



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 7A3P / pdb_00007a3p
Title : Crystal structure of dengue 3 virus envelope glycoprotein in complex with the scFv fragment of the broadly neutralizing human antibody EDE1 C10
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on : 2020-08-18
Resolution : 3.19 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

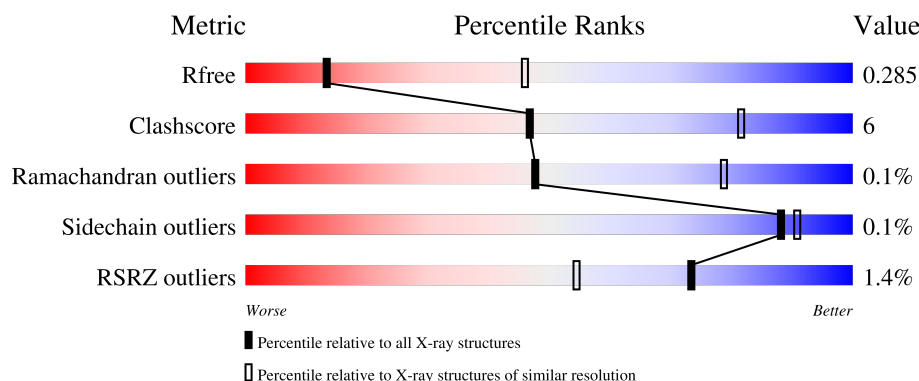
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	428	72% 10% 18%
1	B	428	3% 71% 14% 16%
2	H	144	78% 9% 13%
2	I	144	78% 10% 12%
3	L	154	% 64% 6% 29%

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Mol	Chain	Length	Quality of chain
3	M	154	% 60% 12% 28%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9173 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2721	1725	456	519	21			
1	B	361	Total	C	N	O	S	0	0	0
			2799	1774	473	531	21			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	LEU	-	expression tag	UNP Q07019
A	395	VAL	-	expression tag	UNP Q07019
A	396	PRO	-	expression tag	UNP Q07019
A	397	ARG	-	expression tag	UNP Q07019
A	398	GLY	-	expression tag	UNP Q07019
A	399	SER	-	expression tag	UNP Q07019
A	400	SER	-	expression tag	UNP Q07019
A	401	ALA	-	expression tag	UNP Q07019
A	402	TRP	-	expression tag	UNP Q07019
A	403	SER	-	expression tag	UNP Q07019
A	404	HIS	-	expression tag	UNP Q07019
A	405	PRO	-	expression tag	UNP Q07019
A	406	GLN	-	expression tag	UNP Q07019
A	407	PHE	-	expression tag	UNP Q07019
A	408	GLU	-	expression tag	UNP Q07019
A	409	LYS	-	expression tag	UNP Q07019
A	410	GLY	-	expression tag	UNP Q07019
A	411	GLY	-	expression tag	UNP Q07019
A	412	SER	-	expression tag	UNP Q07019
A	413	GLY	-	expression tag	UNP Q07019
A	414	GLY	-	expression tag	UNP Q07019
A	415	GLY	-	expression tag	UNP Q07019
A	416	SER	-	expression tag	UNP Q07019
A	417	GLY	-	expression tag	UNP Q07019
A	418	GLY	-	expression tag	UNP Q07019

