



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:02 PM UTC

PDB ID : 2Y8T / pdb_00002y8t
Title : Co-structure of AMA1 with a surface exposed region of RON2 from Toxoplasma gondii
Authors : Tonkin, M.L.; Roques, M.; Lamarque, M.H.; Pugniere, M.; Douguet, D.; Crawford, J.; Lebrun, M.; Boulanger, M.J.
Deposited on : 2011-02-10
Resolution : 1.95 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

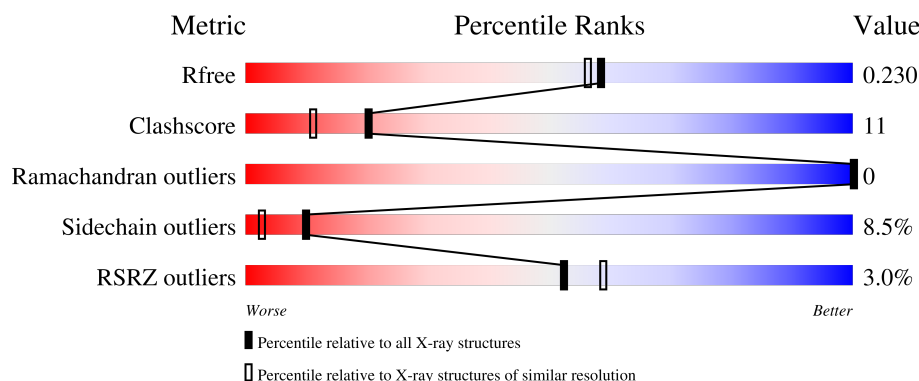
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	432	% 73% 15% • 10%
1	D	432	5% 69% 18% • • 9%
2	B	37	70% 14% 14% •
2	E	37	3% 59% 30% 8% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	9AT	B	1333	-	-	X	-
4	BO3	D	1475	-	X	-	-
4	BO3	D	1476	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7336 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 APICAL MEMBRANE ANTIGEN, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	3	0
			3067	1923	528	594	22			
1	D	395	Total	C	N	O	S	0	0	0
			3117	1962	533	601	21			

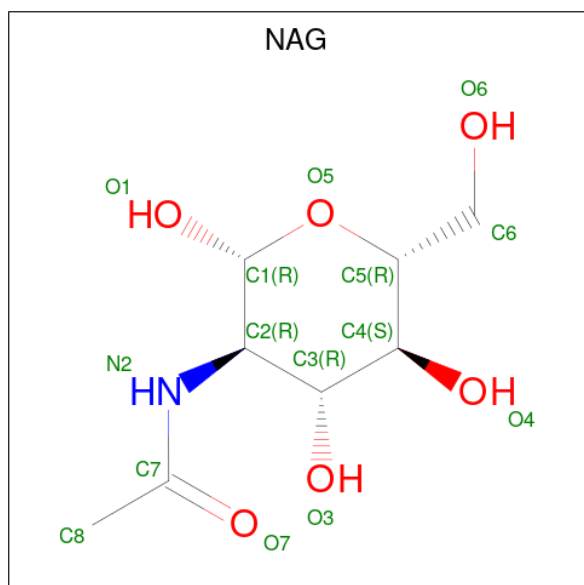
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	expression tag	UNP B9QC59
A	60	SER	-	expression tag	UNP B9QC59
A	61	ALA	-	expression tag	UNP B9QC59
A	62	MET	-	expression tag	UNP B9QC59
A	63	GLY	-	expression tag	UNP B9QC59
A	485	ALA	-	expression tag	UNP B9QC59
A	486	ALA	-	expression tag	UNP B9QC59
A	487	LEU	-	expression tag	UNP B9QC59
A	488	VAL	-	expression tag	UNP B9QC59
A	489	PRO	-	expression tag	UNP B9QC59
A	490	ARG	-	expression tag	UNP B9QC59
D	59	GLY	-	expression tag	UNP B9QC59
D	60	SER	-	expression tag	UNP B9QC59
D	61	ALA	-	expression tag	UNP B9QC59
D	62	MET	-	expression tag	UNP B9QC59
D	63	GLY	-	expression tag	UNP B9QC59
D	485	ALA	-	expression tag	UNP B9QC59
D	486	ALA	-	expression tag	UNP B9QC59
D	487	LEU	-	expression tag	UNP B9QC59
D	488	VAL	-	expression tag	UNP B9QC59
D	489	PRO	-	expression tag	UNP B9QC59
D	490	ARG	-	expression tag	UNP B9QC59

- Molecule 2 is a protein called RHOPTRY NECK PROTEIN 2.

