Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 11:20 PM JST

PDB ID	:	6IEM
Title	:	Argininosuccinate lyase from Mycobacterium tuberculosis
Authors	:	Paul, A.; Mishra, A.; Surolia, A.; Vijayan, M.
Deposited on	:	2018-09-14
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

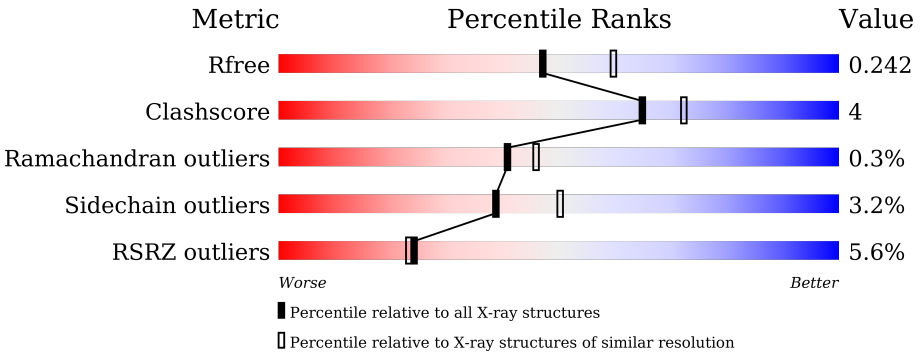
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 88% 7% • •
1	B	470	3% 90% 7% • •
1	C	470	4% 86% 8% • •
1	D	470	4% 84% 11% • •
1	E	470	5% 86% 9% 5%
1	F	470	4% 85% 10% • •

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Mol	Chain	Length	Quality of chain
1	G	470	7% 87% 8%
1	H	470	8% 86% 10%

2 Entry composition (i)

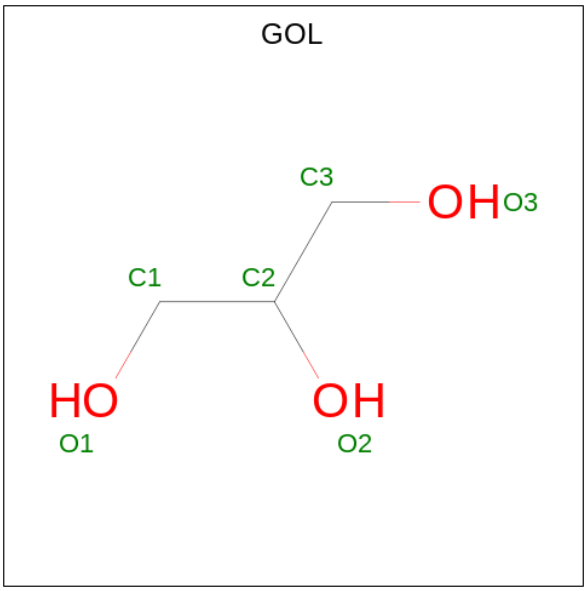
There are 8 unique types of molecules in this entry. The entry contains 27041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

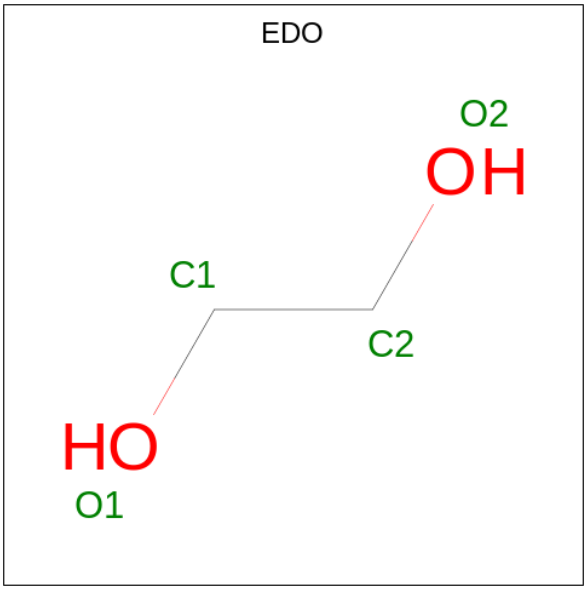
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3255	2046	587	615	7	0	0	0
			Total	C	N	O	S			
1	B	462	3343	2106	597	633	7	0	1	0
			Total	C	N	O	S			
1	C	450	3280	2061	591	621	7	0	0	0
			Total	C	N	O	S			
1	D	454	3325	2086	604	627	8	0	1	0
			Total	C	N	O	S			
1	E	448	3269	2053	586	623	7	0	1	0
			Total	C	N	O	S			
1	F	450	3274	2054	590	623	7	0	0	0
			Total	C	N	O	S			
1	G	449	3224	2026	582	609	7	0	0	0
			Total	C	N	O	S			
1	H	454	3269	2054	587	620	8	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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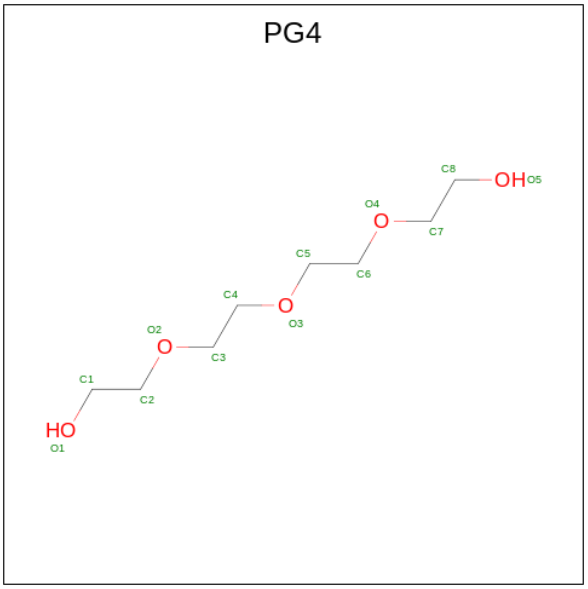
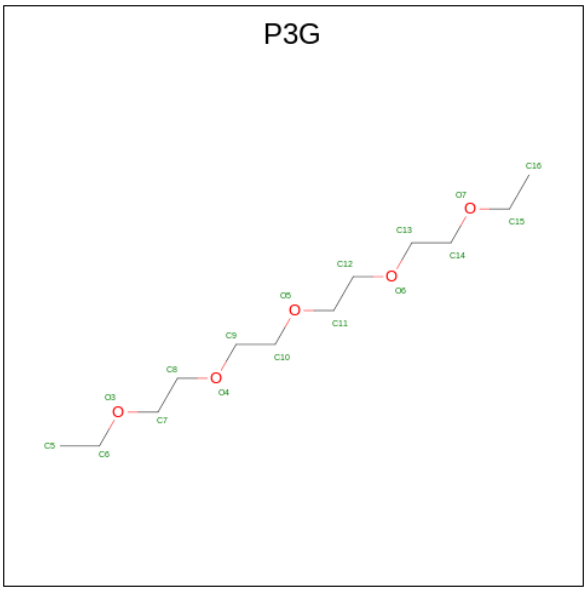
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	E	1	4	2	2	0	0
			Total	C	O		
3	F	1	4	2	2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



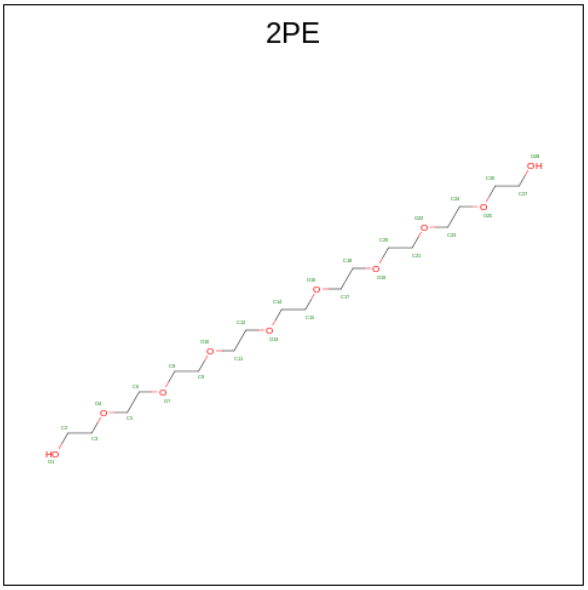
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	13	8	5	0	0
			Total	C	O		
4	C	1	13	8	5	0	0

- Molecule 5 is 3,6,9,12,15-PENTAOXAHEPTADECANE (three-letter code: P3G) (formula: $C_{12}H_{26}O_5$).



