



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 4B3V / pdb_00004b3v
Title : Crystal structure of the Rubella virus glycoprotein E1 in its post-fusion form crystallized in presence of 20mM of Calcium Acetate
Authors : Vaney, M.C.; DuBois, R.M.; Tortorici, M.A.; Rey, F.A.
Deposited on : 2012-07-26
Resolution : 1.98 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

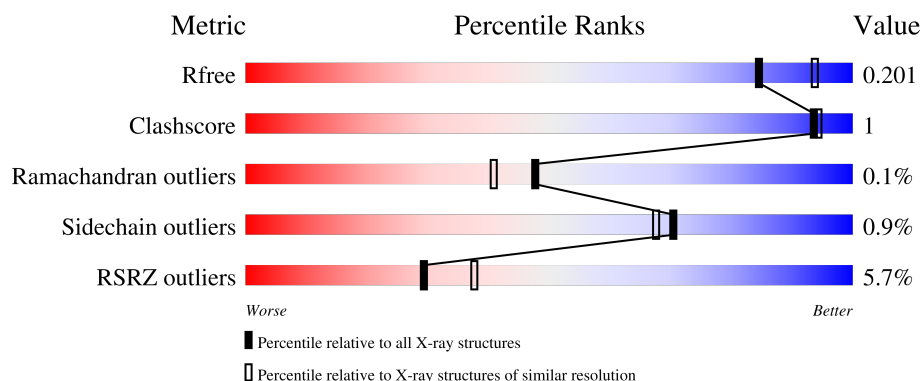
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	5% 87% 9%
1	B	473	5% 86% 5% 9%
1	C	473	5% 87% 5% 9%

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
5	ACT	A	1443	-	-	-	X

2 Entry composition [i](#)

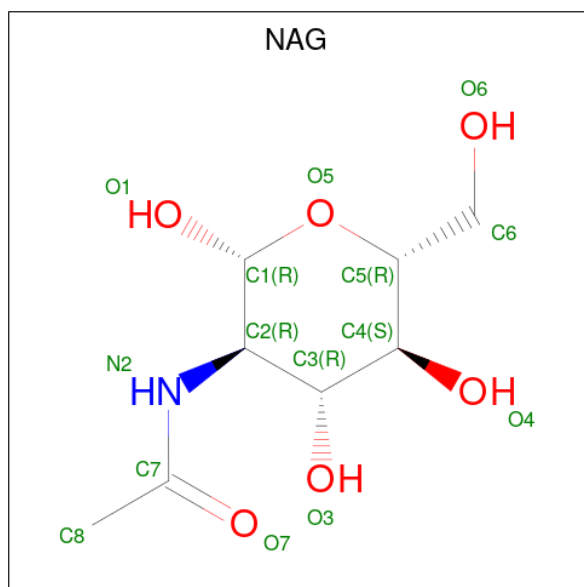
There are 10 unique types of molecules in this entry. The entry contains 11200 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	431	Total	C	N	O	S	0	10	1
			3299	2087	576	613	23			
1	B	432	Total	C	N	O	S	0	5	2
			3270	2067	575	605	23			
1	C	432	Total	C	N	O	S	0	4	2
			3252	2056	571	602	23			

