



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:43 AM UTC

PDB ID : 2Y8S / pdb_00002y8s
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

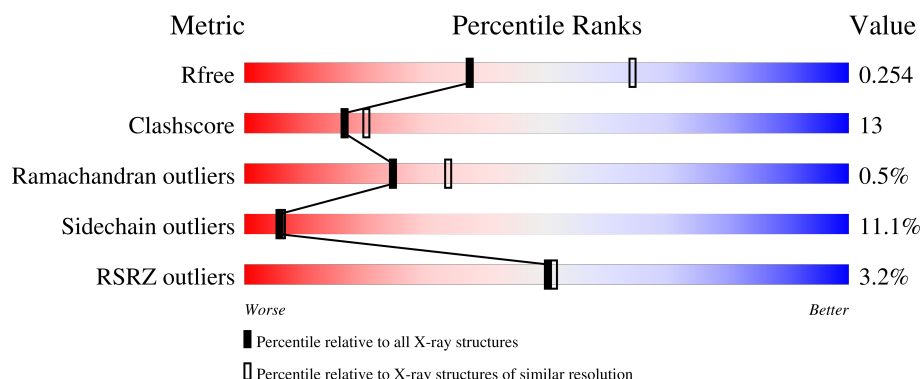
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	2% 67% 19% 11%
1	D	432	3% 61% 25% 9%
2	B	37	5% 54% 32% 8% . .
2	E	37	14% 65% 24% 5% 5%

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
4	BO3	A	1481	-	X	-	-
4	BO3	A	1482	-	X	-	-
5	GOL	A	1484	-	-	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.

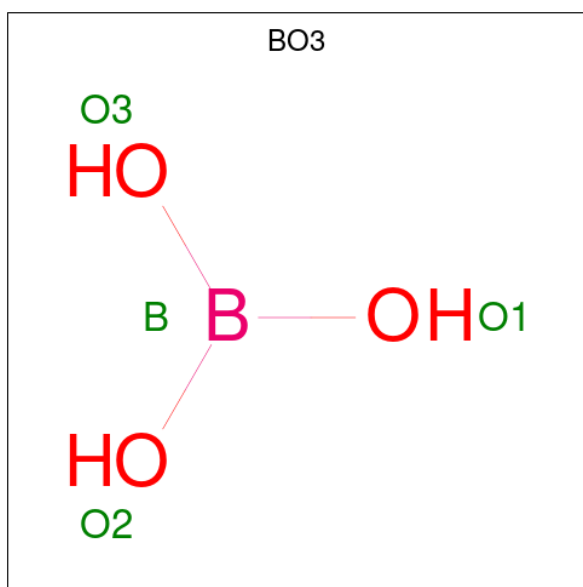
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	0	0	0
			252	156	42	51	3			
2	E	35	Total	C	N	O	S	0	0	0
			245	152	41	49	3			

- Molecule 3 is 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	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 (CCD ID: 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		

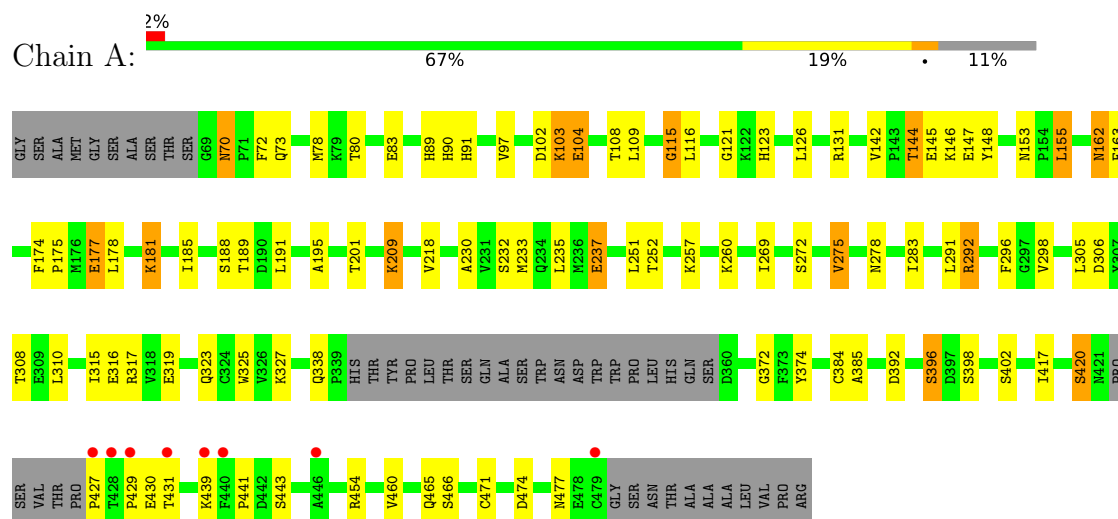
- Molecule 6 is water.

