



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:26 PM UTC

PDB ID : 4ADG / pdb_00004adg
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

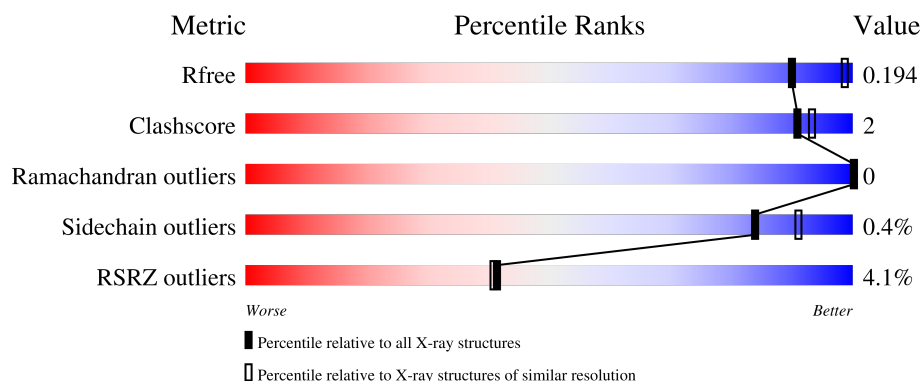
1 Overall quality at a glance

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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 $\leq 5\%$. 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	473	4% 87% 9%
1	B	473	3% 86% 5% 8%
1	C	473	5% 85% 6% 8%

2 Entry composition [i](#)

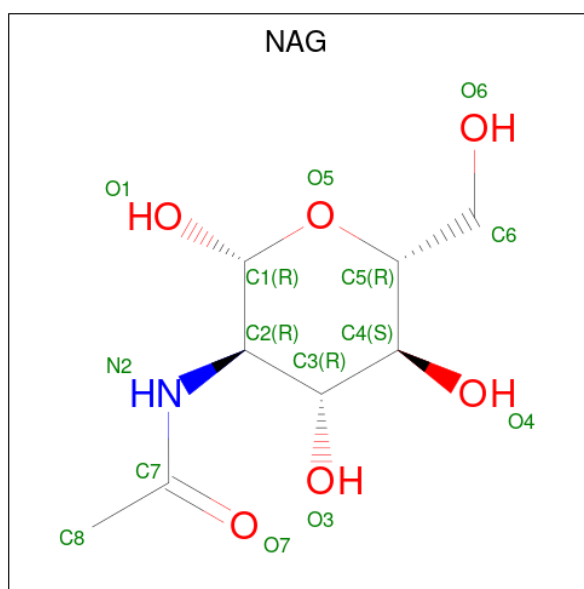
There are 9 unique types of molecules in this entry. The entry contains 11144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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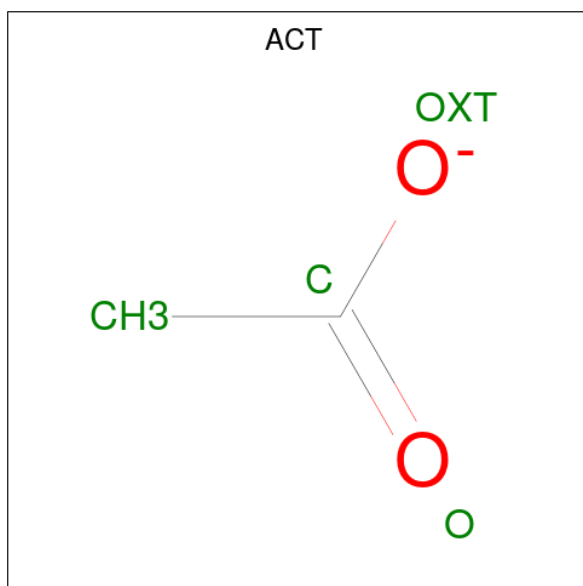
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

