



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:25 AM UTC

PDB ID : 6IEN / pdb_00006ien
Title : Substrate/product bound Argininosuccinate lyase from Mycobacterium tuberculosis
Authors : Paul, A.; Mishra, A.; Surolia, A.; Vijayan, M.
Deposited on : 2018-09-14
Resolution : 2.70 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

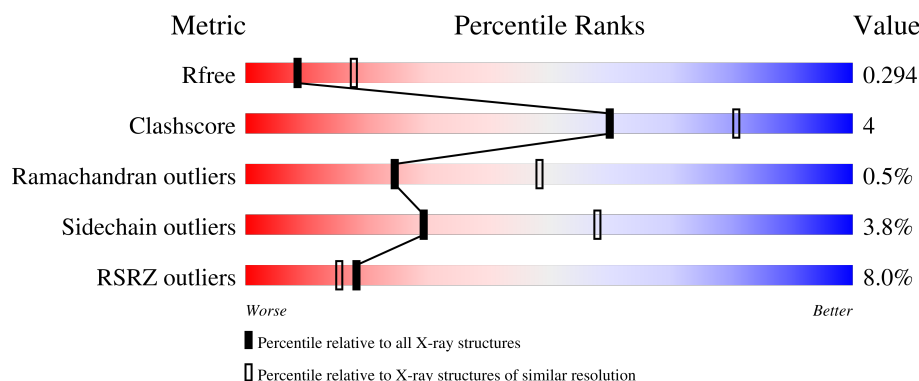
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	470	4% 84% 12% .
1	B	470	5% 84% 12% ..
1	C	470	10% 79% 9% . 11%
1	D	470	11% 76% 11% . 11%

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
2	AS1	A	501	X	-	-	-
2	AS1	B	501	X	-	-	-
2	AS1	D	501	X	-	-	-

2 Entry composition [i](#)

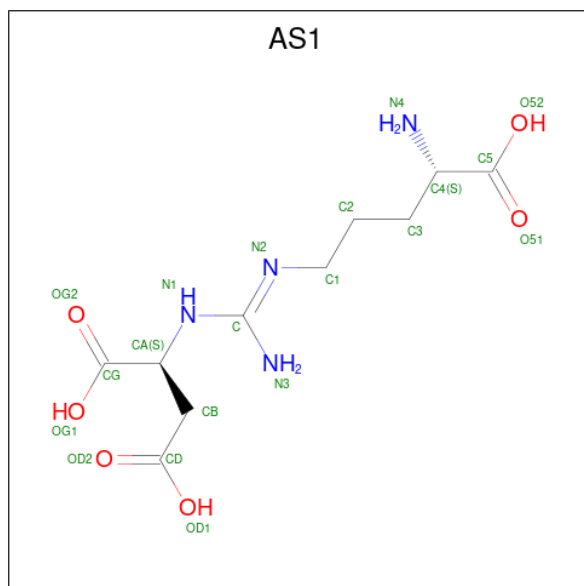
There are 7 unique types of molecules in this entry. The entry contains 13367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Argininosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3365	2103	610	645	7			
1	B	454	Total	C	N	O	S	0	0	0
			3392	2120	615	649	8			
1	C	418	Total	C	N	O	S	0	0	0
			3113	1956	562	587	8			
1	D	416	Total	C	N	O	S	0	0	0
			3097	1946	561	582	8			

- Molecule 2 is ARGININOSUCCINATE (CCD ID: AS1) (formula: C₁₀H₁₈N₄O₆).



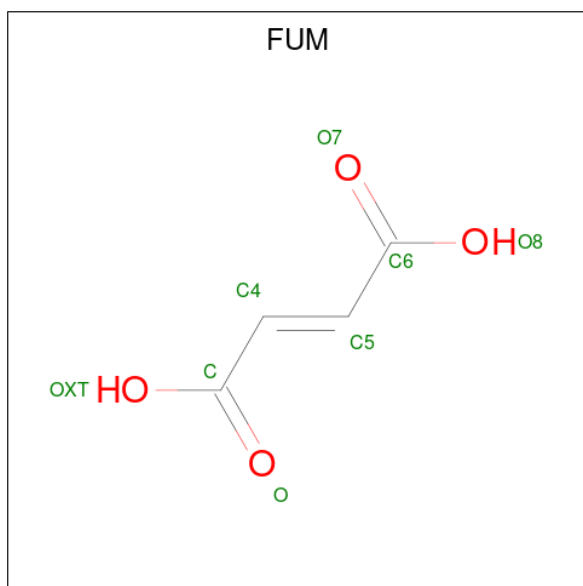
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	10	4	6		
2	B	1	Total	C	N	O	0	0
			20	10	4	6		

Continued on next page...

Continued from previous page...

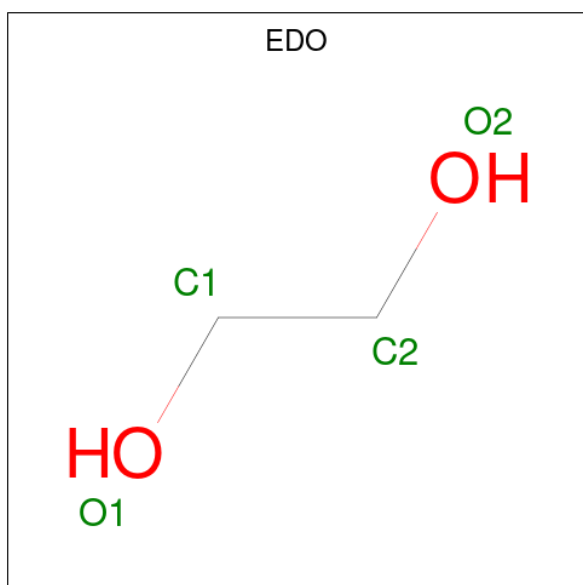
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 3 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



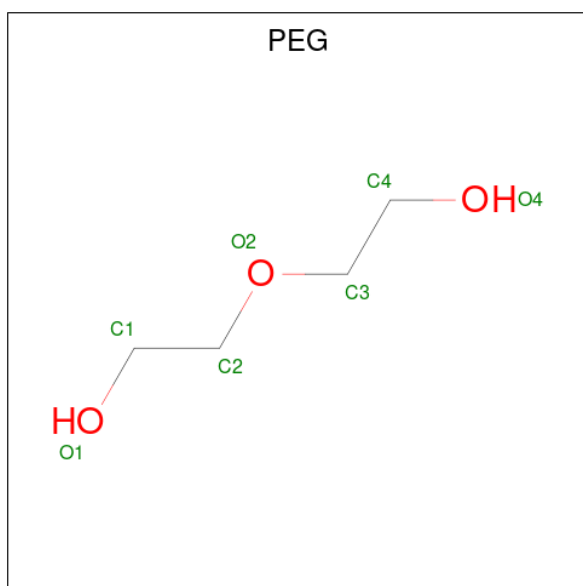
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



