



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:44 am GMT

PDB ID : 2Y8S  
Title : CO-STRUCTURE OF AN AMA1 MUTANT (Y230A) 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 : 2.55 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

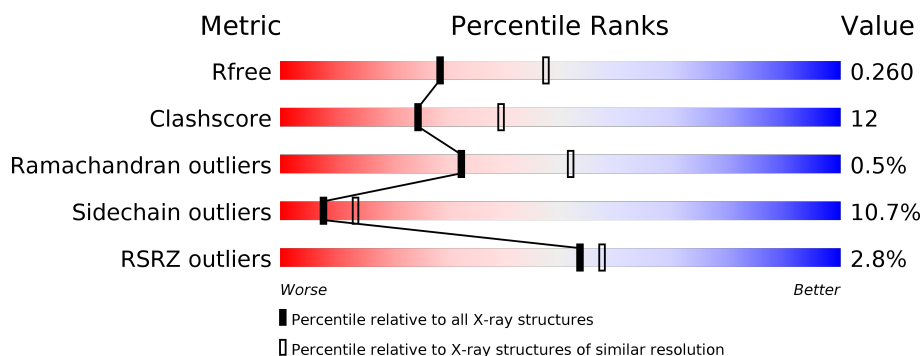
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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  $\geq 3$ , 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>0%</div> <div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	432	<div> <div>3%</div> <div> <div>63%</div> <div>23%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	37	<div> <div>5%</div> <div> <div>62%</div> <div>27%</div> <div>8%</div> <div>•</div> </div> </div>
2	E	37	<div> <div>8%</div> <div> <div>68%</div> <div>24%</div> <div>•</div> <div>5%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BO3	A	1481	-	X	-	-
4	BO3	A	1482	-	X	-	X
5	GOL	A	1484	-	-	X	X
5	GOL	D	1475	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6862 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	386	Total	C	N	O	S	0	0	0
			3023	1894	517	590	22			
1	D	391	Total	C	N	O	S	0	0	0
			3077	1937	527	592	21			

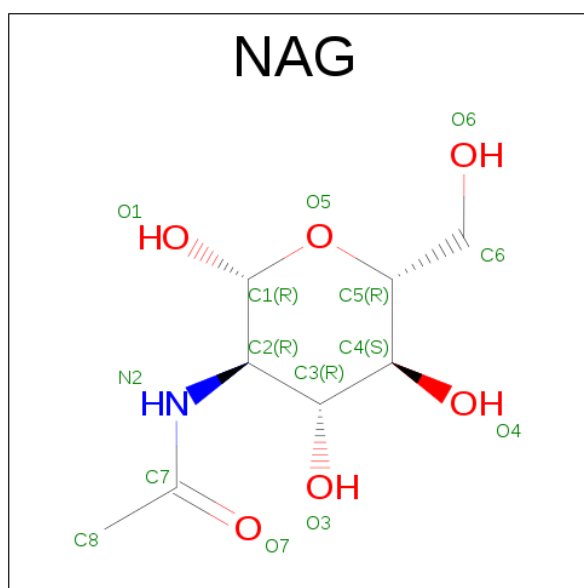
There are 24 discrepancies between the modelled and reference sequences:

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
A	230	ALA	TYR	ENGINEERED MUTATION	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
D	230	ALA	TYR	ENGINEERED MUTATION	UNP B9QC59

