



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:44 AM UTC

PDB ID : 2B7O / pdb_00002b7o
Title : The Structure of 3-Deoxy-D-Arabino-Heptulosonate 7-Phosphate Synthase from Mycobacterium tuberculosis
Authors : Webby, C.J.; Baker, H.M.; Lott, J.S.; Baker, E.N.; Parker, E.J.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2005-10-05
Resolution : 2.30 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

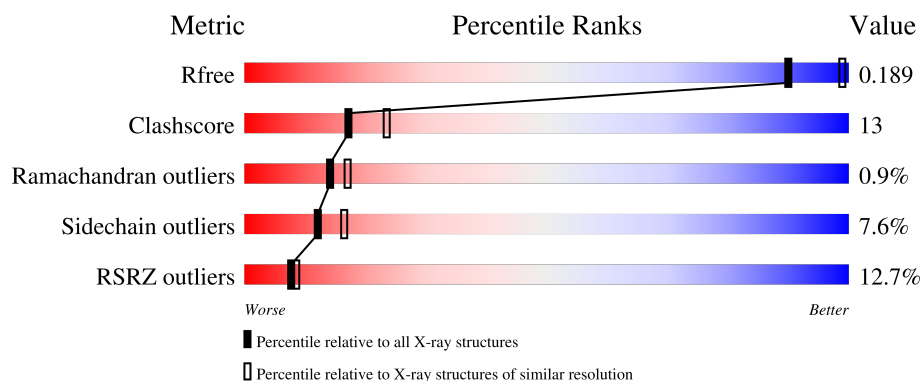
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	464	11% 75% 18% . .
1	B	464	12% 78% 16% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7329 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 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	Se	0	0	0
			3468	2170	630	651	4	13			
1	B	451	Total	C	N	O	S	Se	0	0	0
			3468	2172	629	650	4	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O53512
A	0	ALA	-	expression tag	UNP O53512
B	-1	GLY	-	expression tag	UNP O53512
B	0	ALA	-	expression tag	UNP O53512

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

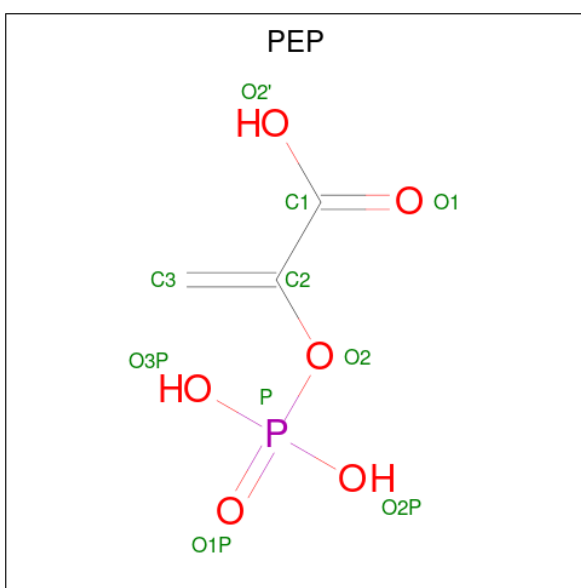
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



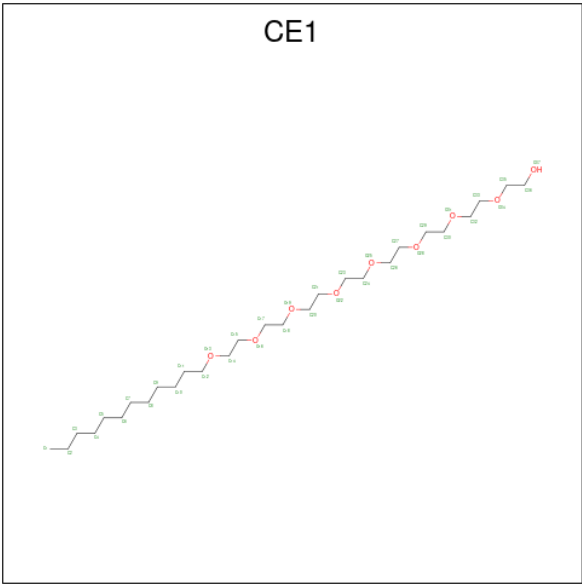
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C₂₈H₅₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	20	5		