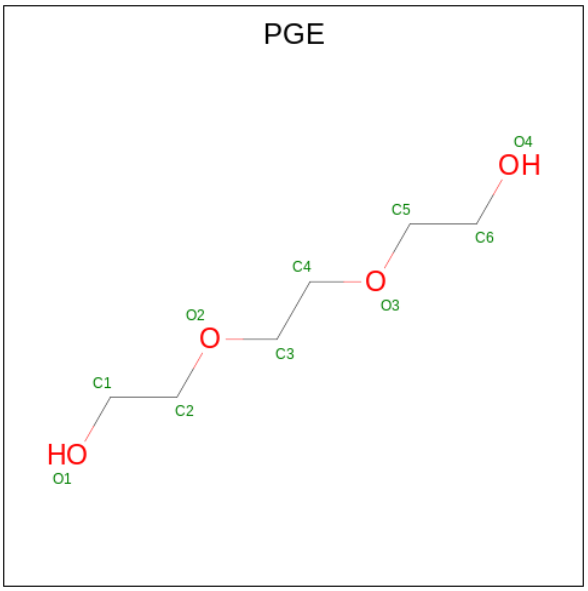
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	D	1	17	12	5	0	0

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	E	1	28	18	10	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	F	1	10	6	4	0	0

- Molecule 8 is water.

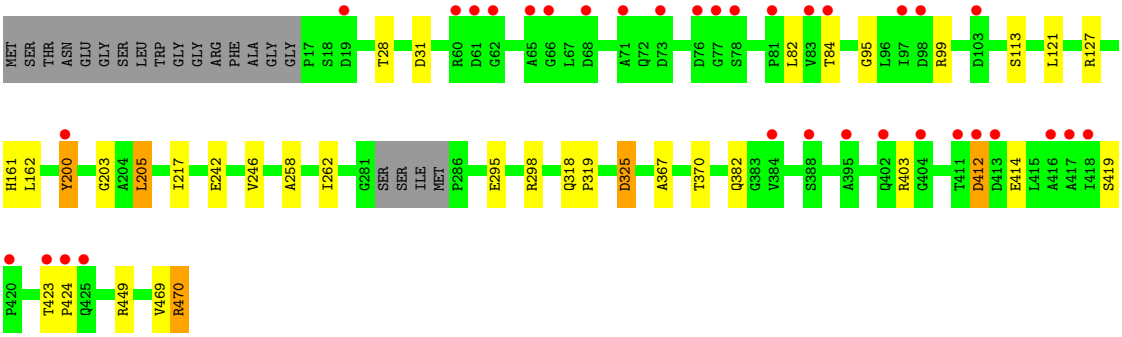
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	78	78	78	0	0
			Total	O		
8	B	99	99	99	0	0
			Total	O		
8	C	87	87	87	0	0
			Total	O		
8	D	96	96	96	0	0
			Total	O		
8	E	95	95	95	0	0
			Total	O		
8	F	88	88	88	0	0
			Total	O		
8	G	67	67	67	0	0
			Total	O		
8	H	71	71	71	0	0

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.

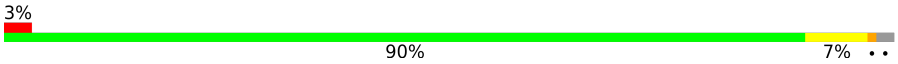
- Molecule 1: Argininosuccinate lyase

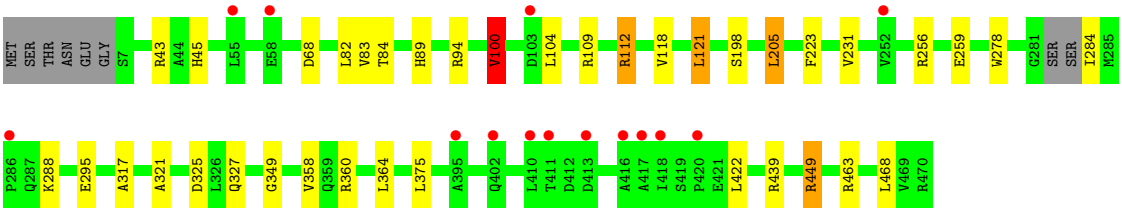
Chain A:



- Molecule 1: Argininosuccinate lyase

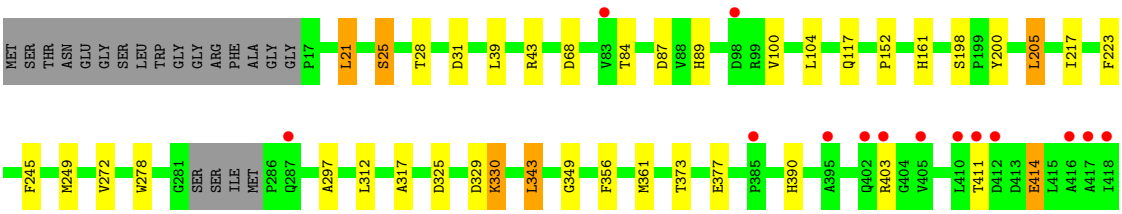
Chain B:



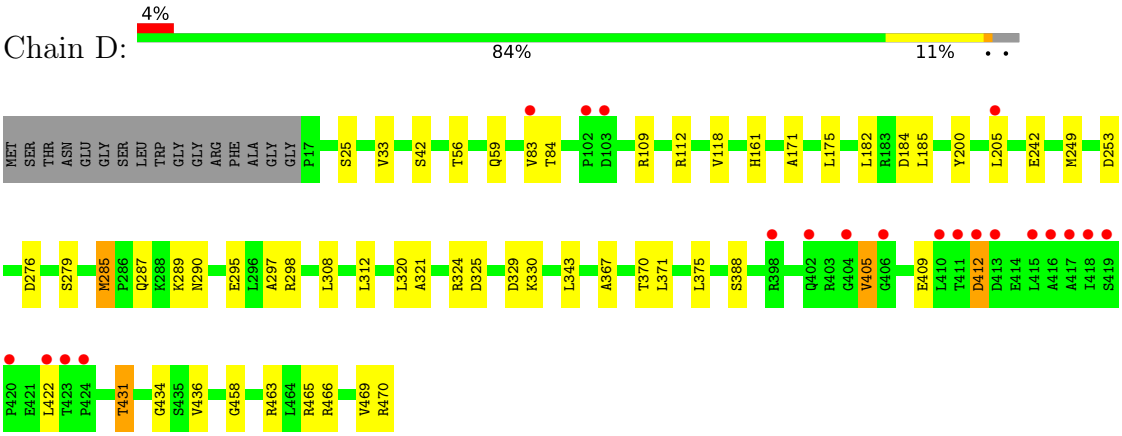


- Molecule 1: Argininosuccinate lyase

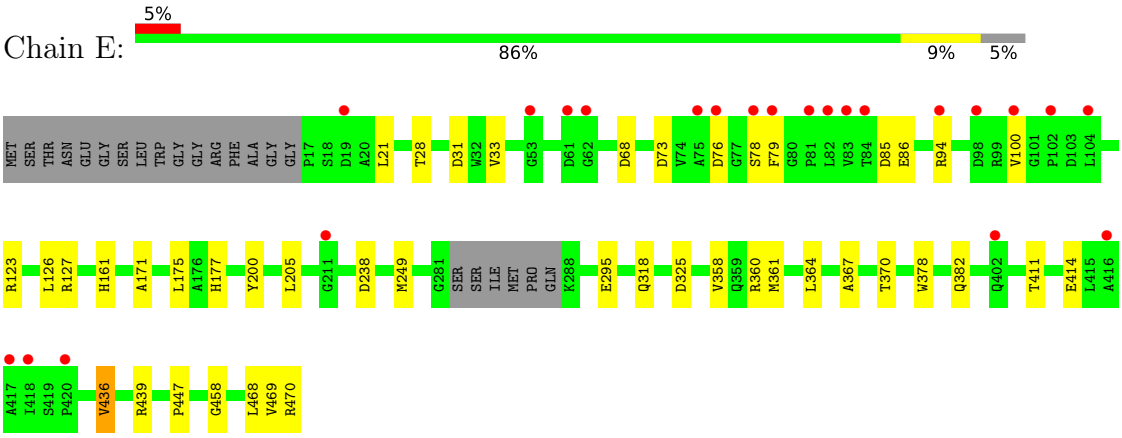
Chain C:



