



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:07 AM UTC

PDB ID : 3NUE / pdb_00003nue
Title : The structure of 3-deoxy-d-arabino-heptulosonate 7-phosphate synthase from mycobacterium tuberculosis complexed with tryptophan
Authors : Parker, E.J.; Jameson, G.B.; Jiao, W.; Webby, C.J.; Baker, E.N.; Baker, H.M.
Deposited on : 2010-07-06
Resolution : 2.50 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

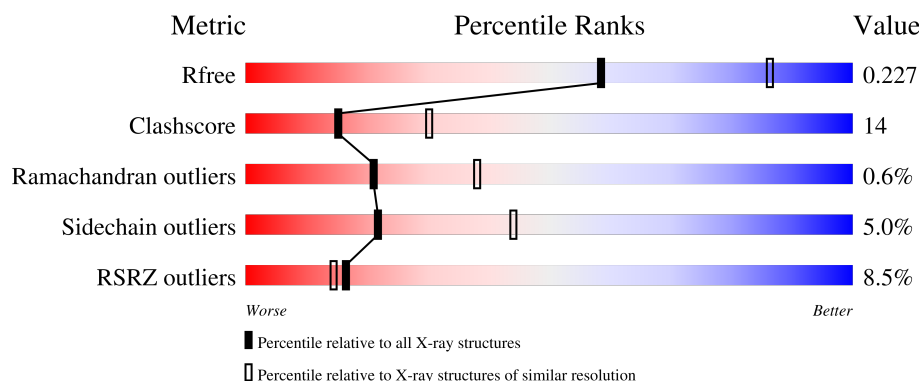
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	9% 74% 20% • •
1	B	464	8% 77% 17% • 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
6	GOL	B	470	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7431 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 Probable 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	7	0
			3533	2210	650	655	18			
1	B	443	Total	C	N	O	S	0	10	0
			3480	2174	636	653	17			

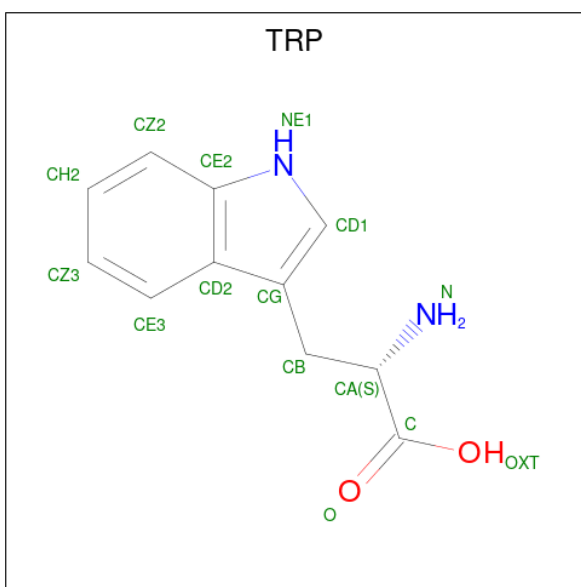
There are 4 discrepancies between the modelled and reference sequences:

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).

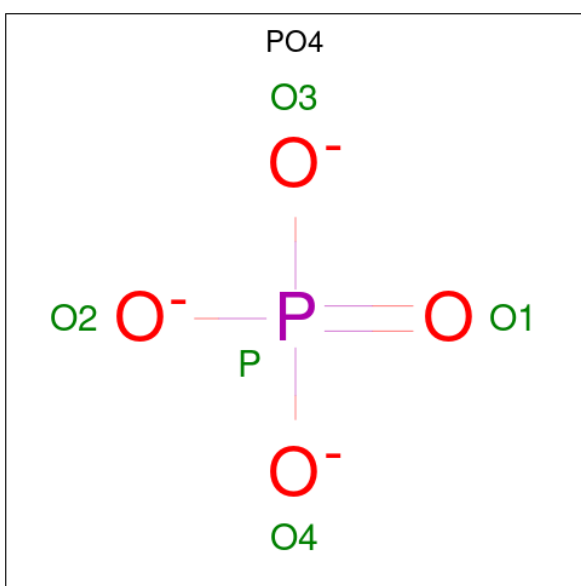
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



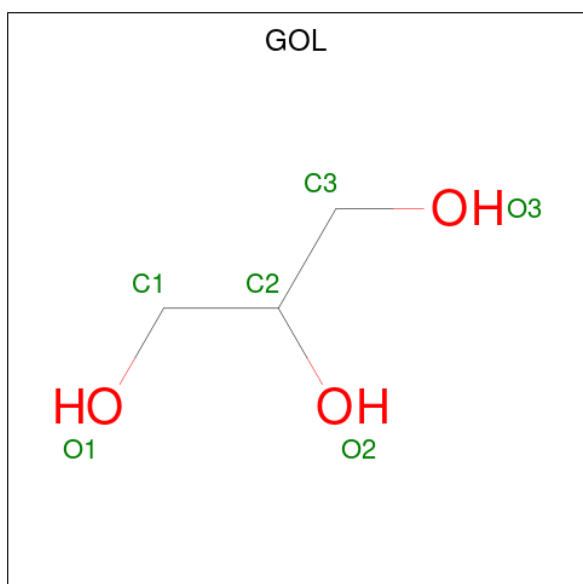
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

