



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 7A3S / pdb_00007a3s
Title : Crystal structure of dengue 3 virus envelope glycoprotein
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.;
Navarro-Sanchez, E.; Rey, F.A.
Deposited on : 2020-08-18
Resolution : 2.80 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

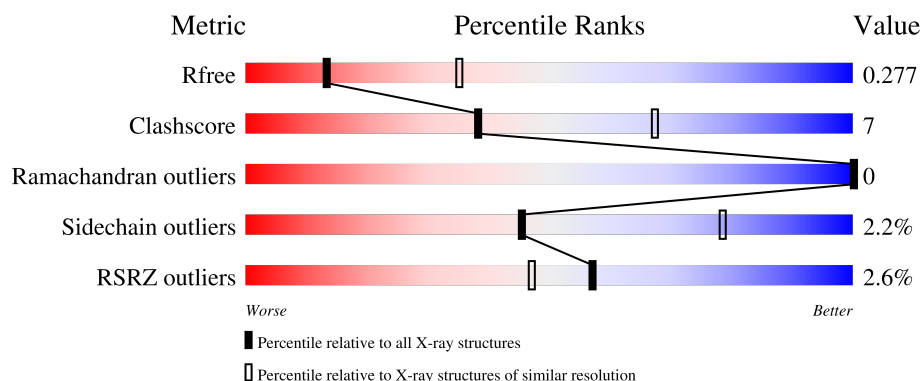
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

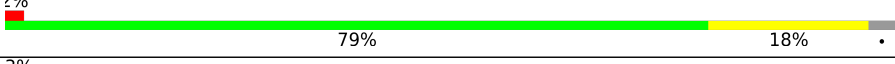
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	394	
1	B	394	
1	C	394	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9114 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.

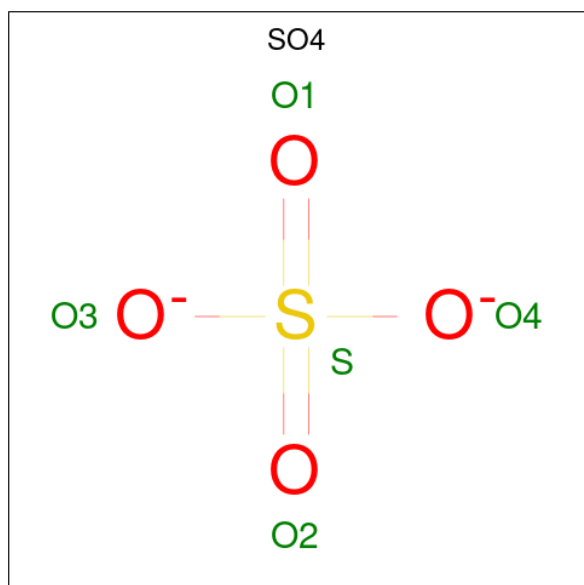
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2966	1871	509	565	21			
1	B	383	Total	C	N	O	S	0	2	0
			2978	1879	514	564	21			
1	C	382	Total	C	N	O	S	0	1	0
			2958	1868	509	560	21			

There are 3 discrepancies between the modelled and reference sequences:

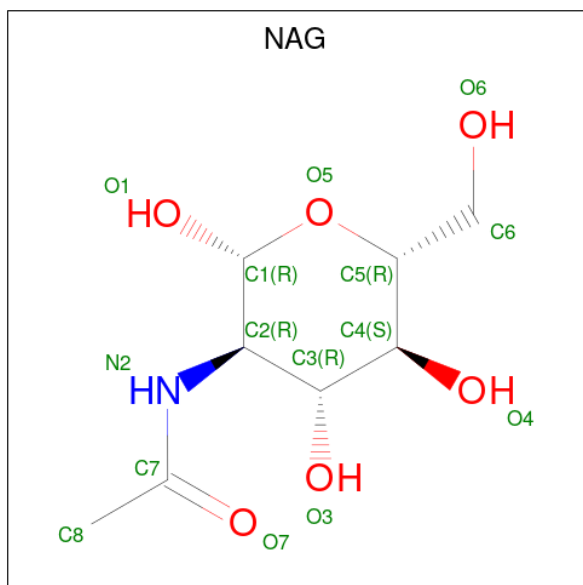
Chain	Residue	Modelled	Actual	Comment	Reference
A	394	PHE	-	expression tag	UNP P27915
B	394	PHE	-	expression tag	UNP P27915
C	394	PHE	-	expression tag	UNP P27915