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



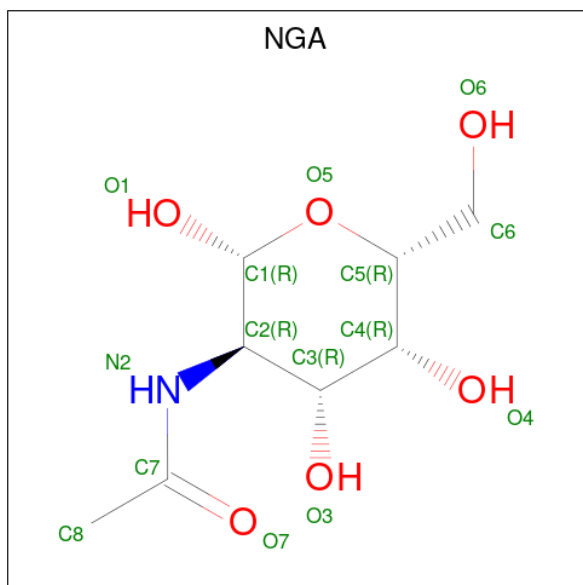
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			12	6	6		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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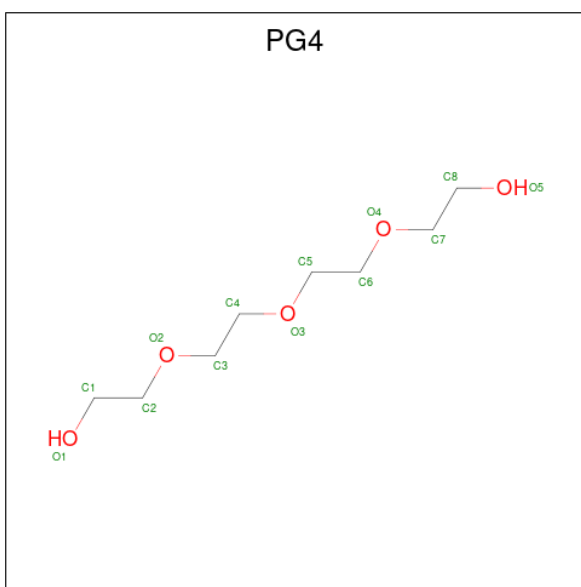
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



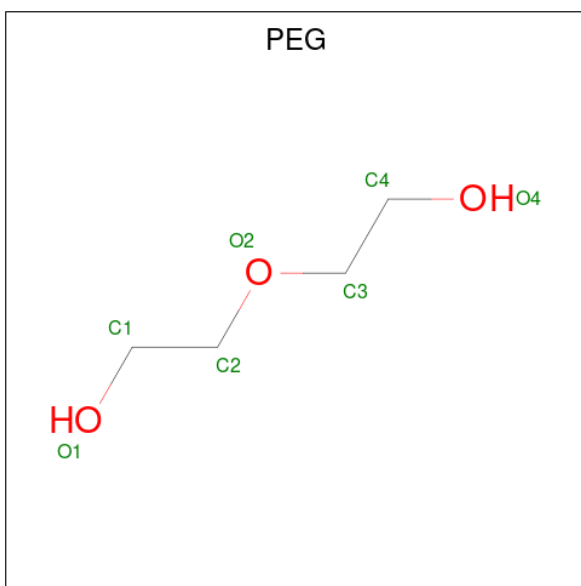
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	5	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	419	Total	O	0	0
			419	419		
10	B	378	Total	O	0	0
			378	378		
10	C	334	Total	O	0	0
			334	334		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.27Å 126.16Å 129.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 1.98 28.99 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.99-1.98) 97.3 (28.99-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.185 , 0.198 0.188 , 0.201	Depositor DCC
R_{free} test set	6752 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11200	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: ACT, GOL, PG4, NA, NAG, NGA, PEG, CA

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	0.66	0/3421	1.04	3/4703 (0.1%)
1	B	0.67	0/3391	1.06	4/4659 (0.1%)
1	C	0.67	0/3372	1.05	3/4635 (0.1%)
All	All	0.66	0/10184	1.05	10/13997 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	HIS	N-CA-C	7.71	122.44	112.89
1	B	236	GLN	N-CA-C	6.10	117.31	108.34
1	C	236	GLN	N-CA-C	5.59	116.56	108.34
1	A	236	GLN	N-CA-C	5.57	116.52	108.34
1	C	218	TRP	N-CA-C	5.53	118.41	109.40
1	B	218	TRP	N-CA-C	5.50	118.36	109.40
1	A	218	TRP	N-CA-C	5.46	118.30	109.40
1	C	222	SER	N-CA-C	5.34	121.61	109.81
1	B	222	SER	N-CA-C	5.28	121.47	109.81
1	A	222	SER	N-CA-C	5.27	121.45	109.81

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	3299	0	3136	8	0
1	B	3270	0	3109	11	0
1	C	3252	0	3096	12	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	28	0	26	0	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
4	A	24	0	32	0	0
4	B	42	0	56	2	0
4	C	30	0	40	1	0
5	A	12	0	9	0	0
5	B	8	0	6	0	0
5	C	8	0	6	1	0
6	A	8	0	9	2	0
7	A	7	0	10	0	0
7	B	7	0	10	0	0
7	C	14	0	20	1	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
10	A	419	0	0	0	0
10	B	378	0	0	0	0
10	C	334	0	0	0	0
All	All	11200	0	9617	28	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 1.