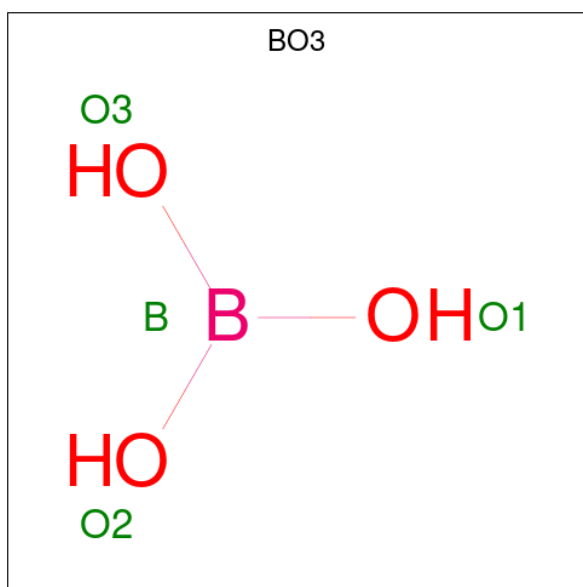
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	37	Total	C	N	O	S	0	0	0
			260	160	44	53	3			
2	E	36	Total	C	N	O	S	0	0	0
			252	156	42	51	3			

- 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	D	1	Total	C	N	O	0	0
			14	8	1	5		

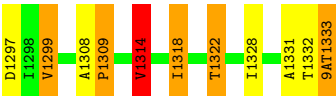
- Molecule 4 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total B O 4 1 3	0	0
4	D	1	Total B O 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	319	Total O 319 319	0	0
5	B	25	Total O 25 25	0	0
5	D	246	Total O 246 246	0	0
5	E	14	Total O 14 14	0	0



● Molecule 2: RHOPTRY NECK PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.86Å 96.38Å 78.35Å 90.00° 115.64° 90.00°	Depositor
Resolution (Å)	39.81 – 1.95 39.81 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-1.95) 99.9 (39.81-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.228 0.171 , 0.230	Depositor DCC
R_{free} test set	3453 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7336	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: 9AT, BO3, 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	1.08	1/3152 (0.0%)	1.11	8/4267 (0.2%)
1	D	1.04	2/3200 (0.1%)	1.16	11/4339 (0.3%)
2	B	1.33	1/255 (0.4%)	1.38	2/349 (0.6%)
2	E	1.04	1/255 (0.4%)	1.37	1/349 (0.3%)
All	All	1.07	5/6862 (0.1%)	1.15	22/9304 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1309	PRO	CA-C	6.96	1.55	1.51
2	E	1309	PRO	CA-C	6.91	1.55	1.51
1	D	417	ILE	CA-CB	6.61	1.61	1.54
1	D	435	CYS	CB-SG	-5.34	1.63	1.81
1	A	449	VAL	CA-CB	5.33	1.61	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ASN	CA-C-N	-11.43	108.01	119.56
1	D	70	ASN	C-N-CA	-11.43	108.01	119.56
2	E	1315	THR	CB-CA-C	-8.45	95.81	109.75
1	A	413	THR	CA-C-N	-7.54	112.92	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	THR	C-N-CA	-7.54	112.92	120.31
1	A	144	THR	N-CA-CB	-7.17	99.39	110.29
1	A	236	MET	CA-CB-CG	-6.87	100.37	114.10
1	D	435	CYS	N-CA-CB	-6.30	99.85	110.49
1	A	311	THR	N-CA-C	6.21	118.56	111.11
1	A	144	THR	OG1-CB-CG2	6.06	121.42	109.30
1	D	248	PRO	CA-C-N	5.98	125.86	119.28
1	D	248	PRO	C-N-CA	5.98	125.86	119.28
2	B	1314	VAL	N-CA-CB	-5.88	101.05	111.93
1	D	435	CYS	CA-C-N	-5.69	115.45	122.84
1	D	435	CYS	C-N-CA	-5.69	115.45	122.84
2	B	1314	VAL	CG1-CB-CG2	5.51	122.92	110.80
1	D	275	VAL	CG1-CB-CG2	5.41	122.71	110.80
1	D	344	LEU	CA-CB-CG	5.37	135.09	116.30
1	D	288	ASN	N-CA-C	5.29	117.05	111.28
1	D	359	SER	N-CA-C	5.13	117.93	109.72
1	A	275	VAL	CA-CB-CG1	5.10	119.08	110.40
1	A	431	THR	N-CA-C	5.02	116.56	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	434	GLN	Peptide
1	D	69	GLY	Peptide

