	350 (100%)	0	100 100
1	C	349/376 (93%)	349 (100%)	0	100 100
All	All	1049/1128 (93%)	1047 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	430	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	398	GLN
1	B	398	GLN
1	B	428	HIS
1	C	189	HIS
1	C	369	HIS
1	C	398	GLN
1	C	428	HIS

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 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
3	GOL	C	1437	-	5,5,5	0.05	0	5,5,5	0.13	0
8	PEG	C	1445	-	6,6,6	0.09	0	5,5,5	0.03	0
2	NAG	B	1001	1	14,14,15	0.27	0	17,19,21	0.42	0
3	GOL	B	1437	-	5,5,5	0.05	0	5,5,5	0.17	0
3	GOL	C	1442	-	5,5,5	0.05	0	5,5,5	0.13	0
2	NAG	C	2001	1	14,14,15	0.26	0	17,19,21	0.56	0
3	GOL	C	1438	-	5,5,5	0.04	0	5,5,5	0.21	0
7	NGA	A	4001	1	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
3	GOL	A	1436	-	5,5,5	0.04	0	5,5,5	0.17	0
5	ACT	A	1438	4	3,3,3	1.09	0	3,3,3	0.92	0
2	NAG	A	1001	1	14,14,15	0.27	0	17,19,21	0.48	0
3	GOL	B	1436	-	5,5,5	0.05	0	5,5,5	0.19	0
3	GOL	C	1441	-	5,5,5	0.04	0	5,5,5	0.13	0
5	ACT	C	1446	4	3,3,3	1.04	0	3,3,3	0.91	0
2	NAG	C	1001	1	14,14,15	0.25	0	17,19,21	0.48	0
5	ACT	B	1440	4	3,3,3	1.10	0	3,3,3	0.91	0
3	GOL	C	1439	-	5,5,5	0.05	0	5,5,5	0.19	0
3	GOL	C	1436	-	5,5,5	0.05	0	5,5,5	0.23	0
3	GOL	C	1443	-	5,5,5	0.03	0	5,5,5	0.12	0
3	GOL	B	1438	-	5,5,5	0.04	0	5,5,5	0.14	0
3	GOL	C	1440	-	5,5,5	0.03	0	5,5,5	0.12	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
2	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
3	GOL	B	1436	-	-	2/4/4/4	-
3	GOL	C	1438	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	1436	-	-	0/4/4/4	-
3	GOL	C	1437	-	-	0/4/4/4	-
3	GOL	C	1439	-	-	0/4/4/4	-
3	GOL	C	1441	-	-	0/4/4/4	-
3	GOL	C	1443	-	-	0/4/4/4	-
7	NGA	A	4001	1	-	4/6/23/26	0/1/1/1
8	PEG	C	1445	-	-	2/4/4/4	-
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	A	1436	-	-	0/4/4/4	-
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	B	1437	-	-	0/4/4/4	-
3	GOL	B	1438	-	-	0/4/4/4	-
3	GOL	C	1442	-	-	0/4/4/4	-
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	C	1440	-	-	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})
7	A	4001	NGA	C1-C2-N2	4.03	117.37	110.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4001	NGA	C8-C7-N2-C2
7	A	4001	NGA	O7-C7-N2-C2
7	A	4001	NGA	O5-C5-C6-O6
7	A	4001	NGA	C4-C5-C6-O6
8	C	1445	PEG	C1-C2-O2-C3
8	C	1445	PEG	C4-C3-O2-C2
3	B	1436	GOL	C1-C2-C3-O3
3	B	1436	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1437	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4001	NGA	1	0
3	B	1436	GOL	1	0
5	C	1446	ACT	1	0
