



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 AM GMT

PDB ID : 2Y8T
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

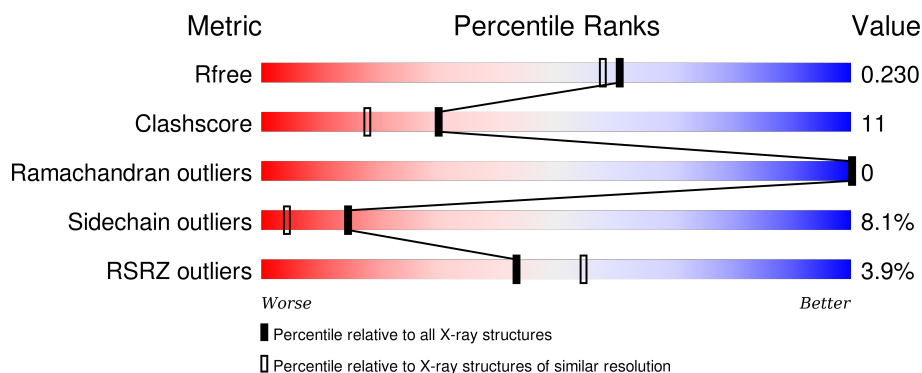
1 Overall quality at a glance

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>73% 13% • • 10%</div> </div>
1	D	432	<div> <div>4%</div> <div>69% 17% • • 9%</div> </div>
2	B	37	<div> <div>70% 19% 8% •</div> </div>
2	E	37	<div> <div>5%</div> <div>59% 32% 5% •</div> </div>

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			

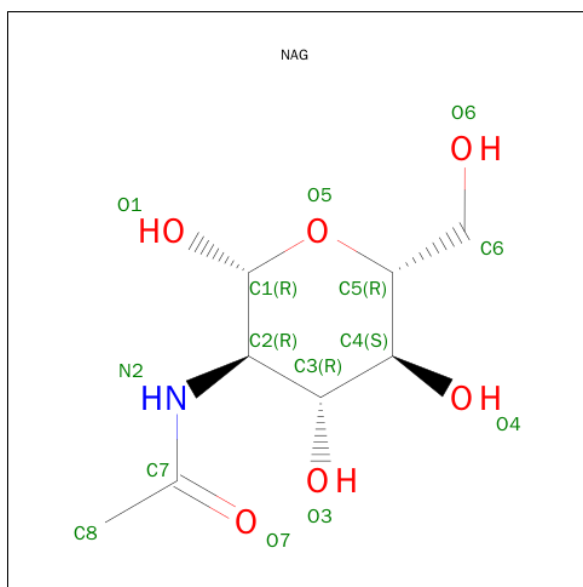
There are 22 discrepancies between the modelled and reference sequences:

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.

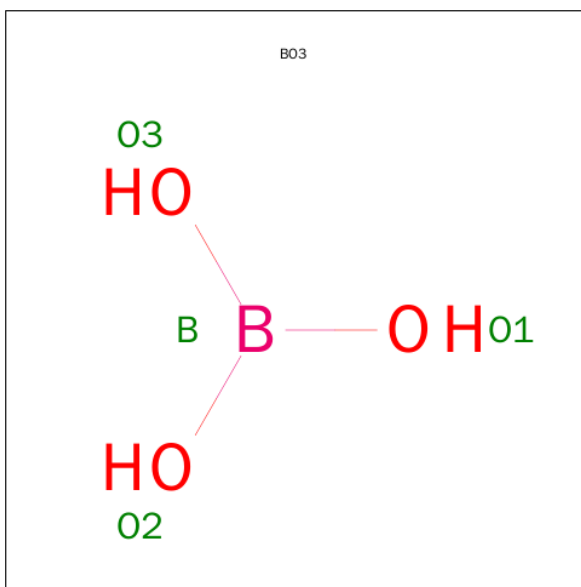
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	37	Total	C	N	O	S	0	0	0
			260	160	44	53	3			
2	E	36	Total	C	N	O	S	0	0	0
			252	156	42	51	3			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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 (three-letter code: 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