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	3067	0	2928	53	0
1	D	3117	0	2959	85	0
2	B	260	0	260	14	0
2	E	252	0	250	15	0
3	A	14	0	13	1	0
3	D	14	0	13	1	0
4	D	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	319	0	0	8	1
5	B	25	0	0	1	0
5	D	246	0	0	15	0
5	E	14	0	0	0	0
All	All	7336	0	6429	148	1

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 11.

All (148) 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)
2:B:1332:THR:C	2:B:1333:9AT:HN2	1.29	1.40
2:B:1332:THR:C	2:B:1333:9AT:N	1.84	1.34
1:A:259[A]:ARG:HD2	5:A:2059:HOH:O	1.43	1.16
1:A:144:THR:HG21	5:B:2022:HOH:O	1.51	1.10
1:D:292:ARG:HD3	1:D:411:GLU:OE1	1.54	1.05
1:D:76:VAL:O	1:D:80:THR:HG23	1.59	1.01
1:A:144:THR:HG22	1:A:147:GLU:H	1.31	0.96
1:A:177:GLU:OE1	1:A:177:GLU:N	2.00	0.93
2:E:1308:ALA:HB1	2:E:1309:PRO:HD2	1.55	0.89
1:D:434:GLN:HB3	5:D:2221:HOH:O	1.72	0.88
1:D:144:THR:HG22	1:D:147:GLU:H	1.41	0.86
1:D:201:THR:CG2	2:E:1314:VAL:HG11	2.05	0.86
1:D:357:HIS:C	1:D:358:GLN:HG2	2.05	0.82
1:A:177:GLU:H	1:A:177:GLU:CD	1.86	0.79
1:D:72:PHE:HA	1:D:78:MET:HG2	1.65	0.78
1:A:259[B]:ARG:HH11	1:A:330:GLU:CD	1.93	0.75
1:D:435:CYS:HB3	1:D:462:GLY:C	2.13	0.74
2:B:1332:THR:C	2:B:1333:9AT:HN1	1.93	0.73
1:D:345:THR:HG22	5:D:2177:HOH:O	1.90	0.70
1:A:96:TYR:OH	1:A:259[B]:ARG:NH2	2.25	0.69
1:D:361:GLN:NE2	2:E:1303:GLU:OE1	2.26	0.68
1:D:441:PRO:O	5:D:2223:HOH:O	2.10	0.68
1:D:345:THR:HG21	1:D:347:GLN:HB2	1.74	0.68
1:A:70:ASN:ND2	1:A:72:PHE:H	1.93	0.67
1:A:436:THR:OG1	1:A:439:LYS:HD2	1.95	0.66
1:A:148:TYR:OH	1:A:153:ASN:ND2	2.30	0.64
1:A:184:ASN:HD21	1:A:200:LYS:HD3	1.62	0.64
1:D:201:THR:HG23	2:E:1314:VAL:HG11	1.78	0.64
3:D:1474:NAG:H83	5:D:2009:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:VAL:HA	1:D:452:CYS:HA	1.81	0.63
1:D:292:ARG:CD	1:D:411:GLU:OE1	2.40	0.63
1:D:201:THR:HG22	2:E:1314:VAL:HG11	1.80	0.63
1:D:450:GLN:OE1	1:D:450:GLN:N	2.25	0.62
1:D:345:THR:HG21	1:D:347:GLN:HE21	1.64	0.62
1:A:162:ASN:HD22	1:A:162:ASN:H	1.48	0.62
1:A:257:LYS:HD2	1:A:259[B]:ARG:HH21	1.64	0.61
1:D:448:ASP:C	1:D:448:ASP:OD1	2.43	0.60
1:D:307:TYR:HA	1:D:310:LEU:HD22	1.83	0.60
1:D:201:THR:HG23	2:E:1314:VAL:CG1	2.31	0.60
1:D:201:THR:CG2	2:E:1314:VAL:CG1	2.77	0.60
1:A:68:SER:HA	1:A:299:TRP:HE1	1.65	0.59
1:D:148:TYR:OH	1:D:252:THR:HG23	2.02	0.59
1:D:69:GLY:N	1:D:72:PHE:H	2.01	0.58