All (28) 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:55:THR:H	7:C:1448:PEG:H21	1.61	0.65
1:B:189:HIS:N	1:B:190:GLY:HA2	2.19	0.57
1:C:178[A]:VAL:HG13	1:C:183:PRO:HA	1.87	0.56
6:A:1447:PG4:H11	1:C:388:ALA:HB3	1.89	0.54
1:B:276:VAL:HG12	1:B:291:ILE:HG12	1.93	0.50
1:A:80:ARG:HH22	1:B:267:THR:HG21	1.76	0.50
1:A:316:TRP:HA	6:A:1447:PG4:H12	1.95	0.49
1:C:167:TRP:HB2	1:C:178[B]:VAL:HG23	1.95	0.48
1:B:344:VAL:HG11	1:B:399:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:HA	4:B:1442[A]:GOL:H2	1.95	0.47
1:A:36:GLY:HA2	1:A:156:ARG:HH21	1.78	0.47
1:C:137:THR:H	5:C:1444:ACT:H3	1.81	0.46
1:C:178[A]:VAL:HG11	1:C:194:VAL:HB	1.98	0.46
1:C:276:VAL:HG12	1:C:291:ILE:HG12	1.96	0.46
1:B:350:TYR:CZ	1:B:394:PRO:HB3	2.51	0.45
1:A:350:TYR:CZ	1:A:394:PRO:HB3	2.51	0.45
1:B:129:ALA:HA	1:B:280:ILE:HA	1.97	0.45
1:A:344:VAL:HG11	1:A:399:VAL:HG11	1.98	0.45
1:A:276:VAL:HG12	1:A:291:ILE:HG12	1.99	0.45
1:C:350:TYR:CZ	1:C:394:PRO:HB3	2.51	0.45
1:C:163[B]:THR:HG21	1:C:203:LEU:HG	2.01	0.43
1:C:129:ALA:HA	1:C:280:ILE:HA	2.01	0.42
1:B:379:ALA:HB3	1:C:8:CYS:HB3	2.01	0.42
1:A:163[B]:THR:HG21	1:A:203:LEU:HG	2.01	0.42
1:B:163[B]:THR:HG21	1:B:203:LEU:HG	2.01	0.42
1:A:252:ARG:HE	1:B:273:GLU:CD	2.29	0.41
1:C:357:LEU:HB2	4:C:1441:GOL:H12	2.03	0.41
1:B:82:CYS:H	4:B:1442[B]:GOL:H32	1.86	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	437/473 (92%)	429 (98%)	6 (1%)	2 (0%)	24	14
1	B	433/473 (92%)	425 (98%)	8 (2%)	0	100	100
1	C	432/473 (91%)	425 (98%)	7 (2%)	0	100	100
All	All	1302/1419 (92%)	1279 (98%)	21 (2%)	2 (0%)	48	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136[A]	ASP
1	A	136[B]	ASP

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	355/376 (94%)	353 (99%)	2 (1%)	78	76
1	B	350/376 (93%)	345 (99%)	5 (1%)	59	54
1	C	349/376 (93%)	347 (99%)	2 (1%)	78	76
All	All	1054/1128 (93%)	1045 (99%)	9 (1%)	70	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	68	THR
1	B	68	THR
1	B	76	ASN
1	B	156	ARG
1	B	189	HIS
1	B	376	ASP
1	C	68	THR
1	C	434	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	308	HIS
1	A	428	HIS
1	B	111	GLN
1	B	150	HIS
1	B	152	HIS
1	B	428	HIS