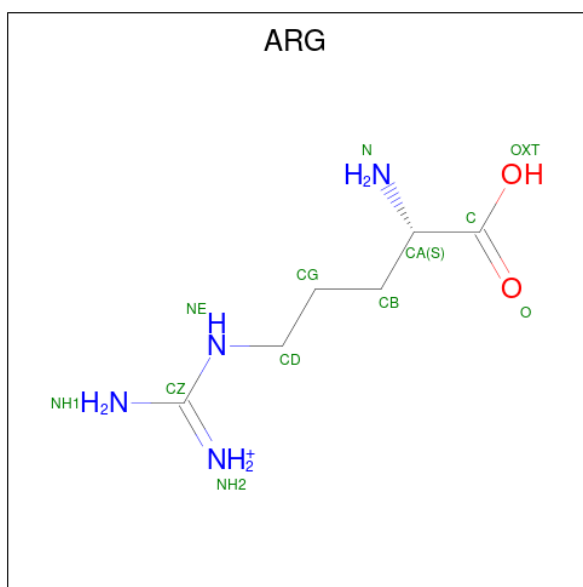
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			12	6	4	2		

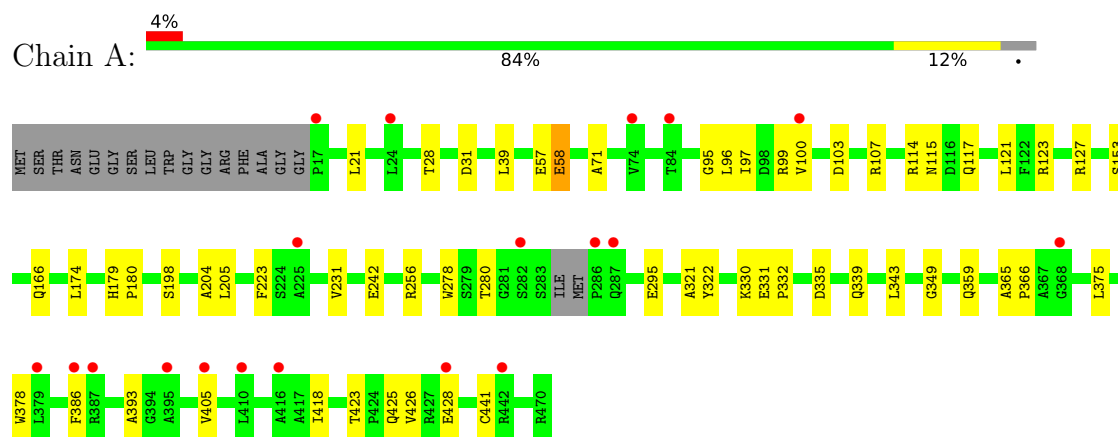
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	93	Total	O	0	0
			93	93		
7	B	73	Total	O	0	0
			73	73		
7	C	61	Total	O	0	0
			61	61		
7	D	66	Total	O	0	0
			66	66		

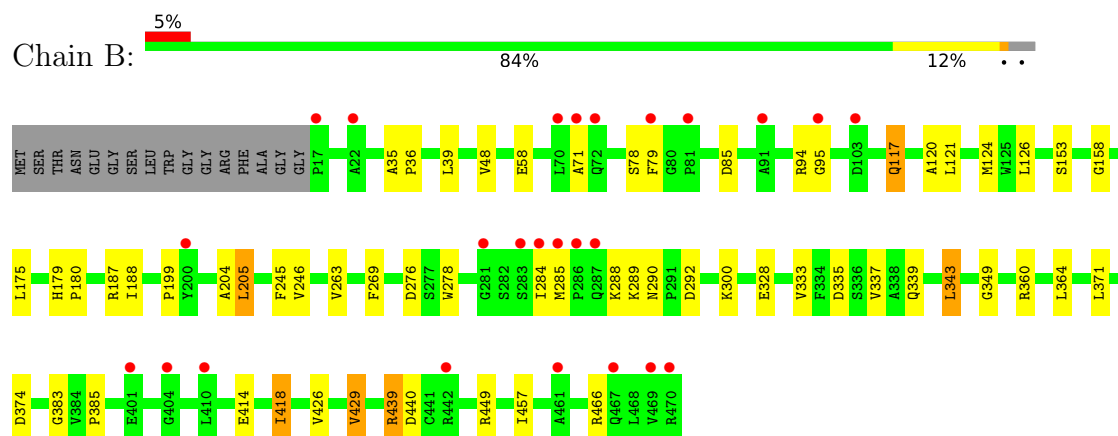
3 Residue-property plots [i](#)

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.