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



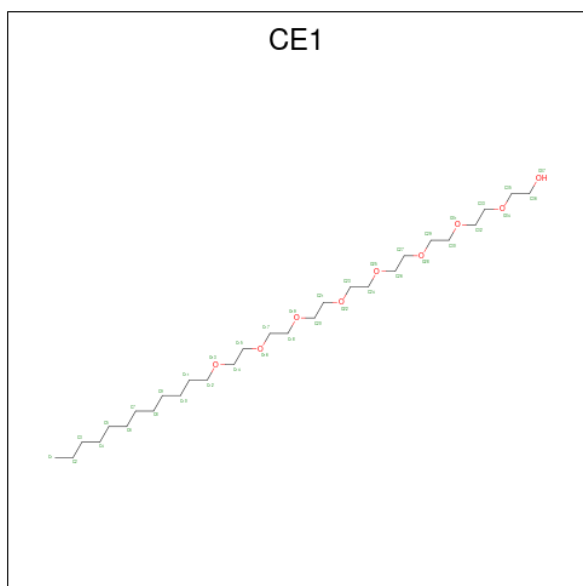
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

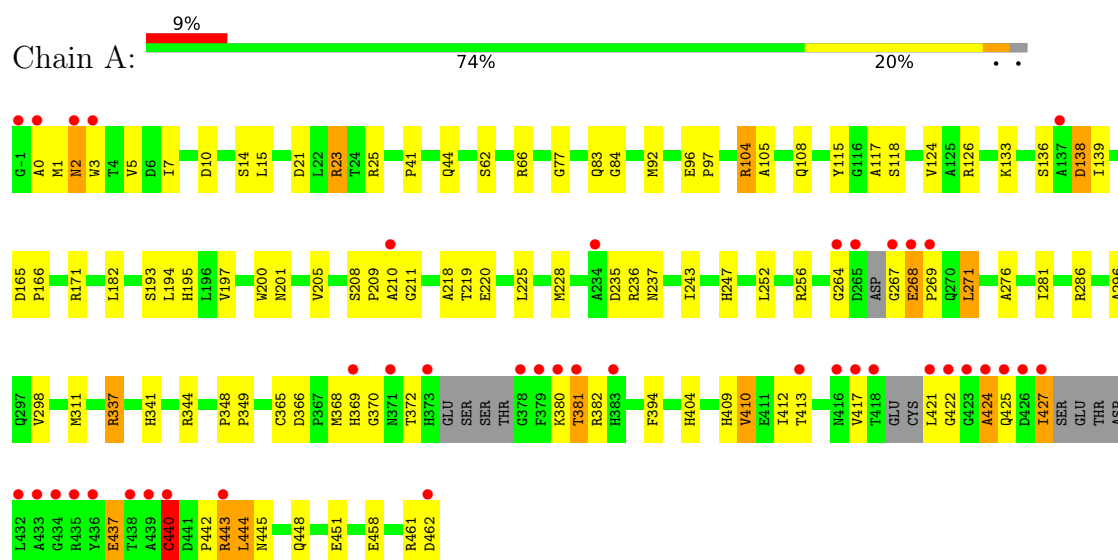
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	135	Total 135	O 135	0	0
9	B	162	Total 162	O 162	0	0

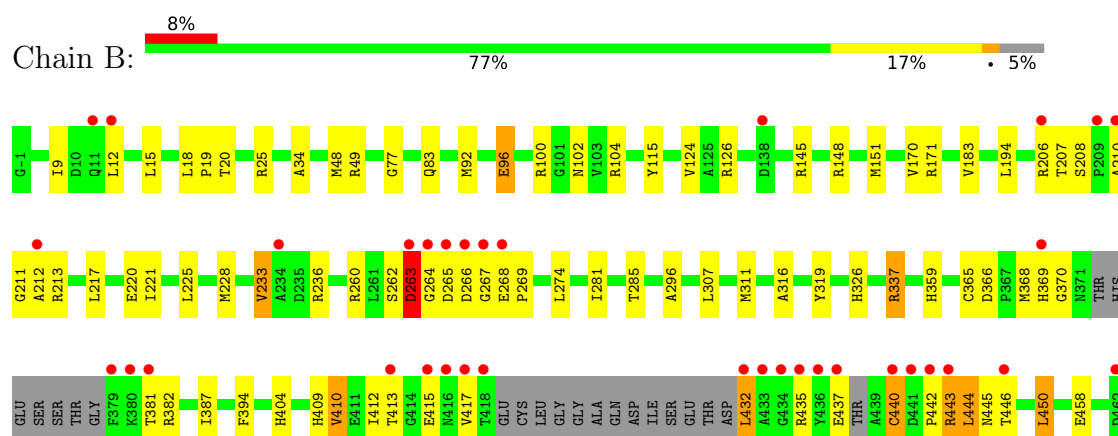
3 Residue-property plots [i](#)

