



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:27 PM EDT

PDB ID : 4YIZ / pdb_00004yiz
Title : Crystal structure of engineered TgAMA1 lacking the DII loop in complex with an Eimeria tenella RON2D3 peptide
Authors : Parker, M.L.; Boulanger, M.J.
Deposited on : 2015-03-02
Resolution : 2.20 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:

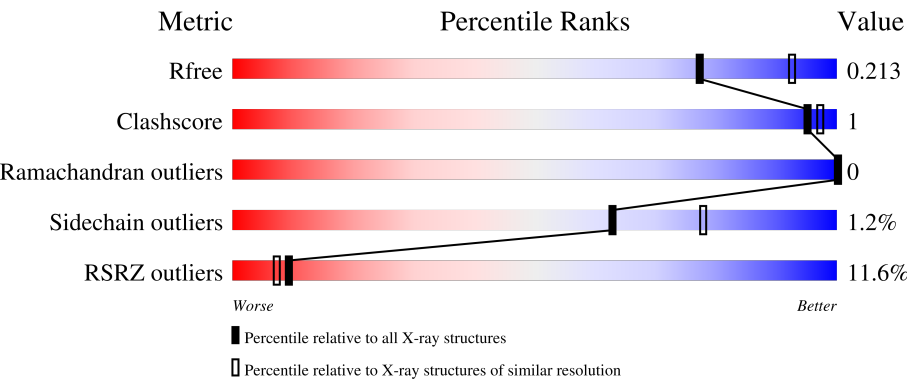
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



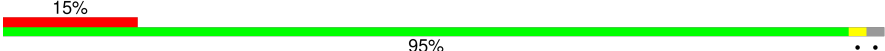
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	419	5% 91% 6%
1	C	419	12% 91% 6%
1	E	419	14% 88% 7%
2	B	40	20% 95%
2	D	40	15% 92% 5%

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Mol	Chain	Length	Quality of chain
2	F	40	 A horizontal bar chart showing the quality of chain F. The bar is primarily green, indicating good quality, with a small red segment at the beginning labeled '15%' and a small yellow segment at the end labeled '95%'. Below the bar, the text '95%' is centered. To the right of the bar, there are two small black dots.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10604 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 AMA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	3	0
			3091	1939	528	602	22			
1	C	392	Total	C	N	O	S	0	2	0
			3085	1935	528	600	22			
1	E	388	Total	C	N	O	S	0	1	0
			3047	1910	521	594	22			