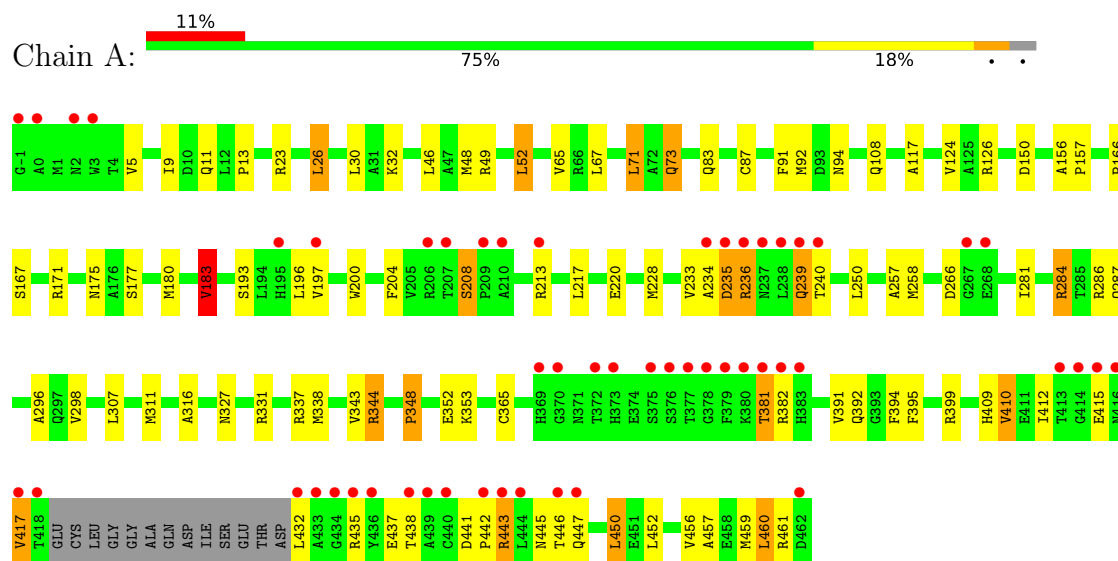
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total	O	0	0
			151	151		
6	B	185	Total	O	0	0
			185	185		

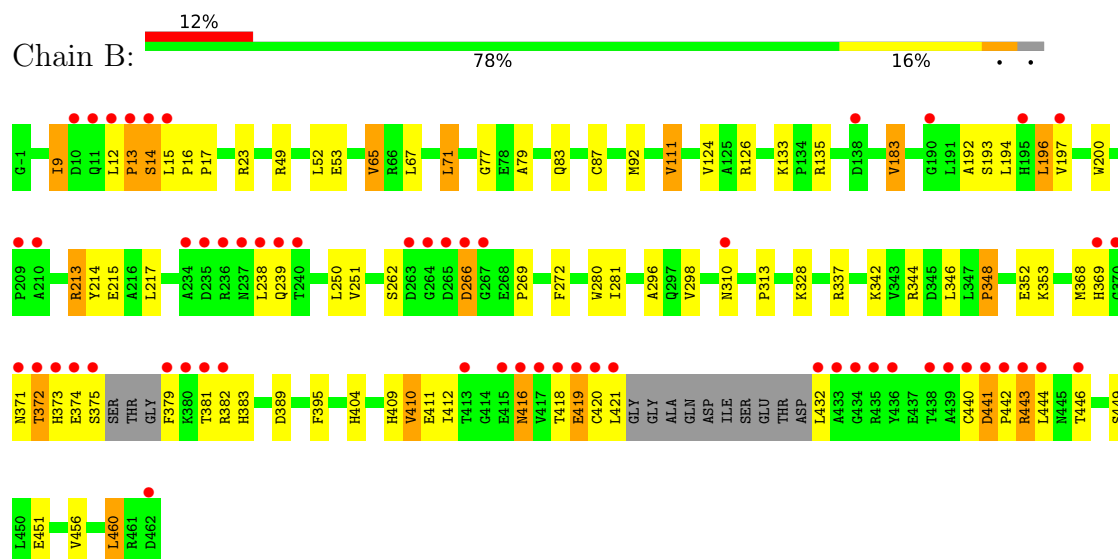
3 Residue-property plots [i](#)

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: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.09 Å 204.09 Å 66.23 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.04 – 2.30 47.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.04-2.30) 100.0 (47.04-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.224 0.187 , 0.189	Depositor DCC
R_{free} test set	3567 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7329	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: CE1, PEP, SO4, MN

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	0.84	0/3528	0.97	7/4780 (0.1%)
1	B	0.94	3/3527 (0.1%)	0.99	7/4777 (0.1%)
All	All	0.90	3/7055 (0.0%)	0.98	14/9557 (0.1%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	VAL	CA-CB	5.96	1.60	1.53
1	B	441	ASP	C-N	5.43	1.39	1.33
1	B	65	VAL	CA-CB	5.06	1.60	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	LEU	N-CA-C	-7.52	97.48	109.59
1	B	9	ILE	CB-CA-C	-6.67	103.54	111.94
1	A	32	LYS	CA-C-N	-6.49	113.29	119.85
1	A	32	LYS	C-N-CA	-6.49	113.29	119.85
1	A	438	THR	N-CA-C	6.43	117.95	111.07
1	B	418	THR	N-CA-C	6.36	113.99	108.78
1	B	183	VAL	N-CA-CB	6.21	118.99	110.54
1	A	183	VAL	N-CA-CB	5.79	118.42	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	VAL	N-CA-CB	5.66	117.17	110.55
1	B	348	PRO	N-CA-C	5.51	117.43	110.70
1	A	240	THR	N-CA-C	-5.38	100.94	109.59
1	A	348	PRO	CA-C-N	-5.24	113.64	119.19
1	A	348	PRO	C-N-CA	-5.24	113.64	119.19
1	B	183	VAL	N-CA-C	5.03	115.75	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLN	Peptide