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	SER	-	expression tag	UNP Q07019
A	420	ALA	-	expression tag	UNP Q07019
A	421	TRP	-	expression tag	UNP Q07019
A	422	SER	-	expression tag	UNP Q07019
A	423	HIS	-	expression tag	UNP Q07019
A	424	PRO	-	expression tag	UNP Q07019
A	425	GLN	-	expression tag	UNP Q07019
A	426	PHE	-	expression tag	UNP Q07019
A	427	GLU	-	expression tag	UNP Q07019
A	428	LYS	-	expression tag	UNP Q07019
B	394	LEU	-	expression tag	UNP Q07019
B	395	VAL	-	expression tag	UNP Q07019
B	396	PRO	-	expression tag	UNP Q07019
B	397	ARG	-	expression tag	UNP Q07019
B	398	GLY	-	expression tag	UNP Q07019
B	399	SER	-	expression tag	UNP Q07019
B	400	SER	-	expression tag	UNP Q07019
B	401	ALA	-	expression tag	UNP Q07019
B	402	TRP	-	expression tag	UNP Q07019
B	403	SER	-	expression tag	UNP Q07019
B	404	HIS	-	expression tag	UNP Q07019
B	405	PRO	-	expression tag	UNP Q07019
B	406	GLN	-	expression tag	UNP Q07019
B	407	PHE	-	expression tag	UNP Q07019
B	408	GLU	-	expression tag	UNP Q07019
B	409	LYS	-	expression tag	UNP Q07019
B	410	GLY	-	expression tag	UNP Q07019
B	411	GLY	-	expression tag	UNP Q07019
B	412	SER	-	expression tag	UNP Q07019
B	413	GLY	-	expression tag	UNP Q07019
B	414	GLY	-	expression tag	UNP Q07019
B	415	GLY	-	expression tag	UNP Q07019
B	416	SER	-	expression tag	UNP Q07019
B	417	GLY	-	expression tag	UNP Q07019
B	418	GLY	-	expression tag	UNP Q07019
B	419	SER	-	expression tag	UNP Q07019
B	420	ALA	-	expression tag	UNP Q07019
B	421	TRP	-	expression tag	UNP Q07019
B	422	SER	-	expression tag	UNP Q07019
B	423	HIS	-	expression tag	UNP Q07019
B	424	PRO	-	expression tag	UNP Q07019
B	425	GLN	-	expression tag	UNP Q07019

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Chain	Residue	Modelled	Actual	Comment	Reference
B	426	PHE	-	expression tag	UNP Q07019
B	427	GLU	-	expression tag	UNP Q07019
B	428	LYS	-	expression tag	UNP Q07019

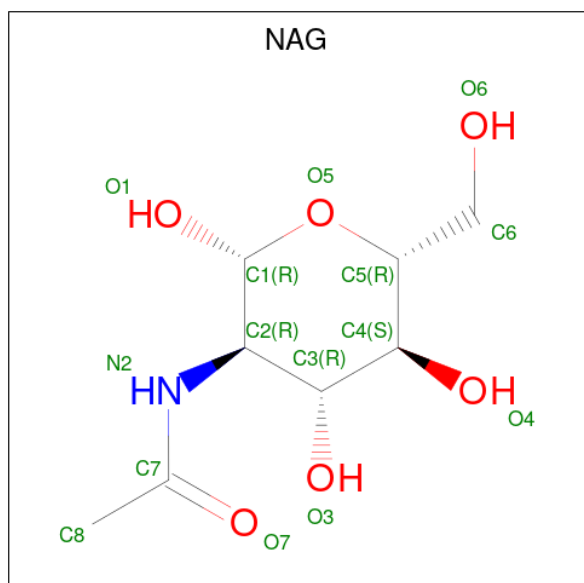
- Molecule 2 is a protein called Single Chain Variable Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	125	Total	C	N	O	S	0	0	0
			1006	642	167	192	5			
2	I	126	Total	C	N	O	S	0	0	0
			1015	647	168	195	5			

- Molecule 3 is a protein called Single Chain Variable Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	109	Total	C	N	O	S	0	0	0
			793	491	135	164	3			
3	M	111	Total	C	N	O	S	0	0	0
			808	499	138	168	3			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

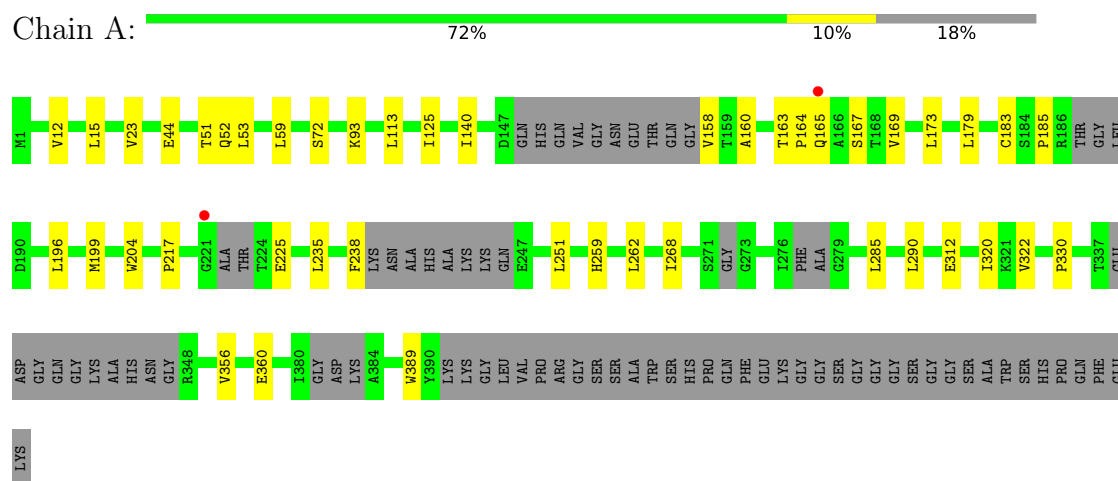
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	2	Total 2	O 2	0	0
5	H	1	Total 1	O 1	0	0
5	L	1	Total 1	O 1	0	0
5	I	3	Total 3	O 3	0	0
5	M	4	Total 4	O 4	0	0