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	expression tag	UNP S8GKS3
A	60	SER	-	expression tag	UNP S8GKS3
A	61	ALA	-	expression tag	UNP S8GKS3
A	62	MET	-	expression tag	UNP S8GKS3
A	63	GLY	-	expression tag	UNP S8GKS3
A	?	-	HIS	deletion	UNP S8GKS3
A	?	-	THR	deletion	UNP S8GKS3
A	?	-	TYR	deletion	UNP S8GKS3
A	?	-	PRO	deletion	UNP S8GKS3
A	?	-	LEU	deletion	UNP S8GKS3
A	?	-	THR	deletion	UNP S8GKS3
A	?	-	SER	deletion	UNP S8GKS3
A	?	-	GLN	deletion	UNP S8GKS3
A	?	-	ALA	deletion	UNP S8GKS3
A	?	-	SER	deletion	UNP S8GKS3
A	?	-	TRP	deletion	UNP S8GKS3
A	?	-	ASN	deletion	UNP S8GKS3
A	?	-	ASP	deletion	UNP S8GKS3
A	353	GLY	TRP	linker	UNP S8GKS3
A	354	SER	TRP	linker	UNP S8GKS3
A	355	GLY	PRO	linker	UNP S8GKS3
A	356	SER	LEU	linker	UNP S8GKS3
A	357	GLY	HIS	linker	UNP S8GKS3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	358	SER	GLN	linker	UNP S8GKS3
A	359	GLY	SER	linker	UNP S8GKS3
A	485	ALA	-	expression tag	UNP S8GKS3
A	486	ALA	-	expression tag	UNP S8GKS3
A	487	LEU	-	expression tag	UNP S8GKS3
A	488	VAL	-	expression tag	UNP S8GKS3
A	489	PRO	-	expression tag	UNP S8GKS3
A	490	ARG	-	expression tag	UNP S8GKS3
C	59	GLY	-	expression tag	UNP S8GKS3
C	60	SER	-	expression tag	UNP S8GKS3
C	61	ALA	-	expression tag	UNP S8GKS3
C	62	MET	-	expression tag	UNP S8GKS3
C	63	GLY	-	expression tag	UNP S8GKS3
C	?	-	HIS	deletion	UNP S8GKS3
C	?	-	THR	deletion	UNP S8GKS3
C	?	-	TYR	deletion	UNP S8GKS3
C	?	-	PRO	deletion	UNP S8GKS3
C	?	-	LEU	deletion	UNP S8GKS3
C	?	-	THR	deletion	UNP S8GKS3
C	?	-	SER	deletion	UNP S8GKS3
C	?	-	GLN	deletion	UNP S8GKS3
C	?	-	ALA	deletion	UNP S8GKS3
C	?	-	SER	deletion	UNP S8GKS3
C	?	-	TRP	deletion	UNP S8GKS3
C	?	-	ASN	deletion	UNP S8GKS3
C	?	-	ASP	deletion	UNP S8GKS3
C	353	GLY	TRP	linker	UNP S8GKS3
C	354	SER	TRP	linker	UNP S8GKS3
C	355	GLY	PRO	linker	UNP S8GKS3
C	356	SER	LEU	linker	UNP S8GKS3
C	357	GLY	HIS	linker	UNP S8GKS3
C	358	SER	GLN	linker	UNP S8GKS3
C	359	GLY	SER	linker	UNP S8GKS3
C	485	ALA	-	expression tag	UNP S8GKS3
C	486	ALA	-	expression tag	UNP S8GKS3
C	487	LEU	-	expression tag	UNP S8GKS3
C	488	VAL	-	expression tag	UNP S8GKS3
C	489	PRO	-	expression tag	UNP S8GKS3
C	490	ARG	-	expression tag	UNP S8GKS3
E	59	GLY	-	expression tag	UNP S8GKS3
E	60	SER	-	expression tag	UNP S8GKS3
E	61	ALA	-	expression tag	UNP S8GKS3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	62	MET	-	expression tag	UNP S8GKS3
E	63	GLY	-	expression tag	UNP S8GKS3
E	?	-	HIS	deletion	UNP S8GKS3
E	?	-	THR	deletion	UNP S8GKS3
E	?	-	TYR	deletion	UNP S8GKS3
E	?	-	PRO	deletion	UNP S8GKS3
E	?	-	LEU	deletion	UNP S8GKS3
E	?	-	THR	deletion	UNP S8GKS3
E	?	-	SER	deletion	UNP S8GKS3
E	?	-	GLN	deletion	UNP S8GKS3
E	?	-	ALA	deletion	UNP S8GKS3
E	?	-	SER	deletion	UNP S8GKS3
E	?	-	TRP	deletion	UNP S8GKS3
E	?	-	ASN	deletion	UNP S8GKS3
E	?	-	ASP	deletion	UNP S8GKS3
E	353	GLY	TRP	linker	UNP S8GKS3
E	354	SER	TRP	linker	UNP S8GKS3
E	355	GLY	PRO	linker	UNP S8GKS3
E	356	SER	LEU	linker	UNP S8GKS3
E	357	GLY	HIS	linker	UNP S8GKS3
E	358	SER	GLN	linker	UNP S8GKS3
E	359	GLY	SER	linker	UNP S8GKS3
E	485	ALA	-	expression tag	UNP S8GKS3
E	486	ALA	-	expression tag	UNP S8GKS3
E	487	LEU	-	expression tag	UNP S8GKS3
E	488	VAL	-	expression tag	UNP S8GKS3
E	489	PRO	-	expression tag	UNP S8GKS3
E	490	ARG	-	expression tag	UNP S8GKS3