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

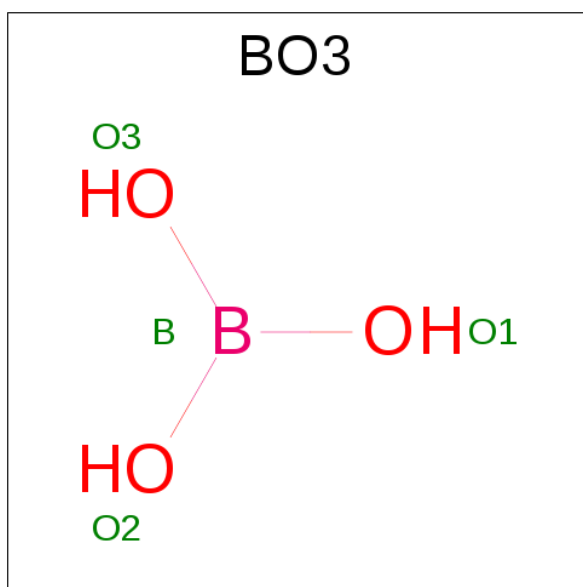
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	0	0	0
			252	156	42	51	3			
2	E	35	Total	C	N	O	S	0	0	0
			245	152	41	49	3			

- 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	A	1	Total	B	O	0	0
			4	1	3		
4	A	1	Total	B	O	0	0
			4	1	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

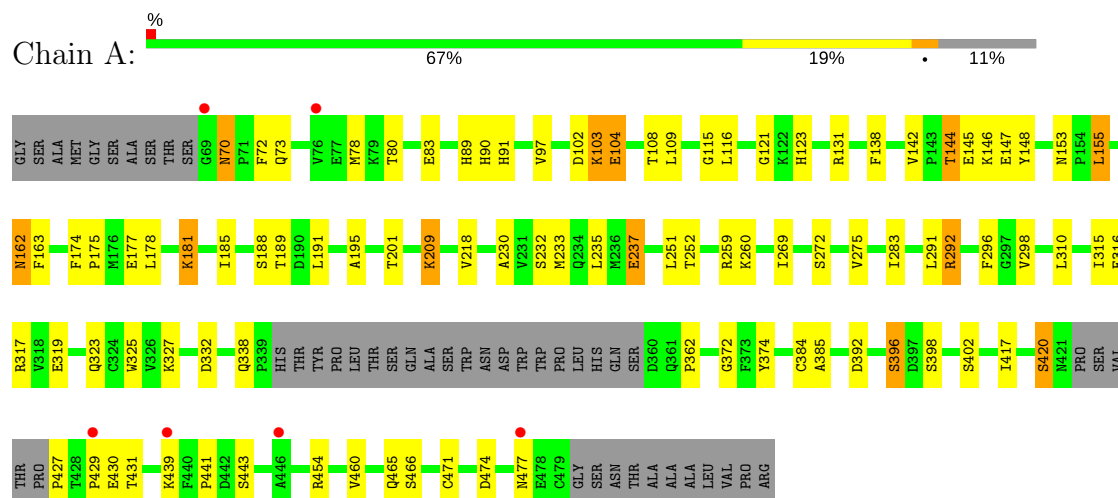
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	103	Total	O	0	0
			103	103		
6	B	13	Total	O	0	0
			13	13		
6	D	90	Total	O	0	0
			90	90		
6	E	5	Total	O	0	0
			5	5		