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	3468	0	3425	102	0
1	B	3468	0	3421	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	2	0
5	A	25	0	41	12	0
6	A	151	0	0	8	0
6	B	185	0	0	5	0
All	All	7329	0	6891	175	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 (175) 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:48:MSE:CE	1:A:167:SER:HA	1.41	1.46
1:A:48:MSE:HE2	1:A:167:SER:CA	1.61	1.28
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.20	1.03
1:A:344:ARG:HD2	6:A:2030:HOH:O	1.59	1.02
1:A:171:ARG:HH21	5:A:1001:CE1:H171	1.22	1.02
1:A:52:LEU:HB3	1:A:258:MSE:CE	1.90	1.00
1:A:311:MSE:HE3	1:A:316:ALA:HB2	1.41	1.00
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.05	0.90
1:A:52:LEU:HB3	1:A:258:MSE:HE1	1.54	0.88
1:A:311:MSE:HE3	1:A:316:ALA:CB	2.02	0.88
1:A:344:ARG:HH11	1:A:344:ARG:CG	1.91	0.84
5:A:1001:CE1:C18	5:A:1001:CE1:H232	2.08	0.83
1:B:133:LYS:HD2	1:B:440:CYS:SG	2.19	0.82
1:A:311:MSE:HE3	1:A:316:ALA:CA	2.09	0.82
1:B:133:LYS:HE3	1:B:135:ARG:HD3	1.59	0.82
1:B:443:ARG:HB2	1:B:443:ARG:NH1	1.96	0.80
1:A:48:MSE:HE2	1:A:167:SER:HA	0.81	0.79
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.48	0.78
1:B:369:HIS:CE1	1:B:411:GLU:OE2	2.36	0.78
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.19	0.78
1:A:48:MSE:CE	1:A:167:SER:CA	2.38	0.78
1:B:12:LEU:N	1:B:13:PRO:HD3	1.99	0.77
1:B:410:VAL:HG13	1:B:412:ILE:HG23	1.67	0.75
1:A:52:LEU:HB3	1:A:258:MSE:HE3	1.68	0.74
5:A:1001:CE1:H232	5:A:1001:CE1:H181	1.70	0.74
1:A:311:MSE:CE	1:A:316:ALA:HA	2.19	0.72
1:A:392:GLN:HA	1:A:459:MSE:CE	2.19	0.72
1:A:48:MSE:HE3	1:A:167:SER:HA	1.63	0.72
1:A:284:ARG:HH11	1:A:284:ARG:HG3	1.55	0.72
1:B:369:HIS:NE2	1:B:411:GLU:OE2	2.22	0.72
1:B:49:ARG:NH1	6:B:2084:HOH:O	2.24	0.71
1:A:395:PHE:CG	1:A:459:MSE:HE2	2.26	0.70
1:B:197:VAL:HA	1:B:200:TRP:CZ3	2.28	0.69
1:B:9:ILE:O	1:B:12:LEU:HB2	1.93	0.68
1:A:311:MSE:CE	1:A:316:ALA:CA	2.70	0.68
1:A:9:ILE:HD13	1:A:48:MSE:HE1	1.75	0.67
1:A:228:MSE:HE3	1:A:233:VAL:HG11	1.75	0.67
1:A:395:PHE:CD1	1:A:459:MSE:HE2	2.29	0.67
1:B:266:ASP:HB2	6:B:2075:HOH:O	1.93	0.66
1:A:392:GLN:HA	1:A:459:MSE:HE3	1.78	0.66
1:B:213:ARG:HH11	1:B:213:ARG:CG	2.08	0.65
1:A:52:LEU:O	1:A:258:MSE:HE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:CD1	1:A:48:MSE:HE1	2.27	0.65
1:A:23:ARG:NH1	6:A:2144:HOH:O	2.29	0.64
1:A:52:LEU:CB	1:A:258:MSE:HE1	2.27	0.64
1:B:313:PRO:HB3	1:B:353:LYS:HG3	1.81	0.63
1:A:126:ARG:HH11	1:A:409:HIS:CE1	2.16	0.62
1:A:443:ARG:H	1:A:443:ARG:HE	1.47	0.62
1:B:383:HIS:CD2	1:B:421:LEU:C	2.78	0.62
1:B:410:VAL:CG1	1:B:412:ILE:HG23	2.29	0.61
1:B:410:VAL:HG13	1:B:412:ILE:CG2	2.30	0.61
1:A:49:ARG:NE	6:A:2015:HOH:O	2.32	0.61
1:A:410:VAL:HG13	1:A:412:ILE:HG23	1.82	0.61
1:A:307:LEU:HD22	1:A:311:MSE:HE2	1.83	0.61
1:B:280:TRP:HE1	4:B:703:PEP:C3	2.14	0.61
5:A:1001:CE1:H232	5:A:1001:CE1:H182	1.82	0.60
1:B:421:LEU:H	1:B:421:LEU:HD23	1.64	0.60
1:A:126:ARG:HH11	1:A:409:HIS:HE1	1.48	0.60
1:B:126:ARG:HH11	1:B:409:HIS:CE1	2.21	0.59
1:A:213:ARG:HH11	1:A:213:ARG:HB2	1.67	0.59
1:A:220:GLU:CD	1:A:461:ARG:HH22	2.11	0.59
1:A:197:VAL:HA	1:A:200:TRP:CZ3	2.37	0.59
1:B:395:PHE:CE2	1:B:460:LEU:HD13	2.37	0.59
1:A:365:CYS:HB2	1:A:394:PHE:CD1	2.39	0.58
1:B:87:CYS:SG	1:B:441:ASP:HB2	2.44	0.57
1:A:382:ARG:HD2	1:A:442:PRO:HG2	1.87	0.57
1:A:171:ARG:NH2	5:A:1001:CE1:H171	2.07	0.57
1:A:257:ALA:C	1:A:258:MSE:HE2	2.29	0.56
1:A:443:ARG:HE	1:A:443:ARG:N	2.03	0.56
1:B:126:ARG:HH11	1:B:409:HIS:HE1	1.51	0.56
1:A:87:CYS:SG	1:A:441:ASP:HB2	2.45	0.56
1:A:92:MSE:O	5:A:1001:CE1:O25	2.24	0.56
1:B:262:SER:HB3	1:B:272:PHE:CE1	2.40	0.56
1:B:371:ASN:O	1:B:372:THR:HG23	2.06	0.55
1:A:395:PHE:HB2	1:A:459:MSE:CE	2.36	0.55
1:A:311:MSE:HE1	1:A:316:ALA:HA	1.88	0.55
1:A:395:PHE:CD1	1:A:459:MSE:CE	2.90	0.54
1:B:395:PHE:HE2	1:B:460:LEU:HD13	1.73	0.54
1:B:67:LEU:HG	1:B:71:LEU:HD22	1.90	0.54
1:B:281:ILE:HD11	1:B:296:ALA:HB2	1.89	0.53
1:B:410:VAL:CG1	1:B:412:ILE:CG2	2.85	0.53
1:A:365:CYS:HB2	1:A:394:PHE:CG	2.43	0.53
1:A:67:LEU:HG	1:A:71:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:HB2	1:B:443:ARG:CZ	2.37	0.53
1:B:443:ARG:HB2	1:B:443:ARG:HH11	1.71	0.53
1:A:437:GLU:H	1:A:443:ARG:HH12	1.56	0.52