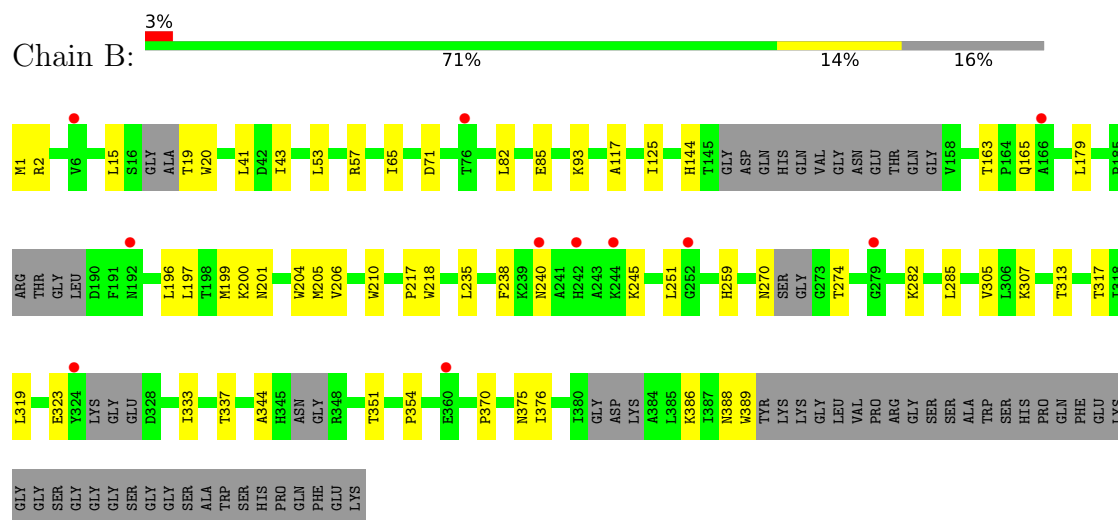
3 Residue-property plots [i](#)

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.

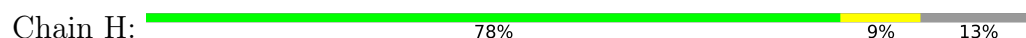
• Molecule 1: Envelope protein E



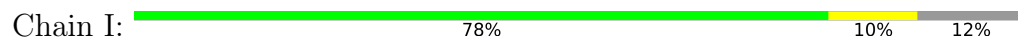
• Molecule 1: Envelope protein E



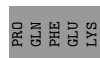
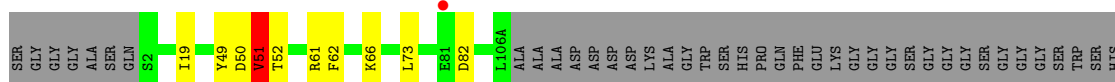
• Molecule 2: Single Chain Variable Fragment



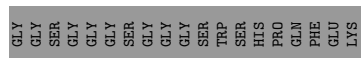
- Molecule 2: Single Chain Variable Fragment