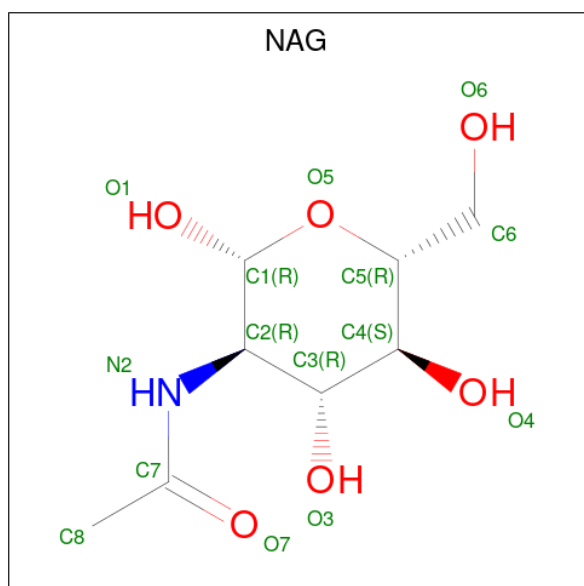
- Molecule 2 is a protein called Rhoptry neck protein 2, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	S	0	1	0
			271	168	45	55	3			
2	D	39	Total	C	N	O	S	0	1	0
			271	168	45	55	3			
2	F	39	Total	C	N	O	S	0	1	0
			271	168	45	55	3			

There are 9 discrepancies between the modelled and reference sequences:

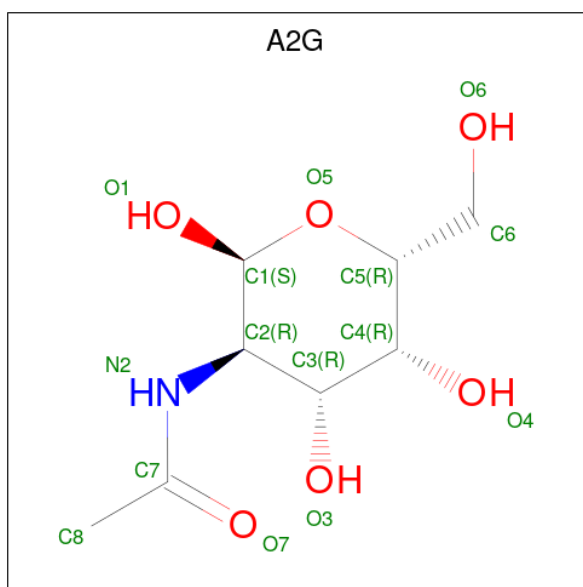
Chain	Residue	Modelled	Actual	Comment	Reference
B	1258	GLY	-	expression tag	UNP U6KQJ2
B	1259	SER	-	expression tag	UNP U6KQJ2
B	1260	ALA	-	expression tag	UNP U6KQJ2
D	1258	GLY	-	expression tag	UNP U6KQJ2
D	1259	SER	-	expression tag	UNP U6KQJ2
D	1260	ALA	-	expression tag	UNP U6KQJ2
F	1258	GLY	-	expression tag	UNP U6KQJ2
F	1259	SER	-	expression tag	UNP U6KQJ2
F	1260	ALA	-	expression tag	UNP U6KQJ2

- 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	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

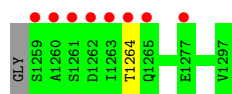
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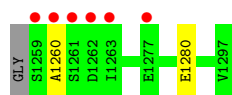
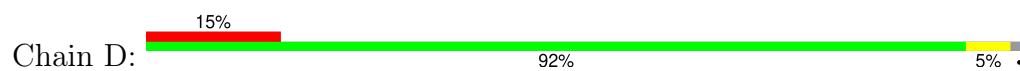
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

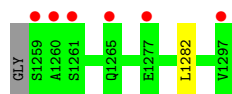
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	C	133	Total	O	0	0
			133	133		
6	E	153	Total	O	0	0
			153	153		
6	B	11	Total	O	0	0
			11	11		
6	D	12	Total	O	0	0
			12	12		
6	F	13	Total	O	0	0
			13	13		



- Molecule 2: Rhoptry neck protein 2, putative



- Molecule 2: Rhoptry neck protein 2, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	265.93Å 265.93Å 94.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.50 – 2.20 59.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (59.50-2.20) 91.7 (59.50-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.207 0.197 , 0.213	Depositor DCC
R_{free} test set	9083 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10604	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, NAG, SO4