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (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	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

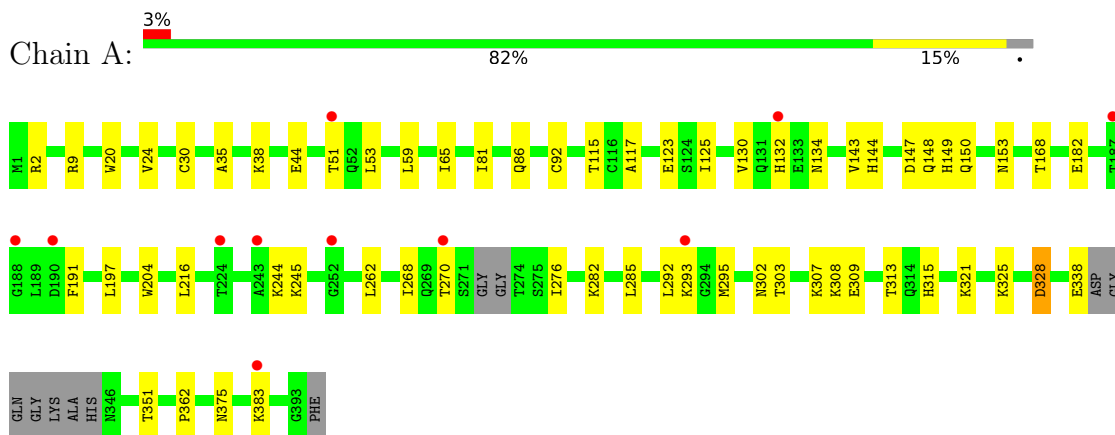
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total 46	O 46	0	0
4	B	35	Total 35	O 35	0	0
4	C	32	Total 32	O 32	0	0

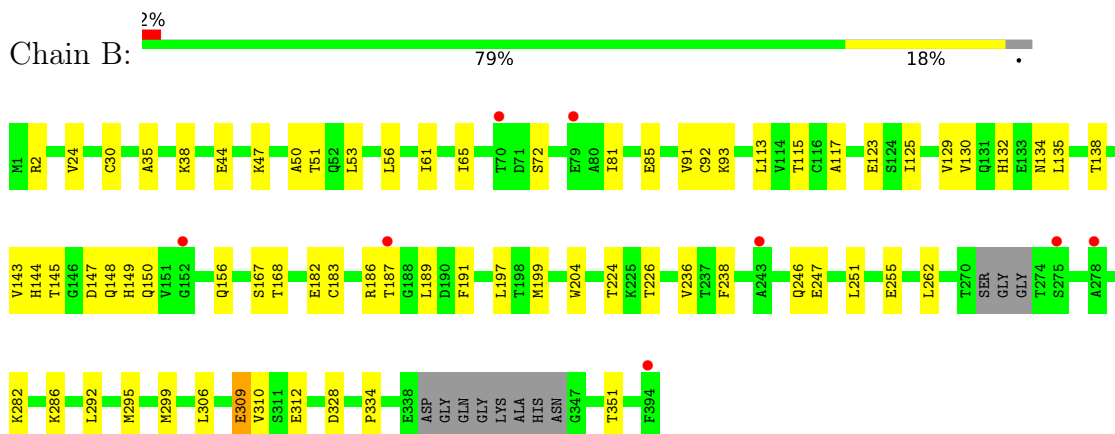
3 Residue-property plots [i](#)

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.