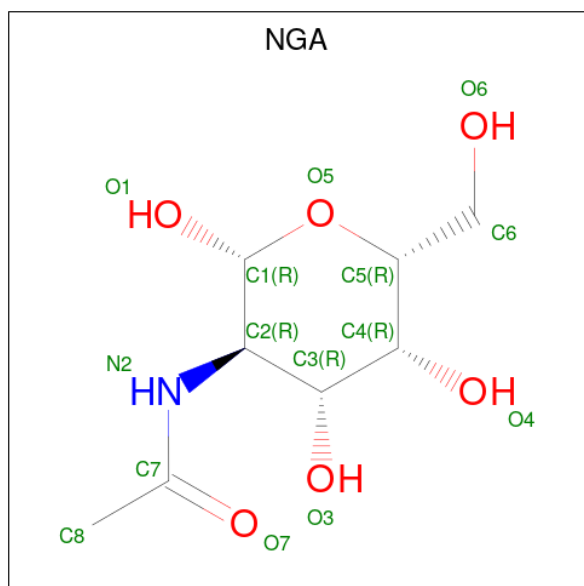


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

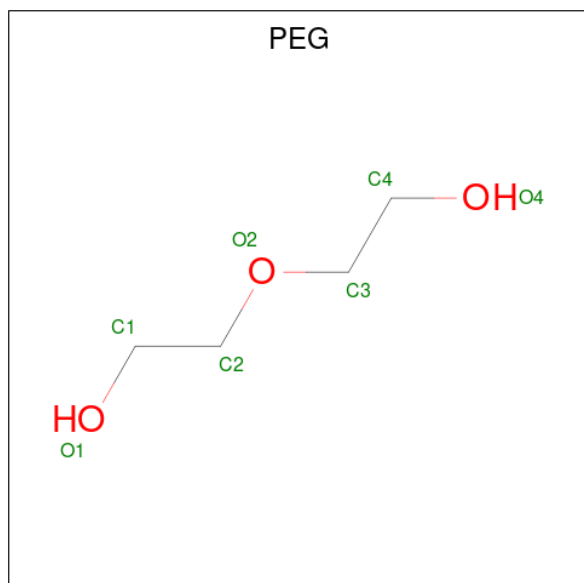
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Cl		0	0
			1	1			

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



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

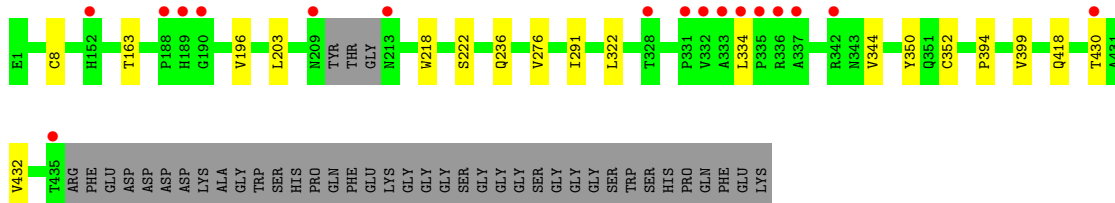
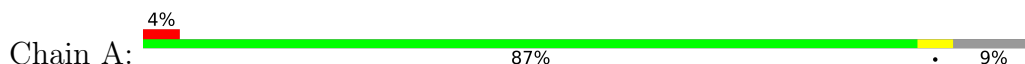
- Molecule 9 is water.

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

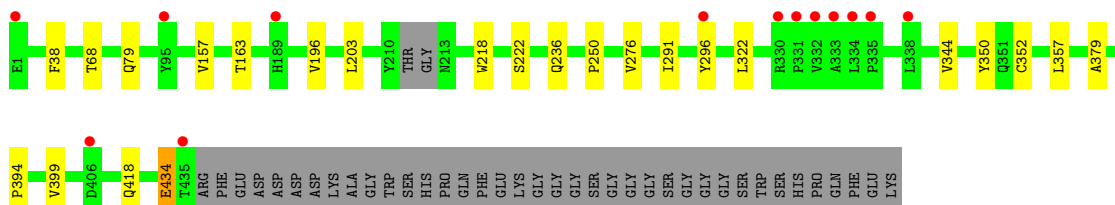
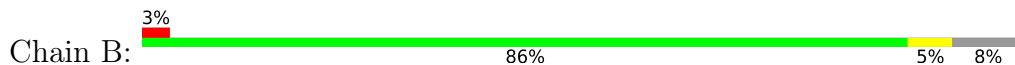
3 Residue-property plots [i](#)

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.