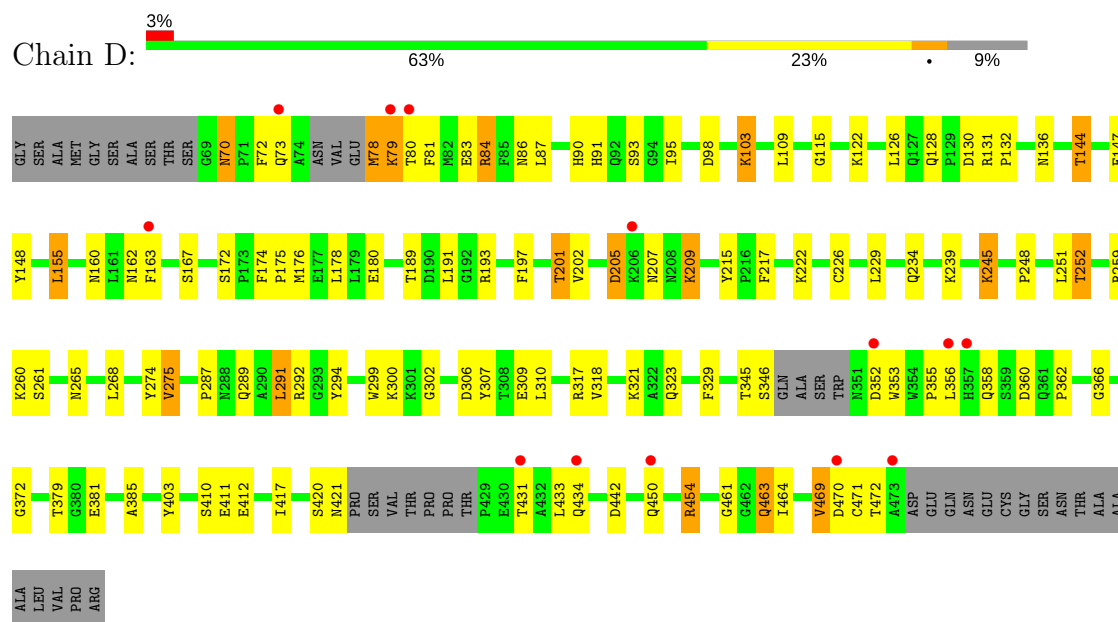
### 3 Residue-property plots [i](#)

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



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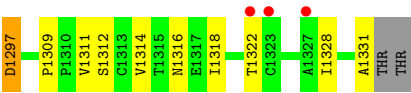


#### • Molecule 2: RHOPTRY NECK PROTEIN 2





● 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, $\alpha$ , $\beta$ , $\gamma$	70.52Å 96.83Å 78.33Å 90.00° 116.75° 90.00°	Depositor
Resolution (Å)	56.70 – 2.55 56.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.70-2.55) 99.9 (56.70-2.55)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.263 0.184 , 0.260	Depositor DCC
$R_{free}$ test set	1548 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.80	0/3097	0.79	0/4194
1	D	0.77	1/3158 (0.0%)	0.81	0/4280
2	B	0.86	0/255	0.87	0/349
2	E	0.65	0/248	0.67	0/339
All	All	0.78	1/6758 (0.0%)	0.80	0/9162

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	226	CYS	CB-SG	-5.15	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3023	0	2873	70	0
1	D	3077	0	2925	83	0
2	B	252	0	250	18	0
2	E	245	0	243	13	0
3	A	14	0	13	1	0
3	D	14	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	6	0	0
5	A	12	0	16	4	0
5	D	6	0	8	0	0
6	A	103	0	0	0	0
6	B	13	0	0	0	0
6	D	90	0	0	1	0
6	E	5	0	0	0	0
All	All	6862	0	6347	160	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 12.

