



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:10 PM UTC

PDB ID : 8HHV / pdb_00008hhv
Title : endo-alpha-D-arabinanase EndoMA1 from Microbacterium arabinogalactanolyticum
Authors : Nakashima, C.; Li, J.; Arakawa, T.; Yamada, C.; Ishiwata, A.; Fujita, K.; Fushinobu, S.
Deposited on : 2022-11-17
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

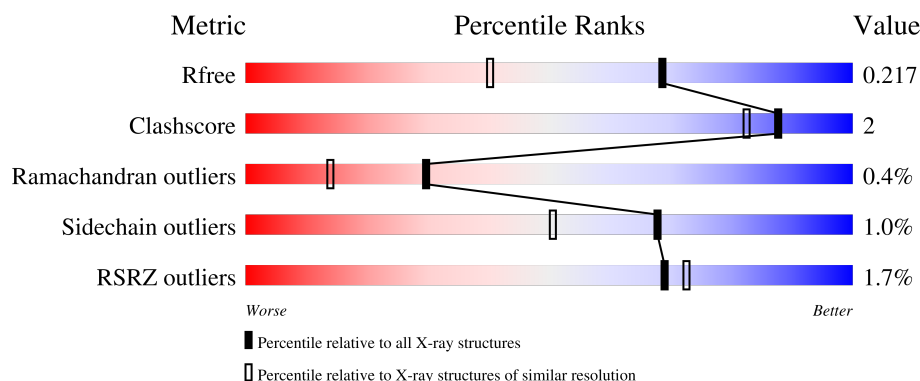
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	488	92% 5% ..
1	B	488	90% 7% ..
1	C	488	4% 91% 7% .
1	D	488	91% 6% .

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	GOL	D	508	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16715 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 endo-alpha-D-arabinanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	2	0
			3720	2347	645	715	13			
1	B	479	Total	C	N	O	S	0	0	0
			3709	2340	645	711	13			
1	C	479	Total	C	N	O	S	0	0	0
			3709	2340	645	711	13			
1	D	479	Total	C	N	O	S	0	0	0
			3709	2340	645	711	13			

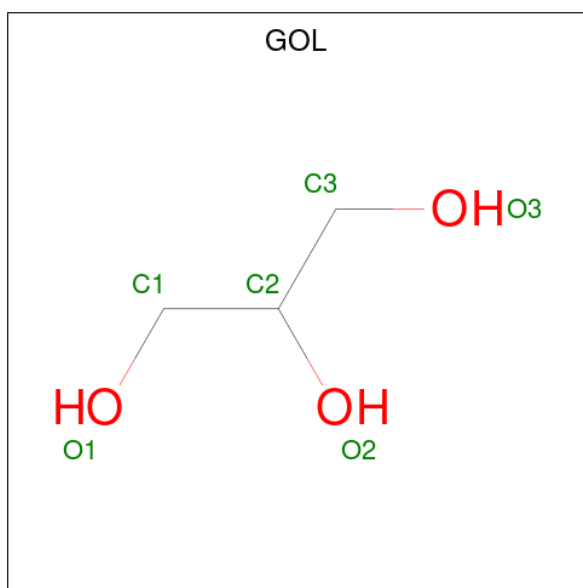
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		
2	D	2	Total	Na	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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

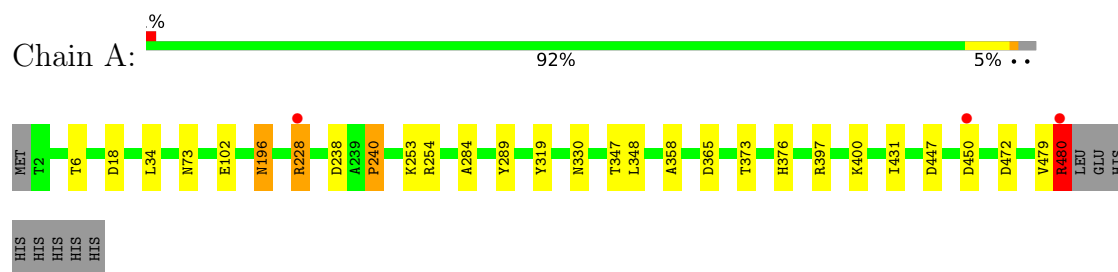
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	458	Total	O	0	0
			458	458		
5	B	491	Total	O	0	0
			491	491		
5	C	361	Total	O	0	0
			361	361		
5	D	450	Total	O	0	0
			450	450		