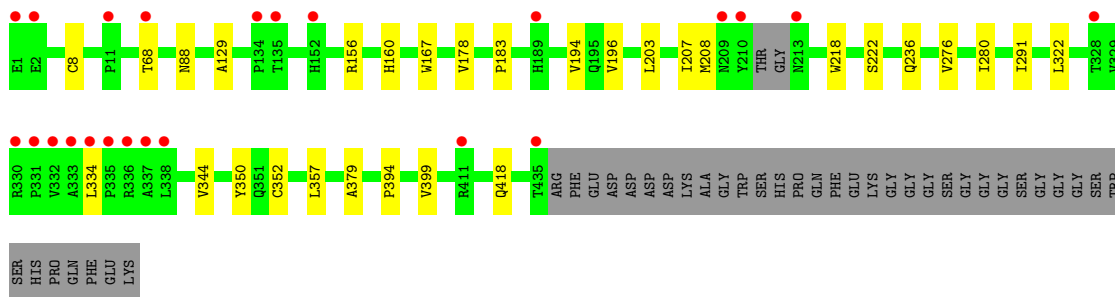
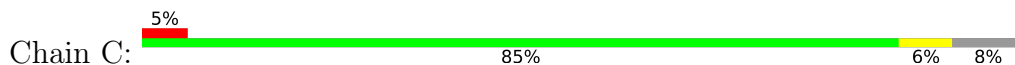
• Molecule 1: E1 ENVELOPE GLYCOPROTEIN



• Molecule 1: E1 ENVELOPE GLYCOPROTEIN



• Molecule 1: E1 ENVELOPE GLYCOPROTEIN



4 Data and refinement statistics

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 20.00 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.18) 98.8 (20.00-2.18)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, NAG, GOL, CA, NGA, ACT

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	0.67	0/3396	1.07	3/4665 (0.1%)
1	B	0.67	0/3402	1.07	4/4677 (0.1%)
1	C	0.67	0/3383	1.08	4/4650 (0.1%)
All	All	0.67	0/10181	1.07	11/13992 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	TRP	N-CA-C	6.00	118.67	108.90
1	C	218	TRP	N-CA-C	5.97	118.63	108.90
1	B	218	TRP	N-CA-C	5.93	118.57	108.90
1	C	236	GLN	N-CA-C	5.48	116.40	108.34
1	B	68	THR	N-CA-C	5.26	117.44	111.02
1	C	222	SER	N-CA-C	5.26	121.43	109.81
1	B	222	SER	N-CA-C	5.23	121.37	109.81
1	C	68	THR	N-CA-C	5.21	117.37	111.02
1	A	236	GLN	N-CA-C	5.18	115.95	108.34
1	A	222	SER	N-CA-C	5.15	121.19	109.81
1	B	236	GLN	N-CA-C	5.09	115.83	108.34

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	3278	0	3110	8	0
1	B	3282	0	3103	12	0
1	C	3268	0	3097	16	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
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	34	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 (34) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:MET:HE2	1:C:208:MET:HB2	1.91	0.43
1:C:196:VAL:HG12	1:C:322:LEU:HD22	2.01	0.43
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	78	87
1	B	350/376 (93%)	349 (100%)	1 (0%)	86	92
1	C	349/376 (93%)	348 (100%)	1 (0%)	86	92
All	All	1049/1128 (93%)	1045 (100%)	4 (0%)	84	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	LEU
1	A	430	THR
1	B	434	GLU
1	C	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS
1	A	398	GLN
1	A	428	HIS
1	B	111	GLN
1	B	152	HIS
1	B	168	GLN
1	B	398	GLN