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



- Molecule 1: Probable 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.71 Å 204.71 Å 66.26 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.69 – 2.50 38.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.69-2.50) 99.9 (38.69-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.228 0.188 , 0.227	Depositor DCC
R_{free} test set	2815 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CL, GOL, CE1, MN, PO4, 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	1.04	1/3603 (0.0%)	1.04	5/4896 (0.1%)
1	B	1.08	1/3551 (0.0%)	1.05	9/4828 (0.2%)
All	All	1.06	2/7154 (0.0%)	1.05	14/9724 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	ALA	C-O	-5.38	1.17	1.24
1	A	105	ALA	CA-CB	-5.36	1.45	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	CYS	N-CA-C	9.17	120.35	108.24
1	A	2	ASN	N-CA-C	7.85	121.35	111.69
1	A	15	LEU	CA-C-N	-7.42	112.74	120.38
1	A	15	LEU	C-N-CA	-7.42	112.74	120.38
1	B	444	LEU	N-CA-C	-6.62	100.48	110.28
1	A	23	ARG	N-CA-C	6.31	118.24	111.36
1	B	233	VAL	O-C-N	6.31	129.90	122.83
1	B	96	GLU	CA-C-N	-5.75	112.58	118.85
1	B	96	GLU	C-N-CA	-5.75	112.58	118.85
1	B	233	VAL	CA-C-N	5.54	131.55	121.97
1	B	233	VAL	C-N-CA	5.54	131.55	121.97
1	B	450	LEU	N-CA-C	-5.38	105.42	111.28
1	A	1	MET	N-CA-C	-5.28	106.69	113.02
1	B	233	VAL	N-CA-CB	5.18	116.75	110.95

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	3533	0	3486	91	0
1	B	3480	0	3419	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	9	0	0
3	B	15	0	9	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	12	0	16	1	0
6	B	30	0	40	9	0
7	A	16	0	29	0	0
8	B	1	0	0	1	0
9	A	135	0	0	8	0
9	B	162	0	0	11	0
All	All	7431	0	7008	193	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 14.