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Mol	Chain	Res	Type
1	C	111	GLN
1	C	152	HIS
1	C	168	GLN
1	C	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 4 are monoatomic - leaving 34 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	$\# Z > 2$
2	NAG	B	1436	1	14,14,15	0.26	0	17,19,21	0.45	0
4	GOL	B	1442[A]	-	5,5,5	0.06	0	5,5,5	0.29	0
2	NAG	A	1436	1	14,14,15	0.28	0	17,19,21	0.50	0
4	GOL	B	1440	-	5,5,5	0.06	0	5,5,5	0.16	0
2	NAG	C	1436	1	14,14,15	0.27	0	17,19,21	0.43	0
4	GOL	B	1437	-	5,5,5	0.06	0	5,5,5	0.21	0
3	NGA	C	1438	1	14,14,15	0.31	0	17,19,21	0.87	2 (11%)
2	NAG	C	1437	1	14,14,15	0.27	0	17,19,21	0.48	0
5	ACT	A	1444	-	3,3,3	1.01	0	3,3,3	1.04	0
7	PEG	B	1446	-	6,6,6	0.13	0	5,5,5	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	B	1444	-	3,3,3	1.13	0	3,3,3	0.94	0
4	GOL	A	1439	-	5,5,5	0.07	0	5,5,5	0.19	0
5	ACT	A	1443	-	3,3,3	1.13	0	3,3,3	0.93	0
4	GOL	B	1439	-	5,5,5	0.04	0	5,5,5	0.14	0
4	GOL	B	1438	-	5,5,5	0.07	0	5,5,5	0.30	0
4	GOL	A	1441	-	5,5,5	0.05	0	5,5,5	0.19	0
4	GOL	A	1440	-	5,5,5	0.05	0	5,5,5	0.14	0
3	NGA	A	1437	1	14,14,15	0.26	0	17,19,21	0.70	0
4	GOL	C	1441	-	5,5,5	0.06	0	5,5,5	0.31	0
7	PEG	C	1448	-	6,6,6	0.12	0	5,5,5	0.02	0
7	PEG	A	1449	-	6,6,6	0.09	0	5,5,5	0.03	0
4	GOL	C	1442	-	5,5,5	0.05	0	5,5,5	0.19	0
5	ACT	A	1445	-	3,3,3	1.04	0	3,3,3	1.05	0
5	ACT	B	1443	9	3,3,3	1.15	0	3,3,3	0.93	0
5	ACT	C	1444	9	3,3,3	1.13	0	3,3,3	0.93	0
7	PEG	C	1447	-	6,6,6	0.11	0	5,5,5	0.07	0
4	GOL	A	1438	-	5,5,5	0.05	0	5,5,5	0.26	0
5	ACT	C	1445	-	3,3,3	1.13	0	3,3,3	0.94	0
4	GOL	B	1441	-	5,5,5	0.06	0	5,5,5	0.20	0
4	GOL	C	1443	-	5,5,5	0.05	0	5,5,5	0.18	0
4	GOL	C	1440	-	5,5,5	0.06	0	5,5,5	0.13	0
6	PG4	A	1447	-	7,7,12	0.40	0	6,6,11	0.84	1 (16%)
4	GOL	B	1442[B]	-	5,5,5	0.05	0	5,5,5	0.32	0
4	GOL	C	1439	-	5,5,5	0.06	0	5,5,5	0.37	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	B	1436	1	-	0/6/23/26	0/1/1/1
4	GOL	B	1442[A]	-	-	0/4/4/4	-
2	NAG	A	1436	1	-	0/6/23/26	0/1/1/1
4	GOL	B	1440	-	-	0/4/4/4	-
2	NAG	C	1436	1	-	0/6/23/26	0/1/1/1
4	GOL	B	1437	-	-	0/4/4/4	-
3	NGA	C	1438	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1437	1	-	0/6/23/26	0/1/1/1
7	PEG	B	1446	-	-	1/4/4/4	-
4	GOL	A	1439	-	-	0/4/4/4	-
4	GOL	B	1439	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1438	-	-	2/4/4/4	-
4	GOL	A	1441	-	-	0/4/4/4	-