All (160) 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:144:THR:HG22	1:A:147:GLU:H	1.26	1.01
1:D:163:PHE:HB3	2:E:1322:THR:HG22	1.46	0.92
1:D:84:ARG:HG2	1:D:84:ARG:HH11	1.39	0.87
1:D:83:GLU:OE2	3:D:1474:NAG:H83	1.76	0.85
1:D:70:ASN:HD22	1:D:72:PHE:H	1.25	0.85
2:E:1309:PRO:HB2	2:E:1311:VAL:HG13	1.59	0.84
1:D:98:ASP:H	1:D:234:GLN:HE22	1.25	0.83
1:A:327:LYS:HZ2	5:A:1484:GOL:H2	1.44	0.80
1:D:163:PHE:CB	2:E:1322:THR:HG22	2.13	0.78
1:A:177:GLU:CD	1:A:177:GLU:H	1.88	0.77
1:D:470:ASP:OD1	1:D:470:ASP:O	2.02	0.75
1:A:327:LYS:HG2	5:A:1484:GOL:H12	1.70	0.74
1:D:292:ARG:HG3	1:D:411:GLU:OE1	1.89	0.73
1:A:185:ILE:HD11	2:B:1318:ILE:CD1	2.19	0.73
1:A:319:GLU:H	1:A:323:GLN:NE2	1.88	0.72
1:A:235:LEU:HD23	1:A:338:GLN:HG2	1.72	0.71
1:D:176:MET:HE1	1:D:193:ARG:HD2	1.72	0.71
1:A:72:PHE:HA	1:A:78:MET:HG2	1.73	0.70
1:D:70:ASN:ND2	1:D:72:PHE:H	1.88	0.70
1:A:319:GLU:H	1:A:323:GLN:HE22	1.40	0.69
2:B:1332:THR:HG22	2:B:1332:THR:O	1.92	0.69
1:D:197:PHE:O	1:D:201:THR:HG22	1.92	0.69
1:A:201:THR:CG2	2:B:1314:VAL:HG11	2.24	0.68
1:D:98:ASP:H	1:D:234:GLN:NE2	1.92	0.67
1:A:439:LYS:O	1:A:441:PRO:HD3	1.95	0.66
1:D:163:PHE:HB3	2:E:1322:THR:CG2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:OE2	3:A:1480:NAG:H83	1.95	0.66
1:D:176:MET:CE	1:D:193:ARG:HD2	2.26	0.66
1:A:327:LYS:NZ	5:A:1484:GOL:H2	2.10	0.66
1:A:153:ASN:HB3	1:A:251:LEU:O	1.97	0.65
1:A:396:SER:HB2	1:A:466:SER:H	1.63	0.63
1:A:144:THR:HB	1:A:147:GLU:OE1	2.01	0.60
2:E:1309:PRO:HB2	2:E:1311:VAL:CG1	2.32	0.59
1:D:205:ASP:HB2	1:D:209:LYS:H	1.67	0.59
1:D:379:THR:OG1	1:D:381:GLU:HG3	2.03	0.59
1:A:323:GLN:O	1:A:327:LYS:HG3	2.03	0.59
1:D:122:LYS:NZ	1:D:234:GLN:HE21	2.01	0.58
1:D:252:THR:HG21	2:E:1331:ALA:HB3	1.85	0.58
1:D:355:PRO:HG3	1:D:360:ASP:HB2	1.85	0.58
1:D:90:HIS:HB2	6:D:2048:HOH:O	2.04	0.58
1:D:215:TYR:HB3	1:D:229:LEU:O	2.04	0.58
1:A:474:ASP:OD1	1:A:474:ASP:N	2.36	0.58
1:A:185:ILE:HD11	2:B:1318:ILE:HD11	1.85	0.57
1:A:454:ARG:HD3	1:A:471:CYS:HA	1.86	0.57
1:D:103:LYS:NZ	1:D:274:TYR:OH	2.37	0.57
1:A:70:ASN:C	1:A:70:ASN:HD22	2.07	0.56
1:A:189:THR:HB	1:A:417:ILE:HA	1.85	0.56
1:A:185:ILE:CD1	2:B:1318:ILE:HD11	2.36	0.56
1:D:345:THR:HG23	1:D:346:SER:N	2.20	0.56
1:D:84:ARG:HG2	1:D:84:ARG:NH1	2.16	0.56
1:A:201:THR:CG2	2:B:1314:VAL:CG1	2.84	0.55
1:D:205:ASP:HB3	1:D:207:ASN:H	1.69	0.55
1:D:155:LEU:HD22	1:D:252:THR:HG22	1.88	0.55
1:A:102:ASP:O	1:A:103:LYS:HD2	2.07	0.55
1:A:162:ASN:HD22	1:A:162:ASN:H	1.55	0.55
2:B:1315:THR:HG23	2:B:1321:VAL:HG22	1.90	0.54