1:B:79:ALA:O	1:B:404:HIS:HE1	1.92	0.52
1:A:175:ASN:HD21	5:A:1001:CE1:H151	1.74	0.52
1:B:12:LEU:N	1:B:13:PRO:CD	2.70	0.52
1:A:220:GLU:OE1	1:A:461:ARG:NH2	2.43	0.52
1:A:457:ALA:O	1:A:461:ARG:HG3	2.10	0.52
1:B:13:PRO:O	1:B:14:SER:HB2	2.09	0.52
1:B:280:TRP:HE1	4:B:703:PEP:H31	1.75	0.52
1:A:344:ARG:CD	6:A:2030:HOH:O	2.34	0.51
1:A:443:ARG:H	1:A:443:ARG:NE	2.07	0.51
1:A:13:PRO:HD2	1:B:92:MSE:HG3	1.91	0.51
1:B:196:LEU:HD13	1:B:200:TRP:CZ2	2.44	0.51
1:B:375:SER:HA	1:B:379:PHE:O	2.10	0.51
1:A:83:GLN:HA	1:A:124:VAL:O	2.11	0.50
1:B:421:LEU:HD21	1:B:432:LEU:HD11	1.93	0.50
1:B:213:ARG:CG	1:B:213:ARG:NH1	2.74	0.50
1:A:48:MSE:HE2	1:A:167:SER:CB	2.39	0.50
1:B:262:SER:HB3	1:B:272:PHE:HE1	1.77	0.50
1:A:410:VAL:HG13	1:A:412:ILE:CG2	2.42	0.50
1:A:126:ARG:HD2	1:A:409:HIS:HE1	1.76	0.50
1:B:310:ASN:ND2	1:B:310:ASN:H	2.09	0.50
1:B:49:ARG:O	1:B:53:GLU:HG3	2.11	0.49
1:A:344:ARG:CG	1:A:344:ARG:NH1	2.61	0.49
1:B:342:LYS:HB3	1:B:346:LEU:HD12	1.96	0.48
1:A:284:ARG:HG3	1:A:284:ARG:NH1	2.27	0.48
5:A:1001:CE1:H142	5:A:1001:CE1:H201	1.96	0.48
1:A:49:ARG:NH2	6:A:2015:HOH:O	2.46	0.48
1:A:52:LEU:CB	1:A:258:MSE:CE	2.78	0.47
1:A:5:VAL:HG13	1:B:9:ILE:HD11	1.96	0.47
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.96	0.47
1:A:409:HIS:HD2	6:A:2081:HOH:O	1.96	0.47
1:B:416:ASN:ND2	1:B:416:ASN:H	2.12	0.47
1:A:410:VAL:CG1	1:A:412:ILE:HG23	2.42	0.47
1:A:26:LEU:HD13	1:A:30:LEU:HD12	1.97	0.47
1:A:171:ARG:HH21	5:A:1001:CE1:C17	2.09	0.47
1:A:281:ILE:HD11	1:A:296:ALA:HB2	1.95	0.47
1:A:204:PHE:O	1:A:208:SER:HB3	2.15	0.46
1:A:395:PHE:O	1:A:399:ARG:HG2	2.16	0.45
1:A:73:GLN:HE21	1:A:73:GLN:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:O	1:A:331:ARG:HD2	2.17	0.45
1:A:417:VAL:HG22	1:A:435:ARG:O	2.17	0.45
1:A:392:GLN:HA	1:A:459:MSE:HE1	1.96	0.44
1:B:13:PRO:O	1:B:14:SER:CB	2.65	0.44
1:A:311:MSE:HE3	1:A:316:ALA:N	2.32	0.44
1:A:417:VAL:HG12	1:A:445:ASN:HB3	1.98	0.44
1:B:269:PRO:HD2	6:B:2076:HOH:O	2.17	0.44
1:A:108:GLN:NE2	1:A:450:LEU:HD21	2.33	0.44
1:B:111:VAL:HG12	1:B:194:LEU:HD22	2.00	0.44
1:B:456:VAL:O	1:B:460:LEU:HD22	2.18	0.43
1:A:48:MSE:HE2	1:A:167:SER:N	2.25	0.43
1:B:77:GLY:HA2	1:B:404:HIS:CG	2.53	0.43
1:A:338:MSE:HG3	1:A:343:VAL:HG23	2.01	0.43
1:A:381:THR:HA	1:A:442:PRO:HG3	2.00	0.43
1:B:373:HIS:CE1	1:B:381:THR:HG23	2.54	0.43
1:B:313:PRO:CB	1:B:353:LYS:HG3	2.46	0.43
1:B:381:THR:HA	1:B:442:PRO:HG3	2.00	0.43
1:A:395:PHE:CE2	1:A:460:LEU:HD13	2.54	0.43
1:B:87:CYS:H	1:B:443:ARG:HD2	1.84	0.43
1:B:126:ARG:HD2	1:B:409:HIS:HE1	1.83	0.43
1:B:12:LEU:H	1:B:13:PRO:HD3	1.82	0.42
1:A:94:ASN:O	5:A:1001:CE1:C21	2.67	0.42
1:A:180:MSE:HE3	1:A:183:VAL:HG22	2.00	0.42
1:B:443:ARG:HH11	1:B:443:ARG:H	1.67	0.42
1:B:83:GLN:HA	1:B:124:VAL:O	2.20	0.42
1:A:410:VAL:CG1	1:A:412:ILE:CG2	2.98	0.42
1:A:48:MSE:HG3	1:A:166:PRO:O	2.20	0.42
1:A:234:ALA:O	1:A:235:ASP:C	2.63	0.41
1:B:214:TYR:CZ	1:B:451:GLU:HG3	2.54	0.41
1:A:91:PHE:CE2	1:A:150:ASP:HB3	2.55	0.41
1:A:286:ARG:O	1:A:287:GLN:C	2.63	0.41
1:A:391:VAL:O	1:A:459:MSE:HE1	2.20	0.41
1:B:16:PRO:HA	1:B:17:PRO:HD3	1.91	0.41
1:B:213:ARG:HD3	1:B:214:TYR:CZ	2.56	0.41
1:B:412:ILE:CG2	1:B:449:SER:OG	2.68	0.41
1:A:409:HIS:CD2	6:A:2081:HOH:O	2.73	0.41
1:B:23:ARG:HD2	6:B:2082:HOH:O	2.21	0.41
1:B:348:PRO:O	1:B:352:GLU:HG3	2.20	0.41
1:A:156:ALA:HA	1:A:157:PRO:HD3	1.96	0.41
1:A:348:PRO:O	1:A:352:GLU:HG3	2.21	0.41
1:A:94:ASN:O	5:A:1001:CE1:H211	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:O	1:A:456:VAL:HG23	2.20	0.41
1:B:344:ARG:NH2	1:B:389:ASP:OD2	2.54	0.41
1:B:368:MSE:HE2	1:B:411:GLU:HB2	2.03	0.41
1:A:213:ARG:HB2	1:A:213:ARG:NH1	2.34	0.41
1:A:399:ARG:NH2	1:A:459:MSE:O	2.53	0.40
5:A:1001:CE1:C18	5:A:1001:CE1:C23	2.90	0.40
1:B:192:ALA:HB3	6:B:2065:HOH:O	2.21	0.40
1:A:117:ALA:HB2	1:A:460:LEU:HG	2.03	0.40
1:A:49:ARG:CZ	6:A:2015:HOH:O	2.69	0.40
1:A:235:ASP:OD2	1:A:236:ARG:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	447/464 (96%)	432 (97%)	12 (3%)	3 (1%)	18	23
1	B	445/464 (96%)	422 (95%)	18 (4%)	5 (1%)	11	13
All	All	892/928 (96%)	854 (96%)	30 (3%)	8 (1%)	14	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	239	GLN
1	A	266	ASP
1	B	14	SER
1	B	419	GLU
1	B	420	CYS
1	B	13	PRO
1	B	374	GLU