- Molecule 3: Single Chain Variable Fragment



- Molecule 3: Single Chain Variable Fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 101.41Å 249.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.19 19.95 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.95-3.19) 96.8 (19.95-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.22Å)	Xtrriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.240 , 0.284 0.242 , 0.285	Depositor DCC
R_{free} test set	1406 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9173	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.41 % 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 5.7289e-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: 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	0/2766	0.45	0/3740
1	B	0.18	0/2847	0.43	0/3850
2	H	0.14	0/1035	0.36	0/1407
2	I	0.19	0/1044	0.45	0/1419
3	L	0.34	0/811	0.46	1/1101 (0.1%)
3	M	0.35	0/826	0.42	0/1121
All	All	0.22	0/9329	0.43	1/12638 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	51	VAL	CB-CA-C	-5.28	102.63	111.29

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	2721	0	2723	27	0
1	B	2799	0	2804	43	0
2	H	1006	0	946	9	0
2	I	1015	0	955	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	793	0	755	6	0
3	M	808	0	771	16	0
4	B	14	0	13	0	0
5	A	6	0	0	0	0
5	B	2	0	0	1	0
5	H	1	0	0	0	0
5	I	3	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	1	0
All	All	9173	0	8967	103	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 6.

All (103) 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:B:375:ASN:HA	1:B:386:LYS:HZ2	1.44	0.82
3:M:92:THR:HG1	3:M:95(A):THR:HG1	1.23	0.81
1:B:370:PRO:HG3	1:B:376:ILE:HD11	1.66	0.77
3:M:33:VAL:HB	3:M:51:VAL:HG22	1.69	0.72
1:A:196:LEU:HD11	1:A:268:ILE:HD11	1.73	0.71
1:B:240:ASN:ND2	1:B:245:LYS:O	2.24	0.71
3:L:50:ASP:O	3:L:52:THR:N	2.25	0.70
1:B:307:LYS:HD3	1:B:323:GLU:HB3	1.78	0.65
1:B:165:GLN:NE2	5:B:602:HOH:O	2.29	0.65
1:B:19:THR:OG1	1:B:20:TRP:N	2.29	0.65
1:B:71:ASP:OD2	3:M:94:ARG:NH1	2.30	0.64
1:A:360:GLU:HB3	3:M:54:ARG:HH12	1.63	0.63
3:M:103:LYS:NZ	5:M:201:HOH:O	2.32	0.63
1:B:41:LEU:HD13	1:B:43:ILE:HD11	1.82	0.61
1:B:217:PRO:HD3	1:B:235:LEU:HD13	1.82	0.61
1:A:93:LYS:HD2	1:A:238:PHE:HB2	1.83	0.60
1:B:163:THR:HG22	1:B:165:GLN:H	1.67	0.60
1:B:245:LYS:HD2	2:I:100(D):TRP:NE1	2.17	0.59
1:A:163:THR:HG22	1:A:165:GLN:H	1.68	0.59
2:I:52(A):ALA:HA	2:I:71:ARG:HD3	1.84	0.59
1:B:375:ASN:CG	1:B:386:LYS:HD3	2.29	0.57
1:A:312:GLU:HB2	1:A:389:TRP:HZ2	1.68	0.57
1:B:386:LYS:HZ1	1:B:388:ASN:HB2	1.69	0.57
1:A:330:PRO:HA	1:A:356:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PRO:CD	1:B:235:LEU:HD13	2.35	0.56
2:H:87:THR:HG23	2:H:110:THR:HA	1.87	0.56
1:A:217:PRO:HD3	1:A:235:LEU:HD13	1.86	0.56
1:B:53:LEU:HD11	1:B:274:THR:HG21	1.87	0.55
2:I:66:ARG:NH2	2:I:86:ASP:OD1	2.40	0.55
1:B:57:ARG:HG2	1:B:218:TRP:CE3	2.42	0.55
1:B:199:MET:HG2	1:B:200:LYS:H	1.72	0.55
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.42	0.54
3:M:94:ARG:HH11	3:M:94:ARG:HG3	1.73	0.54
1:B:245:LYS:HD2	2:I:100(D):TRP:CE2	2.43	0.53
2:I:44:ARG:HD3	3:M:2:SER:HB3	1.89	0.53
1:A:160:ALA:HB1	1:A:169:VAL:HG11	1.91	0.53
1:A:51:THR:HG22	1:A:52:GLN:HG3	1.89	0.53
1:A:320:ILE:HG22	1:A:322:VAL:HG13	1.91	0.52
1:B:386:LYS:NZ	1:B:388:ASN:HB2	2.24	0.52