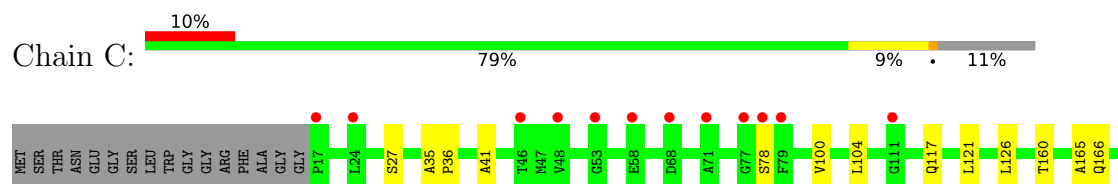
- Molecule 1: Argininosuccinate lyase

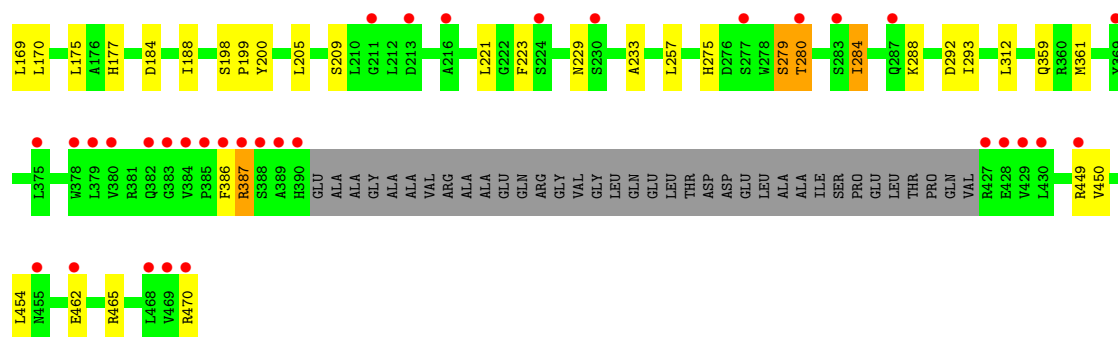


- Molecule 1: Argininosuccinate lyase

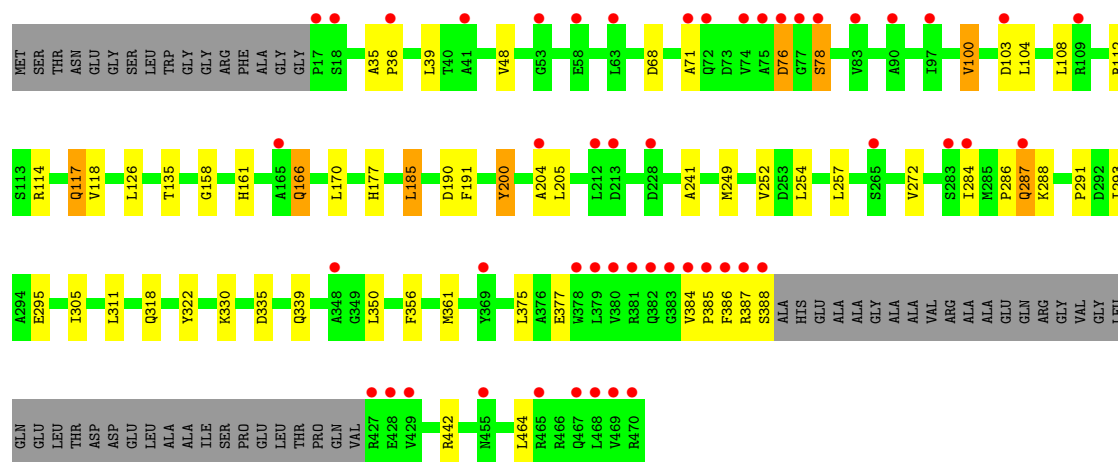
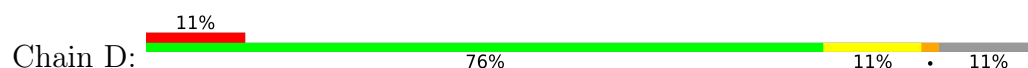


- Molecule 1: Argininosuccinate lyase





• Molecule 1: Argininosuccinate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.18Å 131.35Å 145.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.86 – 2.70 25.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.86-2.70) 99.8 (25.86-2.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.246 , 0.293 0.253 , 0.294	Depositor DCC
R_{free} test set	3056 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.486	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13367	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3206e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, FUM, PEG, AS1

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	0.71	0/3421	0.94	1/4650 (0.0%)
1	B	0.74	0/3450	0.97	0/4691
1	C	0.69	0/3168	0.96	1/4306 (0.0%)
1	D	0.73	0/3151	0.96	2/4282 (0.0%)
All	All	0.72	0/13190	0.96	4/17929 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	LEU	N-CA-C	5.79	117.67	111.36
1	D	318	GLN	CA-C-N	-5.06	114.74	119.85
1	D	318	GLN	C-N-CA	-5.06	114.74	119.85
1	C	288	LYS	N-CA-C	5.01	117.43	109.96

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	3365	0	3346	34	0
1	B	3392	0	3386	37	0
1	C	3113	0	3100	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3097	0	3091	34	0
2	A	20	0	14	5	0
2	B	20	0	14	1	0
2	D	20	0	14	1	0
3	A	8	0	1	0	0
4	A	4	0	6	0	0
4	B	12	0	18	0	0
4	C	4	0	6	0	0
5	A	7	0	10	0	0
6	C	12	0	12	0	0
7	A	93	0	0	1	0
7	B	73	0	0	3	0
7	C	61	0	0	1	0
7	D	66	0	0	0	0
All	All	13367	0	13018	112	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 4.