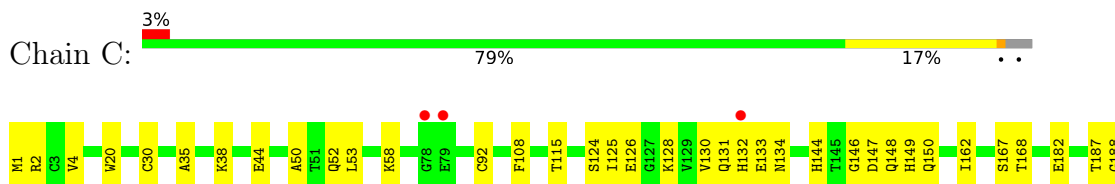
- Molecule 1: Genome polypeptide

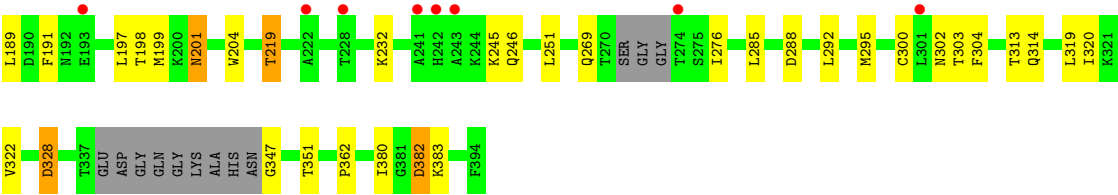


- Molecule 1: Genome polypeptide



- Molecule 1: Genome polypeptide





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.03Å 142.03Å 159.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-2.80) 99.4 (19.93-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.233 , 0.274 0.234 , 0.277	Depositor DCC
R_{free} test set	2537 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9114	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1488e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, NAG

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	0.18	0/3019	0.40	0/4083
1	B	0.16	0/3032	0.37	0/4100
1	C	0.17	0/3012	0.38	0/4074
All	All	0.17	0/9063	0.38	0/12257

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

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	2966	0	2979	38	0
1	B	2978	0	2988	46	0
1	C	2958	0	2972	43	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
3	A	28	0	26	2	0
3	B	28	0	26	1	0
3	C	28	0	26	1	0
4	A	46	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	35	0	0	1	0
4	C	32	0	0	3	0
All	All	9114	0	9017	125	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 7.