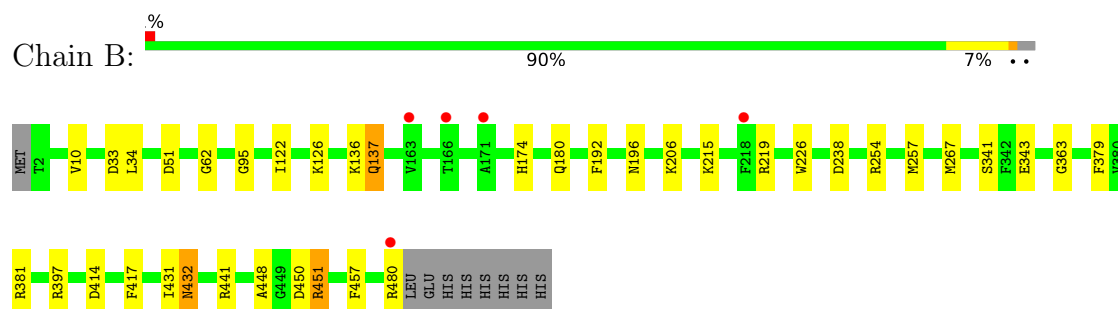
3 Residue-property plots [i](#)

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.

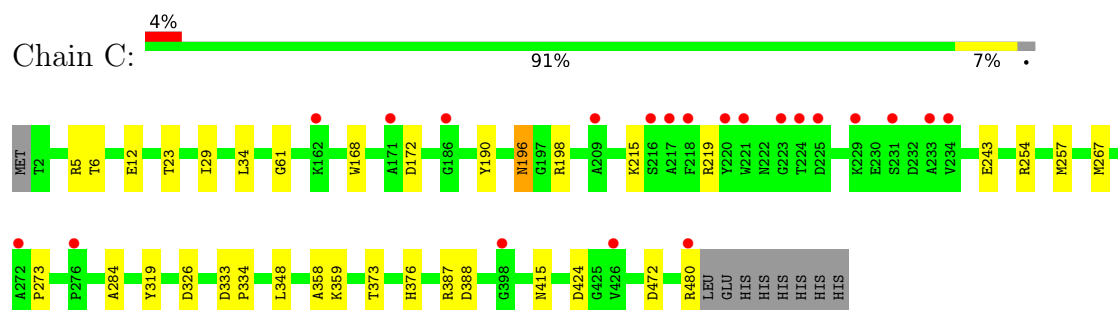
- Molecule 1: endo-alpha-D-arabinanase



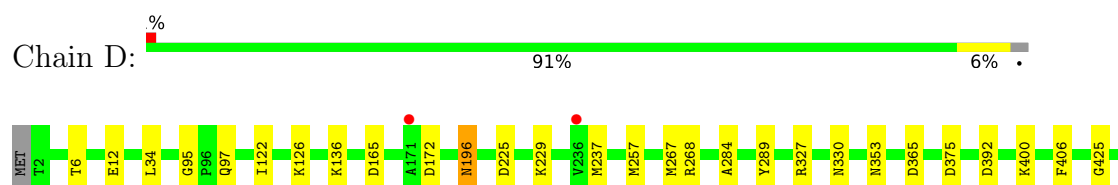
- Molecule 1: endo-alpha-D-arabinanase

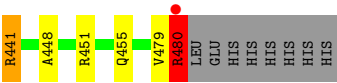


- Molecule 1: endo-alpha-D-arabinanase



- Molecule 1: endo-alpha-D-arabinanase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.28Å 128.30Å 104.02Å 90.00° 109.38° 90.00°	Depositor
Resolution (Å)	46.18 – 1.60 46.18 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.18-1.60) 98.9 (46.18-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.177 , 0.211 0.186 , 0.217	Depositor DCC
R_{free} test set	12950 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16715	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.82% 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: CA, GOL, NA