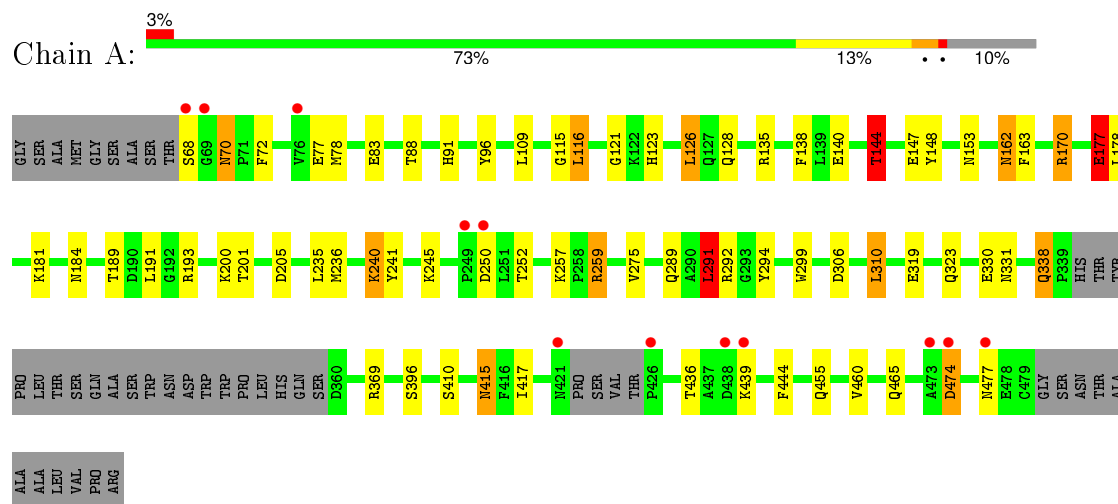
- Molecule 5 is water.

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

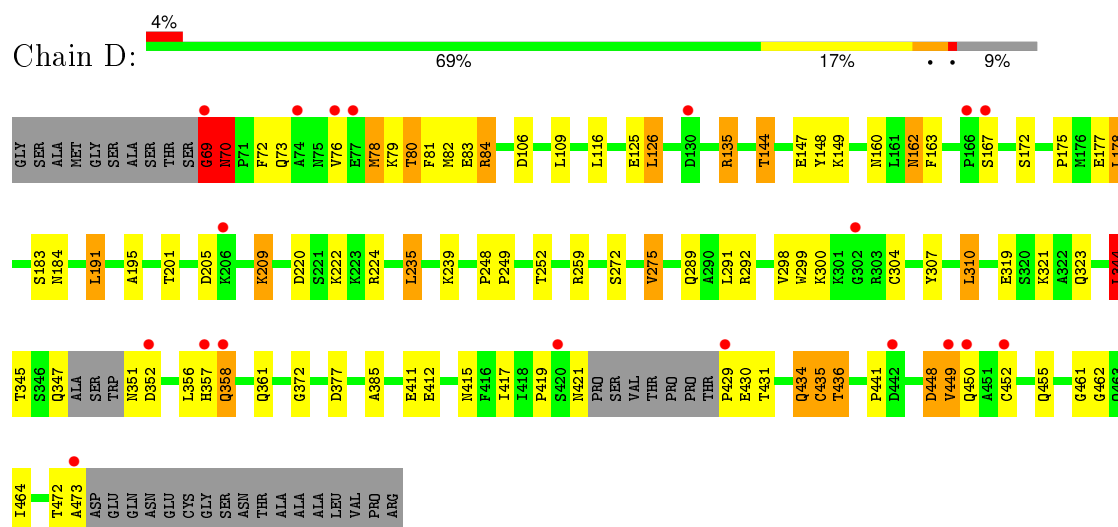
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: APICAL MEMBRANE ANTIGEN, PUTATIVE