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		

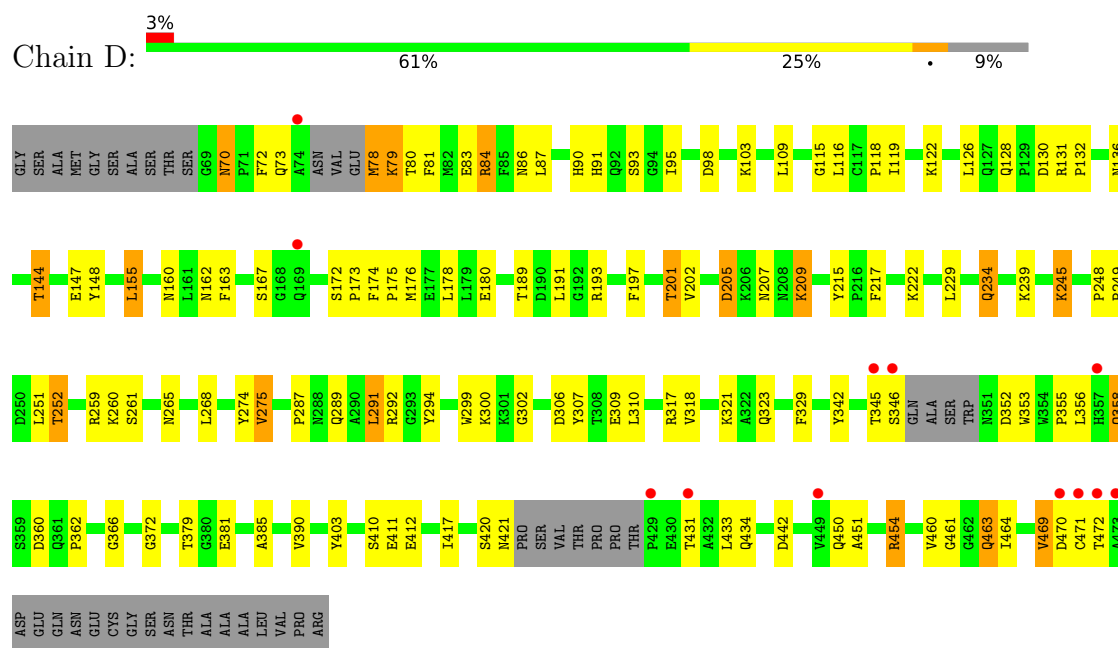
3 Residue-property plots

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.

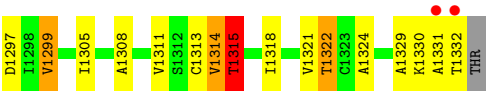
• Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



• 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	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
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.263 (Not available) , 0.254	Depositor DCC
R_{free} test set	1548 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: 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	0.95	0/3097	1.02	4/4194 (0.1%)
1	D	0.91	0/3158	1.08	10/4280 (0.2%)
2	B	1.12	0/255	1.35	4/349 (1.1%)
2	E	0.83	0/248	1.15	0/339
All	All	0.93	0/6758	1.07	18/9162 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1331	ALA	N-CA-C	8.05	118.58	108.19
1	A	257	LYS	N-CA-C	6.55	114.12	108.22
1	D	451	ALA	N-CA-C	-6.11	105.66	113.23
2	B	1308	ALA	CA-C-N	-5.79	114.41	120.38
2	B	1308	ALA	C-N-CA	-5.79	114.41	120.38
1	D	342	TYR	CA-C-N	5.62	125.60	120.03
1	D	342	TYR	C-N-CA	5.62	125.60	120.03
1	A	115	GLY	N-CA-C	5.59	117.90	111.36
1	D	249	PRO	N-CA-C	5.58	121.94	114.18
1	D	234	GLN	N-CA-C	-5.31	107.82	114.56
1	D	358	GLN	N-CA-C	5.29	122.07	110.80
1	A	278	ASN	CA-C-N	5.17	124.83	119.56
1	A	278	ASN	C-N-CA	5.17	124.83	119.56
1	D	317	ARG	CB-CA-C	5.15	118.24	109.80
1	D	342	TYR	N-CA-C	5.11	116.13	109.64
1	D	390	VAL	CA-C-N	-5.05	114.54	119.99
1	D	390	VAL	C-N-CA	-5.05	114.54	119.99
2	B	1315	THR	N-CA-CB	5.04	118.65	110.43

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	3023	0	2873	71	0
1	D	3077	0	2925	89	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
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	167	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 13.