4	GOL	A	1440	-	-	0/4/4/4	-
3	NGA	A	1437	1	-	0/6/23/26	0/1/1/1
4	GOL	C	1441	-	-	1/4/4/4	-
7	PEG	C	1448	-	-	2/4/4/4	-
7	PEG	A	1449	-	-	1/4/4/4	-
4	GOL	C	1442	-	-	0/4/4/4	-
7	PEG	C	1447	-	-	2/4/4/4	-
4	GOL	A	1438	-	-	0/4/4/4	-
4	GOL	B	1441	-	-	0/4/4/4	-
4	GOL	C	1443	-	-	1/4/4/4	-
4	GOL	C	1440	-	-	0/4/4/4	-
6	PG4	A	1447	-	-	4/5/5/10	-
4	GOL	B	1442[B]	-	-	0/4/4/4	-
4	GOL	C	1439	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1438	NGA	C1-O5-C5	2.33	115.31	112.19
3	C	1438	NGA	C1-C2-N2	2.24	113.97	110.43
6	A	1447	PG4	C5-O3-C4	2.04	125.19	112.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1438	GOL	O1-C1-C2-C3
4	C	1441	GOL	O1-C1-C2-C3
7	B	1446	PEG	O1-C1-C2-O2
7	C	1447	PEG	C4-C3-O2-C2
6	A	1447	PG4	C4-C3-O2-C2
7	C	1448	PEG	C4-C3-O2-C2
7	A	1449	PEG	C1-C2-O2-C3
7	C	1447	PEG	C1-C2-O2-C3
7	C	1448	PEG	O1-C1-C2-O2
4	C	1443	GOL	O1-C1-C2-C3
6	A	1447	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1438	GOL	O1-C1-C2-O2
6	A	1447	PG4	C3-C4-O3-C5
6	A	1447	PG4	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1442[A]	GOL	1	0
4	C	1441	GOL	1	0
7	C	1448	PEG	1	0
5	C	1444	ACT	1	0
6	A	1447	PG4	2	0
4	B	1442[B]	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	431/473 (91%)	0.33	23 (5%)	32 41	14, 29, 53, 81	10 (2%)
1	B	432/473 (91%)	0.26	26 (6%)	27 36	13, 28, 51, 74	5 (1%)
1	C	432/473 (91%)	0.17	25 (5%)	29 37	12, 27, 49, 66	5 (1%)
All	All	1295/1419 (91%)	0.25	74 (5%)	29 38	12, 28, 51, 81	20 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	THR	5.2
1	B	189	HIS	5.1
1	B	335	PRO	4.8
1	A	189	HIS	4.7
1	A	332	VAL	4.3
1	A	136[A]	ASP	4.2
1	B	435	THR	4.2
1	A	209	ASN	4.1
1	B	334	LEU	4.1
1	A	135[A]	THR	4.0
1	C	333	ALA	4.0
1	A	335	PRO	4.0
1	A	331	PRO	4.0
1	B	331	PRO	3.8
1	C	213	ASN	3.7
1	B	333	ALA	3.5
1	C	335	PRO	3.4
1	C	189	HIS	3.4
1	B	135	THR	3.4
1	A	188	PRO	3.3
1	B	188	PRO	3.2
1	B	190	GLY	3.2
1	A	336	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	TYR	3.2
1	B	430	THR	3.1
1	A	134[A]	PRO	2.9
1	B	328	THR	2.9
1	B	332	VAL	2.7
1	A	333	ALA	2.7
1	C	308	HIS	2.7
1	B	429	THR	2.6
1	B	304	PRO	2.6
1	C	28	PHE	2.6
1	B	95	TYR	2.5
1	C	11	PRO	2.5
1	A	329	VAL	2.5
1	A	95	TYR	2.5
1	A	334	LEU	2.5
1	C	332	VAL	2.5
1	C	336	ARG	2.4
1	A	430	THR	2.4
1	C	331	PRO	2.4
1	C	17	THR	2.4
1	C	328	THR	2.4
1	B	213	ASN	2.4
1	B	330	ARG	2.3