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	0.33	0/3179	0.64	2/4310 (0.0%)
1	C	0.37	0/3170	0.66	2/4298 (0.0%)
1	E	0.35	0/3126	0.65	3/4233 (0.1%)
2	B	0.38	0/275	0.72	0/380
2	D	0.37	0/275	0.71	1/380 (0.3%)
2	F	0.36	0/275	0.66	0/380
All	All	0.35	0/10300	0.65	8/13981 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	SER	N-CA-C	6.70	118.66	111.36
1	A	260	LYS	N-CA-C	-6.04	99.15	109.24
1	C	260	LYS	N-CA-C	-5.91	99.36	109.24
2	D	1260	ALA	N-CA-C	-5.84	104.87	112.23
1	A	275	VAL	N-CA-C	-5.66	105.37	113.07
1	E	275	VAL	N-CA-C	-5.27	105.90	113.07
1	C	257	LYS	N-CA-C	5.24	112.94	108.22
1	E	260	LYS	N-CA-C	-5.18	100.60	109.24

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	3091	0	2942	6	0
1	C	3085	0	2937	6	0
1	E	3047	0	2892	11	0
2	B	271	0	265	0	0
2	D	271	0	265	1	0
2	F	271	0	265	1	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	1	0
4	A	14	0	12	3	0
5	A	10	0	0	0	0
5	C	10	0	0	0	0
5	E	5	0	0	0	0
6	A	165	0	0	0	0
6	B	11	0	0	0	0
6	C	133	0	0	1	0
6	D	12	0	0	0	0
6	E	153	0	0	1	0
6	F	13	0	0	0	0
All	All	10604	0	9617	23	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 1.

All (23) 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:E:72:PHE:HA	1:E:78:MET:HG2	1.75	0.67
1:E:77:GLU:OE2	1:E:431:THR:HG22	1.92	0.67
1:E:135:ARG:NH1	6:E:708:HOH:O	2.37	0.58
1:C:195:ALA:HB1	1:C:275:VAL:HG22	1.91	0.53
1:E:292:ARG:HB2	1:E:411:GLU:HG2	1.91	0.52
1:E:196:GLU:OE1	1:E:200:LYS:NZ	2.45	0.48
1:C:195:ALA:CB	1:C:275:VAL:HG22	2.44	0.47
1:A:81:PHE:O	1:A:84:ARG:HG2	2.14	0.47
1:C:369[B]:ARG:NH1	6:C:731:HOH:O	2.48	0.47
1:E:448:ASP:O	1:E:452:CYS:N	2.45	0.47
1:A:425:THR:O	4:A:502:A2G:H8A	2.14	0.46
1:E:103:LYS:NZ	1:E:274:TYR:OH	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HB2	1:A:411[A]:GLU:HG2	1.99	0.43
1:A:427:PRO:HD3	4:A:502:A2G:H8	2.01	0.43
1:C:272:SER:O	1:C:275:VAL:HG13	2.19	0.43
1:E:86:ASN:HD22	3:E:501:NAG:H83	1.84	0.43
1:E:77:GLU:OE2	1:E:431:THR:CG2	2.65	0.42
1:A:184:ASN:O	1:A:200:LYS:NZ	2.40	0.41
1:E:260:LYS:HE3	1:E:329:PHE:CG	2.55	0.41
1:E:200:LYS:HG2	2:F:1282:LEU:HD12	2.03	0.41
1:C:204:MET:SD	2:D:1280:GLU:HG2	2.60	0.41
1:C:260:LYS:HE3	1:C:329:PHE:CG	2.56	0.40
1:A:427:PRO:HA	4:A:502:A2G:O7	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	391/419 (93%)	384 (98%)	7 (2%)	0	100	100
1	C	390/419 (93%)	380 (97%)	10 (3%)	0	100	100
1	E	383/419 (91%)	376 (98%)	7 (2%)	0	100	100
2	B	38/40 (95%)	38 (100%)	0	0	100	100
2	D	38/40 (95%)	38 (100%)	0	0	100	100
2	F	38/40 (95%)	38 (100%)	0	0	100	100
All	All	1278/1377 (93%)	1254 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	344/356 (97%)	341 (99%)	3 (1%)	70	84
1	C	343/356 (96%)	340 (99%)	3 (1%)	70	84
1	E	337/356 (95%)	331 (98%)	6 (2%)	51	68
2	B	31/30 (103%)	30 (97%)	1 (3%)	34	47
2	D	31/30 (103%)	31 (100%)	0	100	100
2	F	31/30 (103%)	31 (100%)	0	100	100
All	All	1117/1158 (96%)	1104 (99%)	13 (1%)	63	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	222	LYS
1	A	275	VAL
1	C	275	VAL
1	C	430	GLU
1	C	438	ASP
1	E	77	GLU
1	E	84	ARG
1	E	127	GLN
1	E	222	LYS
1	E	275	VAL
1	E	452	CYS
2	B	1264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	208	ASN
1	A	278	ASN
1	A	476	GLN