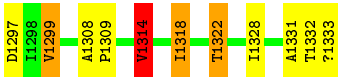


• Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



• Molecule 2: RHOPTRY NECK PROTEIN 2





● 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	69.86 Å 96.38 Å 78.35 Å 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) 100.0 (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 1.95 Å)	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 (5.34%)	DCC
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 , 52.2	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 68139 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.97	1/3152 (0.0%)	0.95	12/4267 (0.3%)
1	D	0.89	2/3200 (0.1%)	0.94	11/4339 (0.3%)
2	B	0.95	0/255	1.14	1/349 (0.3%)
2	E	0.78	0/255	0.92	1/349 (0.3%)
All	All	0.93	3/6862 (0.0%)	0.95	25/9304 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	435	CYS	CB-SG	-10.96	1.63	1.82
1	A	177	GLU	CB-CG	6.25	1.64	1.52
1	D	125	GLU	CG-CD	5.05	1.59	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	LEU	CA-CB-CG	8.60	135.09	115.30
1	A	236	MET	CA-CB-CG	-7.61	100.37	113.30
2	B	1314	VAL	CG1-CB-CG2	7.51	122.92	110.90
1	D	275	VAL	CG1-CB-CG2	7.38	122.71	110.90
1	A	116	LEU	CB-CG-CD1	6.81	122.57	111.00
1	D	235	LEU	CA-CB-CG	6.78	130.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	LEU	CB-CG-CD2	6.77	122.50	111.00
1	A	205	ASP	CB-CG-OD1	6.56	124.21	118.30
1	A	126	LEU	CB-CG-CD1	6.42	121.92	111.00
1	D	126	LEU	CB-CG-CD2	6.19	121.52	111.00
1	D	435	CYS	N-CA-CB	-5.97	99.85	110.60
1	D	344	LEU	CB-CG-CD1	5.95	121.11	111.00
1	A	275	VAL	CG1-CB-CG2	5.85	120.27	110.90
2	E	1315	THR	CB-CA-C	-5.85	95.81	111.60
1	A	170	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	144	THR	N-CA-CB	-5.74	99.39	110.30
1	A	306	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	126	LEU	CB-CG-CD1	5.54	120.42	111.00
1	D	69	GLY	N-CA-C	-5.46	99.44	113.10
1	A	275	VAL	CA-CB-CG1	5.45	119.08	110.90
1	D	235	LEU	CB-CG-CD1	5.16	119.78	111.00
1	D	191	LEU	CB-CG-CD2	5.15	119.76	111.00
1	A	306	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	70	ASN	C-N-CD	5.13	139.17	128.40
1	A	310	LEU	CB-CG-CD1	5.04	119.57	111.00

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 [i](#)