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Mol	Chain	Res	Type
1	B	428	HIS
1	C	152	HIS
1	C	308	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 oligosaccharides 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	$\# Z > 2$
8	PEG	C	1445	-	6,6,6	0.09	0	5,5,5	0.03	0
3	GOL	C	1442	-	5,5,5	0.05	0	5,5,5	0.12	0
3	GOL	C	1441	-	5,5,5	0.04	0	5,5,5	0.12	0
2	NAG	B	1001	1	14,14,15	0.28	0	17,19,21	0.44	0
3	GOL	C	1439	-	5,5,5	0.05	0	5,5,5	0.18	0
2	NAG	A	1001	1	14,14,15	0.28	0	17,19,21	0.50	0
3	GOL	C	1443	-	5,5,5	0.04	0	5,5,5	0.11	0
3	GOL	C	1437	-	5,5,5	0.06	0	5,5,5	0.13	0
3	GOL	C	1438	-	5,5,5	0.04	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	1438	4	3,3,3	1.16	0	3,3,3	0.92	0
5	ACT	B	1440	4	3,3,3	1.17	0	3,3,3	0.91	0
3	GOL	B	1438	-	5,5,5	0.05	0	5,5,5	0.13	0
3	GOL	A	1436	-	5,5,5	0.05	0	5,5,5	0.15	0
2	NAG	C	1001	1	14,14,15	0.26	0	17,19,21	0.50	0
5	ACT	C	1446	4	3,3,3	1.10	0	3,3,3	0.91	0
7	NGA	A	4001	1	14,14,15	0.32	0	17,19,21	1.16	1 (5%)
2	NAG	C	2001	1	14,14,15	0.28	0	17,19,21	0.58	0
3	GOL	C	1436	-	5,5,5	0.05	0	5,5,5	0.24	0
3	GOL	B	1436	-	5,5,5	0.05	0	5,5,5	0.18	0
3	GOL	B	1437	-	5,5,5	0.05	0	5,5,5	0.17	0
3	GOL	C	1440	-	5,5,5	0.04	0	5,5,5	0.11	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
8	PEG	C	1445	-	-	2/4/4/4	-
3	GOL	C	1436	-	-	0/4/4/4	-
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	C	1437	-	-	0/4/4/4	-
3	GOL	B	1436	-	-	2/4/4/4	-
3	GOL	C	1438	-	-	0/4/4/4	-
3	GOL	C	1439	-	-	0/4/4/4	-
3	GOL	C	1442	-	-	0/4/4/4	-
2	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
3	GOL	C	1441	-	-	0/4/4/4	-
3	GOL	B	1437	-	-	0/4/4/4	-
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	A	1436	-	-	0/4/4/4	-
3	GOL	B	1438	-	-	0/4/4/4	-
7	NGA	A	4001	1	-	4/6/23/26	0/1/1/1
3	GOL	C	1440	-	-	0/4/4/4	-
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	C	1443	-	-	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(°)	Ideal(°)
7	A	4001	NGA	C1-C2-N2	4.40	117.37	110.43

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	O5-C5-C6-O6
7	A	4001	NGA	C4-C5-C6-O6
7	A	4001	NGA	O7-C7-N2-C2
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	C	1439	GOL	1	0
5	C	1446	ACT	1	0
7	A	4001	NGA	1	0
3	B	1436	GOL	1	0
3	B	1437	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