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Mol	Chain	Res	Type
1	C	123	HIS
1	C	265	ASN
1	E	169	GLN
1	E	421	ASN
2	F	1266	HIS

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 [i](#)

9 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	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.07	0
3	NAG	E	501	1	14,14,15	0.35	0	17,19,21	0.60	0
4	A2G	A	502	1	14,14,15	0.28	0	17,19,21	0.54	0
5	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.08	0
3	NAG	C	501	1	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	A	501	1	14,14,15	0.34	0	17,19,21	0.62	0
5	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.09	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	C	501	1	-	2/6/23/26	0/1/1/1
3	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	NAG	E	501	1	-	3/6/23/26	0/1/1/1
4	A2G	A	502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C8-C7-N2-C2
3	A	501	NAG	O7-C7-N2-C2
3	C	501	NAG	C8-C7-N2-C2
3	C	501	NAG	O7-C7-N2-C2
3	E	501	NAG	C8-C7-N2-C2
3	E	501	NAG	O7-C7-N2-C2
4	A	502	A2G	C8-C7-N2-C2
4	A	502	A2G	O7-C7-N2-C2
3	E	501	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	NAG	1	0
4	A	502	A2G	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	392/419 (93%)	0.18	22 (5%) 30 27	12, 26, 55, 87	4 (1%)
1	C	392/419 (93%)	0.56	49 (12%) 8 6	12, 30, 88, 117	4 (1%)
1	E	388/419 (92%)	0.68	59 (15%) 5 4	14, 30, 71, 120	2 (0%)
2	B	39/40 (97%)	1.02	8 (20%) 2 2	19, 37, 87, 91	1 (2%)
2	D	39/40 (97%)	0.82	6 (15%) 5 4	16, 32, 78, 80	1 (2%)
2	F	39/40 (97%)	0.78	6 (15%) 5 4	16, 34, 79, 87	1 (2%)
All	All	1289/1377 (93%)	0.51	150 (11%) 9 7	12, 29, 74, 120	13 (1%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	427	PRO	9.4
1	E	429	PRO	8.1
1	C	424	VAL	7.8
1	C	68	SER	6.6
1	E	480	GLY	6.5
1	E	421	ASN	6.4
1	E	430	GLU	6.4
1	C	479	CYS	6.3
1	A	479	CYS	5.8
1	E	435	CYS	5.7
2	F	1259	SER	5.5
1	C	422	PRO	5.5
1	C	423	SER	5.4
2	B	1259	SER	5.4
1	C	425	THR	5.4
1	E	431	THR	5.3
1	E	438	ASP	5.3
1	E	437	ALA	5.3
1	E	68	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	473	ALA	5.1
1	C	426	PRO	5.0
1	E	420	SER	4.8
1	E	441	PRO	4.7
1	C	452	CYS	4.7
1	E	436	THR	4.7
1	E	439	LYS	4.5
2	D	1261	SER	4.5
1	C	427	PRO	4.4
1	E	428	THR	4.4
1	E	464	ILE	4.4
1	C	301	LYS	4.3
1	E	461	GLY	4.3
1	C	181	LYS	4.3
1	E	474	ASP	4.2
1	E	69	GLY	4.0
1	C	446	ALA	4.0
1	C	74	ALA	3.9
1	E	77	GLU	3.8
1	C	311	THR	3.8
2	F	1260	ALA	3.8
1	C	439	LYS	3.8
1	A	69	GLY	3.8