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	0.98	1/3835 (0.0%)	1.25	9/5230 (0.2%)
1	B	1.01	3/3818 (0.1%)	1.31	10/5207 (0.2%)
1	C	0.96	2/3818 (0.1%)	1.24	9/5207 (0.2%)
1	D	0.99	1/3818 (0.0%)	1.25	8/5207 (0.2%)
All	All	0.98	7/15289 (0.0%)	1.26	36/20851 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	2
1	D	0	4
All	All	0	12

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	12	GLU	CD-OE2	6.92	1.38	1.25
1	B	10	VAL	C-N	6.53	1.39	1.33
1	C	376	HIS	CD2-NE2	6.51	1.45	1.37
1	A	18	ASP	CG-OD1	-5.64	1.14	1.25
1	C	12	GLU	CD-OE2	5.53	1.35	1.25
1	B	441	ARG	C-O	5.37	1.30	1.23
1	B	51	ASP	CG-OD2	-5.17	1.15	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	CA-CB-CG	8.21	120.81	112.60
1	A	196	ASN	CA-CB-CG	8.20	120.80	112.60
1	D	172	ASP	CA-CB-CG	7.95	120.55	112.60
1	D	196	ASN	CA-CB-CG	7.18	119.78	112.60
1	B	457	PHE	CA-C-N	6.99	128.10	121.46
1	B	457	PHE	C-N-CA	6.99	128.10	121.46
1	B	414	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	18	ASP	CA-CB-CG	6.72	119.32	112.60
1	D	365	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	330	ASN	CA-CB-CG	-6.31	106.29	112.60
1	B	126	LYS	CB-CA-C	6.14	120.35	110.09
1	B	62	GLY	CA-C-N	-6.05	116.01	122.67
1	B	62	GLY	C-N-CA	-6.05	116.01	122.67
1	C	388	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	254	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	D	165	ASP	CB-CA-C	-5.78	99.13	110.11
1	C	196	ASN	CA-CB-CG	5.77	118.37	112.60
1	D	122	ILE	CA-C-O	-5.76	116.80	120.66
1	B	238	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	254	ARG	CG-CD-NE	-5.60	99.67	112.00
1	A	240	PRO	N-CA-CB	-5.58	96.47	102.60
1	C	326	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	376	HIS	CB-CG-CD2	5.44	138.28	131.20
1	B	33	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	174	HIS	CA-CB-CG	5.43	119.23	113.80
1	A	253	LYS	CB-CA-C	5.43	119.59	111.89
1	D	375	ASP	N-CA-CB	-5.38	102.51	110.53
1	C	415	ASN	CB-CA-C	-5.22	104.25	110.94
1	A	228	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	432	ASN	CA-CB-CG	5.14	117.75	112.60
1	C	172	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	472	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	472	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	61	GLY	CA-C-N	5.04	125.93	120.44
1	C	61	GLY	C-N-CA	5.04	125.93	120.44
1	A	238	ASP	O-C-N	5.04	128.53	122.79

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain
1	A	289	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	480	ARG	Sidechain
1	B	254	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	451	ARG	Sidechain
1	C	219	ARG	Sidechain
1	C	387	ARG	Sidechain
1	D	289	TYR	Sidechain
1	D	327	ARG	Sidechain
1	D	441	ARG	Sidechain
1	D	480	ARG	Sidechain

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	3720	0	3499	12	0
1	B	3709	0	3489	12	0
1	C	3709	0	3489	14	0
1	D	3709	0	3489	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	32	0	0
4	B	18	0	24	1	0
4	C	18	0	23	4	0
4	D	36	0	47	4	0
5	A	458	0	0	1	0
5	B	491	0	0	1	0
5	C	361	0	0	3	0
5	D	450	0	0	12	0
All	All	16715	0	14092	58	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 2.