1:D:441:PRO:HD2	5:D:2223:HOH:O	2.02	0.58
1:D:78:MET:SD	1:D:464:ILE:HD13	2.44	0.57
1:D:106:ASP:OD1	1:D:205:ASP:HB2	2.04	0.57
1:A:123:HIS:HE1	5:A:2057:HOH:O	1.86	0.57
1:A:144:THR:CG2	1:A:147:GLU:H	2.11	0.55
1:D:319:GLU:H	1:D:323:GLN:NE2	2.03	0.55
1:D:175:PRO:HG2	1:D:178:LEU:HD22	1.89	0.55
1:A:396:SER:OG	1:A:465:GLN:HA	2.08	0.54
2:B:1332:THR:CA	2:B:1333:9AT:N	2.65	0.54
1:D:76:VAL:O	1:D:80:THR:CG2	2.47	0.54
1:D:81:PHE:O	1:D:84:ARG:HG3	2.07	0.54
1:D:345:THR:CG2	1:D:347:GLN:HB2	2.38	0.54
1:D:135:ARG:HD3	5:D:2045:HOH:O	2.07	0.53
1:A:235:LEU:HD23	1:A:338:GLN:HG2	1.88	0.53
1:D:81:PHE:O	1:D:84:ARG:CG	2.56	0.53
1:D:239:LYS:HB2	1:D:344:LEU:HG	1.90	0.53
1:D:321:LYS:NZ	5:D:2155:HOH:O	2.40	0.52
1:D:184:ASN:HB2	2:E:1318:ILE:CD1	2.39	0.52
1:D:351:ASN:ND2	5:D:2180:HOH:O	2.14	0.52
1:A:83:GLU:OE2	3:A:1480:NAG:H83	2.09	0.52
1:A:170:ARG:HD2	5:A:2108:HOH:O	2.10	0.52
1:D:377:ASP:OD1	1:D:377:ASP:C	2.52	0.52
1:A:170:ARG:CD	5:A:2108:HOH:O	2.59	0.51
1:D:83:GLU:HG3	5:D:2006:HOH:O	2.10	0.51
1:D:357:HIS:O	1:D:358:GLN:HG2	2.09	0.51
1:A:259[B]:ARG:HD3	1:A:330:GLU:OE2	2.11	0.51
1:D:434:GLN:CB	5:D:2221:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2141:HOH:O	1:D:415:ASN:HB3	2.10	0.51
1:D:448:ASP:OD1	1:D:448:ASP:O	2.29	0.51
1:D:472:THR:OG1	1:D:473:ALA:N	2.44	0.50
1:A:70:ASN:C	1:A:70:ASN:HD22	2.19	0.50
1:A:88:THR:HG21	5:A:2012:HOH:O	2.11	0.50
1:A:201:THR:HG23	2:B:1314:VAL:HG13	1.94	0.50
1:A:410:SER:OG	1:D:412:GLU:OE1	2.17	0.49
1:A:163:PHE:CB	2:B:1322:THR:HG23	2.42	0.49
2:B:1308:ALA:HB1	2:B:1309:PRO:HD2	1.94	0.49
1:A:259[B]:ARG:NH1	1:A:330:GLU:CD	2.66	0.49
1:D:72:PHE:HB3	1:D:82:MET:HG3	1.94	0.49
2:E:1309:PRO:HB2	2:E:1311:VAL:HG23	1.93	0.49
1:A:289:GLN:HE22	1:A:417:ILE:HD11	1.77	0.49
2:B:1314:VAL:HG12	2:B:1322:THR:HG22	1.95	0.49
1:A:144:THR:HG22	1:A:147:GLU:N	2.14	0.49
5:A:2219:HOH:O	1:D:461:GLY:HA2	2.12	0.49
1:D:144:THR:CG2	1:D:147:GLU:H	2.19	0.48
1:D:76:VAL:HG12	5:D:2004:HOH:O	2.12	0.48
1:D:177:GLU:H	1:D:177:GLU:CD	2.22	0.48
1:D:79:LYS:NZ	5:D:2005:HOH:O	2.47	0.47
2:E:1308:ALA:HB1	2:E:1309:PRO:CD	2.38	0.47
1:D:69:GLY:O	1:D:73:GLN:OE1	2.32	0.47
1:A:162:ASN:HD21	2:B:1328:ILE:HD11	1.80	0.47
1:A:162:ASN:HD22	1:A:162:ASN:N	2.10	0.47
1:A:319:GLU:H	1:A:323:GLN:NE2	2.12	0.47
1:A:474:ASP:O	1:A:477:ASN:HB2	2.15	0.47
1:A:91:HIS:CE1	1:A:115:GLY:HA3	2.50	0.47