2	F	1261	SER	3.7
1	C	471	CYS	3.7
1	C	430	GLU	3.7
1	C	450	GLN	3.7
1	E	452	CYS	3.7
1	C	420	SER	3.7
1	C	478	GLU	3.6
2	D	1260	ALA	3.6
2	D	1259	SER	3.6
1	C	474	ASP	3.6
1	C	449	VAL	3.6
1	E	459	CYS	3.5
1	E	74	ALA	3.5
1	A	68	SER	3.4
1	E	463	GLN	3.4
1	C	475	GLU	3.4
1	C	421	ASN	3.3
2	B	1261	SER	3.3
1	A	360	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	434	GLN	3.2
1	C	438	ASP	3.2
1	E	442	ASP	3.2
1	E	440	PHE	3.2
1	A	430	GLU	3.2
1	C	477	ASN	3.2
2	B	1262	ASP	3.2
2	B	1264	THR	3.1
1	C	69	GLY	3.1
1	A	332	ASP	3.1
1	E	465	GLN	3.0
1	E	184	ASN	3.0
1	E	450	GLN	3.0
2	B	1265	GLN	3.0
1	A	77	GLU	3.0
1	C	451	ALA	2.9
1	C	76	VAL	2.9
1	C	447	CYS	2.9
1	E	75	ASN	2.9
1	C	378	THR	2.9
2	B	1277	GLU	2.8
1	E	304	CYS	2.8
1	C	470	ASP	2.8
1	E	73	GLN	2.8
1	C	437	ALA	2.8
1	E	78	MET	2.8
1	C	434	GLN	2.7
2	B	1260	ALA	2.7
1	C	428	THR	2.7
1	C	445	GLY	2.7
1	E	83	GLU	2.7
1	E	183	SER	2.7
1	E	443	SER	2.7
1	E	479	CYS	2.7
1	E	267[A]	HIS	2.7
1	C	444	PHE	2.7
1	A	439	LYS	2.7
1	C	472	THR	2.6
1	A	449	VAL	2.6
1	E	301	LYS	2.6
1	E	447	CYS	2.5
1	A	478	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	1262	ASP	2.5
1	E	80	THR	2.5
1	E	181	LYS	2.5
1	C	453	LYS	2.4
2	F	1297	VAL	2.4
1	C	448	ASP	2.4
1	E	76	VAL	2.4
2	B	1263	ILE	2.4
1	E	90	HIS	2.4
2	F	1277	GLU	2.4
1	E	473	ALA	2.4
1	E	84	ARG	2.4
1	E	250	ASP	2.3
1	C	206	LYS	2.3
1	A	378	THR	2.3
1	A	183	SER	2.3
1	C	77	GLU	2.3
1	C	435	CYS	2.3
1	A	477	ASN	2.3
1	E	432	ALA	2.3
1	E	378	THR	2.3
2	F	1265	GLN	2.3
1	C	443	SER	2.3
1	E	460	VAL	2.3
1	A	473	ALA	2.2
1	A	301	LYS	2.2
1	E	186	LYS	2.2
2	D	1263	ILE	2.2
1	E	412	GLU	2.2
2	D	1277	GLU	2.2
1	E	446	ALA	2.2
1	E	477	ASN	2.1
1	A	209	LYS	2.1
1	C	300	LYS	2.1
1	C	442	ASP	2.1
1	E	275	VAL	2.1
1	E	150	GLN	2.1
1	C	436	THR	2.1
1	A	377	ASP	2.1
1	A	450	GLN	2.1
1	E	462	GLY	2.1
1	A	83	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	250	ASP	2.1
1	A	106	ASP	2.0
1	E	79	LYS	2.0
1	A	475	GLU	2.0
1	C	177	GLU	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(Å ²)	Q<0.9
5	SO4	A	504	5/5	0.83	0.17	53,56,88,91	0
4	A2G	A	502	14/15	0.84	0.18	50,59,66,66	0
5	SO4	A	503	5/5	0.89	0.12	50,66,87,92	0
5	SO4	C	502	5/5	0.89	0.12	42,59,79,86	0
3	NAG	C	501	14/15	0.91	0.10	32,42,47,55	0
3	NAG	E	501	14/15	0.92	0.11	30,37,47,56	0
3	NAG	A	501	14/15	0.93	0.09	23,31,42,43	0
5	SO4	E	502	5/5	0.93	0.10	51,67,72,74	0
5	SO4	C	503	5/5	0.96	0.11	47,51,55,58	5

6.5 Other polymers [i](#)

There are no such residues in this entry.