All (193) 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:B:267[A]:GLY:O	1:B:268[A]:GLU:CG	1.71	1.35
1:B:267[A]:GLY:O	1:B:268[A]:GLU:HG3	1.12	1.25
1:B:267[A]:GLY:C	1:B:268[A]:GLU:HG3	1.64	1.14
1:A:424:ALA:HB2	1:A:448:GLN:HG2	1.12	1.09
1:A:422:GLY:HA2	1:A:427:ILE:HB	1.44	0.98
1:B:96:GLU:HG3	9:B:9038:HOH:O	1.63	0.97
1:B:366:ASP:OD2	1:B:369:HIS:ND1	1.97	0.96
1:A:424:ALA:HB2	1:A:448:GLN:CG	1.95	0.95
1:A:443[B]:ARG:HE	1:A:443[B]:ARG:H	1.05	0.94
1:A:267:GLY:O	1:A:268:GLU:CB	2.18	0.92
1:A:443[B]:ARG:O	1:A:444:LEU:HB2	1.67	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:HD2	9:B:9177:HOH:O	1.76	0.85
1:A:443[B]:ARG:H	1:A:443[B]:ARG:NE	1.75	0.84
1:B:267[A]:GLY:O	1:B:268[A]:GLU:CB	2.27	0.83
1:A:421:LEU:HD23	1:A:442:PRO:HB2	1.61	0.82
1:A:443[B]:ARG:O	1:A:444:LEU:CB	2.28	0.82
1:A:366:ASP:OD2	1:A:369:HIS:ND1	2.13	0.81
1:B:268[A]:GLU:HB3	1:B:269[A]:PRO:CD	2.11	0.81
8:B:469:CL:CL	9:B:9030:HOH:O	2.36	0.80
1:A:2:ASN:O	1:A:3:TRP:HB2	1.82	0.78
1:B:268[A]:GLU:HB3	1:B:269[A]:PRO:HD3	1.65	0.78
1:B:267[A]:GLY:O	1:B:268[A]:GLU:CD	2.28	0.77
1:B:48:MET:CE	1:B:170:VAL:CG2	2.64	0.75
1:B:443:ARG:CZ	1:B:443:ARG:HB2	2.16	0.75
1:B:307:LEU:HD22	1:B:311:MET:HE2	1.68	0.74
1:A:424:ALA:CB	1:A:448:GLN:HG2	2.06	0.73
1:A:382:ARG:HB2	1:A:421:LEU:HD22	1.70	0.73
1:A:421:LEU:CD2	1:A:442:PRO:HB2	2.18	0.73
1:B:25:ARG:HH22	6:B:467:GOL:H11	1.56	0.71
1:A:10:ASP:OD1	1:B:171:ARG:NH2	2.22	0.71
1:B:25:ARG:HH22	6:B:467:GOL:C1	2.06	0.69
1:B:263[B]:ASP:HB2	1:B:269[B]:PRO:HA	1.73	0.69
1:A:5:VAL:HG13	1:B:9:ILE:HD11	1.74	0.68
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.76	0.68
1:B:381:THR:HG22	1:B:382:ARG:N	2.10	0.67
1:B:48:MET:CE	1:B:170:VAL:HG23	2.25	0.66
1:A:366:ASP:CG	1:A:369:HIS:HD1	2.03	0.66
1:B:366:ASP:CG	1:B:369:HIS:HD1	2.02	0.66
1:B:267[A]:GLY:C	1:B:268[A]:GLU:CG	2.42	0.65
1:B:48:MET:CE	1:B:170:VAL:HG21	2.26	0.65
1:B:264[A]:GLY:O	1:B:265[A]:ASP:HB2	1.97	0.64
1:A:92[B]:MET:HA	1:A:92[B]:MET:HE2	1.81	0.63
1:A:382:ARG:HB2	1:A:421:LEU:CD2	2.29	0.62
1:A:0:ALA:HB1	1:A:2:ASN:CB	2.30	0.61
1:B:48:MET:HE3	1:B:170:VAL:CG2	2.31	0.61
1:A:437:GLU:H	1:A:443[B]:ARG:HH12	1.49	0.60
1:A:5:VAL:HG13	1:B:9:ILE:CD1	2.32	0.60
1:A:458:GLU:O	1:A:462:ASP:HB2	2.02	0.60
1:A:413:THR:HG22	1:A:443[B]:ARG:HG3	1.84	0.60
1:B:264[B]:GLY:C	1:B:265[B]:ASP:OD2	2.46	0.59
1:B:311:MET:HE3	1:B:316:ALA:N	2.17	0.59
1:B:311:MET:HE1	1:B:319:TYR:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HG	1:B:225:LEU:HD21	1.85	0.59
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.66	0.59
1:B:381:THR:HA	1:B:442:PRO:HG3	1.85	0.58
1:B:366:ASP:OD2	1:B:369:HIS:CE1	2.56	0.58
1:B:126:ARG:HH11	1:B:409:HIS:CE1	2.22	0.57
1:B:264[B]:GLY:O	1:B:265[B]:ASP:OD2	2.23	0.57
1:B:48:MET:HE2	1:B:170:VAL:HG23	1.85	0.57
1:B:410:VAL:HG13	1:B:412:ILE:HG23	1.86	0.57
1:A:443[B]:ARG:HE	1:A:443[B]:ARG:N	1.89	0.57
1:A:0:ALA:HB1	1:A:2:ASN:HB2	1.86	0.57
1:B:18:LEU:HG	6:B:470:GOL:H2	1.86	0.57
1:B:311:MET:HE1	1:B:319:TYR:CD2	2.41	0.56
1:B:412:ILE:C	1:B:443:ARG:HG2	2.30	0.56
1:A:7:ILE:CD1	1:B:48:MET:HE1	2.36	0.56
1:A:382:ARG:HD2	1:A:442:PRO:HG2	1.87	0.56
1:B:417:VAL:HG11	1:B:443:ARG:HH22	1.71	0.56
1:B:381:THR:HG22	1:B:382:ARG:H	1.69	0.56
1:A:126:ARG:HH11	1:A:409:HIS:HE1	1.54	0.55
1:B:281:ILE:HD11	1:B:296:ALA:HB2	1.89	0.55
1:B:48:MET:HE3	1:B:170:VAL:HG21	1.87	0.55
1:A:236:ARG:HB2	9:A:9019:HOH:O	2.06	0.55
1:A:225:LEU:HD23	1:A:228:MET:HE3	1.89	0.55
1:A:138:ASP:OD1	1:A:138:ASP:N	2.36	0.55
1:A:171:ARG:NH1	9:A:9029:HOH:O	2.39	0.54
1:B:262[B]:SER:O	1:B:263[B]:ASP:HB2	2.06	0.54
1:B:417:VAL:HG11	1:B:443:ARG:NH2	2.22	0.54
1:B:49:ARG:NH1	9:B:9326:HOH:O	2.40	0.54
1:A:7:ILE:HD11	1:B:48:MET:HE1	1.89	0.54
1:B:412:ILE:O	1:B:443:ARG:HG2	2.08	0.54
1:A:220:GLU:OE1	1:A:461:ARG:NH2	2.41	0.53
1:A:10:ASP:CG	1:B:171:ARG:HH21	2.15	0.53
1:B:268[A]:GLU:CB	1:B:269[A]:PRO:CD	2.79	0.52
1:B:417:VAL:HG12	1:B:445:ASN:HB3	1.92	0.52
1:B:265[B]:ASP:O	1:B:266[B]:ASP:CB	2.57	0.52
1:A:83:GLN:HA	1:A:124:VAL:O	2.08	0.52
1:A:133:LYS:NZ	1:A:440:CYS:HB2	2.25	0.52
1:A:421:LEU:HD12	1:A:444:LEU:CD1	2.39	0.52
1:A:252:LEU:O	1:A:256:ARG:HG2	2.10	0.52
1:B:443:ARG:HB3	1:B:444:LEU:O	2.10	0.51
1:B:381:THR:OG1	1:B:432:LEU:HD21	2.10	0.51
1:A:14:SER:HB2	9:A:9016:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HD3	9:B:9153:HOH:O	2.11	0.51
1:A:66:ARG:HD3	9:A:2662:HOH:O	2.11	0.50
1:A:264:GLY:HA2	1:A:269:PRO:HD3	1.93	0.50
1:B:83:GLN:HA	1:B:124:VAL:O	2.10	0.50
1:A:84:GLY:HA2	1:A:410:VAL:O	2.12	0.50
1:B:262[B]:SER:O	1:B:263[B]:ASP:CB	2.59	0.50
1:B:417:VAL:HG21	1:B:443:ARG:HH12	1.75	0.50
1:A:412:ILE:HG22	1:A:444:LEU:HD23	1.93	0.50
1:B:126:ARG:HH11	1:B:409:HIS:HE1	1.56	0.50
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.47	0.50
1:B:410:VAL:CG1	1:B:412:ILE:HG23	2.42	0.50
1:B:337:ARG:O	1:B:337:ARG:HD3	2.12	0.49
1:A:104[B]:ARG:HG2	1:A:200:TRP:CZ3	2.48	0.49
1:B:443:ARG:HD2	9:B:9010:HOH:O	2.12	0.49
1:A:421:LEU:HD12	1:A:444:LEU:HD12	1.95	0.49
1:B:359:HIS:CE1	9:B:9230:HOH:O	2.65	0.49
1:B:115:TYR:OH	1:B:220:GLU:HG2	2.13	0.49
1:A:108:GLN:HG2	1:A:201:ASN:OD1	2.13	0.49
1:B:381:THR:CG2	1:B:382:ARG:N	2.75	0.48
1:A:445:ASN:OD1	1:A:448:GLN:HG3	2.14	0.48
1:A:209:PRO:HG2	1:A:425:GLN:CB	2.43	0.48
1:B:18:LEU:CG	6:B:470:GOL:H2	2.43	0.48
1:A:424:ALA:HB1	1:A:451:GLU:OE1	2.13	0.48
1:B:443:ARG:H	1:B:443:ARG:NE	2.11	0.48
1:B:211:GLY:O	1:B:212:ALA:C	2.57	0.47
6:A:2647:GOL:H32	9:A:2697:HOH:O	2.14	0.47
1:B:381:THR:CG2	1:B:382:ARG:H	2.28	0.47
1:B:264[A]:GLY:O	1:B:265[A]:ASP:CB	2.61	0.47
1:B:368:MET:C	1:B:370:GLY:H	2.21	0.47
1:B:15:LEU:CB	9:B:2681:HOH:O	2.63	0.47
1:B:102:ASN:OD1	1:B:413:THR:HA	2.15	0.47
1:B:210:ALA:O	1:B:211:GLY:C	2.58	0.46
1:A:237[B]:ASN:HD21	1:B:236:ARG:NH2	2.13	0.46
1:B:19:PRO:O	1:B:20:THR:C	2.57	0.46
1:B:145:ARG:NH1	9:B:2691:HOH:O	2.45	0.46
1:A:210:ALA:O	1:A:211:GLY:C	2.59	0.46
1:B:104[A]:ARG:NH1	9:B:2685:HOH:O	2.49	0.46
1:B:365:CYS:HB2	1:B:394:PHE:CD1	2.51	0.45
1:A:421:LEU:HD12	1:A:444:LEU:CA	2.46	0.45
1:A:96[A]:GLU:O	1:A:97:PRO:C	2.57	0.45
1:A:133:LYS:HZ3	1:A:440:CYS:HB2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:CD2	6:B:470:GOL:H2	2.46	0.45
1:A:417:VAL:HG21	1:A:443[B]:ARG:CG	2.47	0.45
1:A:96[A]:GLU:HG2	1:A:182:LEU:HD21	1.97	0.45
1:A:381:THR:HA	1:A:442:PRO:HG3	1.99	0.45
1:A:421:LEU:HD12	1:A:444:LEU:HA	1.98	0.45
1:B:265[B]:ASP:O	1:B:266[B]:ASP:HB2	2.16	0.45
1:A:193:SER:O	1:A:197:VAL:HG23	2.17	0.45
1:A:267:GLY:HA2	9:A:9169:HOH:O	2.15	0.45
1:B:18:LEU:HD21	6:B:470:GOL:H2	1.99	0.45
1:B:311:MET:HE3	1:B:316:ALA:CA	2.46	0.45
6:B:471:GOL:H31	9:B:9195:HOH:O	2.17	0.45
1:B:443:ARG:HB2	1:B:443:ARG:NH2	2.31	0.45
1:A:77:GLY:HA2	1:A:404:HIS:CD2	2.53	0.44
1:A:337:ARG:HD3	1:A:337:ARG:O	2.18	0.44
1:B:15:LEU:CB	6:B:470:GOL:H11	2.47	0.44
1:B:326:HIS:HE1	6:B:467:GOL:H31	1.81	0.44
1:A:344:ARG:HB2	9:A:9253:HOH:O	2.17	0.44
1:A:5:VAL:CG1	1:B:9:ILE:HD11	2.44	0.44
1:B:366:ASP:OD1	1:B:366:ASP:C	2.61	0.44
1:A:194:LEU:HG	1:A:225:LEU:HD21	2.00	0.44
1:B:104[B]:ARG:HH11	1:B:104[B]:ARG:HD2	1.55	0.44
1:A:368:MET:C	1:A:370:GLY:H	2.25	0.44
1:A:126:ARG:HH11	1:A:409:HIS:CE1	2.34	0.44
1:B:206[B]:ARG:HG2	1:B:207:THR:CG2	2.48	0.44
1:B:268[B]:GLU:O	1:B:269[B]:PRO:C	2.60	0.44
1:A:195:HIS:CD2	1:A:225:LEU:HD22	2.53	0.43
1:B:260:ARG:HG3	1:B:274:LEU:HD12	1.99	0.43
1:A:165:ASP:HA	1:A:166:PRO:HD3	1.86	0.43
1:A:341:HIS:ND1	1:A:341:HIS:N	2.65	0.43
1:A:421:LEU:HD12	1:A:444:LEU:CB	2.48	0.43
1:A:365:CYS:HB2	1:A:394:PHE:CD1	2.53	0.43
1:B:77:GLY:HA2	1:B:404:HIS:CD2	2.53	0.43
1:B:225:LEU:HD23	1:B:228:MET:HE3	2.00	0.43
1:A:41:PRO:HG2	1:A:44:GLN:OE1	2.18	0.43
1:A:348:PRO:HB2	1:A:349:PRO:HD3	2.00	0.43
1:B:9:ILE:HA	1:B:12:LEU:HD12	2.00	0.43
1:B:126:ARG:HD2	1:B:409:HIS:HE1	1.84	0.43
1:A:281:ILE:HD11	1:A:296:ALA:HB2	2.00	0.43
1:A:412:ILE:O	1:A:443[A]:ARG:HD2	2.19	0.43
1:B:417:VAL:CG2	1:B:435:ARG:O	2.67	0.42
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ILE:HD13	1:B:444:LEU:HD21	2.00	0.42
1:A:271:LEU:HD23	1:A:298:VAL:HG12	2.01	0.42
1:A:443[A]:ARG:O	1:A:444:LEU:C	2.62	0.42
1:B:458:GLU:OE1	1:B:458:GLU:HA	2.20	0.42
1:A:247:HIS:CE1	1:A:276:ALA:HB2	2.55	0.42
1:B:9:ILE:HA	1:B:12:LEU:CD1	2.50	0.42
1:A:115:TYR:OH	1:A:220:GLU:HG2	2.20	0.42
1:B:206[B]:ARG:HG2	1:B:207:THR:HG23	2.02	0.41
1:A:437:GLU:H	1:A:443[B]:ARG:NH1	2.17	0.41
1:A:117:ALA:O	1:A:118:SER:HB2	2.20	0.41
1:B:151:MET:O	1:B:151:MET:HG2	2.20	0.41
1:A:205:VAL:HG21	1:A:218:ALA:HB2	2.03	0.41
1:A:443[B]:ARG:H	1:A:443[B]:ARG:CD	2.33	0.40
1:A:286:ARG:CZ	1:A:311:MET:HE1	2.51	0.40
1:B:48:MET:HE3	1:B:170:VAL:HG23	1.97	0.40
1:A:25:ARG:NH1	9:A:2705:HOH:O	2.45	0.40
1:A:413:THR:CG2	1:A:443[B]:ARG:HG3	2.49	0.40
1:B:217:LEU:O	1:B:221:ILE:HG13	2.21	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	450/464 (97%)	426 (95%)	20 (4%)	4 (1%)	14	27
1	B	445/464 (96%)	423 (95%)	20 (4%)	2 (0%)	30	49
All	All	895/928 (96%)	849 (95%)	40 (4%)	6 (1%)	21	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	444	LEU
1	B	263[A]	ASP
1	B	263[B]	ASP
1	A	424	ALA
1	A	440	CYS