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	364/363 (100%)	333 (92%)	31 (8%)	10	13
1	B	363/363 (100%)	339 (93%)	24 (7%)	15	21
All	All	727/726 (100%)	672 (92%)	55 (8%)	12	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	26	LEU
1	A	46	LEU
1	A	52	LEU
1	A	65	VAL
1	A	71	LEU
1	A	73	GLN
1	A	177	SER
1	A	183	VAL
1	A	193	SER
1	A	196	LEU
1	A	208	SER
1	A	217	LEU
1	A	236	ARG
1	A	250	LEU
1	A	284	ARG
1	A	298	VAL
1	A	327	ASN
1	A	337	ARG
1	A	344	ARG
1	A	353	LYS
1	A	381	THR
1	A	410	VAL
1	A	415	GLU
1	A	417	VAL
1	A	432	LEU
1	A	443	ARG

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Mol	Chain	Res	Type
1	A	446	THR
1	A	447	GLN
1	A	450	LEU
1	A	460	LEU
1	B	15	LEU
1	B	52	LEU
1	B	65	VAL
1	B	71	LEU
1	B	183	VAL
1	B	193	SER
1	B	196	LEU
1	B	213	ARG
1	B	215	GLU
1	B	217	LEU
1	B	238	LEU
1	B	239	GLN
1	B	250	LEU
1	B	266	ASP
1	B	298	VAL
1	B	328	LYS
1	B	337	ARG
1	B	372	THR
1	B	410	VAL
1	B	416	ASN
1	B	419	GLU
1	B	443	ARG
1	B	446	THR
1	B	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	239	GLN
1	A	360	GLN
1	A	409	HIS
1	A	416	ASN
1	A	447	GLN
1	B	44	GLN
1	B	68	GLN
1	B	392	GLN
1	B	409	HIS