1:D:122:LYS:HZ3	1:D:234:GLN:HE21	1.56	0.54
1:D:291:LEU:HD13	1:D:294:TYR:HB2	1.89	0.54
1:A:148:TYR:OH	1:A:153:ASN:ND2	2.39	0.53
1:D:454:ARG:NH1	1:D:470:ASP:OD1	2.42	0.52
1:A:121:GLY:O	1:A:123:HIS:HD2	1.92	0.52
1:D:81:PHE:O	1:D:84:ARG:HG2	2.09	0.52
1:A:70:ASN:ND2	1:A:72:PHE:H	2.08	0.52
1:D:87:LEU:HD13	1:D:95:ILE:CD1	2.40	0.52
1:A:260:LYS:HD3	1:A:325:TRP:CZ2	2.45	0.52
1:A:155:LEU:HD22	1:A:252:THR:HG22	1.92	0.51
1:A:163:PHE:HB3	2:B:1322:THR:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG11	1:A:230:ALA:HB3	1.93	0.51
1:D:454:ARG:HG2	1:D:471:CYS:HA	1.93	0.51
1:A:145:GLU:HA	1:A:145:GLU:OE1	2.10	0.51
1:A:181:LYS:HD3	1:A:181:LYS:O	2.10	0.51
1:A:372:GLY:HA2	1:A:385:ALA:O	2.10	0.50
1:A:89:HIS:HD2	1:A:90:HIS:CE1	2.29	0.50
1:D:128:GLN:HB2	1:D:136:ASN:OD1	2.12	0.50
1:A:460:VAL:HB	1:A:465:GLN:HG3	1.93	0.49
1:A:97:VAL:HG11	1:A:338:GLN:HE21	1.77	0.49
1:D:163:PHE:CB	2:E:1322:THR:CG2	2.87	0.49
1:A:292:ARG:HG3	1:D:292:ARG:NH1	2.27	0.49
1:D:72:PHE:HA	1:D:78:MET:HE1	1.93	0.49
1:D:83:GLU:OE2	3:D:1474:NAG:C8	2.55	0.49
1:A:201:THR:HG22	2:B:1314:VAL:HG11	1.95	0.49
1:D:420:SER:O	1:D:421:ASN:OD1	2.30	0.49
1:D:144:THR:HG22	1:D:147:GLU:H	1.77	0.48
1:A:163:PHE:CB	2:B:1322:THR:HG23	2.43	0.48
1:D:130:ASP:OD2	1:D:245:LYS:HE3	2.13	0.48
1:D:289:GLN:HE22	1:D:417:ILE:HD11	1.79	0.48
2:B:1297:ASP:OD2	2:B:1299:VAL:HG13	2.14	0.48
1:D:93:SER:O	1:D:366:GLY:HA2	2.14	0.48
1:D:372:GLY:HA2	1:D:385:ALA:O	2.14	0.47
1:A:201:THR:HG22	2:B:1314:VAL:CG1	2.43	0.47
1:D:454:ARG:NH2	1:D:472:THR:HG22	2.30	0.47
1:A:145:GLU:OE1	2:B:1329:ALA:HA	2.14	0.47
1:D:292:ARG:HG3	1:D:411:GLU:CD	2.34	0.47
1:D:248:PRO:HG2	1:D:251:LEU:CD1	2.44	0.47
1:A:218:VAL:HA	1:A:269:ILE:O	2.15	0.46
1:D:454:ARG:HD2	1:D:469:VAL:HG12	1.98	0.46
1:A:91:HIS:CE1	1:A:115:GLY:HA3	2.51	0.46
1:D:201:THR:HB	2:E:1316:ASN:HD22	1.80	0.46
1:A:175:PRO:CB	1:A:177:GLU:OE1	2.64	0.46
1:D:248:PRO:HG2	1:D:251:LEU:HD12	1.98	0.46
1:D:84:ARG:HD3	1:D:287:PRO:HA	1.97	0.46
1:A:298:VAL:HA	1:A:392:ASP:OD1	2.16	0.46
1:D:176:MET:O	1:D:180:GLU:HG2	2.17	0.45
1:D:433:LEU:O	1:D:463:GLN:HG3	2.16	0.45
1:D:217:PHE:HE1	1:D:275:VAL:HG13	1.81	0.45
1:D:201:THR:OG1	2:E:1314:VAL:HG11	2.16	0.45
1:A:174:PHE:HA	1:A:175:PRO:HD3	1.85	0.45
1:D:160:ASN:ND2	1:D:172:SER:OG	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:CE2	1:A:402:SER:HB3	2.52	0.45
1:D:454:ARG:HH22	1:D:472:THR:HG22	1.81	0.45
1:A:427:PRO:HB2	1:A:429:PRO:HD3	1.98	0.44
1:A:89:HIS:CD2	1:A:90:HIS:CE1	3.04	0.44