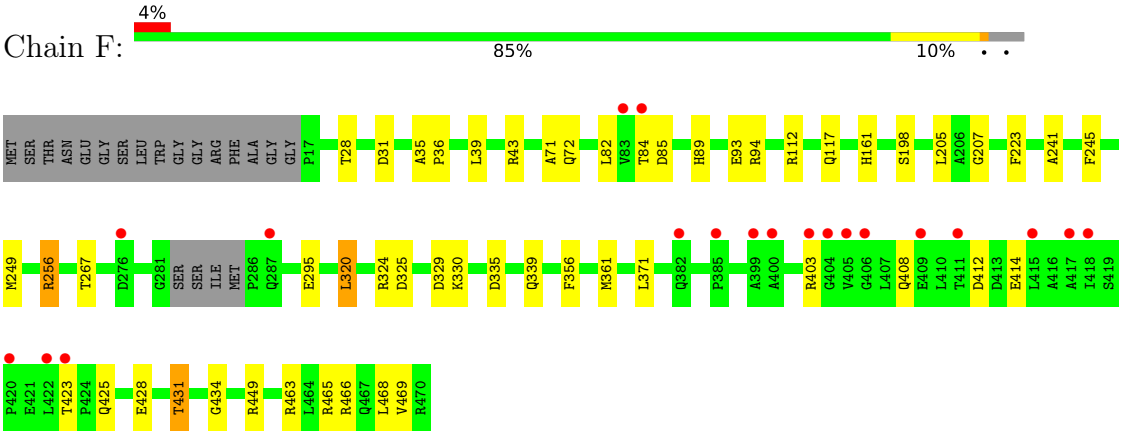
• Molecule 1: Argininosuccinate lyase



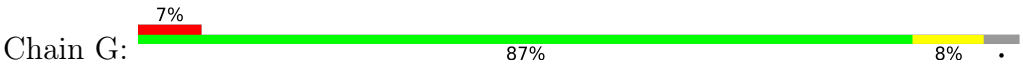
• Molecule 1: Argininosuccinate lyase

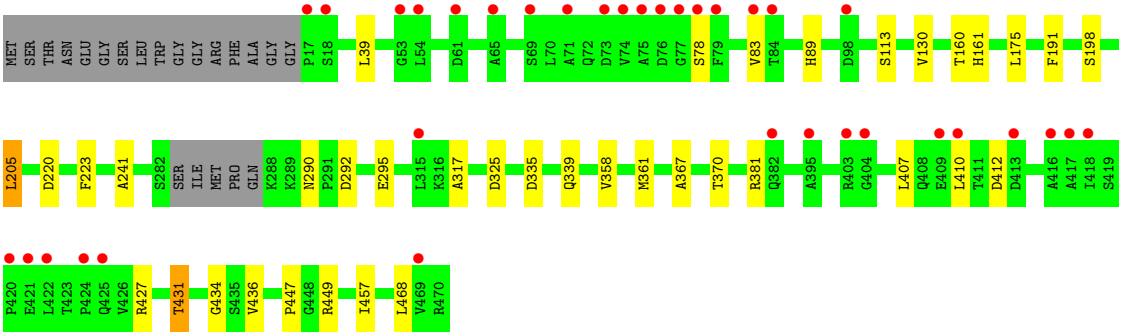


• Molecule 1: Argininosuccinate lyase



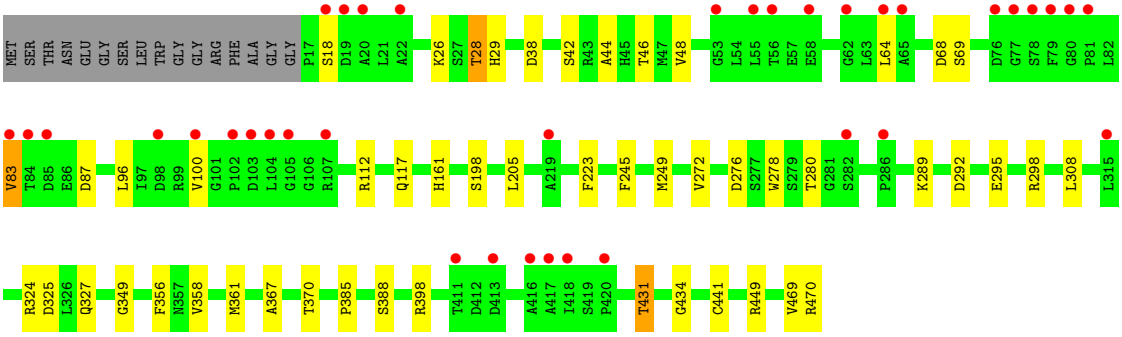
• Molecule 1: Argininosuccinate lyase





- Molecule 1: Argininosuccinate lyase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.55Å 183.82Å 190.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.48 – 2.20 40.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.48-2.20) 100.0 (40.42-2.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.203 , 0.244 0.203 , 0.242	Depositor DCC
R_{free} test set	11347 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27041	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PGE, EDO, PG4, P3G, 2PE

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	0.47	0/3312	0.65	0/4517
1	B	0.49	0/3406	0.69	0/4645
1	C	0.49	0/3337	0.66	0/4548
1	D	0.47	0/3382	0.67	0/4607
1	E	0.47	0/3324	0.66	0/4529
1	F	0.48	0/3331	0.65	0/4541
1	G	0.43	0/3279	0.62	0/4476
1	H	0.44	0/3328	0.63	0/4541
All	All	0.47	0/26699	0.65	0/36404

There are no bond length outliers.

There are no bond angle outliers.