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Mol	Chain	Res	Type
1	B	416	ASN
1	B	447	GLN
1	B	448	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 [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	PEP	B	703	-	9,9,9	2.65	3 (33%)	11,13,13	2.21	5 (45%)
4	PEP	A	702	-	9,9,9	4.19	1 (11%)	11,13,13	3.19	3 (27%)
3	SO4	A	2001	-	4,4,4	0.26	0	6,6,6	0.31	0
3	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.18	0
5	CE1	A	1001	-	24,24,36	0.50	0	23,23,35	0.62	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	PEP	B	703	-	-	4/9/9/9	-
5	CE1	A	1001	-	-	13/22/22/34	-
4	PEP	A	702	-	-	4/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	PEP	C2-C1	-12.21	1.37	1.49
4	B	703	PEP	P-O2	-6.21	1.48	1.59
4	B	703	PEP	O2-C2	-3.23	1.30	1.39
4	B	703	PEP	C2-C1	2.94	1.52	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	PEP	C3-C2-C1	-7.33	109.17	122.73
4	A	702	PEP	O2'-C1-C2	5.03	122.48	113.91
4	A	702	PEP	O1-C1-C2	-4.75	114.63	121.79
4	B	703	PEP	O2-C2-C3	-4.50	116.25	124.85
4	B	703	PEP	O2'-C1-O1	-3.08	116.57	123.90
4	B	703	PEP	O1-C1-C2	2.73	125.90	121.79
4	B	703	PEP	C3-C2-C1	-2.10	118.84	122.73
4	B	703	PEP	O2P-P-O1P	2.01	118.68	110.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	PEP	O1-C1-C2-C3
4	A	702	PEP	O2'-C1-C2-C3
4	B	703	PEP	O1-C1-C2-C3
4	B	703	PEP	O1-C1-C2-O2
4	B	703	PEP	O2'-C1-C2-C3
4	B	703	PEP	O2'-C1-C2-O2
5	A	1001	CE1	C14-C15-O16-C17
5	A	1001	CE1	C10-C11-C12-O13
5	A	1001	CE1	C5-C6-C7-C8
5	A	1001	CE1	O13-C14-C15-O16
5	A	1001	CE1	O16-C17-C18-O19
5	A	1001	CE1	O22-C23-C24-O25
5	A	1001	CE1	C7-C8-C9-C10