1:D:372:GLY:CA	1:D:385:ALA:O	2.65	0.44
1:D:189:THR:HB	1:D:417:ILE:HA	1.99	0.44
2:E:1297:ASP:C	2:E:1297:ASP:OD1	2.56	0.44
1:D:189:THR:O	1:D:193:ARG:HG3	2.17	0.44
1:D:78:MET:O	1:D:81:PHE:HB3	2.18	0.44
1:D:174:PHE:HA	1:D:175:PRO:HD3	1.83	0.44
1:A:315:ILE:HA	1:A:384:CYS:O	2.18	0.44
1:A:195:ALA:HB1	1:A:275:VAL:HG22	1.99	0.43
1:A:474:ASP:O	1:A:477:ASN:HB2	2.18	0.43
1:A:195:ALA:CB	1:A:275:VAL:HG22	2.47	0.43
1:D:433:LEU:O	1:D:464:ILE:HG13	2.19	0.43
1:D:176:MET:CE	1:D:193:ARG:CD	2.94	0.43
1:D:265:ASN:HB3	1:D:268:LEU:HD12	2.00	0.43
1:A:272:SER:O	1:A:275:VAL:HG13	2.19	0.43
1:A:374:TYR:OH	1:D:461:GLY:HA3	2.19	0.43
1:A:292:ARG:NH2	1:A:398:SER:HB2	2.34	0.43
1:D:70:ASN:HD21	1:D:72:PHE:HB2	1.84	0.43
1:D:299:TRP:CZ2	1:D:302:GLY:O	2.72	0.43
1:D:84:ARG:HH11	1:D:84:ARG:CG	2.18	0.42
2:E:1309:PRO:C	2:E:1311:VAL:H	2.22	0.42
1:A:283:ILE:HG22	1:A:427:PRO:HB3	2.01	0.42
1:A:327:LYS:HZ2	5:A:1484:GOL:C2	2.24	0.42
1:D:148:TYR:CE2	2:E:1331:ALA:HB2	2.54	0.42
1:A:233:MET:HG2	2:B:1305:ILE:O	2.19	0.42
1:D:91:HIS:CE1	1:D:115:GLY:HA3	2.55	0.42
1:A:201:THR:HG23	2:B:1314:VAL:CG1	2.49	0.42
1:A:70:ASN:C	1:A:70:ASN:ND2	2.72	0.42
1:A:209:LYS:HA	1:A:209:LYS:HD2	1.91	0.42
1:D:79:LYS:HG2	1:D:80:THR:N	2.35	0.42
1:D:84:ARG:NH1	1:D:84:ARG:CG	2.80	0.42
1:D:86:ASN:HD22	3:D:1474:NAG:H83	1.85	0.41
2:B:1313:CYS:HA	2:B:1322:THR:O	2.20	0.41
1:D:202:VAL:O	2:E:1314:VAL:HG13	2.21	0.41
1:D:318:VAL:HG12	1:D:323:GLN:HG3	2.01	0.41
2:B:1314:VAL:HB	2:B:1322:THR:HG22	2.03	0.41
1:D:176:MET:CE	1:D:193:ARG:HB2	2.50	0.41
1:D:307:TYR:C	1:D:309:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LYS:HD2	1:D:329:PHE:CG	2.56	0.41
1:A:144:THR:HG22	1:A:147:GLU:N	2.11	0.41
1:A:235:LEU:HD11	1:A:237:GLU:CG	2.51	0.41
1:D:131:ARG:O	1:D:132:PRO:C	2.59	0.41
1:D:352:ASP:HB3	1:D:353:TRP:CD1	2.56	0.41
1:D:321:LYS:HB3	1:D:403:TYR:OH	2.22	0.40
1:D:360:ASP:OD1	1:D:362:PRO:HD3	2.21	0.40
1:A:163:PHE:CE1	2:B:1324:ALA:HB2	2.56	0.40
1:A:70:ASN:HD21	1:A:72:PHE:HB2	1.86	0.40
1:D:81:PHE:CZ	1:D:433:LEU:HD11	2.56	0.40
1:A:104:GLU:HA	1:A:108:THR:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/432 (88%)	360 (95%)	19 (5%)	1 (0%)	44	64
1	D	383/432 (89%)	359 (94%)	21 (6%)	3 (1%)	22	38
2	B	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
2	E	33/37 (89%)	30 (91%)	3 (9%)	0	100	100
All	All	830/938 (88%)	781 (94%)	45 (5%)	4 (0%)	32	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	GLN
1	D	442	ASP
1	A	420	SER
1	D	205	ASP