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	3255	0	3185	24	0
1	B	3343	0	3265	20	0
1	C	3280	0	3225	42	0
1	D	3325	0	3284	44	0
1	E	3269	0	3204	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3274	0	3209	43	0
1	G	3224	0	3142	24	0
1	H	3269	0	3186	33	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
4	B	13	0	18	0	0
4	C	13	0	18	0	0
5	D	17	0	26	1	0
6	E	28	0	38	1	0
7	F	10	0	14	0	0
8	A	78	0	0	1	0
8	B	99	0	0	1	0
8	C	87	0	0	1	0
8	D	96	0	0	5	0
8	E	95	0	0	0	0
8	F	88	0	0	2	0
8	G	67	0	0	1	0
8	H	71	0	0	0	0
All	All	27041	0	25872	215	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 (215) 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:G:431:THR:HG22	1:G:434:GLY:H	1.21	1.04
1:E:249:MET:HE1	1:F:241:ALA:HB3	1.48	0.94
1:C:87:ASP:OD2	1:C:89:HIS:HD2	1.54	0.89
1:G:431:THR:HG22	1:G:434:GLY:N	2.01	0.74
1:A:203:GLY:HA3	2:A:501:GOL:H32	1.70	0.71
1:E:249:MET:CE	1:F:241:ALA:HB3	2.20	0.71
1:D:405:VAL:HG13	1:D:409:GLU:HB2	1.71	0.71
1:C:87:ASP:OD2	1:C:89:HIS:CD2	2.42	0.68
1:C:312:LEU:HD21	1:D:249:MET:CE	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:THR:HG23	1:H:434:GLY:H	1.57	0.66
1:F:249:MET:SD	8:F:677:HOH:O	2.54	0.66
1:G:160:THR:HG23	1:H:205:LEU:HD23	1.78	0.66
1:D:56:THR:HG23	1:D:59:GLN:H	1.61	0.65
1:A:469:VAL:O	1:A:470:ARG:HB2	1.96	0.65
1:C:373:THR:HG22	1:C:377:GLU:OE1	1.97	0.65
1:E:469:VAL:O	1:E:470[B]:ARG:HB2	1.97	0.64
1:G:241:ALA:HB3	1:H:249:MET:HE3	1.79	0.64
1:F:423:THR:HG22	1:F:425:GLN:H	1.61	0.63
1:A:318:GLN:NE2	1:A:325:ASP:HB2	2.13	0.63
1:C:411:THR:OG1	1:C:414:GLU:HG3	1.98	0.63
1:C:297:ALA:HA	1:C:343:LEU:HD11	1.81	0.63
1:D:375:LEU:HD21	1:D:422:LEU:HD21	1.80	0.63
1:D:469:VAL:O	1:D:470[A]:ARG:HB2	1.99	0.62
1:C:312:LEU:HD21	1:D:249:MET:HE2	1.81	0.61
1:D:458:GLY:HA3	5:D:503:P3G:H92	1.83	0.61
1:A:318:GLN:HE22	1:A:325:ASP:HB2	1.65	0.60
1:H:431:THR:CG2	1:H:434:GLY:H	2.13	0.60
1:A:127:ARG:HH22	1:A:470:ARG:NH2	1.99	0.60
1:D:276:ASP:HA	1:D:289:LYS:HE3	1.83	0.60
1:G:431:THR:CG2	1:G:434:GLY:H	2.07	0.60
1:C:469:VAL:HG11	1:F:466:ARG:HH21	1.67	0.59
1:F:431:THR:HG22	1:F:434:GLY:H	1.65	0.59
2:A:501:GOL:H2	1:B:439:ARG:NH1	2.18	0.58
1:C:249:MET:CE	1:D:312:LEU:HD21	2.33	0.58
1:B:284:ILE:CB	1:B:288:LYS:HG3	2.33	0.58
1:B:43:ARG:NH1	1:B:68:ASP:OD1	2.37	0.58
1:D:367:ALA:O	1:D:370:THR:HG23	2.03	0.58
1:A:470:ARG:NH1	8:A:601:HOH:O	2.36	0.58
1:E:411:THR:HG23	1:E:414:GLU:OE2	2.02	0.57
1:D:25:SER:HB2	1:D:324:ARG:HH12	1.70	0.57
1:B:295:GLU:OE2	1:C:161:HIS:HA	2.04	0.57
1:D:469:VAL:O	1:D:470[B]:ARG:HB2	2.01	0.57
1:E:238:ASP:HB2	1:F:249:MET:HE3	1.87	0.57
1:H:245:PHE:CZ	1:H:249:MET:HE2	2.40	0.57
1:A:423:THR:HB	1:A:424:PRO:HD2	1.87	0.56
1:A:28:THR:HA	1:A:31:ASP:OD1	2.05	0.56
1:F:245:PHE:HZ	1:F:249:MET:HE1	1.70	0.56
1:H:358:VAL:HA	1:H:361:MET:HE2	1.87	0.56
1:C:312:LEU:HD21	1:D:249:MET:HE1	1.87	0.56
1:F:329:ASP:OD1	1:F:330:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:99:ARG:HD2	2.08	0.54
1:C:100:VAL:HB	1:C:104:LEU:HD23	1.89	0.54
1:A:403:ARG:NH1	1:A:414:GLU:OE2	2.40	0.54
1:C:469:VAL:CG1	1:F:466:ARG:NH2	2.70	0.54
1:F:431:THR:CG2	1:F:434:GLY:H	2.20	0.54
1:E:458:GLY:HA3	6:E:501:2PE:H82	1.90	0.54
1:B:327:GLN:HG2	3:B:503:EDO:O2	2.08	0.54
1:E:73:ASP:HB3	1:E:79:PHE:HB2	1.90	0.53
1:F:161:HIS:HA	1:G:295:GLU:OE2	2.09	0.53
1:D:182:LEU:HD23	1:D:185:LEU:HD12	1.91	0.53
1:B:375:LEU:HD21	1:B:422:LEU:HD21	1.90	0.52
1:C:469:VAL:HG11	1:F:466:ARG:NH2	2.24	0.52
1:G:198:SER:HB2	1:G:223:PHE:CD2	2.44	0.52
1:C:28:THR:HA	1:C:31:ASP:OD1	2.09	0.52
1:C:312:LEU:CD2	1:D:249:MET:HE2	2.40	0.52
1:E:360:ARG:CZ	1:E:364:LEU:HD11	2.40	0.52
1:C:249:MET:HE2	1:D:312:LEU:HD21	1.92	0.52
1:C:272:VAL:HG12	1:C:356:PHE:CD1	2.45	0.52
1:E:295:GLU:OE1	1:H:161:HIS:ND1	2.37	0.51
1:F:403:ARG:NH1	1:F:414:GLU:OE2	2.42	0.51
1:E:171:ALA:O	1:E:175:LEU:HG	2.10	0.51
1:A:82:LEU:CB	1:A:84:THR:HG22	2.41	0.51
1:H:26:LYS:NZ	1:H:83:VAL:HA	2.26	0.51
1:D:83:VAL:HG23	8:D:676:HOH:O	2.10	0.51
1:G:367:ALA:O	1:G:370:THR:HG23	2.11	0.51
1:C:43:ARG:NH1	1:C:68:ASP:OD1	2.44	0.51
1:C:439:ARG:HH11	1:C:439:ARG:HG2	1.76	0.51
1:D:42:SER:OG	1:D:112:ARG:NH1	2.43	0.51
1:A:161:HIS:HA	1:D:295:GLU:OE2	2.11	0.51
1:E:295:GLU:OE2	1:H:161:HIS:HA	2.11	0.51
1:E:177:HIS:NE2	1:F:320:LEU:HD22	2.25	0.50
1:D:285:MET:HG2	1:D:287:GLN:HE22	1.77	0.50
1:D:109:ARG:O	1:D:112:ARG:HB2	2.11	0.50
1:D:329:ASP:OD1	1:D:330:LYS:N	2.45	0.50
1:H:26:LYS:O	1:H:29:HIS:HE1	1.95	0.49
1:D:42:SER:HA	1:D:112:ARG:NH1	2.27	0.49
1:C:356:PHE:HB3	1:C:361:MET:HE1	1.95	0.49
1:H:42:SER:HA	1:H:112:ARG:NH1	2.27	0.49
1:H:367:ALA:O	1:H:370:THR:HG23	2.13	0.49
1:C:462:GLU:HG2	1:F:469:VAL:HG11	1.94	0.49
1:H:38:ASP:OD1	1:H:117:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:THR:HG23	1:H:292:ASP:OD2	2.13	0.49
1:G:175:LEU:HD22	1:G:457:ILE:CD1	2.43	0.49
1:F:330:LYS:HE3	8:F:655:HOH:O	2.13	0.49
1:A:258:ALA:O	1:A:262:ILE:HG13	2.12	0.48
1:F:28:THR:HA	1:F:31:ASP:OD1	2.13	0.48
1:C:465:ARG:HE	1:F:465:ARG:NH1	2.12	0.48
1:G:358:VAL:HA	1:G:361:MET:HE3	1.95	0.48
1:A:382:GLN:OE1	1:A:382:GLN:HA	2.12	0.48
1:E:318:GLN:O	1:F:256:ARG:NH1	2.47	0.48
1:E:85:ASP:OD2	1:E:94:ARG:NH2	2.37	0.47
1:E:28:THR:HA	1:E:31:ASP:OD1	2.14	0.47
1:E:367:ALA:O	1:E:370:THR:HG23	2.13	0.47
1:B:109:ARG:O	1:B:112:ARG:HB2	2.14	0.47
1:C:245:PHE:CE1	1:C:249:MET:HE3	2.49	0.47
1:C:249:MET:HE1	1:D:312:LEU:HD21	1.97	0.47
1:C:469:VAL:CG1	1:F:466:ARG:HH21	2.28	0.47
1:D:285:MET:CG	1:D:287:GLN:HE22	2.27	0.47