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	367/376 (98%)	344 (94%)	23 (6%)	16	34
1	B	363/376 (96%)	347 (96%)	16 (4%)	25	50
All	All	730/752 (97%)	691 (95%)	39 (5%)	22	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	23	ARG
1	A	62	SER
1	A	104[A]	ARG
1	A	104[B]	ARG
1	A	136	SER
1	A	138	ASP
1	A	139	ILE
1	A	208	SER
1	A	219	THR
1	A	235	ASP
1	A	243	ILE
1	A	271	LEU
1	A	337	ARG
1	A	372	THR
1	A	380	LYS
1	A	381	THR
1	A	410	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	427	ILE
1	A	437	GLU
1	A	440	CYS
1	A	443[A]	ARG
1	A	443[B]	ARG
1	B	92	MET
1	B	183	VAL
1	B	208	SER
1	B	233	VAL
1	B	263[A]	ASP
1	B	263[B]	ASP
1	B	285	THR
1	B	337	ARG
1	B	410	VAL
1	B	415	GLU
1	B	432	LEU
1	B	437	GLU
1	B	440	CYS
1	B	443	ARG
1	B	446	THR
1	B	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	340	ASN
1	A	373	HIS
1	A	392	GLN
1	A	409	HIS
1	B	195	HIS
1	B	239	GLN
1	B	326	HIS
1	B	409	HIS
1	B	447	GLN