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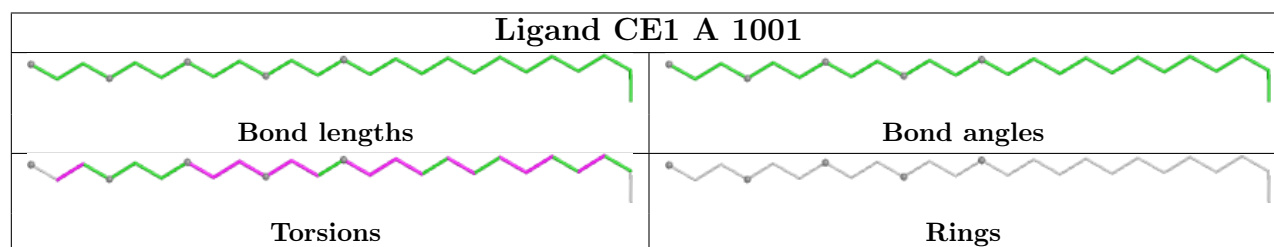
Mol	Chain	Res	Type	Atoms
5	A	1001	CE1	C9-C10-C11-C12
5	A	1001	CE1	C2-C3-C4-C5
5	A	1001	CE1	C17-C18-O19-C20
5	A	1001	CE1	C18-C17-O16-C15
4	A	702	PEP	O1-C1-C2-O2
5	A	1001	CE1	C11-C12-O13-C14
5	A	1001	CE1	C4-C5-C6-C7
4	A	702	PEP	O2'-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	PEP	2	0
5	A	1001	CE1	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	438/464 (94%)	0.45	53 (12%) 8 9	25, 41, 80, 97	0
1	B	438/464 (94%)	0.30	58 (13%) 7 8	23, 35, 77, 95	0
All	All	876/928 (94%)	0.38	111 (12%) 8 8	23, 38, 79, 97	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	LEU	7.3
1	B	421	LEU	7.0
1	B	237	ASN	6.9
1	B	11	GLN	6.7
1	B	13	PRO	6.5
1	B	379	PHE	6.3
1	A	438	THR	6.1
1	A	377	THR	5.9
1	B	432	LEU	5.6
1	A	418	THR	5.3
1	B	418	THR	5.2
1	A	379	PHE	5.2
1	B	375	SER	5.2
1	A	416	ASN	5.0
1	A	443	ARG	4.8
1	B	15	LEU	4.8
1	B	436	TYR	4.6
1	A	237	ASN	4.6
1	A	234	ALA	4.6
1	B	12	LEU	4.5
1	B	420	CYS	4.5
1	B	380	LYS	4.4
1	A	439	ALA	4.3
1	A	378	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	3	TRP	4.2
1	A	413	THR	4.2
1	A	434	GLY	4.1
1	B	238	LEU	4.1
1	A	381	THR	4.0
1	B	413	THR	4.0
1	A	238	LEU	4.0
1	A	436	TYR	3.9
1	B	240	THR	3.9
1	A	440	CYS	3.9
1	B	14	SER	3.9
1	B	373	HIS	3.9
1	A	442	PRO	3.8
1	A	417	VAL	3.8
1	B	372	THR	3.8
1	A	433	ALA	3.7
1	A	375	SER	3.7
1	A	380	LYS	3.6
1	A	376	SER	3.6
1	B	310	ASN	3.6
1	B	415	GLU	3.5
1	B	446	THR	3.4
1	A	239	GLN	3.4
1	A	235	ASP	3.4
1	B	239	GLN	3.4
1	A	236	ARG	3.4
1	B	438	THR	3.3
1	B	234	ALA	3.3
1	B	265	ASP	3.3
1	B	416	ASN	3.3
1	A	210	ALA	3.2
1	B	236	ARG	3.2
1	A	-1	GLY	3.2
1	B	267	GLY	3.1
1	A	0	ALA	3.1
1	A	373	HIS	3.1
1	B	442	PRO	3.1
1	B	462	ASP	3.0
1	B	441	ASP	3.0
1	B	433	ALA	3.0
1	B	439	ALA	3.0
1	B	440	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	267	GLY	3.0
1	B	417	VAL	2.9
1	A	240	THR	2.9
1	A	369	HIS	2.9
1	B	444	LEU	2.9
1	B	419	GLU	2.8
1	B	443	ARG	2.7
1	B	381	THR	2.7
1	B	266	ASP	2.7
1	A	370	GLY	2.7
1	A	435	ARG	2.7
1	A	415	GLU	2.7
1	B	374	GLU	2.7
1	B	195	HIS	2.6
1	A	462	ASP	2.6
1	B	235	ASP	2.6
1	A	207	THR	2.6
1	A	195	HIS	2.6
1	A	2	ASN	2.6
1	A	209	PRO	2.5
1	B	371	ASN	2.5
1	A	197	VAL	2.4
1	B	434	GLY	2.4
1	A	444	LEU	2.4
1	B	435	ARG	2.4
1	B	263	ASP	2.3
1	A	446	THR	2.3
1	A	383	HIS	2.3
1	B	209	PRO	2.3
1	B	190	GLY	2.3
1	B	264	GLY	2.3
1	A	372	THR	2.3
1	A	382	ARG	2.3
1	B	369	HIS	2.3
1	B	370	GLY	2.2
1	A	213	ARG	2.2
1	A	414	GLY	2.2
1	B	382	ARG	2.2
1	B	138	ASP	2.1
1	B	197	VAL	2.1
1	A	447	GLN	2.1
1	B	10	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	206	ARG	2.1
1	B	210	ALA	2.1
1	A	268	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](#)