1:D:25:SER:HB2	1:D:324:ARG:NH1	2.29	0.47
1:E:123:ARG:O	1:E:127:ARG:HG3	2.15	0.47
1:F:35:ALA:HB3	1:F:36:PRO:HD3	1.97	0.47
1:H:449:ARG:HA	1:H:449:ARG:HD3	1.71	0.47
1:D:279:SER:HB2	1:D:290:ASN:O	2.14	0.46
1:F:198:SER:HB2	1:F:223:PHE:CD2	2.50	0.46
1:B:278:TRP:CH2	1:B:349:GLY:HA3	2.50	0.46
1:F:356:PHE:HB3	1:F:361:MET:HE1	1.98	0.46
1:G:335:ASP:O	1:G:339:GLN:HG2	2.15	0.46
1:C:21:LEU:O	1:C:25:SER:OG	2.33	0.46
1:C:39:LEU:O	1:C:43:ARG:HG3	2.16	0.46
1:H:385:PRO:HG2	1:H:388:SER:HB2	1.97	0.46
1:H:26:LYS:HE2	1:H:28:THR:OG1	2.16	0.46
1:F:449:ARG:HA	1:F:449:ARG:HD3	1.64	0.45
1:E:436:VAL:HG13	1:E:447:PRO:HD3	1.97	0.45
1:E:249:MET:CE	1:F:241:ALA:CB	2.92	0.45
1:C:278:TRP:CH2	1:C:349:GLY:HA3	2.51	0.45
1:G:175:LEU:HD22	1:G:457:ILE:HD13	1.98	0.45
1:D:465:ARG:NH2	8:D:603:HOH:O	2.47	0.45
1:A:295:GLU:OE2	1:D:161:HIS:HA	2.16	0.45
1:A:319:PRO:HD3	1:B:259:GLU:HG2	1.99	0.45
1:G:89:HIS:HB3	8:G:565:HOH:O	2.15	0.45
1:D:466:ARG:HG2	8:D:603:HOH:O	2.16	0.45
1:G:241:ALA:HB3	1:H:249:MET:CE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:449:ARG:HA	1:G:449:ARG:HD3	1.75	0.45
1:H:276:ASP:OD1	1:H:289:LYS:HE3	2.17	0.45
1:E:161:HIS:HA	1:H:295:GLU:OE2	2.17	0.44
1:D:470[A]:ARG:NH1	8:D:604:HOH:O	2.49	0.44
1:H:96:LEU:O	1:H:100:VAL:HG22	2.17	0.44
1:A:449:ARG:HA	1:A:449:ARG:HD3	1.85	0.44
1:C:200:TYR:CD2	1:C:217:ILE:HG21	2.53	0.44
1:B:100:VAL:HG13	1:B:104:LEU:HB3	2.00	0.44
1:B:360:ARG:CZ	1:B:364:LEU:HD11	2.48	0.44
1:F:245:PHE:CZ	1:F:249:MET:CE	3.01	0.44
1:A:298:ARG:HG3	1:B:317:ALA:HB2	1.99	0.44
1:G:290:ASN:HB2	1:G:292:ASP:OD1	2.18	0.44
1:B:449:ARG:HA	1:B:449:ARG:HD3	1.72	0.44
1:H:272:VAL:HG12	1:H:356:PHE:CD1	2.53	0.44
1:F:295:GLU:OE2	1:G:161:HIS:HA	2.18	0.43
1:C:198:SER:HB2	1:C:223:PHE:CD2	2.53	0.43
1:D:171:ALA:O	1:D:175:LEU:HG	2.18	0.43
1:E:177:HIS:CE1	1:F:320:LEU:HD22	2.53	0.43
1:A:367:ALA:O	1:A:370:THR:HG23	2.18	0.43
1:B:45:HIS:NE2	1:B:112:ARG:HG2	2.33	0.43
1:A:412:ASP:OD2	1:A:424:PRO:HB3	2.18	0.43
1:D:184:ASP:OD2	1:D:253:ASP:OD2	2.36	0.43
1:F:82:LEU:HB2	1:F:84:THR:HG22	2.00	0.43
1:F:335:ASP:O	1:F:339:GLN:HG2	2.17	0.43
1:H:44:ALA:O	1:H:48:VAL:HG23	2.18	0.43
1:F:324:ARG:HB3	1:H:295:GLU:HB2	2.00	0.43
1:F:428:GLU:O	1:F:434:GLY:HA3	2.18	0.43
1:D:431:THR:HG23	1:D:434:GLY:H	1.83	0.43
1:H:198:SER:HB2	1:H:223:PHE:CD2	2.54	0.43
1:C:89:HIS:HB3	8:C:683:HOH:O	2.18	0.43
1:D:276:ASP:HA	1:D:289:LYS:CE	2.46	0.43
1:G:381:ARG:HH21	1:G:381:ARG:HG3	1.85	0.42
1:G:130:VAL:HG11	1:G:191:PHE:CE2	2.55	0.42
1:H:278:TRP:CH2	1:H:349:GLY:HA3	2.53	0.42
1:C:245:PHE:CZ	1:C:249:MET:HE3	2.54	0.42
1:F:85:ASP:OD2	1:F:94:ARG:NH2	2.52	0.42
1:B:198:SER:HB2	1:B:223:PHE:CG	2.55	0.42
1:C:152:PRO:HD2	1:F:72:GLN:HB2	2.02	0.42
1:F:112:ARG:NH2	1:F:117:GLN:OE1	2.51	0.42
1:G:436:VAL:HG12	1:G:447:PRO:HD3	2.02	0.42
1:A:127:ARG:HH22	1:A:470:ARG:HH21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:468:LEU:HD12	1:G:468:LEU:HA	1.82	0.42
1:B:231:VAL:HG13	1:B:321:ALA:HB2	2.01	0.42
1:E:378:TRP:O	1:E:382:GLN:HG2	2.19	0.42
1:A:200:TYR:HD2	1:A:217:ILE:HG21	1.85	0.41
1:G:317:ALA:HB2	1:H:298:ARG:HG3	2.01	0.41
1:D:412:ASP:N	1:D:412:ASP:OD1	2.52	0.41
1:B:256:ARG:HD3	8:B:694:HOH:O	2.20	0.41
1:F:468:LEU:HD23	1:F:468:LEU:HA	1.92	0.41
1:H:324:ARG:NE	1:H:327:GLN:OE1	2.52	0.41
1:C:343:LEU:HD23	1:C:343:LEU:HA	1.93	0.41
1:C:449:ARG:HA	1:C:449:ARG:HD3	1.85	0.41
1:E:358:VAL:HA	1:E:361:MET:HE2	2.03	0.41
1:F:39:LEU:HD13	1:F:71:ALA:HA	2.02	0.41
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.95	0.41
1:D:56:THR:HG22	1:D:59:GLN:OE1	2.20	0.41
1:D:463:ARG:HH11	1:D:463:ARG:HG2	1.86	0.41
1:B:89:HIS:HE1	1:B:121:LEU:HD23	1.85	0.41
1:B:278:TRP:CZ3	1:B:349:GLY:HA3	2.56	0.41
1:C:403:ARG:HE	1:C:403:ARG:HB3	1.60	0.41
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.87	0.41
1:C:245:PHE:CZ	1:D:242:GLU:HA	2.56	0.41
1:C:249:MET:HE3	1:C:249:MET:HB2	1.86	0.41
1:F:89:HIS:CD2	1:F:89:HIS:H	2.39	0.41
1:C:465:ARG:HE	1:F:465:ARG:CZ	2.34	0.41
1:H:26:LYS:HZ1	1:H:83:VAL:HA	1.86	0.41
1:H:245:PHE:HA	1:H:308:LEU:HD22	2.03	0.41
1:C:317:ALA:HB2	1:D:298:ARG:HG3	2.02	0.40
1:C:329:ASP:OD1	1:C:330:LYS:N	2.54	0.40
1:D:297:ALA:HA	1:D:343:LEU:HD21	2.02	0.40
1:D:320:LEU:HB3	1:D:321:ALA:HA	2.04	0.40
1:F:245:PHE:HZ	1:F:249:MET:CE	2.33	0.40
1:G:410:LEU:O	1:G:427:ARG:NH2	2.44	0.40
1:H:441:CYS:O	1:H:449:ARG:HG3	2.21	0.40
1:D:249:MET:HB2	1:D:249:MET:HE3	1.85	0.40
1:D:470[A]:ARG:NH2	8:D:605:HOH:O	2.55	0.40
1:F:39:LEU:O	1:F:43:ARG:HG3	2.22	0.40
1:H:46:THR:HG21	1:H:64:LEU:HG	2.04	0.40
1:H:28:THR:HG23	1:H:87:ASP:HA	2.03	0.40
1:A:242:GLU:O	1:A:246:VAL:HG23	2.22	0.40
1:B:82:LEU:HG	1:B:94:ARG:CZ	2.51	0.40
1:E:439:ARG:HD3	1:F:207:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:LEU:HD23	1:E:468:LEU:HA	1.96	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	446/470 (95%)	431 (97%)	14 (3%)	1 (0%)	47	55
1	B	459/470 (98%)	448 (98%)	9 (2%)	2 (0%)	34	37
1	C	446/470 (95%)	436 (98%)	9 (2%)	1 (0%)	47	55
1	D	452/470 (96%)	444 (98%)	7 (2%)	1 (0%)	47	55
1	E	444/470 (94%)	426 (96%)	16 (4%)	2 (0%)	29	31
1	F	446/470 (95%)	433 (97%)	12 (3%)	1 (0%)	47	55
1	G	445/470 (95%)	430 (97%)	13 (3%)	2 (0%)	34	37
1	H	453/470 (96%)	441 (97%)	10 (2%)	2 (0%)	34	37
All	All	3591/3760 (96%)	3489 (97%)	90 (2%)	12 (0%)	41	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	18	SER
1	A	205	LEU
1	C	205	LEU
1	E	205	LEU
1	F	205	LEU
1	G	205	LEU
1	B	205	LEU
1	B	100	VAL
1	D	205	LEU