All (125) 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:A:149:HIS:HB3	3:A:403:NAG:H82	1.59	0.83
1:C:147:ASP:HB3	1:C:150:GLN:HB2	1.66	0.77
1:B:143:VAL:O	1:B:150:GLN:NE2	2.23	0.71
1:C:328:ASP:OD1	1:C:328:ASP:N	2.23	0.68
1:B:145:THR:H	1:B:150:GLN:HE22	1.41	0.67
1:A:51:THR:HG22	1:A:134:ASN:HB3	1.76	0.67
1:C:149:HIS:HB3	3:C:403:NAG:H2	1.75	0.67
1:C:2:ARG:NH1	1:C:44:GLU:OE1	2.28	0.66
1:C:201:ASN:N	1:C:201:ASN:OD1	2.28	0.66
1:A:125:ILE:HD12	1:A:197:LEU:HD11	1.77	0.66
1:C:144:HIS:HB3	1:C:351:THR:HG23	1.77	0.66
1:A:143:VAL:O	1:A:150:GLN:NE2	2.29	0.65
1:A:144:HIS:HA	1:A:150:GLN:HE22	1.62	0.64
1:C:58:LYS:HB3	1:C:219:THR:HG22	1.79	0.64
1:B:144:HIS:HB3	1:B:351:THR:HG23	1.78	0.63
1:A:24:VAL:HG22	1:A:282:LYS:HG2	1.79	0.63
2:A:401:SO4:S	4:A:501:HOH:O	2.55	0.63
1:B:150:GLN:HG3	1:B:156:GLN:OE1	2.00	0.61
1:B:51:THR:O	4:B:501:HOH:O	2.16	0.61
1:B:167:SER:OG	1:B:183:CYS:O	2.18	0.61
1:C:146:GLY:H	1:C:150:GLN:HE22	1.49	0.61
1:A:144:HIS:HB3	1:A:351:THR:HG23	1.83	0.60
1:C:128:LYS:NZ	4:C:502:HOH:O	2.32	0.60
1:C:168:THR:HG22	1:C:182:GLU:HA	1.83	0.59
1:B:72:SER:HB3	1:B:113:LEU:HD13	1.84	0.59
1:C:131:GLN:NE2	4:C:503:HOH:O	2.36	0.59
1:A:153:ASN:ND2	3:A:403:NAG:H83	2.17	0.59
1:B:199:MET:HE2	1:B:255:GLU:HG3	1.86	0.57
1:C:58:LYS:HE2	1:C:124:SER:OG	2.05	0.57
1:A:308:LYS:HB2	1:A:321:LYS:HD2	1.87	0.57
1:B:93:LYS:HD2	1:B:238:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASP:OD1	1:C:382:ASP:N	2.39	0.55
1:B:132:HIS:HB2	1:B:187:THR:HG21	1.88	0.55
1:B:186:ARG:HH21	1:B:282:LYS:NZ	2.05	0.55
1:C:125:ILE:HD12	1:C:197:LEU:HD11	1.89	0.53
1:C:269:GLN:HB3	1:C:276:ILE:HB	1.90	0.53
1:C:20:TRP:HA	1:C:285:LEU:O	2.09	0.52
1:A:303:THR:HG23	1:A:383:LYS:HD3	1.92	0.52
1:C:232:LYS:NZ	2:C:401:SO4:O4	2.37	0.52
1:B:130:VAL:O	1:B:191:PHE:HB3	2.10	0.51
1:B:224:THR:HG22	1:B:226:THR:H	1.76	0.51
1:A:65:ILE:HG23	1:A:117:ALA:HB1	1.93	0.51
1:A:9:ARG:HB3	1:A:315:HIS:CE1	2.46	0.50
1:A:168:THR:HG22	1:A:182:GLU:HA	1.93	0.50
1:B:306:LEU:HD21	1:B:310:VAL:HG23	1.93	0.50
1:C:347:GLY:N	4:C:506:HOH:O	2.44	0.50
1:A:59:LEU:HD23	1:A:216:LEU:HD12	1.93	0.50
1:C:303:THR:HG22	1:C:383:LYS:HB2	1.94	0.49
1:A:147:ASP:HB3	1:A:150:GLN:HB2	1.95	0.49
1:A:313:THR:HG22	1:A:315:HIS:H	1.78	0.49
1:B:182:GLU:OE1	1:B:286:LYS:NZ	2.34	0.48
1:C:50:ALA:HB1	1:C:53:LEU:HD21	1.95	0.48
1:C:35:ALA:HB3	1:C:38:LYS:HB2	1.95	0.48
1:A:309:GLU:H	1:A:309:GLU:CD	2.21	0.48
1:B:299:MET:HG3	1:B:334:PRO:HG3	1.95	0.48
1:A:81:ILE:HD13	1:B:129:VAL:HG11	1.94	0.48
1:C:199:MET:HB2	1:C:204:TRP:HZ3	1.79	0.48
1:A:148:GLN:HG3	1:A:362:PRO:HD2	1.95	0.47
1:B:65:ILE:HG23	1:B:117:ALA:HB1	1.96	0.47
1:A:2:ARG:NH1	1:A:44:GLU:OE1	2.48	0.47
1:A:244:LYS:HG2	1:A:245:LYS:HG3	1.97	0.47
1:A:328:ASP:OD1	1:A:328:ASP:N	2.36	0.47
1:B:292:LEU:HB3	1:B:295:MET:HG2	1.96	0.47
1:B:61:ILE:HD13	1:B:199:MET:HE3	1.96	0.46
1:A:92:CYS:HA	1:A:115:THR:O	2.16	0.46
1:C:92:CYS:HA	1:C:115:THR:O	2.15	0.46
1:C:245:LYS:HG3	1:C:246:GLN:H	1.80	0.46
1:A:204:TRP:CE3	1:A:262:LEU:HD13	2.51	0.46
1:B:51:THR:OG1	1:B:134:ASN:O	2.31	0.46
1:A:130:VAL:O	1:A:191:PHE:HB3	2.15	0.45
1:B:53:LEU:HD22	1:B:130:VAL:HG22	1.98	0.45
1:B:328:ASP:OD1	1:B:328:ASP:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HB3	1:C:295:MET:HG2	1.99	0.45