5.3.3 RNA ⓘ

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 19 ligands modelled in this entry, 3 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	$\# Z > 2$
6	GOL	A	2647	-	5,5,5	0.30	0	5,5,5	1.09	0
5	SO4	B	464	-	4,4,4	0.27	0	6,6,6	0.40	0
6	GOL	B	470	-	5,5,5	0.36	0	5,5,5	0.84	0
5	SO4	A	466	-	4,4,4	0.30	0	6,6,6	0.50	0
5	SO4	B	465	-	4,4,4	0.54	0	6,6,6	1.04	1 (16%)
6	GOL	B	471	-	5,5,5	0.45	0	5,5,5	1.30	0
4	PO4	B	463	-	4,4,4	1.24	0	6,6,6	1.11	0
3	TRP	B	9004	-	15,16,16	1.04	1 (6%)	18,22,22	0.94	1 (5%)
7	CE1	A	1001	-	15,15,36	0.66	0	14,14,35	0.54	0
3	TRP	A	9004	-	15,16,16	1.13	1 (6%)	18,22,22	0.75	0
6	GOL	A	467	-	5,5,5	0.59	0	5,5,5	0.77	0
4	PO4	A	464	-	4,4,4	0.95	0	6,6,6	1.40	0
6	GOL	B	468	-	5,5,5	0.47	0	5,5,5	0.47	0
6	GOL	B	467	-	5,5,5	0.49	0	5,5,5	1.04	0
5	SO4	A	465	-	4,4,4	0.23	0	6,6,6	0.58	0
6	GOL	B	2647	-	5,5,5	0.63	0	5,5,5	0.55	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
6	GOL	A	2647	-	-	2/4/4/4	-
6	GOL	B	470	-	-	1/4/4/4	-
6	GOL	B	471	-	-	4/4/4/4	-
7	CE1	A	1001	-	-	7/13/13/34	-
3	TRP	B	9004	-	-	0/8/8/8	0/2/2/2
3	TRP	A	9004	-	-	0/8/8/8	0/2/2/2
6	GOL	A	467	-	-	2/4/4/4	-
6	GOL	B	468	-	-	2/4/4/4	-
6	GOL	B	467	-	-	2/4/4/4	-
6	GOL	B	2647	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9004	TRP	OXT-C	-2.63	1.22	1.30
3	A	9004	TRP	OXT-C	-2.57	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9004	TRP	OXT-C-O	-3.45	116.25	124.08
5	B	465	SO4	O4-S-O2	-2.06	98.79	109.56