1:A:121:GLY:O	1:A:123:HIS:HD2	1.97	0.46
1:A:331:ASN:OD1	1:A:369[A]:ARG:HD2	2.14	0.46
5:A:2279:HOH:O	1:D:222:LYS:HD2	2.16	0.46
1:D:431:THR:O	1:D:434:GLN:HG2	2.16	0.46
1:D:429:PRO:HB2	1:D:430:GLU:H	1.52	0.45
1:A:68:SER:HA	1:A:299:TRP:NE1	2.30	0.45
1:D:220:ASP:OD1	1:D:220:ASP:C	2.59	0.45
1:D:201:THR:HG22	2:E:1314:VAL:CG1	2.44	0.45
1:A:128:GLN:O	1:A:245:LYS:HD3	2.15	0.45
1:A:240:LYS:HG2	1:A:241:TYR:CE2	2.51	0.45
1:A:460:VAL:CG2	1:A:465:GLN:HG3	2.46	0.45
1:D:78:MET:CE	1:D:464:ILE:HD13	2.47	0.45
1:D:298:VAL:O	1:D:298:VAL:HG23	2.16	0.45
1:D:71:PRO:O	1:D:78:MET:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:THR:HG22	5:D:2222:HOH:O	2.16	0.45
1:A:163:PHE:HB3	2:B:1322:THR:HG23	1.99	0.44
1:A:72:PHE:O	1:A:78:MET:HG3	2.17	0.44
1:D:435:CYS:CB	1:D:462:GLY:C	2.89	0.44
1:A:292[A]:ARG:HD2	1:D:292:ARG:HD2	1.98	0.44
1:D:70:ASN:HB3	1:D:299:TRP:CZ2	2.53	0.44
1:D:224:ARG:NH1	5:D:2100:HOH:O	2.50	0.44
1:D:73:GLN:HA	1:D:79:LYS:HG3	2.00	0.44
1:D:272:SER:O	1:D:275:VAL:HG13	2.18	0.44
1:D:344:LEU:HD13	1:D:344:LEU:O	2.18	0.44
1:D:289:GLN:HE22	1:D:417:ILE:HD11	1.83	0.43
1:D:248:PRO:HA	1:D:249:PRO:HD3	1.69	0.43
1:D:163:PHE:CB	2:E:1322:THR:HG23	2.49	0.43
1:D:345:THR:CG2	1:D:347:GLN:HE21	2.30	0.43
5:D:2171:HOH:O	2:E:1301:HIS:HE1	2.02	0.43
1:A:268:LEU:C	1:A:269:ILE:HG13	2.43	0.43
1:D:304:CYS:H	1:D:455:GLN:NE2	2.18	0.42
1:A:415:ASN:HD22	1:A:415:ASN:N	2.16	0.42
1:D:160:ASN:ND2	1:D:172:SER:OG	2.44	0.42
1:D:81:PHE:O	1:D:84:ARG:HG2	2.20	0.42
1:D:163:PHE:HB3	2:E:1322:THR:HG23	2.01	0.42
1:D:435:CYS:O	1:D:462:GLY:HA2	2.19	0.42
1:D:209:LYS:HA	1:D:209:LYS:HE3	2.01	0.42
1:A:184:ASN:HB3	2:B:1318:ILE:HD11	2.02	0.41
1:D:372:GLY:HA2	1:D:385:ALA:O	2.20	0.41
1:D:162:ASN:HD21	2:E:1328:ILE:HD11	1.85	0.41
1:A:252:THR:HG21	2:B:1331:ALA:CB	2.51	0.41
1:D:344:LEU:O	1:D:344:LEU:CD1	2.69	0.41
1:D:347:GLN:HB2	1:D:347:GLN:HE21	1.76	0.41
1:A:135:ARG:NH1	1:A:140:GLU:OE2	2.54	0.41
1:A:189:THR:O	1:A:193:ARG:HG3	2.20	0.41
2:B:1297:ASP:OD2	2:B:1299:VAL:HG13	2.21	0.41
1:D:195:ALA:CB	1:D:275:VAL:HG22	2.51	0.40
1:A:163:PHE:HB2	2:B:1322:THR:HG23	2.03	0.40
1:D:345:THR:HG23	1:D:347:GLN:N	2.37	0.40
1:A:291:LEU:HD13	1:A:294:TYR:HB2	2.03	0.40
1:A:444:PHE:HA	1:A:455:GLN:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2131:HOH:O	5:A:2249:HOH:O[2_555]	2.02	0.18