1:A:292:LEU:HB3	1:A:295:MET:HG2	1.98	0.45
1:B:125:ILE:HD12	1:B:197:LEU:HD11	1.98	0.45
1:A:53:LEU:HD22	1:A:130:VAL:HG22	1.98	0.45
1:B:149:HIS:HB3	3:B:403:NAG:H2	1.99	0.45
1:C:1:MET:HG3	1:C:150:GLN:NE2	2.32	0.45
1:A:86:GLN:HG3	1:B:56:LEU:HD23	1.98	0.44
1:C:52:GLN:HB3	1:C:134:ASN:ND2	2.32	0.44
1:C:313:THR:HG22	1:C:314:GLN:N	2.32	0.44
1:B:147:ASP:HB3	1:B:150:GLN:HB2	1.99	0.44
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.80	0.44
1:C:125:ILE:CG2	1:C:199:MET:HG2	2.48	0.44
1:C:199:MET:HB3	1:C:199:MET:HE2	1.75	0.44
1:A:307:LYS:HA	1:A:307:LYS:HD2	1.72	0.44
1:B:91:VAL:HG11	1:B:236:VAL:HG11	1.98	0.44
1:C:162:ILE:HG23	1:C:167:SER:HA	1.99	0.44
1:B:147:ASP:OD1	1:B:148:GLN:N	2.51	0.44
1:C:130:VAL:O	1:C:191:PHE:HB3	2.17	0.44
1:B:47:LYS:HG2	1:B:138:THR:HB	2.00	0.44
1:C:380:ILE:HD12	1:C:380:ILE:HA	1.83	0.43
1:C:1:MET:HE2	1:C:4:VAL:HG21	1.99	0.43
1:B:251:LEU:HD12	1:B:251:LEU:HA	1.86	0.43
1:A:20:TRP:HA	1:A:285:LEU:O	2.18	0.43
1:A:35:ALA:HB3	1:A:38:LYS:HB2	2.01	0.43
1:B:309:GLU:CD	1:B:309:GLU:H	2.26	0.43
1:C:126:GLU:HB2	1:C:198:THR:CG2	2.48	0.43
1:B:24:VAL:HG22	1:B:282:LYS:HG2	2.01	0.43
1:B:92:CYS:HA	1:B:115:THR:O	2.18	0.43
1:A:303:THR:HG22	1:A:383:LYS:HB2	2.00	0.43
1:B:199:MET:HB3	1:B:204:TRP:HZ3	1.84	0.43
1:A:302:ASN:HB3	1:A:303:THR:H	1.57	0.42
1:B:35:ALA:HB3	1:B:38:LYS:HB2	2.01	0.42
1:A:293:LYS:HB3	4:A:525:HOH:O	2.18	0.42
1:B:2:ARG:NH1	1:B:44:GLU:OE1	2.52	0.42
1:A:268:ILE:HG23	1:A:276:ILE:O	2.19	0.42
1:B:81:ILE:HA	1:B:85:GLU:OE2	2.19	0.42
1:C:148:GLN:HG3	1:C:362:PRO:HD2	2.02	0.42
1:A:303:THR:OG1	1:A:325:LYS:HB2	2.19	0.41
1:B:145:THR:H	1:B:150:GLN:NE2	2.15	0.41
1:B:168:THR:HG22	1:B:182:GLU:HA	2.01	0.41
1:C:300:CYS:SG	1:C:304:PHE:HZ	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLN:HA	1:B:156:GLN:NE2	2.35	0.41
1:B:312:GLU:O	1:C:108:PHE:HB2	2.20	0.41
1:B:50:ALA:HB1	1:B:53:LEU:HD21	2.02	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.91	0.41
1:A:338:GLU:HB2	1:A:375:ASN:HB2	2.03	0.40
1:A:197:LEU:HD23	1:A:262:LEU:HD21	2.02	0.40
1:B:204:TRP:CD2	1:B:262:LEU:HD13	2.56	0.40
1:C:53:LEU:HD22	1:C:130:VAL:HG22	2.02	0.40
1:C:302:ASN:HB3	1:C:303:THR:H	1.58	0.40
1:C:133:GLU:H	1:C:133:GLU:HG3	1.73	0.40
1:C:187:THR:OG1	1:C:188:GLY:N	2.54	0.40
1:C:320:ILE:HG22	1:C:322:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	378/394 (96%)	370 (98%)	8 (2%)	0	100	100
1	B	379/394 (96%)	371 (98%)	8 (2%)	0	100	100
1	C	377/394 (96%)	368 (98%)	9 (2%)	0	100	100
All	All	1134/1182 (96%)	1109 (98%)	25 (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	327/332 (98%)	322 (98%)	5 (2%)	57	84
1	B	327/332 (98%)	321 (98%)	6 (2%)	51	82
1	C	325/332 (98%)	315 (97%)	10 (3%)	35	70
All	All	979/996 (98%)	958 (98%)	21 (2%)	45	79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	123	GLU
1	A	132	HIS
1	A	270	THR
1	A	328	ASP
1	B	30	CYS
1	B	123	GLU
1	B	189	LEU
1	B	246	GLN
1	B	247	GLU
1	B	309	GLU
1	C	30	CYS
1	C	132	HIS
1	C	189	LEU
1	C	201	ASN
1	C	219	THR
1	C	251	LEU
1	C	288	ASP
1	C	319	LEU
1	C	328	ASP
1	C	382	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	132	HIS
1	A	150	GLN
1	A	240	ASN
1	A	242	HIS