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Mol	Chain	Res	Type
1	H	83	VAL
1	E	100	VAL
1	G	83	VAL

5.3.2 Protein sidechains (i)

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	312/352 (89%)	304 (97%)	8 (3%)	46	58
1	B	320/352 (91%)	308 (96%)	12 (4%)	33	42
1	C	317/352 (90%)	306 (96%)	11 (4%)	36	46
1	D	324/352 (92%)	311 (96%)	13 (4%)	31	40
1	E	316/352 (90%)	306 (97%)	10 (3%)	39	50
1	F	317/352 (90%)	307 (97%)	10 (3%)	39	50
1	G	305/352 (87%)	297 (97%)	8 (3%)	46	58
1	H	311/352 (88%)	303 (97%)	8 (3%)	46	58
All	All	2522/2816 (90%)	2442 (97%)	80 (3%)	39	50

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	121	LEU
1	A	200	TYR
1	A	205	LEU
1	A	325	ASP
1	A	412	ASP
1	A	419	SER
1	A	470	ARG
1	B	83	VAL
1	B	84	THR
1	B	100	VAL
1	B	112	ARG

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Mol	Chain	Res	Type
1	B	118	VAL
1	B	121	LEU
1	B	205	LEU
1	B	325	ASP
1	B	358	VAL
1	B	449	ARG
1	B	463	ARG
1	B	468	LEU
1	C	21	LEU
1	C	25	SER
1	C	84	THR
1	C	117	GLN
1	C	205	LEU
1	C	325	ASP
1	C	330	LYS
1	C	343	LEU
1	C	390	HIS
1	C	414	GLU
1	C	469	VAL
1	D	33	VAL
1	D	84	THR
1	D	118	VAL
1	D	200	TYR
1	D	285	MET
1	D	308	LEU
1	D	325	ASP
1	D	371	LEU
1	D	388	SER
1	D	405	VAL
1	D	412	ASP
1	D	431	THR
1	D	436	VAL
1	E	21	LEU
1	E	33	VAL
1	E	68	ASP
1	E	76	ASP
1	E	78	SER
1	E	86	GLU
1	E	126	LEU
1	E	200	TYR
1	E	325	ASP
1	E	436	VAL

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Mol	Chain	Res	Type
1	F	93	GLU
1	F	256	ARG
1	F	267	THR
1	F	320	LEU
1	F	325	ASP
1	F	371	LEU
1	F	408	GLN
1	F	412	ASP
1	F	431	THR
1	F	463	ARG
1	G	78	SER
1	G	113	SER
1	G	205	LEU
1	G	220	ASP
1	G	325	ASP
1	G	407	LEU
1	G	412	ASP
1	G	431	THR
1	H	28	THR
1	H	68	ASP
1	H	69	SER
1	H	325	ASP
1	H	398	ARG
1	H	431	THR
1	H	469	VAL
1	H	470	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	HIS
1	C	89	HIS
1	D	287	GLN
1	E	390	HIS
1	F	382	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
3	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	B	503	-	3,3,3	0.55	0	2,2,2	0.14	0
4	PG4	C	501	-	12,12,12	0.48	0	11,11,11	0.33	0
5	P3G	D	503	-	16,16,16	0.59	0	15,15,15	0.23	0
7	PGE	F	501	-	9,9,9	0.50	0	8,8,8	0.35	0
2	GOL	A	501	-	5,5,5	0.40	0	5,5,5	1.01	0
3	EDO	A	502	-	3,3,3	0.66	0	2,2,2	0.13	0
3	EDO	F	502	-	3,3,3	0.68	0	2,2,2	0.24	0
3	EDO	E	502	-	3,3,3	0.55	0	2,2,2	0.44	0
6	2PE	E	501	-	27,27,27	0.56	0	26,26,26	0.34	0
3	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PG4	B	501	-	12,12,12	0.45	0	11,11,11	0.62	0
3	EDO	D	502	-	3,3,3	0.49	0	2,2,2	0.52	0
2	GOL	B	502	-	5,5,5	0.40	0	5,5,5	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	503	-	-	1/1/1/1	-
4	PG4	C	501	-	-	8/10/10/10	-
5	P3G	D	503	-	-	6/14/14/14	-
7	PGE	F	501	-	-	4/7/7/7	-
2	GOL	A	501	-	-	3/4/4/4	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	F	502	-	-	0/1/1/1	-
3	EDO	E	502	-	-	1/1/1/1	-
6	2PE	E	501	-	-	16/25/25/25	-
3	EDO	C	502	-	-	1/1/1/1	-
4	PG4	B	501	-	-	6/10/10/10	-
3	EDO	D	502	-	-	1/1/1/1	-
2	GOL	B	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	GOL	C1-C2-C3-O3
4	C	501	PG4	O2-C3-C4-O3
7	F	501	PGE	O2-C3-C4-O3
5	D	503	P3G	O5-C11-C12-O6
5	D	503	P3G	O6-C13-C14-O7
4	B	501	PG4	O2-C3-C4-O3
5	D	503	P3G	O3-C7-C8-O4
6	E	501	2PE	O7-C8-C9-O10
6	E	501	2PE	O13-C14-C15-O16
4	B	501	PG4	O1-C1-C2-O2
6	E	501	2PE	O19-C20-C21-O22
4	B	501	PG4	O4-C7-C8-O5
2	A	501	GOL	O1-C1-C2-C3
2	A	501	GOL	C1-C2-C3-O3
6	E	501	2PE	O25-C26-C27-O28
4	B	501	PG4	O3-C5-C6-O4
6	E	501	2PE	O22-C23-C24-O25
3	C	502	EDO	O1-C1-C2-O2
3	E	502	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	501	PG4	O4-C7-C8-O5
7	F	501	PGE	O1-C1-C2-O2
7	F	501	PGE	O3-C5-C6-O4
5	D	503	P3G	O5-C10-C9-O4
2	B	502	GOL	O2-C2-C3-O3
2	A	501	GOL	O1-C1-C2-O2
4	C	501	PG4	O3-C5-C6-O4
5	D	503	P3G	C8-C7-O3-C6
5	D	503	P3G	C12-C11-O5-C10
4	C	501	PG4	C6-C5-O3-C4
4	C	501	PG4	O1-C1-C2-O2
6	E	501	2PE	C27-C26-O25-C24
6	E	501	2PE	C12-C11-O10-C9
6	E	501	2PE	C14-C15-O16-C17
6	E	501	2PE	C21-C20-O19-C18
4	C	501	PG4	C4-C3-O2-C2
4	C	501	PG4	C3-C4-O3-C5
7	F	501	PGE	C1-C2-O2-C3
6	E	501	2PE	C11-C12-O13-C14
6	E	501	2PE	O10-C11-C12-O13
6	E	501	2PE	C17-C18-O19-C20
4	C	501	PG4	C5-C6-O4-C7
3	B	503	EDO	O1-C1-C2-O2
4	B	501	PG4	C6-C5-O3-C4
6	E	501	2PE	C24-C23-O22-C21
6	E	501	2PE	C23-C24-O25-C26
6	E	501	2PE	C18-C17-O16-C15
3	D	501	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
4	B	501	PG4	C8-C7-O4-C6
3	D	502	EDO	O1-C1-C2-O2
6	E	501	2PE	C2-C3-O4-C5

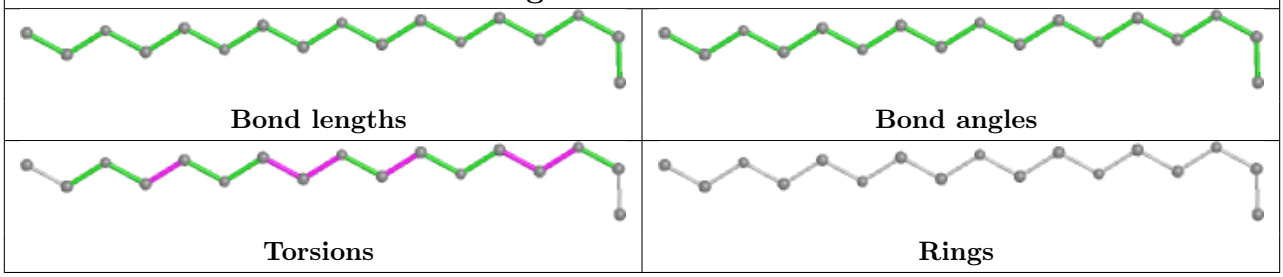
There are no ring outliers.