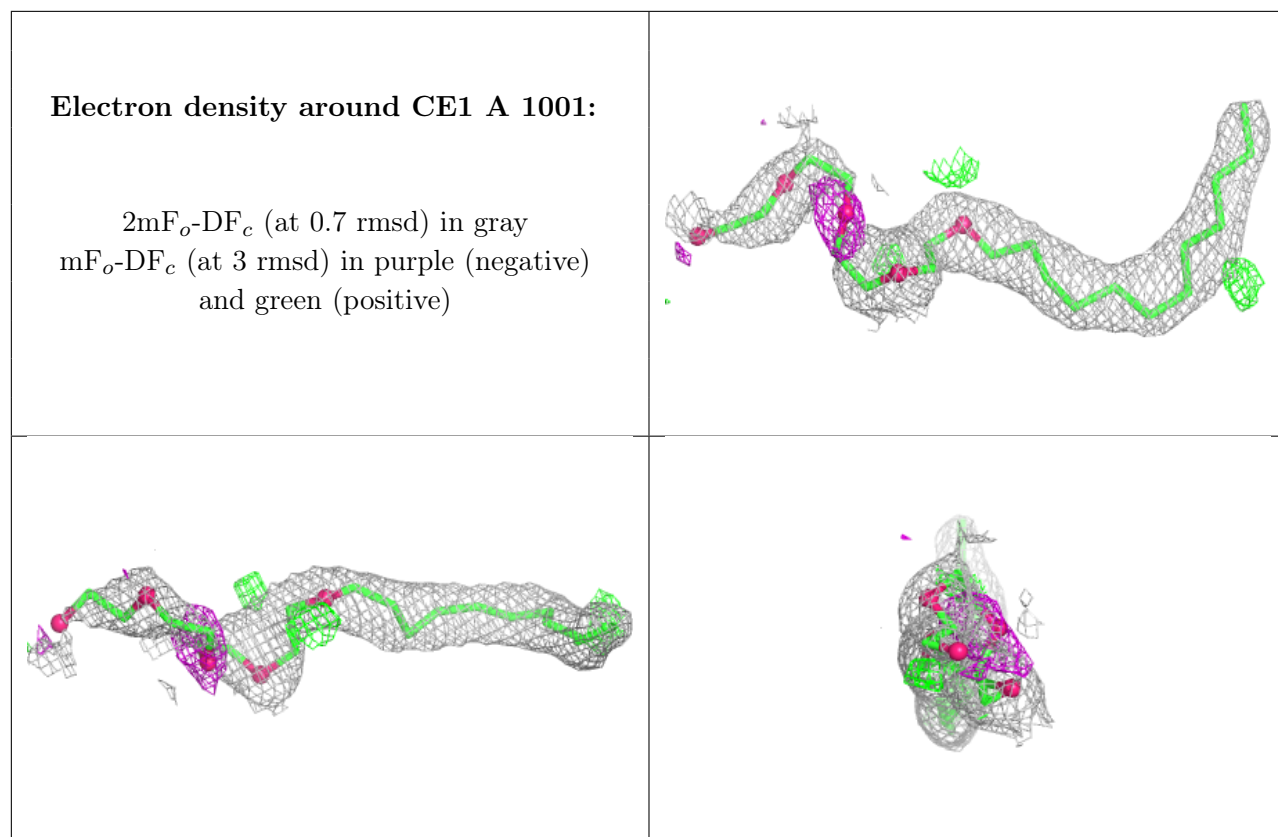
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	SO4	B	2002	5/5	0.80	0.20	68,68,69,69	5
4	PEP	A	702	10/10	0.80	0.22	45,48,50,52	10
3	SO4	A	2001	5/5	0.82	0.17	53,54,55,56	5
4	PEP	B	703	10/10	0.85	0.17	34,40,43,44	10
5	CE1	A	1001	25/37	0.87	0.22	50,56,65,66	0
2	MN	B	701	1/1	0.93	0.08	57,57,57,57	1
2	MN	A	700	1/1	0.97	0.06	55,55,55,55	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.