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/371 (90%)	301 (90%)	33 (10%)	9	16
1	D	339/371 (91%)	302 (89%)	37 (11%)	7	13
2	B	28/29 (97%)	24 (86%)	4 (14%)	4	6
2	E	27/29 (93%)	23 (85%)	4 (15%)	3	5
All	All	728/800 (91%)	650 (89%)	78 (11%)	8	13

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	73	GLN
1	A	80	THR
1	A	103	LYS
1	A	104	GLU
1	A	109	LEU
1	A	116	LEU
1	A	131	ARG
1	A	138	PHE
1	A	144	THR
1	A	146	LYS
1	A	155	LEU
1	A	162	ASN
1	A	178	LEU
1	A	181	LYS
1	A	188	SER
1	A	191	LEU
1	A	209	LYS
1	A	232	SER
1	A	237	GLU
1	A	259	ARG
1	A	291	LEU
1	A	292	ARG
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	316	GLU
1	A	317	ARG
1	A	332	ASP
1	A	362	PRO
1	A	396	SER
1	A	420	SER
1	A	430	GLU
1	A	431	THR
1	A	443	SER
2	B	1299	VAL
2	B	1311	VAL
2	B	1315	THR
2	B	1322	THR
1	D	70	ASN
1	D	73	GLN
1	D	78	MET
1	D	79	LYS
1	D	84	ARG
1	D	103	LYS
1	D	109	LEU
1	D	126	LEU
1	D	144	THR
1	D	155	LEU
1	D	162	ASN
1	D	167	SER
1	D	178	LEU
1	D	191	LEU
1	D	201	THR
1	D	209	LYS
1	D	222	LYS
1	D	239	LYS
1	D	245	LYS
1	D	252	THR
1	D	259	ARG
1	D	261	SER
1	D	275	VAL
1	D	291	LEU
1	D	300	LYS
1	D	306	ASP
1	D	310	LEU
1	D	317	ARG
1	D	356	LEU