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2647	GOL	O1-C1-C2-O2
6	A	2647	GOL	O1-C1-C2-C3
6	A	467	GOL	C1-C2-C3-O3
6	B	467	GOL	O1-C1-C2-C3
6	B	468	GOL	C1-C2-C3-O3
6	B	471	GOL	C1-C2-C3-O3
6	B	471	GOL	O2-C2-C3-O3
6	A	467	GOL	O2-C2-C3-O3
7	A	1001	CE1	C10-C11-C12-O13
6	B	471	GOL	O1-C1-C2-C3
7	A	1001	CE1	C9-C10-C11-C12
6	B	468	GOL	O2-C2-C3-O3
7	A	1001	CE1	O13-C14-C15-O16
6	B	471	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

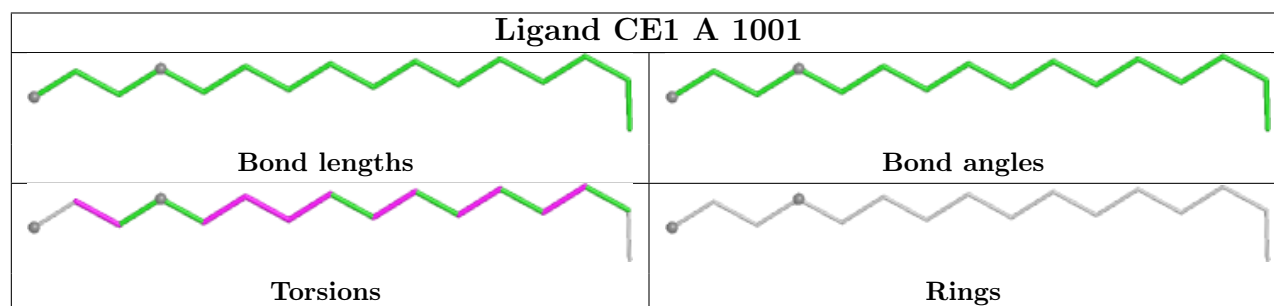
Mol	Chain	Res	Type	Atoms
7	A	1001	CE1	C4-C5-C6-C7
6	B	467	GOL	O1-C1-C2-O2
7	A	1001	CE1	C11-C10-C9-C8
7	A	1001	CE1	C2-C3-C4-C5
6	B	470	GOL	O2-C2-C3-O3
7	A	1001	CE1	C6-C7-C8-C9

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2647	GOL	1	0
6	B	470	GOL	5	0
6	B	471	GOL	1	0
6	B	467	GOL	3	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	453/464 (97%)	0.03	41 (9%) 15 13	8, 25, 69, 86	7 (1%)
1	B	443/464 (95%)	-0.17	35 (7%) 18 16	11, 22, 56, 79	10 (2%)
All	All	896/928 (96%)	-0.07	76 (8%) 16 14	8, 23, 61, 86	17 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	GLY	6.3
1	A	427	ILE	5.8
1	B	379	PHE	5.8
1	A	443[A]	ARG	5.7
1	B	432	LEU	5.7
1	B	380	LYS	5.5
1	A	433	ALA	5.4
1	B	267[A]	GLY	5.3
1	B	265[A]	ASP	5.3
1	B	263[A]	ASP	5.3
1	A	432	LEU	5.0
1	A	380	LYS	4.8
1	A	0	ALA	4.8
1	B	433	ALA	4.8
1	B	266[A]	ASP	4.8
1	A	265	ASP	4.8
1	B	436	TYR	4.6
1	A	378	GLY	4.5
1	A	421	LEU	4.5
1	B	413	THR	4.3
1	A	379	PHE	4.3
1	B	418	THR	4.3
1	A	3	TRP	4.3
1	B	381	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	426	ASP	4.2
1	B	210	ALA	4.0
1	B	434	GLY	4.0
1	A	373	HIS	4.0
1	A	425	GLN	3.9
1	B	441	ASP	3.9
1	B	11	GLN	3.9
1	B	437	GLU	3.8
1	A	436	TYR	3.8
1	A	418	THR	3.7
1	A	424	ALA	3.7
1	A	413	THR	3.6
1	B	234	ALA	3.6
1	A	422	GLY	3.5
1	A	434	GLY	3.5
1	A	381	THR	3.4
1	B	443	ARG	3.4
1	B	416	ASN	3.4
1	B	138	ASP	3.3
1	B	268[A]	GLU	3.3
1	A	438	THR	3.2
1	A	423	GLY	3.2
1	A	268	GLU	3.1
1	B	417	VAL	3.1
1	A	416	ASN	3.0
1	B	264[A]	GLY	3.0
1	A	440	CYS	3.0
1	B	442	PRO	3.0
1	B	440	CYS	2.9
1	A	264	GLY	2.8
1	A	417	VAL	2.8
1	A	383	HIS	2.7
1	A	267	GLY	2.7
1	A	234	ALA	2.6
1	A	210	ALA	2.5
1	A	439	ALA	2.5
1	B	435	ARG	2.5
1	A	137	ALA	2.4
1	B	369	HIS	2.4
1	B	212	ALA	2.4
1	A	435	ARG	2.4
1	A	369	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	371	ASN	2.3
1	B	209	PRO	2.3
1	A	269	PRO	2.2
1	B	446	THR	2.1
1	B	206[A]	ARG	2.1
1	A	462	ASP	2.1
1	A	2	ASN	2.1
1	B	415	GLU	2.0
1	B	462	ASP	2.0
1	B	12	LEU	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.