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	385/432 (89%)	377 (98%)	8 (2%)	0	100	100
1	D	389/432 (90%)	376 (97%)	13 (3%)	0	100	100
2	B	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
2	E	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	843/938 (90%)	820 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/372 (91%)	319 (94%)	21 (6%)	16	6
1	D	344/372 (92%)	311 (90%)	33 (10%)	8	2
2	B	28/28 (100%)	24 (86%)	4 (14%)	3	0
2	E	28/28 (100%)	22 (79%)	6 (21%)	1	0
All	All	740/800 (92%)	676 (91%)	64 (9%)	10	2

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	109	LEU
1	A	116	LEU
1	A	126	LEU
1	A	144	THR
1	A	162	ASN
1	A	177	GLU
1	A	178	LEU
1	A	181	LYS
1	A	191	LEU
1	A	236	MET
1	A	240	LYS
1	A	250	ASP
1	A	259[A]	ARG
1	A	259[B]	ARG
1	A	275	VAL
1	A	291	LEU
1	A	310	LEU
1	A	338	GLN
1	A	415	ASN
1	A	474	ASP
2	B	1299	VAL
2	B	1314	VAL
2	B	1318	ILE
2	B	1322	THR
1	D	70	ASN
1	D	78	MET
1	D	80	THR
1	D	84	ARG
1	D	109	LEU
1	D	116	LEU
1	D	126	LEU
1	D	135	ARG
1	D	144	THR
1	D	149	LYS
1	D	162	ASN
1	D	167	SER
1	D	178	LEU
1	D	183	SER
1	D	191	LEU
1	D	209	LYS
1	D	235	LEU
1	D	245	LYS

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Mol	Chain	Res	Type
1	D	264	GLU
1	D	275	VAL
1	D	291	LEU
1	D	300	LYS
1	D	305	LEU
1	D	310	LEU
1	D	344	LEU
1	D	352	ASP
1	D	356	LEU
1	D	358	GLN
1	D	421	ASN
1	D	436	THR
1	D	448	ASP
1	D	449	VAL
1	D	463	GLN
2	E	1297	ASP
2	E	1299	VAL
2	E	1312	SER
2	E	1315	THR
2	E	1322	THR
2	E	1330	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ASN
1	A	123	HIS
1	A	153	ASN
1	A	162	ASN
1	A	184	ASN
1	A	208	ASN
1	A	323	GLN
1	A	338	GLN
1	A	389	GLN
1	A	415	ASN
1	A	465	GLN
1	A	476	GLN
1	D	92	GLN
1	D	101	GLN
1	D	153	ASN
1	D	160	ASN

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Mol	Chain	Res	Type
1	D	162	ASN
1	D	289	GLN
1	D	323	GLN
1	D	347	GLN
1	D	455	GLN
2	E	1301	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
2	9AT	B	1333	-	7,7,7	0.67	0	9,9,9	1.54	2 (22%)