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Mol	Chain	Res	Type
1	D	410	SER
1	D	412	GLU
1	D	431	THR
1	D	434	GLN
1	D	450	GLN
1	D	454	ARG
1	D	463	GLN
1	D	469	VAL
2	E	1297	ASP
2	E	1312	SER
2	E	1318	ILE
2	E	1328	ILE

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	123	HIS
1	A	153	ASN
1	A	160	ASN
1	A	162	ASN
1	A	169	GLN
1	A	208	ASN
1	A	265	ASN
1	A	323	GLN
1	A	338	GLN
1	A	389	GLN
1	A	434	GLN
1	D	70	ASN
1	D	73	GLN
1	D	123	HIS
1	D	153	ASN
1	D	160	ASN
1	D	162	ASN
1	D	207	ASN
1	D	227	HIS
1	D	234	GLN
1	D	289	GLN
1	D	434	GLN
2	E	1300	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	0.57	0	15,19,21	2.40	6 (40%)
4	BO3	A	1481	-	3,3,3	4.85	3 (100%)	3,3,3	0.70	0
4	BO3	A	1482	-	3,3,3	5.14	3 (100%)	3,3,3	0.38	0
5	GOL	A	1483	-	5,5,5	0.40	0	5,5,5	0.39	0
5	GOL	A	1484	-	5,5,5	0.69	0	5,5,5	0.93	0
3	NAG	D	1474	1	14,14,15	0.46	0	15,19,21	1.41	2 (13%)
5	GOL	D	1475	-	5,5,5	0.51	0	5,5,5	0.39	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
4	BO3	A	1481	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BO3	A	1482	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1483	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1484	-	-	0/4/4/4	0/0/0/0
3	NAG	D	1474	1	-	0/6/23/26	0/1/1/1
5	GOL	D	1475	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1481	BO3	B-O2	4.59	1.52	1.36
4	A	1481	BO3	B-O1	4.83	1.52	1.36
4	A	1482	BO3	B-O1	5.00	1.53	1.36
4	A	1482	BO3	B-O3	5.05	1.53	1.36
4	A	1481	BO3	B-O3	5.13	1.54	1.36
4	A	1482	BO3	B-O2	5.37	1.54	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1474	NAG	O5-C1-C2	-3.26	106.94	111.47
3	A	1480	NAG	C4-C3-C2	-2.99	106.64	111.02
3	D	1474	NAG	O7-C7-C8	-2.55	117.42	122.06
3	A	1480	NAG	O7-C7-C8	-2.19	118.07	122.06
3	A	1480	NAG	C3-C4-C5	-2.12	106.49	110.22
3	A	1480	NAG	C2-N2-C7	2.45	126.51	122.94
3	A	1480	NAG	C8-C7-N2	3.23	121.95	116.11
3	A	1480	NAG	C1-O5-C5	6.42	121.01	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1480	NAG	1	0
5	A	1484	GOL	4	0
3	D	1474	NAG	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	386/432 (89%)	0.15	6 (1%) 72 74	10, 25, 60, 76	5 (1%)
1	D	391/432 (90%)	0.31	13 (3%) 47 51	11, 35, 57, 75	5 (1%)
2	B	36/37 (97%)	0.18	2 (5%) 25 27	19, 28, 50, 54	0
2	E	35/37 (94%)	0.99	3 (8%) 11 11	32, 49, 71, 73	0
All	All	848/938 (90%)	0.26	24 (2%) 53 57	10, 30, 59, 76	10 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	HIS	3.9
1	D	352	ASP	3.5
1	A	69	GLY	2.9
1	D	450	GLN	2.9
1	A	439	LYS	2.7
1	D	80	THR	2.6
1	A	477	ASN	2.6
1	A	446	ALA	2.6
1	D	434	GLN	2.6
2	E	1327	ALA	2.6
1	D	206	LYS	2.5
1	D	356	LEU	2.4
1	D	470	ASP	2.4
2	E	1322	THR	2.3
1	D	73	GLN	2.3
1	D	79	LYS	2.2
2	E	1323	CYS	2.2
1	D	473	ALA	2.2
1	A	429	PRO	2.2
1	D	163	PHE	2.2
1	A	76	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1331	ALA	2.1
1	D	431	THR	2.1
2	B	1328	ILE	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	A	1484	6/6	0.81	0.22	8.36	40,42,43,43	0
5	GOL	D	1475	6/6	0.63	0.30	6.65	51,53,54,55	0
4	BO3	A	1482	4/4	0.87	0.29	3.39	40,41,41,42	0
4	BO3	A	1481	4/4	0.94	0.19	0.43	31,33,35,36	0
5	GOL	A	1483	6/6	0.84	0.18	0.33	55,57,58,59	0
3	NAG	A	1480	14/15	0.93	0.16	-0.35	26,38,45,46	0
3	NAG	D	1474	14/15	0.94	0.17	-0.53	38,40,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.