All (112) 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:C:275:HIS:O	1:C:279:SER:HB2	1.79	0.80
1:B:117:GLN:O	1:B:121:LEU:HG	1.87	0.74
1:A:242:GLU:OE1	1:B:187:ARG:NH1	2.24	0.68
1:A:322:TYR:OH	2:A:501:AS1:H12	1.96	0.66
1:B:284:ILE:HD11	1:D:204:ALA:HB2	1.78	0.65
1:B:120:ALA:O	1:B:124:MET:HG3	1.96	0.65
1:D:76:ASP:HB3	1:D:78:SER:OG	1.96	0.63
1:D:286:PRO:O	1:D:287:GLN:CB	2.47	0.63
1:C:462:GLU:OE1	1:C:465:ARG:NH1	2.32	0.62
1:C:117:GLN:O	1:C:121:LEU:HG	1.99	0.62
1:A:114:ARG:HB3	2:A:501:AS1:H21	1.81	0.60
1:A:117:GLN:O	1:A:121:LEU:HG	2.03	0.59
1:D:100:VAL:HG22	1:D:104:LEU:HD23	1.84	0.58
1:D:385:PRO:O	1:D:387:ARG:N	2.37	0.57
1:B:39:LEU:HD13	1:B:71:ALA:HA	1.87	0.57
1:A:97:ILE:O	1:A:100:VAL:O	2.22	0.56
1:D:286:PRO:O	1:D:287:GLN:CG	2.53	0.56
2:B:501:AS1:HB1	2:B:501:AS1:N3	2.21	0.55
1:B:333:VAL:O	1:B:337:VAL:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:TRP:CD2	1:A:426:VAL:HG23	2.42	0.54
1:B:440:ASP:O	1:B:449:ARG:NE	2.38	0.54
7:C:607:HOH:O	1:D:442:ARG:HD2	2.06	0.54
1:B:204:ALA:HB2	1:D:284:ILE:HD11	1.88	0.53
1:A:295:GLU:OE2	1:D:161:HIS:HA	2.08	0.53
1:A:95:GLY:O	1:A:99:ARG:NH1	2.39	0.53
1:B:175:LEU:HD22	1:B:457:ILE:HD13	1.91	0.53
1:C:386:PHE:O	1:C:387:ARG:CB	2.57	0.53
1:A:423:THR:OG1	1:A:425:GLN:CD	2.52	0.53
1:B:35:ALA:HB3	1:B:36:PRO:HD3	1.91	0.53
1:D:286:PRO:O	1:D:287:GLN:HB3	2.09	0.53
1:A:256:ARG:HD2	7:B:664:HOH:O	2.08	0.52
1:A:57:GLU:O	1:A:58:GLU:CB	2.57	0.52
1:A:295:GLU:OE1	1:D:161:HIS:ND1	2.43	0.51
1:A:57:GLU:O	1:A:58:GLU:HB3	2.11	0.51
1:B:285:MET:SD	1:C:165:ALA:HB1	2.51	0.51
1:B:85:ASP:OD2	1:B:94:ARG:NH2	2.45	0.50
1:B:278:TRP:CH2	1:B:349:GLY:HA3	2.46	0.50
1:C:41:ALA:HA	1:C:221:LEU:HD21	1.93	0.50
1:C:175:LEU:HD21	1:C:454:LEU:HD13	1.92	0.50
1:D:286:PRO:O	1:D:287:GLN:CD	2.55	0.50
1:D:322:TYR:CZ	2:D:501:AS1:H11	2.46	0.50
1:D:272:VAL:HG12	1:D:356:PHE:CD1	2.47	0.50
1:A:204:ALA:HB2	1:C:284:ILE:HD11	1.93	0.49
1:B:335:ASP:O	1:B:339:GLN:HG2	2.12	0.49
1:D:387:ARG:O	1:D:388:SER:CB	2.60	0.49
1:C:312:LEU:HB3	1:D:305:ILE:HG12	1.95	0.49
1:B:276:ASP:OD1	1:B:289:LYS:HE3	2.13	0.49
1:A:441:CYS:HB2	7:A:665:HOH:O	2.13	0.48
1:B:284:ILE:CG2	1:D:112:ARG:O	2.62	0.48
1:B:371:LEU:O	1:B:374:ASP:HB2	2.15	0.47
1:A:322:TYR:CZ	2:A:501:AS1:H12	2.50	0.47
1:D:39:LEU:HD13	1:D:71:ALA:HA	1.98	0.46
1:D:170:LEU:HD22	1:D:361:MET:HE1	1.96	0.46
1:B:288:LYS:NZ	1:C:160:THR:OG1	2.47	0.46
1:B:290:ASN:HB2	1:B:292:ASP:OD1	2.16	0.46
1:A:335:ASP:O	1:A:339:GLN:HG2	2.15	0.46
1:D:190:ASP:O	1:D:191:PHE:C	2.59	0.46
1:A:386:PHE:CZ	1:D:284:ILE:HG22	2.51	0.46
1:A:115:ASN:OD1	2:A:501:AS1:N1	2.49	0.45
1:B:426:VAL:O	1:B:429:VAL:HG22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:O	1:A:127:ARG:HG3	2.17	0.45
1:A:375:LEU:HD22	1:A:393:ALA:HA	1.98	0.45
1:C:209:SER:CB	1:D:377:GLU:OE1	2.64	0.45
1:D:158:GLY:N	1:D:166:GLN:O	2.46	0.45
1:C:100:VAL:HB	1:C:104:LEU:HD23	1.99	0.45
1:B:120:ALA:HB2	1:B:199:PRO:HG2	1.98	0.45
1:B:439:ARG:NH1	7:B:608:HOH:O	2.49	0.44
1:C:199:PRO:HB3	1:C:233:ALA:HB1	1.98	0.44
1:A:242:GLU:HA	1:B:245:PHE:CZ	2.53	0.44
1:C:198:SER:HB2	1:C:223:PHE:CG	2.53	0.44
1:C:280:THR:HB	1:C:292:ASP:OD1	2.18	0.44
1:D:177:HIS:CE1	1:D:257:LEU:HA	2.53	0.44
1:D:293:ILE:HB	1:D:350:LEU:HD22	2.00	0.43
1:D:117:GLN:OE1	1:D:200:TYR:OH	2.28	0.43
1:A:107:ARG:HG2	1:B:385:PRO:HB3	2.00	0.43
1:D:241:ALA:HA	1:D:311:LEU:HD23	2.00	0.43
1:A:39:LEU:HD13	1:A:71:ALA:HA	2.01	0.43
1:B:374:ASP:OD1	1:B:439:ARG:NH2	2.49	0.43
1:C:169:LEU:HD12	1:C:450:VAL:HG21	1.99	0.43
1:D:185:LEU:HB3	1:D:464:LEU:HD13	2.01	0.43
1:A:28:THR:HA	1:A:31:ASP:OD1	2.19	0.43
1:A:198:SER:HB2	1:A:223:PHE:CG	2.53	0.42
1:B:300:LYS:HD2	1:B:343:LEU:HD11	2.01	0.42
1:D:114:ARG:O	1:D:118:VAL:HG12	2.18	0.42
1:B:263:VAL:CG1	1:B:269:PHE:CZ	3.02	0.42
1:B:284:ILE:HG21	1:D:112:ARG:O	2.20	0.42
1:A:21:LEU:HD13	1:C:293:ILE:HD11	2.02	0.42
1:A:278:TRP:CZ3	1:A:349:GLY:HA3	2.54	0.42
1:D:335:ASP:O	1:D:339:GLN:HG2	2.20	0.42
1:B:360:ARG:CZ	1:B:364:LEU:HD11	2.49	0.42
1:C:35:ALA:HB3	1:C:36:PRO:HD3	2.02	0.42
1:A:179:HIS:HB2	1:A:180:PRO:HD3	2.02	0.41
1:A:231:VAL:HG13	1:A:321:ALA:HB2	2.01	0.41
1:D:35:ALA:N	1:D:36:PRO:CD	2.83	0.41
1:A:331:GLU:N	1:A:332:PRO:HD2	2.34	0.41
1:C:184:ASP:O	1:C:188:ILE:HG13	2.19	0.41
1:B:175:LEU:HD22	1:B:457:ILE:CD1	2.49	0.41
2:A:501:AS1:HB1	2:A:501:AS1:N3	2.35	0.41
1:D:249:MET:HE3	1:D:252:VAL:HB	2.02	0.41
1:C:198:SER:HA	1:C:199:PRO:HD3	1.84	0.41
1:C:177:HIS:CE1	1:C:257:LEU:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HB2	1:B:205:LEU:HD21	2.03	0.41
1:B:158:GLY:HA2	7:B:615:HOH:O	2.21	0.41
1:C:170:LEU:HD22	1:C:361:MET:HE1	2.03	0.41
1:B:179:HIS:N	1:B:180:PRO:CD	2.84	0.40
1:A:107:ARG:NH2	1:B:383:GLY:O	2.53	0.40
1:B:79:PHE:CZ	1:B:95:GLY:HA3	2.57	0.40
1:C:229:ASN:OD1	1:C:229:ASN:C	2.63	0.40
1:B:414:GLU:O	1:B:418:ILE:HG13	2.22	0.40
1:D:291:PRO:O	1:D:295:GLU:HG3	2.21	0.40
1:A:365:ALA:HB3	1:A:366:PRO:HD3	2.04	0.40
1:B:188:ILE:HG13	1:B:246:VAL:HG11	2.04	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	448/470 (95%)	432 (96%)	14 (3%)	2 (0%)	30	54
1	B	452/470 (96%)	437 (97%)	13 (3%)	2 (0%)	30	54
1	C	414/470 (88%)	404 (98%)	8 (2%)	2 (0%)	24	48
1	D	412/470 (88%)	397 (96%)	12 (3%)	3 (1%)	18	41
All	All	1726/1880 (92%)	1670 (97%)	47 (3%)	9 (0%)	24	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	D	386	PHE
1	B	205	LEU
1	B	328	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	205	LEU
1	A	205	LEU
1	C	387	ARG
1	D	287	GLN
1	C	205	LEU