1	C	334	LEU	2.3
1	B	186	ASN	2.3
1	A	328	THR	2.3
1	C	135	THR	2.3
1	C	429	THR	2.3
1	A	213	ASN	2.3
1	B	338	LEU	2.3
1	C	430	THR	2.3
1	A	112	TYR	2.2
1	B	336	ARG	2.2
1	C	329	VAL	2.2
1	A	222	SER	2.2
1	C	405	SER	2.2
1	C	304	PRO	2.2
1	A	290	HIS	2.1
1	A	337	ALA	2.1
1	B	326	PHE	2.1
1	C	214	GLN	2.1
1	C	12	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	112	TYR	2.0
1	B	134	PRO	2.0
1	C	352	CYS	2.0
1	B	2	GLU	2.0
1	C	222	SER	2.0
1	C	68	THR	2.0
1	B	209	ASN	2.0
1	C	209	ASN	2.0
1	A	386	VAL	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 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
5	ACT	A	1443	4/4	0.30	0.40	47,48,48,48	4
3	NGA	C	1438	14/15	0.41	0.22	74,77,80,80	0
3	NGA	A	1437	14/15	0.43	0.25	76,78,80,80	0
2	NAG	C	1437	14/15	0.56	0.18	73,74,76,76	0
5	ACT	B	1443	4/4	0.56	0.25	65,65,65,65	0
5	ACT	B	1444	4/4	0.56	0.36	77,77,77,78	0
6	PG4	A	1447	8/13	0.61	0.34	65,66,67,67	0
5	ACT	C	1445	4/4	0.62	0.37	80,80,80,80	0
5	ACT	C	1444	4/4	0.63	0.29	71,71,71,71	0
5	ACT	A	1444	4/4	0.68	0.22	62,62,62,62	0
7	PEG	B	1446	7/7	0.71	0.24	45,49,52,52	0
4	GOL	B	1442[A]	6/6	0.74	0.25	42,45,45,46	6
4	GOL	B	1442[B]	6/6	0.74	0.25	26,29,29,29	6
4	GOL	C	1441	6/6	0.75	0.22	57,58,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PEG	C	1448	7/7	0.75	0.20	41,45,48,48	0
4	GOL	B	1438	6/6	0.77	0.19	50,50,52,52	0
5	ACT	A	1445	4/4	0.77	0.34	84,84,84,84	0
4	GOL	B	1439	6/6	0.77	0.19	51,54,55,56	0
7	PEG	C	1447	7/7	0.78	0.31	82,83,83,83	0
4	GOL	B	1440	6/6	0.78	0.21	60,61,61,61	0
7	PEG	A	1449	7/7	0.79	0.21	62,63,63,63	0
4	GOL	A	1441	6/6	0.79	0.21	70,71,71,71	0
4	GOL	A	1440	6/6	0.80	0.21	66,67,67,67	0
2	NAG	B	1436	14/15	0.80	0.12	45,47,50,51	0
4	GOL	C	1442	6/6	0.80	0.28	69,70,70,71	0
4	GOL	B	1441	6/6	0.80	0.23	69,70,70,70	0
4	GOL	A	1438	6/6	0.80	0.20	49,51,51,51	0
4	GOL	C	1443	6/6	0.81	0.22	74,74,75,75	0
4	GOL	A	1439	6/6	0.83	0.19	59,61,61,61	0
2	NAG	C	1436	14/15	0.84	0.12	43,47,50,50	0
2	NAG	A	1436	14/15	0.85	0.11	42,45,47,48	0
4	GOL	C	1440	6/6	0.86	0.14	39,39,39,40	0
4	GOL	C	1439	6/6	0.86	0.12	33,36,37,39	0
4	GOL	B	1437	6/6	0.87	0.16	33,34,35,35	0
8	NA	A	1450	1/1	0.97	0.03	41,41,41,41	1
9	CA	B	1445	1/1	0.98	0.09	36,36,36,36	0
9	CA	A	1451	1/1	0.99	0.03	33,33,33,33	1
9	CA	C	1446	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.