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	9AT	B	1333	-	-	0/7/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1333	9AT	CA-C-NXT	-2.55	113.01	117.02
2	B	1333	9AT	O-C-CA	2.16	123.17	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1333	9AT	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	NAG	D	1474	1	14,14,15	0.48	0	17,19,21	1.32	2 (11%)
3	NAG	A	1480	1	14,14,15	0.72	0	17,19,21	2.14	7 (41%)
4	BO3	D	1475	-	3,3,3	5.25	3 (100%)	3,3,3	0.77	0
4	BO3	D	1476	-	3,3,3	5.21	3 (100%)	3,3,3	0.22	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
3	NAG	D	1474	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1480	1	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1475	BO3	B-O3	5.57	1.54	1.36
4	D	1476	BO3	B-O3	5.38	1.54	1.36
4	D	1475	BO3	B-O1	5.30	1.53	1.36
4	D	1476	BO3	B-O1	5.13	1.53	1.36
4	D	1476	BO3	B-O2	5.11	1.53	1.36
4	D	1475	BO3	B-O2	4.83	1.52	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	NAG	C8-C7-N2	4.29	123.23	116.12
3	A	1480	NAG	O5-C5-C4	-3.33	102.73	110.83
3	A	1480	NAG	O5-C1-C2	-3.21	106.32	111.29
3	A	1480	NAG	O7-C7-C8	-2.71	117.22	122.05
3	D	1474	NAG	C1-C2-N2	2.66	114.63	110.43
3	A	1480	NAG	C6-C5-C4	-2.54	106.78	113.02
3	A	1480	NAG	O5-C5-C6	2.50	112.53	107.66
3	D	1474	NAG	O5-C5-C6	2.36	112.26	107.66
3	A	1480	NAG	O3-C3-C2	-2.33	104.56	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1480	NAG	O5-C5-C6-O6
3	A	1480	NAG	C8-C7-N2-C2
3	A	1480	NAG	O7-C7-N2-C2
3	D	1474	NAG	C8-C7-N2-C2
3	D	1474	NAG	O7-C7-N2-C2
3	D	1474	NAG	C4-C5-C6-O6
3	D	1474	NAG	O5-C5-C6-O6
3	A	1480	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1474	NAG	1	0
3	A	1480	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1332:THR	C	1333:9AT	N	1.84

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	388/432 (89%)	-0.29	4 (1%) 79 84	8, 17, 39, 51	8 (2%)
1	D	395/432 (91%)	0.11	21 (5%) 32 37	9, 22, 44, 65	5 (1%)
2	B	36/37 (97%)	-0.28	0 100 100	10, 20, 33, 37	0
2	E	36/37 (97%)	0.58	1 (2%) 55 62	14, 30, 45, 46	0
All	All	855/938 (91%)	-0.07	26 (3%) 52 59	8, 20, 43, 65	13 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	473	ALA	6.5
1	D	449	VAL	5.6
1	D	429	PRO	4.9
1	A	68	SER	4.3
1	D	69	GLY	3.9
1	D	472	THR	3.5
1	D	76	VAL	3.4
1	A	426	PRO	2.8
1	D	471	CYS	2.8
1	D	451	ALA	2.7
1	D	352	ASP	2.5
1	D	442	ASP	2.5
1	D	345	THR	2.5
1	D	452	CYS	2.5
1	A	430	GLU	2.4
1	D	441	PRO	2.4
1	D	448	ASP	2.3
1	D	77	GLU	2.3
1	D	132	PRO	2.2
1	A	250	ASP	2.2
1	D	447	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	70	ASN	2.2
1	D	435	CYS	2.2
1	D	357	HIS	2.1
1	D	74	ALA	2.1
2	E	1331	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	9AT	B	1333	8/8	0.79	0.16	42,44,45,45	0

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
4	BO3	D	1475	4/4	0.81	0.11	41,42,42,43	0
4	BO3	D	1476	4/4	0.83	0.16	44,45,45,48	0
3	NAG	D	1474	14/15	0.90	0.08	22,29,33,36	0
3	NAG	A	1480	14/15	0.92	0.09	17,21,29,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.