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	337/352 (96%)	327 (97%)	10 (3%)	36	66
1	B	342/352 (97%)	331 (97%)	11 (3%)	34	64
1	C	310/352 (88%)	299 (96%)	11 (4%)	32	61
1	D	310/352 (88%)	292 (94%)	18 (6%)	18	42
All	All	1299/1408 (92%)	1249 (96%)	50 (4%)	29	58

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	103	ASP
1	A	153	SER
1	A	174	LEU
1	A	280	THR
1	A	330	LYS
1	A	359	GLN
1	A	405	VAL
1	A	418	ILE
1	A	428	GLU
1	B	48	VAL
1	B	58	GLU
1	B	78	SER
1	B	117	GLN
1	B	126	LEU
1	B	153	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	343	LEU
1	B	418	ILE
1	B	429	VAL
1	B	439	ARG
1	B	466	ARG
1	C	27	SER
1	C	78	SER
1	C	126	LEU
1	C	166	GLN
1	C	200	TYR
1	C	279	SER
1	C	280	THR
1	C	284	ILE
1	C	359	GLN
1	C	449	ARG
1	C	470	ARG
1	D	48	VAL
1	D	68	ASP
1	D	76	ASP
1	D	78	SER
1	D	100	VAL
1	D	103	ASP
1	D	108	LEU
1	D	117	GLN
1	D	126	LEU
1	D	135	THR
1	D	166	GLN
1	D	185	LEU
1	D	200	TYR
1	D	254	LEU
1	D	288	LYS
1	D	330	LYS
1	D	375	LEU
1	D	384	VAL

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	117	GLN
1	A	166	GLN
1	A	275	HIS
1	B	89	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	HIS
1	C	290	ASN
1	C	323	ASN
1	C	357	ASN
1	C	467	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
2	AS1	D	501	-	18,19,19	1.30	3 (16%)	19,24,24	1.95	4 (21%)
4	EDO	B	504	-	3,3,3	0.56	0	2,2,2	0.22	0
2	AS1	A	501	-	18,19,19	1.37	3 (16%)	19,24,24	2.28	6 (31%)
2	AS1	B	501	-	18,19,19	1.34	2 (11%)	19,24,24	1.63	3 (15%)
6	ARG	C	501	-	10,11,11	0.88	1 (10%)	9,13,13	1.06	1 (11%)
4	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.51	0
5	PEG	A	504	-	6,6,6	0.45	0	5,5,5	0.36	0
4	EDO	B	503	-	3,3,3	0.60	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUM	A	502	-	7,7,7	1.27	2 (28%)	8,8,8	0.86	0
4	EDO	B	502	-	3,3,3	0.49	0	2,2,2	0.28	0
4	EDO	C	502	-	3,3,3	0.54	0	2,2,2	0.36	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
2	AS1	D	501	-	1/1/6/7	4/21/23/23	-
4	EDO	B	504	-	-	1/1/1/1	-
2	AS1	A	501	-	1/1/6/7	11/21/23/23	-
2	AS1	B	501	-	1/1/6/7	9/21/23/23	-
6	ARG	C	501	-	-	4/11/11/11	-
4	EDO	A	503	-	-	1/1/1/1	-
5	PEG	A	504	-	-	2/4/4/4	-
4	EDO	B	503	-	-	1/1/1/1	-
3	FUM	A	502	-	-	0/5/5/5	-
4	EDO	B	502	-	-	1/1/1/1	-
4	EDO	C	502	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	AS1	C-N2	3.16	1.36	1.28
2	B	501	AS1	C-N3	-3.14	1.26	1.34
2	A	501	AS1	C-N2	3.03	1.36	1.28
2	A	501	AS1	C-N3	-2.81	1.27	1.34
6	C	501	ARG	OXT-C	-2.62	1.22	1.30
2	D	501	AS1	C-N3	-2.58	1.28	1.34
2	B	501	AS1	C-N2	2.56	1.35	1.28
3	A	502	FUM	O8-C6	-2.14	1.25	1.30
3	A	502	FUM	OXT-C	-2.09	1.25	1.30
2	A	501	AS1	O52-C5	-2.04	1.24	1.30
2	D	501	AS1	OG1-CG	-2.00	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AS1	C2-C1-N2	6.15	121.55	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	AS1	C2-C1-N2	5.81	120.96	110.67
2	A	501	AS1	N1-C-N2	-4.59	113.88	125.00
2	B	501	AS1	CG-CA-N1	4.26	120.44	110.57
2	A	501	AS1	CB-CA-N1	3.25	116.84	110.64
2	D	501	AS1	C1-N2-C	3.14	129.08	121.86
2	B	501	AS1	N1-C-N2	-2.91	117.94	125.00
2	D	501	AS1	CB-CA-CG	-2.90	105.00	110.79
2	B	501	AS1	CB-CA-N1	2.77	115.92	110.64
2	A	501	AS1	OD1-CD-CB	2.30	121.15	114.00
6	C	501	ARG	OXT-C-O	-2.29	118.88	124.08
2	A	501	AS1	OG2-CG-CA	-2.27	114.95	122.26
2	A	501	AS1	OG1-CG-CA	2.25	121.12	113.51
2	D	501	AS1	N3-C-N1	-2.17	114.71	118.86

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	AS1	CA
2	B	501	AS1	CA
2	D	501	AS1	CA