1:A:158:VAL:HG21	1:A:173:LEU:HD23	1.91	0.52
1:A:72:SER:HB3	1:A:113:LEU:HD12	1.90	0.52
1:B:313:THR:OG1	1:B:317:THR:OG1	2.28	0.52
2:I:36:TRP:CE2	2:I:80:MET:HB2	2.45	0.51
1:A:44:GLU:HB3	1:A:140:ILE:HG23	1.93	0.51
1:A:15:LEU:H	1:A:15:LEU:HD23	1.75	0.51
1:A:59:LEU:HB2	1:A:125:ILE:HG12	1.92	0.50
3:M:92:THR:OG1	3:M:95(A):THR:OG1	2.13	0.50
1:B:125:ILE:HD12	1:B:197:LEU:HD21	1.94	0.49
2:H:65:ASP:OD1	2:H:65:ASP:N	2.44	0.49
1:A:225:GLU:HA	1:A:225:GLU:OE2	2.11	0.49
2:H:66:ARG:NH2	2:H:86:ASP:OD1	2.46	0.49
1:A:53:LEU:HD12	1:A:53:LEU:O	2.13	0.48
2:I:100(H):LEU:O	3:M:49:TYR:HB2	2.13	0.48
1:B:333:ILE:HD12	1:B:354:PRO:HB2	1.96	0.48
2:I:100(H):LEU:HD13	3:M:50:ASP:OD2	2.14	0.48
2:H:52(A):ALA:HA	2:H:71:ARG:HD3	1.96	0.48
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.96	0.47
3:L:62:PHE:HD1	3:L:73:LEU:HD11	1.78	0.47
3:M:32:TYR:O	3:M:90:SER:HA	2.14	0.47
2:I:100(B):ASP:HB3	2:I:100(D):TRP:CD1	2.50	0.47
1:A:204:TRP:CE3	1:A:262:LEU:HD13	2.50	0.46
1:B:93:LYS:HB2	1:B:238:PHE:CD2	2.51	0.46
1:B:206:VAL:HG21	1:B:210:TRP:CE3	2.51	0.46
3:M:61:ARG:NH1	3:M:82:ASP:OD2	2.43	0.46
1:A:12:VAL:HG21	1:A:23:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASN:O	1:B:389:TRP:HB2	2.17	0.45
3:M:94:ARG:NH1	3:M:94:ARG:HG3	2.30	0.45
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.79	0.45
1:B:337:THR:HG23	1:B:344:ALA:HB3	1.99	0.44
1:B:144:HIS:HB3	1:B:351:THR:HG23	1.98	0.44
1:B:313:THR:HG21	1:B:319:LEU:HD13	2.00	0.44
2:H:100(H):LEU:O	3:L:49:TYR:HB2	2.17	0.44
1:B:125:ILE:HG22	1:B:199:MET:HG3	1.99	0.44
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.27	0.44
1:A:179:LEU:HD21	1:A:285:LEU:HD22	1.99	0.43
1:B:201:ASN:O	1:B:270:ASN:HB3	2.18	0.43
1:A:164:PRO:HG3	1:A:185:PRO:HG2	2.00	0.43
2:I:36:TRP:HB3	2:I:48:MET:HE3	2.00	0.43
1:B:199:MET:SD	1:B:259:HIS:NE2	2.92	0.42
1:B:65:ILE:HG23	1:B:117:ALA:HB1	2.01	0.42
1:B:179:LEU:HD21	1:B:285:LEU:HD22	2.01	0.42
2:I:65:ASP:OD1	2:I:65:ASP:N	2.52	0.42
1:B:1:MET:HG3	1:B:2:ARG:H	1.85	0.42
1:B:305:VAL:HB	1:B:323:GLU:HG2	2.02	0.42
1:A:173:LEU:HD12	1:A:290:LEU:HD11	2.02	0.41
2:I:100(H):LEU:HD13	3:M:50:ASP:CG	2.45	0.41
1:A:167:SER:OG	1:A:183:CYS:O	2.38	0.41
1:B:282:LYS:HE3	1:B:282:LYS:HB2	1.71	0.41
2:H:6:GLU:OE1	2:H:6:GLU:N	2.50	0.41
3:M:66:LYS:HA	3:M:71:ALA:HA	2.03	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.91	0.41
3:M:79:GLN:O	3:M:106:VAL:HG21	2.21	0.41
1:A:259:HIS:ND1	1:B:251:LEU:O	2.54	0.41
1:B:53:LEU:CD1	1:B:274:THR:HG21	2.50	0.41
3:L:19:ILE:HD12	3:L:19:ILE:HA	1.89	0.41
2:H:47:TRP:HZ2	2:H:50:TRP:HD1	1.68	0.41
1:A:199:MET:HE3	1:A:204:TRP:HZ3	1.87	0.40
1:B:82:LEU:HB2	1:B:85:GLU:HG3	2.02	0.40
1:B:205:MET:HE3	1:B:205:MET:HB3	1.96	0.40
1:B:196:LEU:HD12	1:B:204:TRP:O	2.22	0.40
2:H:47:TRP:HZ2	2:H:50:TRP:CD1	2.40	0.40
3:L:51:VAL:HG11	3:L:66:LYS:HB2	2.03	0.40
1:A:251:LEU:O	1:B:259:HIS:ND1	2.51	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	333/428 (78%)	321 (96%)	12 (4%)	0	100	100
1	B	345/428 (81%)	326 (94%)	19 (6%)	0	100	100
2	H	123/144 (85%)	119 (97%)	4 (3%)	0	100	100
2	I	124/144 (86%)	120 (97%)	4 (3%)	0	100	100
3	L	107/154 (70%)	105 (98%)	1 (1%)	1 (1%)	14	47
3	M	109/154 (71%)	105 (96%)	4 (4%)	0	100	100
All	All	1141/1452 (79%)	1096 (96%)	44 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	VAL