4 monomers are involved in 5 short contacts:

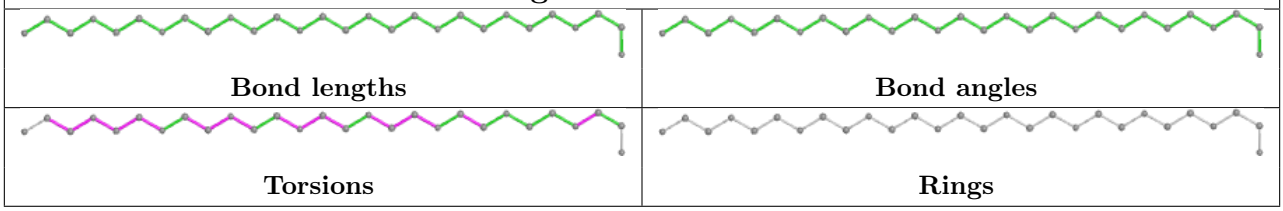
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	EDO	1	0
5	D	503	P3G	1	0
2	A	501	GOL	2	0
6	E	501	2PE	1	0

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 then 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 P3G D 503



Ligand 2PE E 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	450/470 (95%)	0.23	34 (7%)	13	12	15, 32, 63, 76	0
1	B	462/470 (98%)	-0.01	14 (3%)	50	48	14, 28, 60, 78	0
1	C	450/470 (95%)	-0.00	19 (4%)	36	34	14, 28, 56, 80	0
1	D	454/470 (96%)	0.02	21 (4%)	32	31	16, 29, 54, 65	0
1	E	448/470 (95%)	0.10	23 (5%)	28	26	14, 30, 62, 83	0
1	F	450/470 (95%)	0.08	20 (4%)	34	32	14, 30, 58, 74	0
1	G	449/470 (95%)	0.22	35 (7%)	13	11	17, 37, 65, 76	0
1	H	454/470 (96%)	0.34	37 (8%)	12	10	18, 36, 65, 76	0
All	All	3617/3760 (96%)	0.12	203 (5%)	24	23	14, 31, 62, 83	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	5.8
1	F	83	VAL	5.2
1	H	420	PRO	5.2
1	A	420	PRO	5.2
1	H	78	SER	5.1
1	G	420	PRO	4.9
1	H	418	ILE	4.9
1	E	84	THR	4.8
1	A	413	ASP	4.8
1	F	405	VAL	4.7
1	A	65	ALA	4.7
1	H	84	THR	4.6
1	F	404	GLY	4.4
1	F	417	ALA	4.4
1	H	76	ASP	4.3
1	G	76	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	420	PRO	4.2
1	C	385	PRO	4.2
1	A	404	GLY	4.0
1	G	78	SER	4.0
1	B	417	ALA	4.0
1	F	409	GLU	4.0
1	C	287	GLN	3.9
1	C	411	THR	3.9
1	G	75	ALA	3.9
1	H	105	GLY	3.8
1	A	78	SER	3.8
1	A	418	ILE	3.8
1	E	98	ASP	3.8
1	H	18	SER	3.8
1	G	65	ALA	3.7
1	E	53	GLY	3.6
1	C	470	ARG	3.6
1	A	417	ALA	3.6
1	G	469	VAL	3.5
1	A	61	ASP	3.5
1	H	98	ASP	3.5
1	D	398	ARG	3.5
1	B	418	ILE	3.5
1	D	418	ILE	3.5
1	G	424	PRO	3.5
1	H	416	ALA	3.5
1	A	77	GLY	3.4
1	C	405	VAL	3.4
1	G	382	GLN	3.4
1	A	76	ASP	3.4
1	A	19	ASP	3.3
1	H	77	GLY	3.3
1	G	416	ALA	3.3
1	C	395	ALA	3.3
1	G	53	GLY	3.2
1	H	282	SER	3.2
1	C	417	ALA	3.2
1	E	76	ASP	3.2
1	E	78	SER	3.2
1	A	97	ILE	3.2
1	F	385	PRO	3.1
1	H	58	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	412	ASP	3.1
1	E	62	GLY	3.1
1	G	425	GLN	3.1
1	A	395	ALA	3.1
1	G	84	THR	3.1
1	H	62	GLY	3.1
1	G	79	PHE	3.1
1	H	103	ASP	3.0
1	C	418	ILE	3.0
1	D	416	ALA	3.0
1	B	416	ALA	3.0
1	C	416	ALA	3.0
1	H	65	ALA	3.0
1	E	211	GLY	3.0
1	A	388	SER	2.9
1	H	81	PRO	2.9
1	F	422	LEU	2.9
1	H	417	ALA	2.9
1	A	62	GLY	2.9
1	H	286	PRO	2.9
1	G	413	ASP	2.9
1	H	107	ARG	2.9
1	H	20	ALA	2.9
1	D	102	PRO	2.9
1	G	403	ARG	2.9
1	D	424	PRO	2.8
1	A	68	ASP	2.8
1	D	412	ASP	2.8
1	C	423	THR	2.8
1	E	75	ALA	2.8
1	E	19	ASP	2.8
1	D	402	GLN	2.8
1	F	420	PRO	2.8
1	H	56	THR	2.8
1	G	73	ASP	2.7
1	D	103	ASP	2.7
1	D	415	LEU	2.7
1	A	411	THR	2.7
1	B	411	THR	2.7
1	E	81	PRO	2.7
1	H	104	LEU	2.7
1	H	85	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	84	THR	2.7
1	A	73	ASP	2.7
1	E	104	LEU	2.7
1	F	423	THR	2.7
1	H	102	PRO	2.6
1	A	416	ALA	2.6
1	A	384	VAL	2.6
1	G	98	ASP	2.6
1	D	205	LEU	2.6
1	G	418	ILE	2.6
1	D	419	SER	2.6
1	E	79	PHE	2.6
1	H	64	LEU	2.6
1	E	418	ILE	2.6
1	A	424	PRO	2.6
1	B	420	PRO	2.6
1	A	81	PRO	2.5
1	B	402	GLN	2.5
1	H	413	ASP	2.5
1	B	286	PRO	2.5
1	H	55	LEU	2.5
1	H	83	VAL	2.5
1	D	417	ALA	2.5
1	A	200	TYR	2.5
1	C	402	GLN	2.5
1	D	422	LEU	2.5
1	E	416	ALA	2.4
1	G	395	ALA	2.4
1	C	98	ASP	2.4
1	F	400	ALA	2.4
1	D	411	THR	2.4
1	B	103	ASP	2.4
1	E	417	ALA	2.4
1	F	411	THR	2.4
1	G	71	ALA	2.4
1	H	79	PHE	2.4
1	A	60	ARG	2.3
1	E	61	ASP	2.3
1	G	409	GLU	2.3
1	A	402	GLN	2.3
1	F	382	GLN	2.3
1	F	399	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	54	LEU	2.3
1	H	22	ALA	2.3
1	C	420	PRO	2.3
1	A	71	ALA	2.3
1	F	84	THR	2.3
1	A	423	THR	2.3
1	F	418	ILE	2.3
1	B	55	LEU	2.3
1	E	402	GLN	2.3
1	F	406	GLY	2.3
1	H	411	THR	2.2
1	E	82	LEU	2.2
1	C	424	PRO	2.2
1	G	417	ALA	2.2
1	B	410	LEU	2.2
1	A	83	VAL	2.2
1	C	83	VAL	2.2
1	G	74	VAL	2.2
1	H	100	VAL	2.2
1	G	404	GLY	2.2
1	G	83	VAL	2.2
1	B	58	GLU	2.2
1	H	19	ASP	2.2
1	B	395	ALA	2.2
1	C	419	SER	2.2
1	G	61	ASP	2.2
1	E	102	PRO	2.2
1	A	66	GLY	2.2
1	F	287	GLN	2.2
1	C	410	LEU	2.1
1	E	420	PRO	2.1
1	H	80	GLY	2.1
1	E	94	ARG	2.1
1	A	98	ASP	2.1
1	G	422	LEU	2.1
1	B	252	VAL	2.1
1	D	406	GLY	2.1
1	F	415	LEU	2.1
1	G	410	LEU	2.1
1	A	412	ASP	2.1
1	D	423	THR	2.1
1	F	403	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	403	ARG	2.1
1	G	421	GLU	2.1
1	D	404	GLY	2.1
1	H	53	GLY	2.1
1	H	315	LEU	2.1
1	E	100	VAL	2.1
1	G	315	LEU	2.0
1	G	17	PRO	2.0
1	B	413	ASP	2.0
1	G	77	GLY	2.0
1	G	18	SER	2.0
1	H	219	ALA	2.0
1	D	83	VAL	2.0
1	D	410	LEU	2.0
1	A	425	GLN	2.0
1	A	103	ASP	2.0
1	D	413	ASP	2.0
1	F	276	ASP	2.0
1	G	69	SER	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 monosaccharides 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
3	EDO	D	501	4/4	0.61	0.16	52,56,57,58	0
3	EDO	F	502	4/4	0.69	0.20	40,44,47,47	0
3	EDO	D	502	4/4	0.73	0.21	59,61,65,65	0
5	P3G	D	503	17/17	0.83	0.16	51,59,67,69	0