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AS1	C2-C3-C4-C5
2	A	501	AS1	N2-C1-C2-C3
2	A	501	AS1	CB-CA-N1-C
2	B	501	AS1	CB-CA-N1-C
2	D	501	AS1	C2-C1-N2-C
6	C	501	ARG	N-CA-CB-CG
2	D	501	AS1	C1-C2-C3-C4
4	B	503	EDO	O1-C1-C2-O2
2	B	501	AS1	N1-CA-CG-OG2
2	B	501	AS1	N1-CA-CG-OG1
2	D	501	AS1	CA-CB-CD-OD1
2	D	501	AS1	CA-CB-CD-OD2
2	A	501	AS1	N1-CA-CG-OG2
2	A	501	AS1	N1-CA-CG-OG1
5	A	504	PEG	O1-C1-C2-O2
2	A	501	AS1	N3-C-N1-CA
2	B	501	AS1	N3-C-N1-CA
4	B	502	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	504	EDO	O1-C1-C2-O2
2	A	501	AS1	N2-C-N1-CA
2	A	501	AS1	CB-CA-CG-OG2
2	A	501	AS1	CB-CA-CG-OG1
2	B	501	AS1	CG-CA-CB-CD
4	A	503	EDO	O1-C1-C2-O2
2	B	501	AS1	CB-CA-CG-OG2
2	B	501	AS1	N4-C4-C5-O52
2	B	501	AS1	CB-CA-CG-OG1
5	A	504	PEG	C1-C2-O2-C3
6	C	501	ARG	C-CA-CB-CG
4	C	502	EDO	O1-C1-C2-O2
2	A	501	AS1	C1-C2-C3-C4
2	A	501	AS1	C2-C3-C4-N4
6	C	501	ARG	OXT-C-CA-N
2	B	501	AS1	N4-C4-C5-O51
6	C	501	ARG	O-C-CA-N

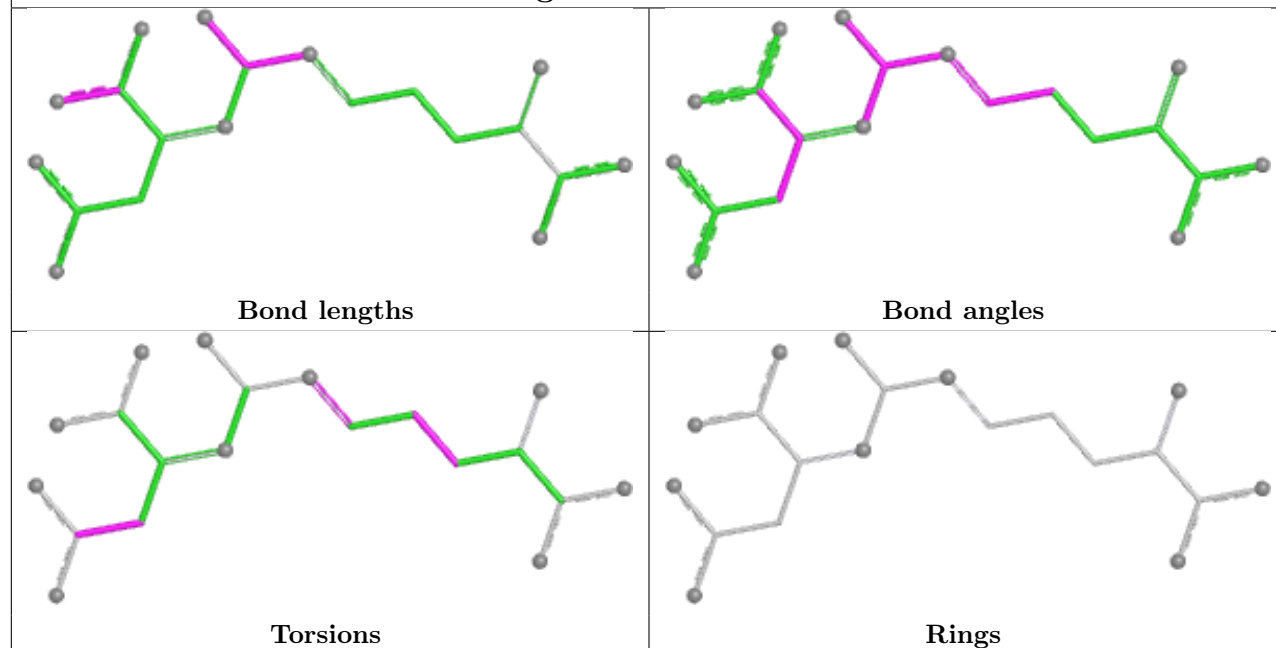
There are no ring outliers.

3 monomers are involved in 7 short contacts:

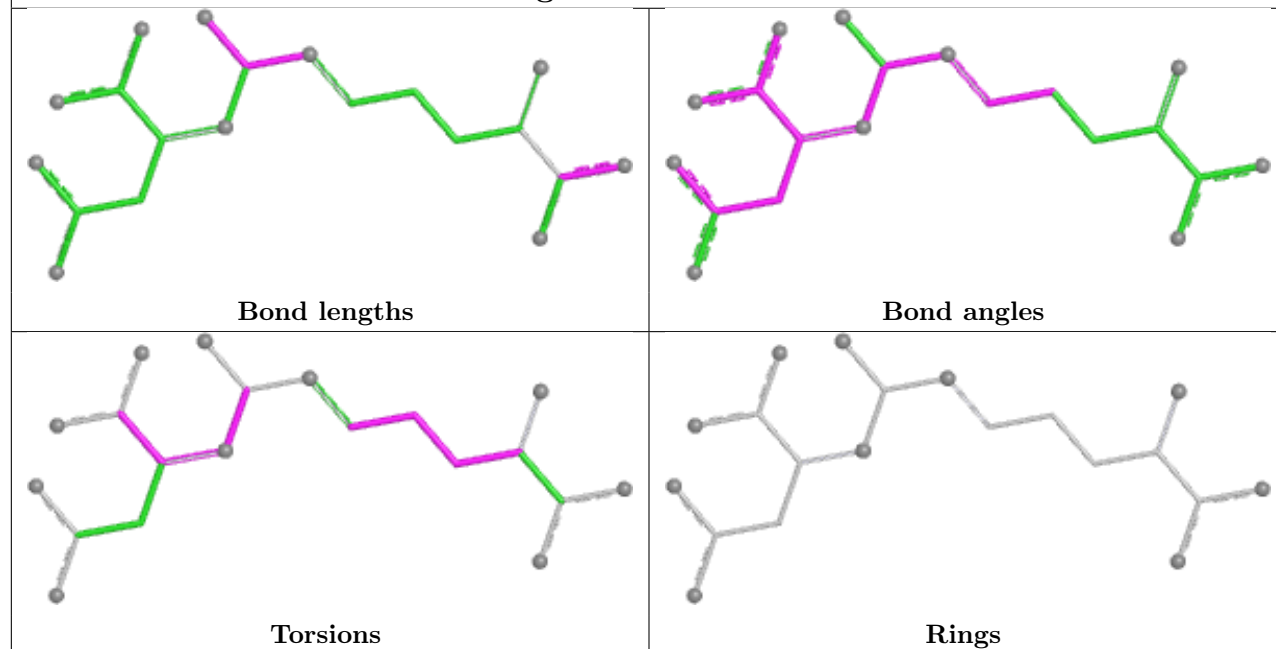
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	AS1	1	0
2	A	501	AS1	5	0
2	B	501	AS1	1	0