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Mol	Chain	Res	Type
1	A	259	HIS
1	A	315	HIS
1	B	52	GLN
1	B	134	ASN
1	B	149	HIS
1	B	150	GLN
1	B	207	HIS
1	B	353	ASN
1	C	134	ASN
1	C	149	HIS
1	C	230	ASN
1	C	353	ASN

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](#)

9 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	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.14	0
3	NAG	C	403	1	14,14,15	0.33	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	403	1	14,14,15	0.46	0	17,19,21	0.39	0
2	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.12	0
3	NAG	C	402	1	14,14,15	0.87	1 (7%)	17,19,21	0.59	0
2	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.08	0
3	NAG	A	403	1	14,14,15	0.87	1 (7%)	17,19,21	1.54	2 (11%)
3	NAG	B	402	1	14,14,15	1.41	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	A	402	1	14,14,15	0.24	0	17,19,21	1.10	2 (11%)

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
3	NAG	C	403	1	-	0/6/23/26	0/1/1/1
3	NAG	B	403	1	-	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	3/6/23/26	0/1/1/1
3	NAG	A	403	1	-	4/6/23/26	0/1/1/1
3	NAG	B	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAG	O5-C1	-3.63	1.37	1.43
3	B	402	NAG	C1-C2	3.31	1.56	1.52
3	A	403	NAG	C1-C2	2.91	1.56	1.52
3	C	402	NAG	C1-C2	2.77	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAG	C2-N2-C7	4.10	128.39	122.90
3	A	403	NAG	C1-O5-C5	4.07	117.64	112.19
3	A	402	NAG	C1-O5-C5	3.09	116.33	112.19
3	B	402	NAG	C4-C3-C2	2.76	115.07	111.02
3	A	402	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	NAG	C4-C5-C6-O6
3	A	403	NAG	C8-C7-N2-C2
3	A	403	NAG	O7-C7-N2-C2
3	C	402	NAG	C8-C7-N2-C2
3	C	402	NAG	O7-C7-N2-C2
3	A	403	NAG	O5-C5-C6-O6
3	A	402	NAG	O5-C5-C6-O6
3	A	402	NAG	C3-C2-N2-C7
3	C	402	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	NAG	1	0
3	B	403	NAG	1	0
2	C	401	SO4	1	0
2	A	401	SO4	1	0
3	A	403	NAG	2	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	384/394 (97%)	0.10	11 (2%) 53 43	43, 72, 137, 218	0
1	B	383/394 (97%)	-0.01	8 (2%) 63 54	29, 69, 130, 167	2 (0%)
1	C	382/394 (96%)	0.26	11 (2%) 53 43	35, 86, 136, 182	1 (0%)
All	All	1149/1182 (97%)	0.12	30 (2%) 57 47	29, 76, 137, 218	3 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	THR	3.6
1	A	224	THR	3.4
1	B	275	SER	3.2
1	A	243	ALA	3.1
1	C	193	GLU	3.0
1	C	243	ALA	2.8
1	A	252	GLY	2.8
1	C	79	GLU	2.8
1	A	270	THR	2.7
1	B	243	ALA	2.6
1	A	187	THR	2.6
1	B	152	GLY	2.5
1	B	278	ALA	2.5
1	C	241	ALA	2.5
1	A	293	LYS	2.4
1	A	51	THR	2.4
1	C	228	THR	2.4
1	C	242	HIS	2.3
1	C	222	ALA	2.3
1	B	70	THR	2.3
1	B	394	PHE	2.2
1	C	132	HIS	2.2
1	A	190	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	132	HIS	2.1
1	C	301	LEU	2.1
1	A	383	LYS	2.1
1	A	188	GLY	2.1
1	B	79	GLU	2.0
1	C	78	GLY	2.0
1	C	274	THR	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
3	NAG	A	402	14/15	0.42	0.16	127,145,151,151	0
3	NAG	B	402	14/15	0.49	0.13	112,126,130,131	0
3	NAG	B	403	14/15	0.64	0.16	115,121,131,134	0
3	NAG	C	402	14/15	0.69	0.11	109,123,127,127	0
3	NAG	A	403	14/15	0.70	0.13	84,111,124,125	0
2	SO4	C	401	5/5	0.71	0.13	86,104,107,112	0
2	SO4	B	401	5/5	0.76	0.15	130,133,135,136	0
3	NAG	C	403	14/15	0.79	0.12	105,116,122,122	0
2	SO4	A	401	5/5	0.83	0.14	73,105,109,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.