3	C	1439	GOL	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 (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	A	432/473 (91%)	-0.05	23 (5%)	26	27	16, 27, 51, 76	0
1	B	433/473 (91%)	-0.09	18 (4%)	36	37	16, 25, 48, 63	0
1	C	433/473 (91%)	-0.11	22 (5%)	28	29	15, 25, 48, 71	0
All	All	1298/1419 (91%)	-0.09	63 (4%)	29	31	15, 25, 49, 76	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	9.6
1	B	333	ALA	8.8
1	C	335	PRO	7.7
1	B	332	VAL	7.1
1	A	189	HIS	6.8
1	C	332	VAL	6.5
1	A	335	PRO	6.3
1	C	334	LEU	6.2
1	A	332	VAL	5.6
1	A	333	ALA	5.3
1	B	335	PRO	5.3
1	A	334	LEU	5.1
1	C	336	ARG	4.8
1	B	334	LEU	4.7
1	B	135	THR	4.5
1	C	213	ASN	4.5
1	A	213	ASN	4.3
1	C	209	ASN	4.3
1	A	328	THR	4.2
1	B	210	TYR	4.2
1	B	435	THR	4.0
1	A	435	THR	3.7
1	C	331	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	1	GLU	3.6
1	A	336	ARG	3.6
1	C	210	TYR	3.6
1	A	135	THR	3.6
1	B	209	ASN	3.4
1	A	330	ARG	3.4
1	B	213	ASN	3.3
1	B	134	PRO	3.1
1	A	1	GLU	3.1
1	C	135	THR	3.1
1	A	331	PRO	3.0
1	B	328	THR	3.0
1	A	134	PRO	3.0
1	A	214	GLN	2.9
1	C	2	GLU	2.9
1	B	331	PRO	2.8
1	B	411	ARG	2.7
1	A	188	PRO	2.6
1	B	60	GLU	2.6
1	B	215	GLN	2.6
1	C	11	PRO	2.5
1	C	365	GLY	2.4
1	C	134	PRO	2.4
1	C	214	GLN	2.4
1	A	209	ASN	2.4
1	A	152	HIS	2.4
1	A	404	GLU	2.4
1	B	214	GLN	2.4
1	C	328	THR	2.4
1	B	1	GLU	2.3
1	C	411	ARG	2.3
1	C	338	LEU	2.3
1	A	365	GLY	2.2
1	A	411	ARG	2.1
1	C	215	GLN	2.1
1	A	338	LEU	2.1
1	A	60	GLU	2.1
1	B	186	ASN	2.0
1	C	68	THR	2.0
1	C	404	GLU	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, 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	C	1441	6/6	0.56	0.37	80,80,81,81	0
3	GOL	C	1442	6/6	0.58	0.45	90,90,91,91	0
7	NGA	A	4001	14/15	0.61	0.51	58,60,62,62	0
3	GOL	C	1443	6/6	0.65	0.38	81,82,82,82	0
3	GOL	C	1436	6/6	0.65	0.25	46,47,49,50	0
3	GOL	C	1440	6/6	0.67	0.29	69,70,70,70	0
3	GOL	B	1437	6/6	0.68	0.29	62,62,62,62	0
3	GOL	B	1438	6/6	0.69	0.30	64,66,66,66	0
2	NAG	C	2001	14/15	0.71	0.42	66,68,69,69	0
3	GOL	C	1438	6/6	0.78	0.25	56,57,57,57	0
8	PEG	C	1445	7/7	0.78	0.19	74,75,75,75	0
3	GOL	C	1439	6/6	0.79	0.34	55,56,56,56	0
3	GOL	B	1436	6/6	0.81	0.27	48,49,49,49	0
3	GOL	A	1436	6/6	0.81	0.28	69,70,70,70	0
3	GOL	C	1437	6/6	0.83	0.24	53,54,55,55	0
2	NAG	B	1001	14/15	0.84	0.23	41,43,46,47	0
2	NAG	C	1001	14/15	0.86	0.26	40,43,47,47	0
2	NAG	A	1001	14/15	0.86	0.28	38,42,45,45	0
5	ACT	B	1440	4/4	0.88	0.15	41,42,42,43	0
5	ACT	C	1446	4/4	0.90	0.14	39,39,40,41	0
5	ACT	A	1438	4/4	0.95	0.14	43,43,43,44	0
6	CL	A	1439	1/1	0.97	0.13	47,47,47,47	0
4	CA	C	1444	1/1	0.98	0.03	28,28,28,28	0
4	CA	B	1439	1/1	0.99	0.03	27,27,27,27	0
4	CA	A	1437	1/1	0.99	0.02	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.