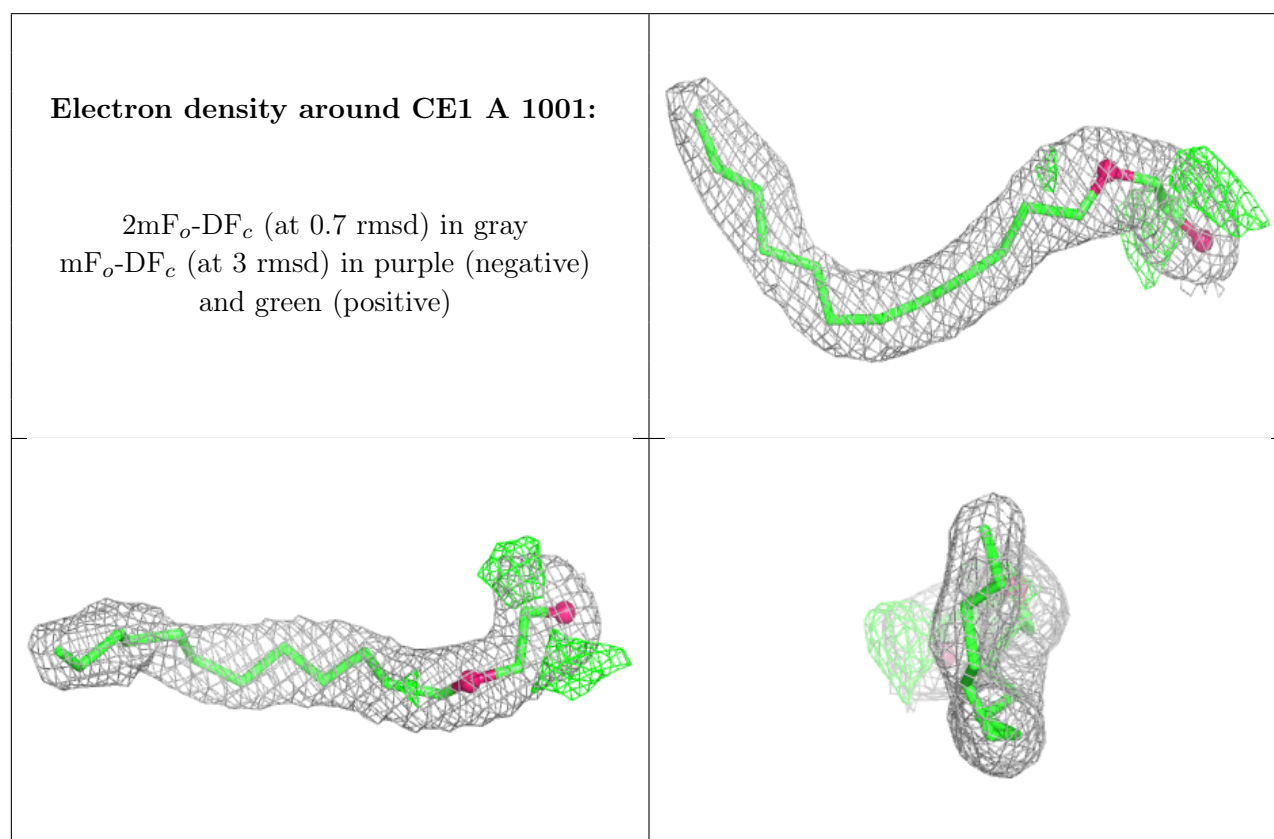
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	466	5/5	0.77	0.19	88,88,90,91	0
5	SO4	A	465	5/5	0.84	0.20	70,77,80,83	0
6	GOL	B	467	6/6	0.84	0.15	37,46,48,55	0
6	GOL	B	471	6/6	0.87	0.14	18,32,34,36	0
6	GOL	B	470	6/6	0.89	0.16	34,43,47,51	0
2	MN	B	466	1/1	0.90	0.08	55,55,55,55	1
7	CE1	A	1001	16/37	0.91	0.14	16,31,35,37	0
2	MN	A	463	1/1	0.93	0.07	48,48,48,48	1
5	SO4	B	465	5/5	0.94	0.12	26,29,37,39	0
6	GOL	A	2647	6/6	0.95	0.10	26,30,33,36	0
6	GOL	A	467	6/6	0.95	0.10	25,34,36,40	0
5	SO4	B	464	5/5	0.95	0.08	41,41,42,43	5
6	GOL	B	468	6/6	0.97	0.06	23,28,32,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRP	B	9004	15/15	0.98	0.05	11,15,17,21	0
4	PO4	A	464	5/5	0.98	0.06	29,29,33,38	0
6	GOL	B	2647	6/6	0.98	0.05	18,22,24,26	0
3	TRP	A	9004	15/15	0.98	0.05	14,19,26,26	0
8	CL	B	469	1/1	0.98	0.05	37,37,37,37	0
4	PO4	B	463	5/5	0.99	0.06	22,23,26,27	0

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.