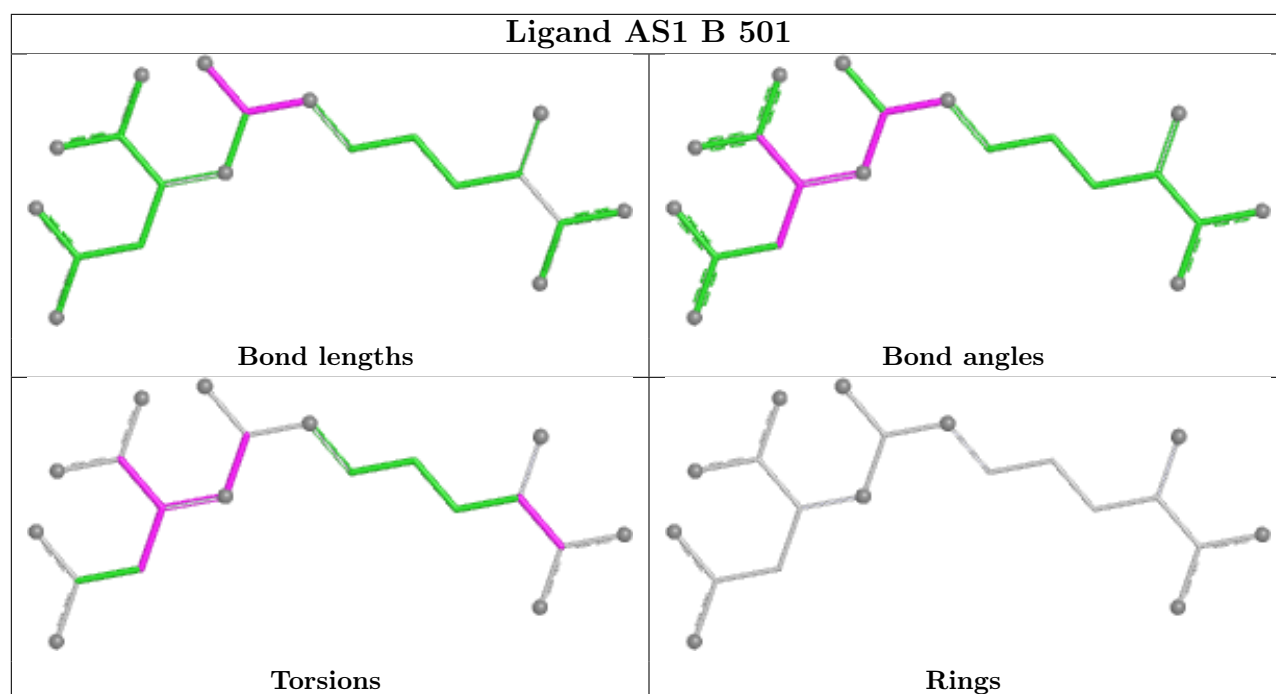
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand AS1 D 501



Ligand AS1 A 501





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	452/470 (96%)	0.47	19 (4%) 40 37	6, 20, 39, 62	0
1	B	454/470 (96%)	0.53	25 (5%) 30 27	8, 21, 41, 68	0
1	C	418/470 (88%)	0.73	45 (10%) 11 9	9, 24, 58, 84	0
1	D	416/470 (88%)	0.85	50 (12%) 9 7	10, 24, 58, 87	0
All	All	1740/1880 (92%)	0.64	139 (7%) 18 15	6, 22, 51, 87	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	ILE	6.8
1	C	469	VAL	6.4
1	D	388	SER	6.0
1	D	470	ARG	6.0
1	A	286	PRO	5.6
1	C	390	HIS	5.5
1	D	387	ARG	5.1
1	D	429	VAL	5.1
1	D	382	GLN	4.9
1	C	77	GLY	4.7
1	C	369	TYR	4.7
1	C	470	ARG	4.5
1	C	387	ARG	4.4
1	C	428	GLU	4.4
1	D	469	VAL	4.4
1	C	111	GLY	4.3
1	D	385	PRO	4.2
1	D	383	GLY	4.1
1	A	287	GLN	4.1
1	D	378	TRP	4.0
1	A	405	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	380	VAL	4.0
1	D	379	LEU	3.8
1	C	378	TRP	3.8
1	C	78	SER	3.8
1	C	427	ARG	3.7
1	B	72	GLN	3.6
1	D	76	ASP	3.5
1	C	384	VAL	3.5
1	C	429	VAL	3.5
1	D	384	VAL	3.4
1	B	285	MET	3.4
1	D	381	ARG	3.4
1	B	22	ALA	3.4
1	D	428	GLU	3.3
1	C	216	ALA	3.3
1	C	382	GLN	3.3
1	D	369	TYR	3.3
1	D	74	VAL	3.3
1	A	428	GLU	3.2
1	C	455	ASN	3.2
1	C	71	ALA	3.2
1	C	383	GLY	3.2
1	D	427	ARG	3.1
1	A	387	ARG	3.1
1	B	91	ALA	3.0
1	C	379	LEU	3.0
1	A	84	THR	3.0
1	D	41	ALA	3.0
1	C	58	GLU	2.9
1	C	287	GLN	2.9
1	A	386	PHE	2.9
1	B	81	PRO	2.9
1	C	375	LEU	2.9
1	D	71	ALA	2.9
1	D	348	ALA	2.8
1	C	53	GLY	2.8
1	C	211	GLY	2.8
1	D	77	GLY	2.8
1	A	395	ALA	2.8
1	B	469	VAL	2.8
1	D	204	ALA	2.8
1	B	283	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	212	LEU	2.7
1	A	368	GLY	2.7
1	B	281	GLY	2.7
1	B	286	PRO	2.7
1	C	283	SER	2.7
1	C	386	PHE	2.7
1	B	79	PHE	2.6
1	B	103	ASP	2.6
1	C	389	ALA	2.6
1	D	386	PHE	2.6
1	C	430	LEU	2.6
1	B	470	ARG	2.6
1	D	75	ALA	2.6
1	B	401	GLU	2.6
1	D	103	ASP	2.5
1	D	468	LEU	2.5
1	B	17	PRO	2.5
1	D	228	ASP	2.5
1	D	465	ARG	2.5
1	D	17	PRO	2.5
1	A	442	ARG	2.5
1	C	388	SER	2.4
1	B	95	GLY	2.4
1	C	24	LEU	2.4
1	A	17	PRO	2.4
1	B	461	ALA	2.4
1	B	71	ALA	2.4
1	B	200	TYR	2.4
1	D	97	ILE	2.4
1	D	455	ASN	2.4
1	C	449	ARG	2.4
1	C	280	THR	2.3
1	A	416	ALA	2.3
1	D	284	ILE	2.3
1	C	48	VAL	2.3
1	C	468	LEU	2.3
1	D	90	ALA	2.3
1	C	46	THR	2.3
1	C	224	SER	2.3
1	D	78	SER	2.3
1	B	442	ARG	2.2
1	A	100	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	287	GLN	2.2
1	D	467	GLN	2.2
1	C	68	ASP	2.2
1	C	230	SER	2.2
1	C	79	PHE	2.2
1	D	283	SER	2.2
1	D	287	GLN	2.2
1	B	70	LEU	2.2
1	B	410	LEU	2.2
1	D	265	SER	2.2
1	A	225	ALA	2.1
1	D	165	ALA	2.1
1	C	17	PRO	2.1
1	A	410	LEU	2.1
1	C	277	SER	2.1
1	A	379	LEU	2.1
1	C	380	VAL	2.1
1	C	462	GLU	2.1
1	D	58	GLU	2.1
1	B	467	GLN	2.1
1	D	72	GLN	2.1
1	B	404	GLY	2.1
1	D	83	VAL	2.1
1	C	213	ASP	2.1
1	A	282	SER	2.1
1	D	63	LEU	2.1
1	D	213	ASP	2.0
1	D	18	SER	2.0
1	C	385	PRO	2.0
1	D	36	PRO	2.0
1	A	24	LEU	2.0
1	A	74	VAL	2.0
1	D	109	ARG	2.0
1	D	53	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