All (58) 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)
4:D:508:GOL:H32	5:D:639:HOH:O	1.54	1.06
4:D:508:GOL:H2	5:D:651:HOH:O	1.68	0.93
4:D:508:GOL:C3	5:D:639:HOH:O	2.23	0.77
1:A:397:ARG:NH1	1:A:450:ASP:OD1	2.23	0.71
1:D:353:ASN:HB3	5:D:602:HOH:O	1.93	0.67
1:B:136:LYS:HE2	1:B:137:GLN:HE22	1.60	0.65
1:C:6:THR:HG23	1:C:284:ALA:HA	1.83	0.61
1:D:400:LYS:NZ	5:D:604:HOH:O	2.35	0.60
1:D:479:VAL:O	1:D:480:ARG:HB2	2.03	0.57
1:D:353:ASN:CB	5:D:602:HOH:O	2.50	0.56
1:D:237:MET:HG2	1:D:268:ARG:NH1	2.20	0.56
1:C:257:MET:O	1:C:267:MET:HA	2.07	0.55
1:C:198:ARG:NH2	4:C:505:GOL:H11	2.22	0.55
4:D:508:GOL:C2	5:D:651:HOH:O	2.41	0.55
1:A:479:VAL:O	1:A:480:ARG:HB2	2.08	0.52
1:B:448:ALA:O	1:B:451:ARG:NH1	2.37	0.52
1:D:225:ASP:HB2	5:D:796:HOH:O	2.11	0.51
1:D:6:THR:HG23	1:D:284:ALA:HA	1.93	0.50
1:B:397:ARG:NH1	1:B:450:ASP:OD1	2.42	0.50
1:C:198:ARG:HH22	4:C:505:GOL:C1	2.25	0.49
1:B:206:LYS:HE2	1:B:226:TRP:CG	2.48	0.49
1:A:348:LEU:HD13	1:A:358:ALA:HB3	1.94	0.48
1:C:198:ARG:HH22	4:C:505:GOL:H11	1.77	0.47
1:C:359:LYS:HE2	5:C:620:HOH:O	2.15	0.47
1:C:5:ARG:HD2	5:C:741:HOH:O	2.15	0.46
1:D:257:MET:O	1:D:267:MET:HA	2.16	0.46
4:B:505:GOL:H2	5:B:922:HOH:O	2.16	0.46
1:A:6:THR:HG23	1:A:284:ALA:HA	1.98	0.46
1:D:136:LYS:NZ	5:D:616:HOH:O	2.49	0.46
1:B:417:PHE:CE2	1:B:432:ASN:HB2	2.51	0.45
1:C:254:ARG:HD3	5:C:682:HOH:O	2.15	0.45
1:A:431:ILE:HD12	1:A:431:ILE:C	2.42	0.45
1:C:333:ASP:N	1:C:334:PRO:CD	2.80	0.45
1:D:425:GLY:O	5:D:601:HOH:O	2.21	0.45
1:C:319:TYR:CE2	1:C:373:THR:HG22	2.52	0.45
1:A:330:ASN:ND2	5:A:601:HOH:O	2.23	0.44
1:A:348:LEU:CD1	1:A:358:ALA:HB3	2.47	0.44
1:D:353:ASN:CG	5:D:602:HOH:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASP:OD1	1:D:455:GLN:HG2	2.18	0.43
1:C:190:TYR:CE1	1:C:273:PRO:HG2	2.54	0.43
1:B:257:MET:O	1:B:267:MET:HA	2.18	0.43
1:B:180:GLN:HA	1:B:192:PHE:O	2.19	0.43
1:B:341:SER:HB3	1:B:343:GLU:HG2	2.00	0.43
1:B:397:ARG:HD3	1:B:450:ASP:OD1	2.19	0.42
1:A:347:THR:CG2	4:C:504:GOL:H31	2.50	0.42
1:D:97:GLN:HG2	5:D:993:HOH:O	2.18	0.42
1:B:363:GLY:HA3	1:B:379:PHE:CE2	2.54	0.42
1:B:219:ARG:HB3	1:B:226:TRP:HB3	2.02	0.41
1:A:365:ASP:O	1:A:376:HIS:HA	2.21	0.41
1:D:448:ALA:O	1:D:451:ARG:NH1	2.45	0.41
1:B:431:ILE:C	1:B:431:ILE:HD12	2.46	0.40
1:C:168:TRP:CD1	1:C:215:LYS:HE3	2.57	0.40
1:A:319:TYR:CE2	1:A:373:THR:HG22	2.57	0.40
1:C:23:THR:HB	1:C:29:ILE:HB	2.04	0.40
1:C:348:LEU:HD13	1:C:358:ALA:HB3	2.03	0.40
1:D:406:PHE:CE2	1:D:441:ARG:HB2	2.56	0.40
1:A:73:ASN:O	1:A:102:GLU:HA	2.21	0.40
1:A:400:LYS:HG2	1:A:447:ASP:OD1	2.22	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	479/488 (98%)	466 (97%)	12 (2%)	1 (0%)	43	24
1	B	477/488 (98%)	460 (96%)	15 (3%)	2 (0%)	30	14
1	C	477/488 (98%)	456 (96%)	19 (4%)	2 (0%)	30	14
1	D	477/488 (98%)	458 (96%)	17 (4%)	2 (0%)	30	14
All	All	1910/1952 (98%)	1840 (96%)	63 (3%)	7 (0%)	30	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	B	34	LEU
1	D	34	LEU
1	C	34	LEU
1	C	243	GLU
1	B	95	GLY
1	D	95	GLY