All (167) 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:HH11	1:D:84:ARG:HG2	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
1:A:327:LYS:HZ2	5:A:1484:GOL:H2	1.42	0.84
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:177:GLU:H	1:A:177:GLU:CD	1.88	0.81
1:D:176:MET:HE1	1:D:193:ARG:CB	2.11	0.81
1:D:163:PHE:CB	2:E:1322:THR:HG22	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ASP:O	1:D:470:ASP:OD1	2.02	0.75
1:A:327:LYS:HG2	5:A:1484:GOL:H12	1.70	0.74
1:D:176:MET:HE1	1:D:193:ARG:HB2	1.68	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: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
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:70:ASN:C	1:A:70:ASN:HD22	2.07	0.61
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:90:HIS:HB2	6:D:2048:HOH:O	2.04	0.58
1:D:355:PRO:HG3	1:D:360:ASP:HB2	1.85	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:D:176:MET:HE2	1:D:193:ARG:HD2	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:176:MET:HE1	1:D:193:ARG:HB3	1.89	0.55
2:B:1315:THR:HG23	2:B:1321:VAL:HG22	1.90	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:D:292:ARG:HG3	1:D:411:GLU:CD	2.34	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
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:O	1:A:181:LYS:HD3	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:97:VAL:HG11	1:A:338:GLN:HE21	1.77	0.49
1:A:460:VAL:HB	1:A:465:GLN:HG3	1.93	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:83:GLU:OE2	3:D:1474:NAG:C8	2.55	0.49
2:E:1297:ASP:C	2:E:1297:ASP:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:1309:PRO:C	2:E:1311:VAL:H	2.22	0.47
1:D:122:LYS:HZ1	1:D:234:GLN:HE21	1.62	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:A:327:LYS:HZ2	5:A:1484:GOL:C2	2.18	0.46
1:D:307:TYR:C	1:D:309:GLU:H	2.23	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:A:306:ASP:OD1	1:A:308:THR:OG1	2.22	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:84:ARG:HD3	1:D:287:PRO:HA	1.97	0.46
1:D:248:PRO:HG2	1:D:251:LEU:HD12	1.98	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:131:ARG:O	1:D:132:PRO:C	2.59	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
1:A:296:PHE:CE2	1:A:402:SER:HB3	2.52	0.45
1:D:70:ASN:HD22	1:D:70:ASN:C	2.24	0.45
1:D:454:ARG:HH22	1:D:472:THR:HG22	1.81	0.45
1:A:89:HIS:CD2	1:A:90:HIS:CE1	3.04	0.44
1:A:427:PRO:HB2	1:A:429:PRO:HD3	1.98	0.44
1:D:118:PRO:C	1:D:119:ILE:HD13	2.41	0.44
1:D:189:THR:HB	1:D:417:ILE:HA	1.99	0.44
1:D:372:GLY:CA	1:D:385:ALA:O	2.65	0.44
1:D:78:MET:O	1:D:81:PHE:HB3	2.18	0.44
1:D:189:THR:O	1:D:193:ARG:HG3	2.17	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:D:460:VAL:O	1:D:461:GLY:C	2.59	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:70:ASN:C	1:A:70:ASN:ND2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:SER:HA	1:D:173:PRO:C	2.43	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
1:D:78:MET:O	1:D:79:LYS:C	2.61	0.42
1:A:283:ILE:HG22	1:A:427:PRO:HB3	2.01	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:209:LYS:HD2	1:A:209:LYS:HA	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: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: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:70:ASN:HD21	1:A:72:PHE:HB2	1.86	0.40
1:A:163:PHE:CE1	2:B:1324:ALA:HB2	2.56	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%)	36	45
1	D	383/432 (89%)	359 (94%)	21 (6%)	3 (1%)	16	22
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%)	24	34

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 [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	334/371 (90%)	301 (90%)	33 (10%)	7	9
1	D	339/371 (91%)	303 (89%)	36 (11%)	6	7
2	B	28/29 (97%)	22 (79%)	6 (21%)	1	1
2	E	27/29 (93%)	21 (78%)	6 (22%)	1	1
All	All	728/800 (91%)	647 (89%)	81 (11%)	6	6

All (81) 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	126	LEU
1	A	131	ARG
1	A	144	THR
1	A	146	LYS
1	A	155	LEU
1	A	162	ASN
1	A	177	GLU
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	275	VAL
1	A	291	LEU
1	A	292	ARG
1	A	305	LEU
1	A	310	LEU
1	A	316	GLU
1	A	317	ARG
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	1314	VAL
2	B	1315	THR
2	B	1322	THR
2	B	1330	LYS
1	D	70	ASN
1	D	73	GLN
1	D	78	MET