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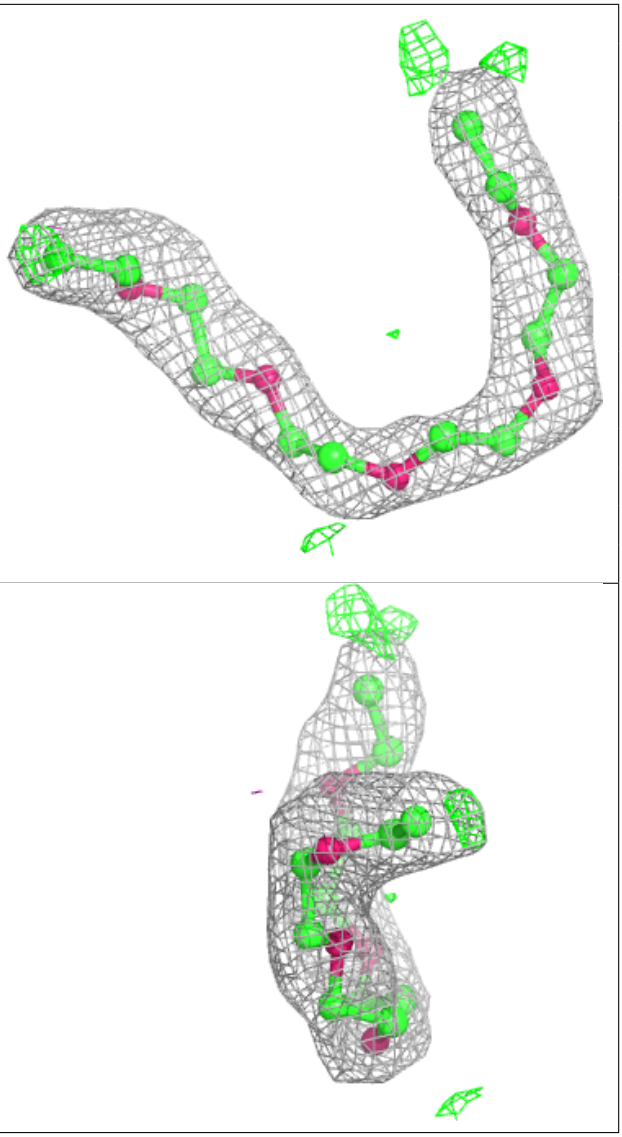
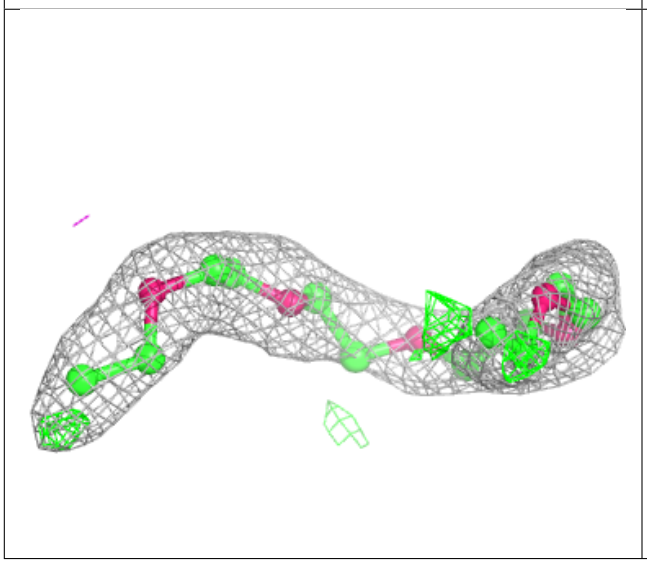
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	502	4/4	0.85	0.19	57,60,60,61	0
6	2PE	E	501	28/28	0.86	0.18	46,56,65,67	0
3	EDO	A	502	4/4	0.87	0.14	33,38,39,40	0
3	EDO	E	502	4/4	0.88	0.11	37,41,42,46	0
4	PG4	C	501	13/13	0.89	0.14	48,55,62,64	0
7	PGE	F	501	10/10	0.89	0.12	43,52,54,57	0
2	GOL	B	502	6/6	0.90	0.16	36,37,41,44	0
4	PG4	B	501	13/13	0.91	0.16	41,47,52,52	0
2	GOL	A	501	6/6	0.93	0.16	37,44,47,47	0
3	EDO	B	503	4/4	0.96	0.23	41,43,43,44	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 P3G D 503:

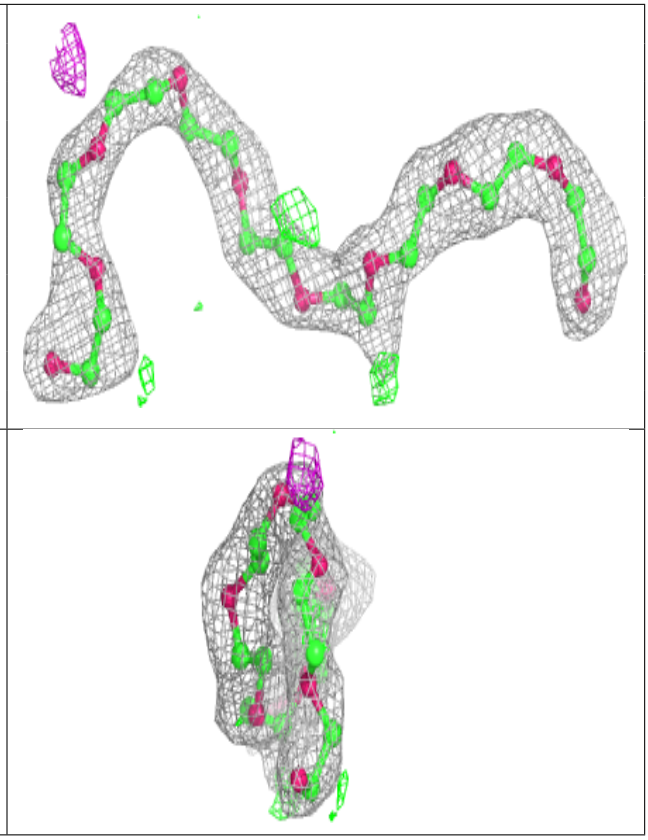
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around 2PE E 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.