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	385/392 (98%)	382 (99%)	3 (1%)	73	59
1	B	383/392 (98%)	378 (99%)	5 (1%)	61	40
1	C	383/392 (98%)	380 (99%)	3 (1%)	73	59
1	D	383/392 (98%)	379 (99%)	4 (1%)	68	50
All	All	1534/1568 (98%)	1519 (99%)	15 (1%)	68	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	240	PRO
1	A	480	ARG
1	B	122	ILE
1	B	137	GLN
1	B	196	ASN
1	B	215	LYS
1	B	480	ARG
1	C	196	ASN
1	C	424	ASP
1	C	480	ARG
1	D	126	LYS
1	D	196	ASN

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Mol	Chain	Res	Type
1	D	229	LYS
1	D	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	B	97	GLN
1	B	137	GLN
1	D	366	ASN

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](#)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 for Mogul analysis.

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	$\# Z > 2$
4	GOL	B	505	-	5,5,5	0.26	0	5,5,5	0.72	0
4	GOL	D	504	-	5,5,5	0.30	0	5,5,5	0.45	0
4	GOL	D	506	2	5,5,5	0.30	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	507	-	5,5,5	0.35	0	5,5,5	0.67	0
4	GOL	C	504	-	5,5,5	0.38	0	5,5,5	0.47	0
4	GOL	B	506	-	5,5,5	0.21	0	5,5,5	0.70	0
4	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.72	0
4	GOL	A	506	-	5,5,5	0.31	0	5,5,5	0.77	0
4	GOL	D	509	-	5,5,5	0.39	0	5,5,5	0.49	0
4	GOL	B	504	-	5,5,5	0.48	0	5,5,5	0.27	0
4	GOL	D	505	-	5,5,5	0.18	0	5,5,5	0.37	0
4	GOL	A	505	-	5,5,5	0.17	0	5,5,5	0.79	0
4	GOL	C	505	2	5,5,5	0.10	0	5,5,5	0.83	0
4	GOL	D	508	-	5,5,5	0.25	0	5,5,5	0.75	0
4	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.24	0
4	GOL	C	506	-	5,5,5	0.26	0	5,5,5	1.08	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
4	GOL	B	505	-	-	3/4/4/4	-
4	GOL	D	504	-	-	0/4/4/4	-
4	GOL	D	506	2	-	4/4/4/4	-
4	GOL	D	507	-	-	0/4/4/4	-
4	GOL	C	504	-	-	0/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
4	GOL	A	507	-	-	2/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	D	509	-	-	2/4/4/4	-
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
4	GOL	C	505	2	-	2/4/4/4	-
4	GOL	D	508	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	C	506	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	507	GOL	O1-C1-C2-C3
4	C	506	GOL	O1-C1-C2-C3
4	D	506	GOL	C1-C2-C3-O3
4	D	506	GOL	O2-C2-C3-O3
4	D	508	GOL	O1-C1-C2-C3
4	D	509	GOL	O1-C1-C2-C3
4	D	509	GOL	O1-C1-C2-O2
4	A	506	GOL	O1-C1-C2-C3
4	B	505	GOL	O1-C1-C2-C3
4	B	506	GOL	O1-C1-C2-C3
4	C	505	GOL	O1-C1-C2-C3
4	D	506	GOL	O1-C1-C2-C3
4	A	507	GOL	O1-C1-C2-O2
4	D	508	GOL	O1-C1-C2-O2
4	A	506	GOL	O1-C1-C2-O2