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	52	0
1	D	3117	0	2959	84	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	6	0	0
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	146	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 (146) 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	1.35
2:B:1332:THR:C	2:B:1333:9AT:N	1.84	1.29
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:N	1:A:177:GLU:OE1	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:72:PHE:HA	1:D:78:MET:HG2	1.65	0.78
1:D:357:HIS:C	1:D:358:GLN:HG2	2.05	0.77
1:A:177:GLU:CD	1:A:177:GLU:H	1.86	0.74
1:A:259[B]:ARG:HH11	1:A:330:GLU:CD	1.93	0.70
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:435:CYS:HB3	1:D:462:GLY:C	2.13	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:N	1:D:450:GLN:OE1	2.25	0.62
2:B:1332:THR:C	2:B:1333:9AT:HN1	1.93	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: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
2:B:1332:THR:CA	2:B:1333:9AT:N	2.65	0.57
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:D:78:MET:HE1	1:D:464:ILE:HD13	1.86	0.56
1:A:410:SER:OG	1:D:412:GLU:OE1	2.17	0.56
1:D:448:ASP:C	1:D:448:ASP:OD1	2.43	0.56
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
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:357:HIS:O	1:D:358:GLN:HG2	2.09	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:448:ASP:O	1:D:448:ASP:OD1	2.29	0.51
5:A:2141:HOH:O	1:D:415:ASN:HB3	2.10	0.51
1:D:472:THR:OG1	1:D:473:ALA:N	2.44	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: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
2:E:1309:PRO:HB2	2:E:1311:VAL:HG23	1.93	0.49
1:D:72:PHE:HB3	1:D:82:MET:HG3	1.94	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
2:E:1308:ALA:HB1	2:E:1309:PRO:CD	2.38	0.47
1:D:79:LYS:NZ	5:D:2005:HOH:O	2.47	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:D:377:ASP:C	1:D:377:ASP:OD1	2.52	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
1:D:431:THR:O	1:D:434:GLN:HG2	2.16	0.46
5:A:2279:HOH:O	1:D:222:LYS:HD2	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:201:THR:HG22	2:E:1314:VAL:CG1	2.44	0.45
1:A:259[B]:ARG:NH1	1:A:330:GLU:CD	2.66	0.45
1:A:128:GLN:O	1:A:245:LYS:HD3	2.15	0.45
1:A:460:VAL:CG2	1:A:465:GLN:HG3	2.46	0.45
1:A:240:LYS:HG2	1:A:241:TYR:CE2	2.51	0.45
1:D:298:VAL:HG23	1:D:298:VAL:O	2.16	0.45
1:D:78:MET:CE	1:D:464:ILE:HD13	2.47	0.45
1:D:436:THR:HG22	5:D:2222:HOH:O	2.16	0.45
1:A:70:ASN:C	1:A:70:ASN:HD22	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:344:LEU:O	1:D:344:LEU:HD13	2.18	0.44
1:D:272:SER:O	1:D:275:VAL:HG13	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:177:GLU:H	1:D:177:GLU:CD	2.22	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:D:304:CYS:H	1:D:455:GLN:NE2	2.18	0.42
1:D:160:ASN:ND2	1:D:172:SER:OG	2.44	0.42
1:A:415:ASN:HD22	1:A:415:ASN:N	2.16	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:HE3	1:D:209:LYS:HA	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:220:ASP:C	1:D:220:ASP:OD1	2.59	0.41
1:D:347:GLN:HE21	1:D:347:GLN:HB2	1.76	0.41
1:D:344:LEU:O	1:D:344:LEU:CD1	2.69	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:D:345:THR:HG23	1:D:347:GLN:N	2.37	0.40
1:A:163:PHE:HB2	2:B:1322:THR:HG23	2.03	0.40
1:A:444:PHE:HA	1:A:455:GLN:O	2.22	0.40
1:A:291:LEU:HD13	1:A:294:TYR:HB2	2.03	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%)	23	8
1	D	344/372 (92%)	314 (91%)	30 (9%)	13	3
2	B	28/28 (100%)	24 (86%)	4 (14%)	4	1
2	E	28/28 (100%)	22 (79%)	6 (21%)	1	0
All	All	740/800 (92%)	679 (92%)	61 (8%)	15	4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	GLU
1	A	109	LEU
1	A	116	LEU
1	A	126	LEU
1	A	138	PHE
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	240	LYS
1	A	250	ASP
1	A	259[A]	ARG
1	A	259[B]	ARG
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	259	ARG

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Mol	Chain	Res	Type
1	D	291	LEU
1	D	300	LYS
1	D	310	LEU
1	D	344	LEU
1	D	352	ASP
1	D	356	LEU
1	D	358	GLN
1	D	419	PRO
1	D	421	ASN
1	D	436	THR
1	D	448	ASP
1	D	449	VAL
2	E	1297	ASP
2	E	1299	VAL
2	E	1312	SER
2	E	1315	THR
2	E	1322	THR
2	E	1330	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	92	GLN
1	A	101	GLN
1	A	123	HIS
1	A	153	ASN
1	A	160	ASN
1	A	162	ASN
1	A	184	ASN
1	A	208	ASN
1	A	323	GLN
1	A	338	GLN
1	A	415	ASN
1	A	463	GLN
1	D	92	GLN
1	D	101	GLN
1	D	153	ASN
1	D	160	ASN
1	D	162	ASN
1	D	207	ASN
1	D	289	GLN