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	432/473 (91%)	0.01	17 (3%) 43 42	12, 27, 51, 76	6 (1%)
1	B	433/473 (91%)	-0.02	13 (3%) 52 52	11, 25, 48, 63	7 (1%)
1	C	433/473 (91%)	-0.05	23 (5%) 32 31	11, 25, 48, 71	4 (0%)
All	All	1298/1419 (91%)	-0.02	53 (4%) 41 41	11, 25, 49, 76	17 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	5.7
1	B	333	ALA	5.6
1	C	335	PRO	5.4
1	B	332	VAL	5.3
1	C	332	VAL	5.3
1	A	435	THR	5.0
1	A	334	LEU	4.6
1	C	331	PRO	4.6
1	A	189	HIS	4.6
1	B	334	LEU	4.4
1	A	335	PRO	4.3
1	A	332	VAL	4.3
1	C	336	ARG	4.0
1	A	336	ARG	3.9
1	B	335	PRO	3.7
1	A	328	THR	3.5
1	A	333	ALA	3.5
1	C	210	TYR	3.5
1	C	435	THR	3.4
1	C	334	LEU	3.3
1	B	435	THR	3.1
1	A	213	ASN	3.0
1	C	2	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	342[A]	ARG	2.8
1	C	213	ASN	2.8
1	C	338	LEU	2.8
1	C	189	HIS	2.8
1	B	95	TYR	2.8
1	C	330	ARG	2.7
1	A	337	ALA	2.7
1	C	209	ASN	2.6
1	B	189	HIS	2.5
1	C	337	ALA	2.4
1	A	152	HIS	2.4
1	C	11	PRO	2.4
1	C	411	ARG	2.4
1	B	331	PRO	2.4
1	A	331	PRO	2.4
1	C	68	THR	2.3
1	B	330	ARG	2.3
1	B	296[A]	TYR	2.3
1	C	152	HIS	2.2
1	C	135	THR	2.2
1	C	328	THR	2.2
1	B	338	LEU	2.2
1	C	1	GLU	2.1
1	A	188	PRO	2.1
1	B	406	ASP	2.1
1	A	190	GLY	2.1
1	B	1	GLU	2.0
1	A	209	ASN	2.0
1	A	430	THR	2.0
1	C	134	PRO	2.0

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 oligosaccharides 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
7	NGA	A	4001	14/15	0.44	0.23	58,60,62,62	0
2	NAG	C	2001	14/15	0.56	0.18	66,68,69,69	0
3	GOL	C	1443	6/6	0.66	0.34	81,82,82,82	0
8	PEG	C	1445	7/7	0.69	0.26	74,75,75,75	0
3	GOL	C	1442	6/6	0.76	0.30	90,90,91,91	0
3	GOL	C	1438	6/6	0.76	0.21	56,57,57,57	0
3	GOL	A	1436	6/6	0.78	0.18	69,70,70,70	0
3	GOL	C	1439	6/6	0.78	0.26	55,56,56,56	0
3	GOL	C	1436	6/6	0.78	0.20	46,47,49,50	0
3	GOL	C	1441	6/6	0.79	0.25	80,80,81,81	0
5	ACT	B	1440	4/4	0.79	0.16	41,42,42,43	0
3	GOL	C	1437	6/6	0.80	0.18	53,54,55,55	0
3	GOL	C	1440	6/6	0.80	0.17	69,70,70,70	0
3	GOL	B	1438	6/6	0.82	0.18	64,66,66,66	0
2	NAG	C	1001	14/15	0.82	0.12	40,43,47,47	0
3	GOL	B	1437	6/6	0.82	0.21	62,62,62,62	0
2	NAG	A	1001	14/15	0.83	0.11	38,42,45,45	0
5	ACT	C	1446	4/4	0.83	0.15	39,39,40,41	0
2	NAG	B	1001	14/15	0.84	0.12	41,43,46,47	0
3	GOL	B	1436	6/6	0.84	0.20	48,49,49,49	0
5	ACT	A	1438	4/4	0.85	0.16	43,43,43,44	0
6	CL	A	1439	1/1	0.96	0.06	47,47,47,47	0
4	CA	A	1437	1/1	0.99	0.03	30,30,30,30	0
4	CA	B	1439	1/1	0.99	0.03	27,27,27,27	0
4	CA	C	1444	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.