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	304/357 (85%)	304 (100%)	0	100	100
1	B	311/357 (87%)	311 (100%)	0	100	100
2	H	105/112 (94%)	105 (100%)	0	100	100
2	I	106/112 (95%)	106 (100%)	0	100	100
3	L	89/116 (77%)	88 (99%)	1 (1%)	65	79
3	M	91/116 (78%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1006/1170 (86%)	1005 (100%)	1 (0%)	88 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	375	ASN
1	B	86	GLN
1	B	240	ASN
1	B	246	GLN
1	B	375	ASN
2	I	64	GLN

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 ⓘ

1 ligand is 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	$\# Z > 2$
4	NAG	B	501	1	14,14,15	1.14	1 (7%)	17,19,21	2.34	5 (29%)

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
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	NAG	O5-C1	3.08	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	NAG	C1-C2-N2	5.18	118.59	110.43
4	B	501	NAG	C2-N2-C7	4.91	129.48	122.90
4	B	501	NAG	C1-O5-C5	4.18	117.79	112.19
4	B	501	NAG	C4-C3-C2	-3.29	106.20	111.02
4	B	501	NAG	O4-C4-C3	2.25	115.68	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C3-C2-N2-C7
4	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	351/428 (82%)	0.37	2 (0%) 85 73	44, 66, 94, 107	0
1	B	361/428 (84%)	0.44	11 (3%) 52 33	38, 75, 107, 121	0
2	H	125/144 (86%)	0.19	0 100 100	46, 69, 85, 92	0
2	I	126/144 (87%)	0.20	0 100 100	37, 52, 66, 89	0
3	L	109/154 (70%)	0.24	1 (0%) 81 64	47, 66, 96, 100	0
3	M	111/154 (72%)	0.14	2 (1%) 67 48	36, 48, 66, 84	0
All	All	1183/1452 (81%)	0.32	16 (1%) 73 54	36, 65, 98, 121	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	THR	3.0
3	L	81	GLU	2.9
1	B	192	ASN	2.9
3	M	81	GLU	2.7
1	B	166	ALA	2.7
1	A	221	GLY	2.5
1	B	240	ASN	2.4
1	B	242	HIS	2.4
3	M	106(A)	LEU	2.3
1	B	360	GLU	2.2
1	B	252	GLY	2.2
1	B	6	VAL	2.2
1	B	244	LYS	2.2
1	A	165	GLN	2.1
1	B	279	GLY	2.1
1	B	324	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
4	NAG	B	501	14/15	0.53	0.18	89,96,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.