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Mol	Chain	Res	Type
1	D	79	LYS
1	D	84	ARG
1	D	109	LEU
1	D	116	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	356	LEU
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	1303	GLU
2	E	1311	VAL
2	E	1312	SER
2	E	1318	ILE
2	E	1328	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	101	GLN
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	323	GLN
1	A	338	GLN
1	A	389	GLN
1	A	434	GLN
1	A	476	GLN
2	B	1316	ASN
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	361	GLN
1	D	389	GLN
1	D	434	GLN
1	D	450	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
5	GOL	A	1484	-	5,5,5	0.73	0	5,5,5	1.03	0
3	NAG	A	1480	1	14,14,15	0.56	0	17,19,21	2.35	6 (35%)
4	BO3	A	1482	-	3,3,3	5.39	3 (100%)	3,3,3	0.38	0
4	BO3	A	1481	-	3,3,3	5.08	3 (100%)	3,3,3	0.70	0
3	NAG	D	1474	1	14,14,15	0.47	0	17,19,21	1.47	3 (17%)
5	GOL	D	1475	-	5,5,5	0.56	0	5,5,5	0.38	0
5	GOL	A	1483	-	5,5,5	0.45	0	5,5,5	0.37	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
5	GOL	A	1484	-	-	2/4/4/4	-
3	NAG	A	1480	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1474	1	-	2/6/23/26	0/1/1/1
5	GOL	D	1475	-	-	0/4/4/4	-
5	GOL	A	1483	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1482	BO3	B-O2	5.63	1.54	1.36
4	A	1481	BO3	B-O3	5.37	1.54	1.36
4	A	1482	BO3	B-O3	5.29	1.53	1.36
4	A	1482	BO3	B-O1	5.24	1.53	1.36
4	A	1481	BO3	B-O1	5.06	1.52	1.36
4	A	1481	BO3	B-O2	4.80	1.52	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	NAG	C1-O5-C5	6.58	121.01	112.19
3	A	1480	NAG	C8-C7-N2	3.51	121.95	116.12
3	A	1480	NAG	C4-C3-C2	-2.99	106.64	111.02
3	D	1474	NAG	O5-C1-C2	-2.81	106.94	111.29
3	A	1480	NAG	C2-N2-C7	2.70	126.51	122.90
3	D	1474	NAG	O7-C7-C8	-2.60	117.42	122.05
3	A	1480	NAG	O7-C7-C8	-2.24	118.07	122.05
3	D	1474	NAG	C8-C7-N2	2.11	119.62	116.12
3	A	1480	NAG	C3-C4-C5	-2.07	106.49	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
5	A	1484	GOL	O1-C1-C2-O2
5	A	1484	GOL	O2-C2-C3-O3
5	A	1483	GOL	O1-C1-C2-C3
5	A	1483	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1484	GOL	4	0
3	A	1480	NAG	1	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, 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	386/432 (89%)	-0.24	8 (2%) 63 64	10, 24, 60, 76	5 (1%)
1	D	391/432 (90%)	0.09	12 (3%) 51 52	11, 35, 57, 75	5 (1%)
2	B	36/37 (97%)	-0.04	2 (5%) 30 29	19, 28, 50, 54	0
2	E	35/37 (94%)	0.89	5 (14%) 6 5	32, 49, 71, 73	0
All	All	848/938 (90%)	-0.03	27 (3%) 50 51	10, 30, 59, 76	10 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	473	ALA	5.0
1	D	429	PRO	4.4
1	A	427	PRO	3.7
1	A	429	PRO	3.3
1	D	431	THR	3.3
2	B	1331	ALA	3.2
1	D	357	HIS	3.0
1	A	446	ALA	2.9
1	D	74	ALA	2.8
1	A	428	THR	2.8
2	E	1322	THR	2.5
1	D	470	ASP	2.5
1	D	169	GLN	2.5
2	B	1332	THR	2.5
1	D	472	THR	2.5
1	D	346	SER	2.3
1	D	471	CYS	2.3
2	E	1331	ALA	2.3
2	E	1313	CYS	2.3
1	A	479	CYS	2.2
1	A	440	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	1329	ALA	2.2
1	A	431	THR	2.2
1	D	449	VAL	2.1
1	D	345	THR	2.1
2	E	1323	CYS	2.0
1	A	439	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	D	1475	6/6	0.82	0.15	51,53,54,55	0
5	GOL	A	1483	6/6	0.87	0.12	55,57,58,59	0
5	GOL	A	1484	6/6	0.87	0.12	40,42,43,43	0
3	NAG	A	1480	14/15	0.87	0.10	26,38,45,46	0
3	NAG	D	1474	14/15	0.88	0.09	38,40,42,44	0
4	BO3	A	1482	4/4	0.90	0.10	40,41,41,42	0
4	BO3	A	1481	4/4	0.95	0.08	31,33,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.