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Mol	Chain	Res	Type
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	-	6,7,7	0.38	0	5,9,9	1.63	1 (20%)

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	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1333	9AT	CG2-CB-CA	-2.65	108.63	112.53

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 carbohydrates 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	A	1480	1	14,14,15	0.70	0	15,19,21	1.89	6 (40%)
3	NAG	D	1474	1	14,14,15	0.47	0	15,19,21	1.17	1 (6%)
4	BO3	D	1475	-	3,3,3	7.92	3 (100%)	3,3,3	0.92	0
4	BO3	D	1476	-	3,3,3	7.86	3 (100%)	3,3,3	0.28	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	A	1480	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1474	1	-	0/6/23/26	0/1/1/1
4	BO3	D	1475	-	-	0/0/0/0	0/0/0/0
4	BO3	D	1476	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1475	BO3	B-O2	7.30	1.52	1.36
4	D	1476	BO3	B-O2	7.72	1.53	1.36
4	D	1476	BO3	B-O1	7.75	1.53	1.36
4	D	1475	BO3	B-O1	8.00	1.53	1.36
4	D	1476	BO3	B-O3	8.11	1.54	1.36
4	D	1475	BO3	B-O3	8.41	1.54	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	NAG	O7-C7-C8	-2.64	117.22	122.06
3	A	1480	NAG	C6-C5-C4	-2.53	106.78	113.02
3	A	1480	NAG	C3-C2-N2	-2.32	105.00	110.56
3	A	1480	NAG	O3-C3-C2	-2.30	104.56	109.11
3	D	1474	NAG	O5-C5-C6	2.27	112.26	107.35
3	A	1480	NAG	O5-C5-C6	2.39	112.53	107.35
3	A	1480	NAG	C8-C7-N2	3.72	123.23	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1480	NAG	1	0
3	D	1474	NAG	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	388/432 (89%)	-0.08	12 (3%)	52	62	8, 17, 39, 51	5 (1%)
1	D	395/432 (91%)	0.17	19 (4%)	34	45	9, 22, 44, 65	5 (1%)
2	B	36/37 (97%)	-0.23	0	100	100	10, 20, 33, 37	0
2	E	36/37 (97%)	0.62	2 (5%)	28	39	14, 30, 45, 46	0
All	All	855/938 (91%)	0.06	33 (3%)	43	54	8, 20, 43, 65	10 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	6.6
1	D	450	GLN	3.8
2	E	1331	ALA	3.7
1	D	76	VAL	3.6
1	D	473	ALA	3.4
1	D	74	ALA	3.3
1	D	449	VAL	3.3
1	A	250	ASP	3.2
1	A	439	LYS	3.2
1	A	421	ASN	3.2
1	A	438	ASP	3.1
1	D	77	GLU	2.9
1	A	76	VAL	2.9
1	D	358	GLN	2.8
1	A	473	ALA	2.7
1	D	357	HIS	2.7
1	D	352	ASP	2.6
1	D	166	PRO	2.5
1	D	69	GLY	2.4
1	A	426	PRO	2.4
1	D	429	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	420	SER	2.3
1	D	442	ASP	2.3
1	D	302	GLY	2.3
1	A	69	GLY	2.2
2	E	1332	THR	2.2
1	D	167	SER	2.2
1	A	477	ASN	2.1
1	A	474	ASP	2.1
1	D	452	CYS	2.1
1	A	249	PRO	2.1
1	D	130	ASP	2.0
1	D	206	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	9AT	B	1333	8/8	0.84	0.18	-	42,44,45,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1480	14/15	0.94	0.13	0.89	17,21,29,36	0
3	NAG	D	1474	14/15	0.93	0.09	-0.52	22,29,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BO3	D	1476	4/4	0.82	0.12	-	44,45,45,48	0
4	BO3	D	1475	4/4	0.87	0.12	-	41,42,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.