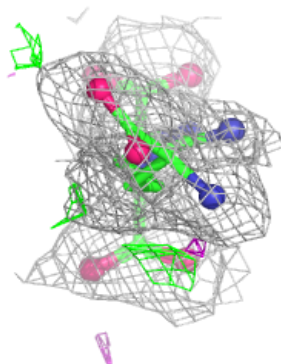
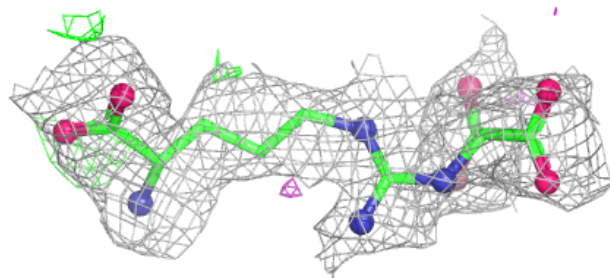
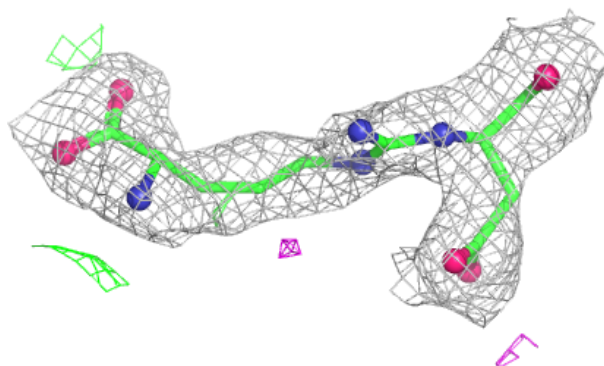
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	C	502	4/4	0.43	0.35	33,35,36,38	0
4	EDO	B	504	4/4	0.74	0.23	47,48,50,50	0
5	PEG	A	504	7/7	0.75	0.18	45,46,47,48	0
4	EDO	B	503	4/4	0.77	0.19	20,21,21,21	0
4	EDO	A	503	4/4	0.77	0.17	40,41,42,43	0
2	AS1	D	501	20/20	0.81	0.16	29,42,46,48	0
4	EDO	B	502	4/4	0.84	0.14	39,40,40,41	0
6	ARG	C	501	12/12	0.88	0.13	27,28,32,32	0
3	FUM	A	502	8/8	0.89	0.11	35,37,37,39	0
2	AS1	B	501	20/20	0.90	0.11	20,23,24,25	0
2	AS1	A	501	20/20	0.92	0.10	17,22,22,23	0

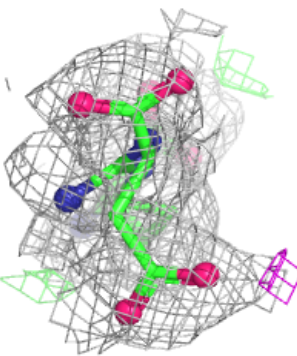
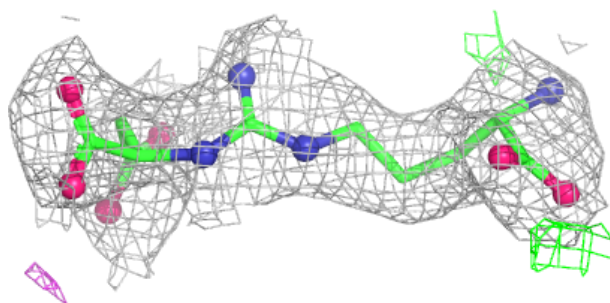
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AS1 D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

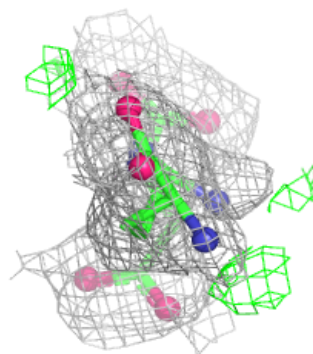
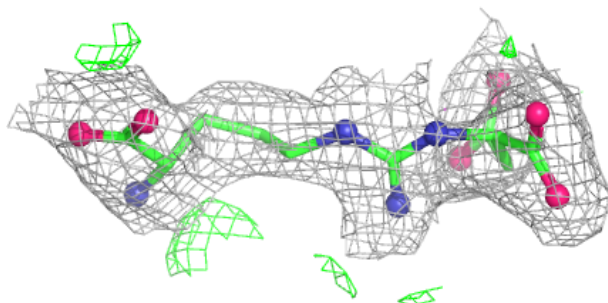
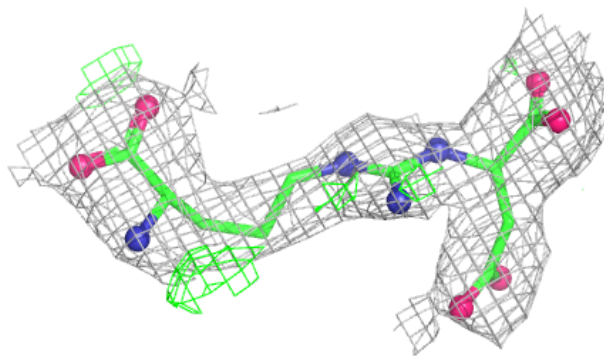
**Electron density around AS1 B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AS1 A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.