4	C	506	GOL	O1-C1-C2-O2
4	D	506	GOL	O1-C1-C2-O2
4	B	505	GOL	O2-C2-C3-O3
4	C	506	GOL	O2-C2-C3-O3
4	C	505	GOL	O2-C2-C3-O3
4	B	505	GOL	O1-C1-C2-O2
4	B	506	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	GOL	1	0
4	C	504	GOL	1	0
4	C	505	GOL	3	0
4	D	508	GOL	4	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	479/488 (98%)	-0.11	3 (0%) 85 88	10, 16, 29, 64	2 (0%)
1	B	479/488 (98%)	0.04	5 (1%) 79 83	11, 17, 32, 55	0
1	C	479/488 (98%)	0.25	21 (4%) 39 40	11, 19, 37, 66	0
1	D	479/488 (98%)	-0.01	3 (0%) 85 88	11, 17, 31, 56	0
All	All	1916/1952 (98%)	0.04	32 (1%) 69 72	10, 17, 33, 66	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	ALA	4.6
1	B	171	ALA	3.5
1	C	480	ARG	3.4
1	A	480	ARG	3.1
1	C	233	ALA	3.1
1	D	480	ARG	3.0
1	C	221	TRP	3.0
1	C	234	VAL	2.9
1	C	171	ALA	2.8
1	C	209	ALA	2.6
1	C	276	PRO	2.6
1	B	163	VAL	2.4
1	C	224	THR	2.4
1	A	450	ASP	2.4
1	C	398	GLY	2.4
1	C	162	LYS	2.3
1	B	480	ARG	2.3
1	C	229	LYS	2.3
1	C	223	GLY	2.2
1	C	217	ALA	2.2
1	C	218	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	272	ALA	2.1
1	C	186	GLY	2.1
1	C	225	ASP	2.1
1	C	216	SER	2.1
1	A	228	ARG	2.1
1	C	231	SER	2.0
1	C	426	VAL	2.0
1	B	166	THR	2.0
1	B	218	PHE	2.0
1	C	220	TYR	2.0
1	D	236	VAL	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
4	GOL	A	507	6/6	0.83	0.14	29,33,36,37	0
4	GOL	B	506	6/6	0.83	0.13	33,36,38,40	0
4	GOL	D	509	6/6	0.86	0.12	26,32,32,34	0
4	GOL	D	506	6/6	0.87	0.15	22,36,39,43	0
4	GOL	C	505	6/6	0.88	0.14	23,36,40,41	0
4	GOL	D	508	6/6	0.90	0.11	23,29,31,33	0
4	GOL	C	506	6/6	0.91	0.10	22,29,31,32	0
4	GOL	D	507	6/6	0.91	0.10	18,23,26,26	0
4	GOL	A	506	6/6	0.94	0.09	19,24,30,31	0
4	GOL	C	504	6/6	0.94	0.08	17,22,24,24	0
4	GOL	B	505	6/6	0.95	0.08	25,27,29,30	0
4	GOL	A	505	6/6	0.96	0.06	17,18,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	504	6/6	0.96	0.08	16,19,22,23	0
4	GOL	B	504	6/6	0.97	0.05	13,14,15,16	0
4	GOL	D	504	6/6	0.97	0.05	14,15,16,17	0
2	NA	B	502	1/1	0.98	0.07	18,18,18,18	0
4	GOL	D	505	6/6	0.98	0.05	18,20,21,21	0
2	NA	C	502	1/1	0.98	0.06	20,20,20,20	0
2	NA	A	501	1/1	0.99	0.03	11,11,11,11	0
2	NA	C	501	1/1	0.99	0.06	15,15,15,15	0
2	NA	A	502	1/1	0.99	0.05	16,16,16,16	0
2	NA	D	501	1/1	0.99	0.07	18,18,18,18	0
2	NA	B	501	1/1	0.99	0.03	11,11,11,11	0
3	CA	A	503	1/1	1.00	0.02	12,12,12,12	0
3	CA	B	503	1/1	1.00	0.02	11,11,11,11	0
3	CA	C	503	1/1	1.00	0.03	15,15,15,15	0
3	CA	D	503	1/1	1.00	0.04	11,11,11,11	0
2	NA	D	502	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.