



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:56 PM UTC

PDB ID : 6IEM / pdb_00006iem
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 ⓘ 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:

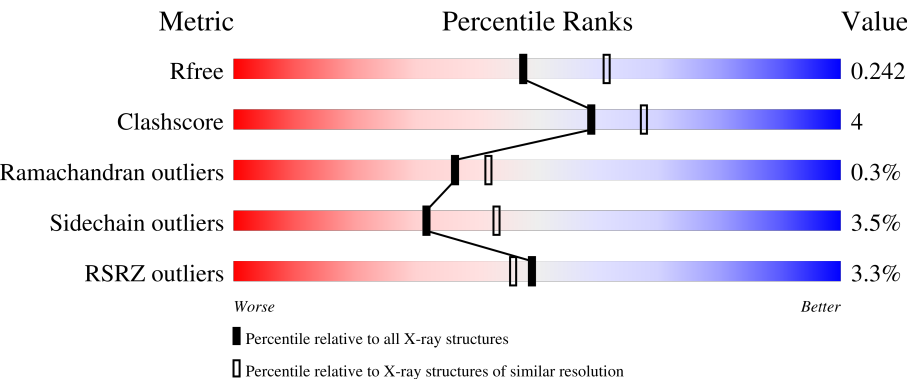
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	3% 87% 8% .
1	B	470	5% 89% 8% ..
1	C	470	3% 86% 8% ..
1	D	470	2% 84% 11% ..
1	E	470	% 86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	470	3% 84% 10%
1	G	470	4% 87% 8%
1	H	470	5% 85% 11%

2 Entry composition

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

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



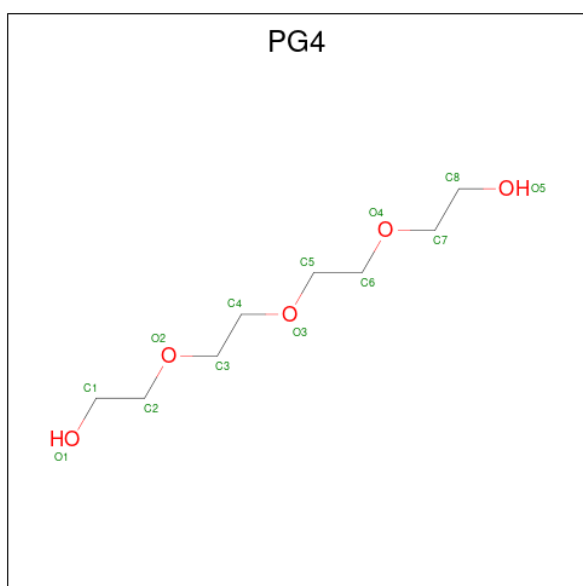
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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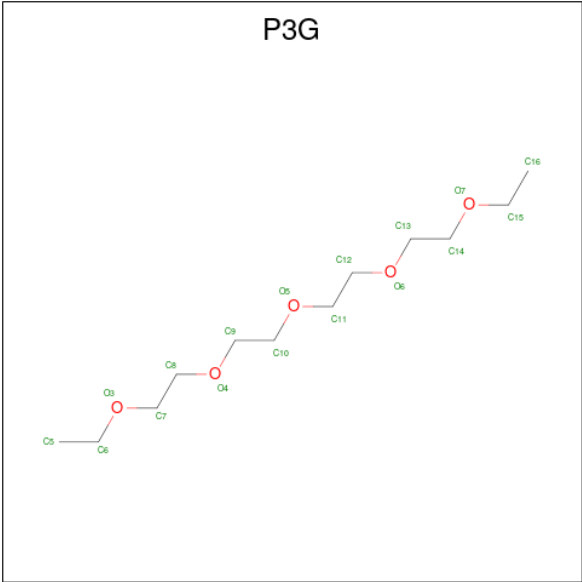
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



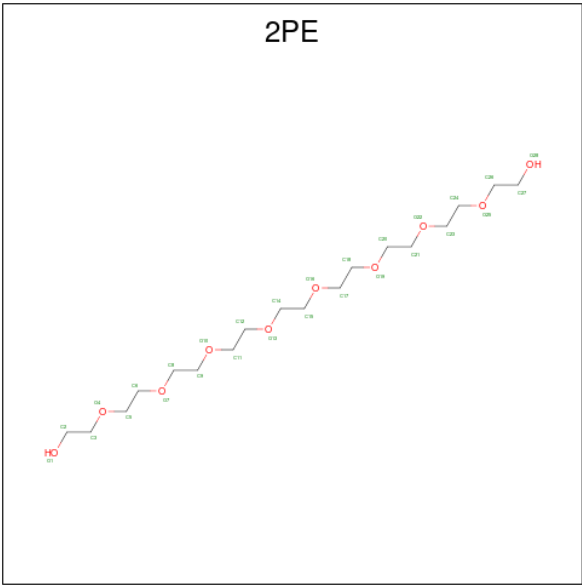
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0

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



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

- Molecule 6 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



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

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

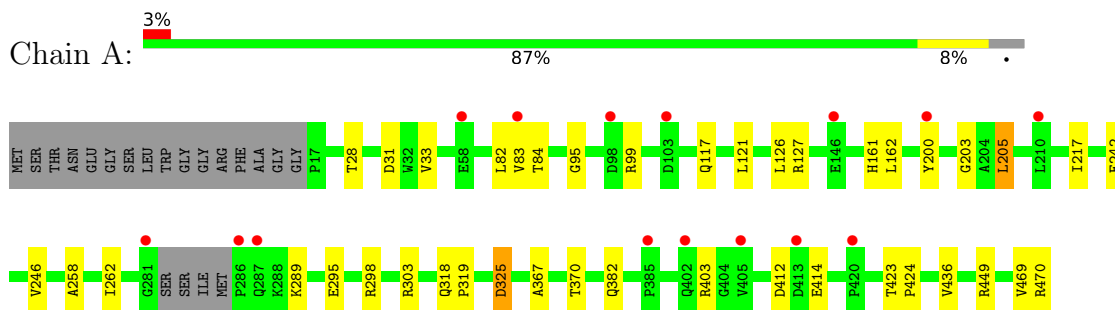
- Molecule 8 is water.

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

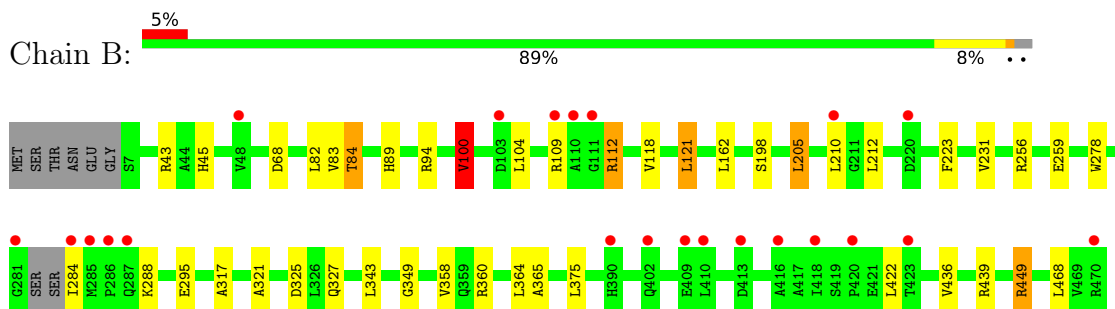
3 Residue-property plots [i](#)

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.

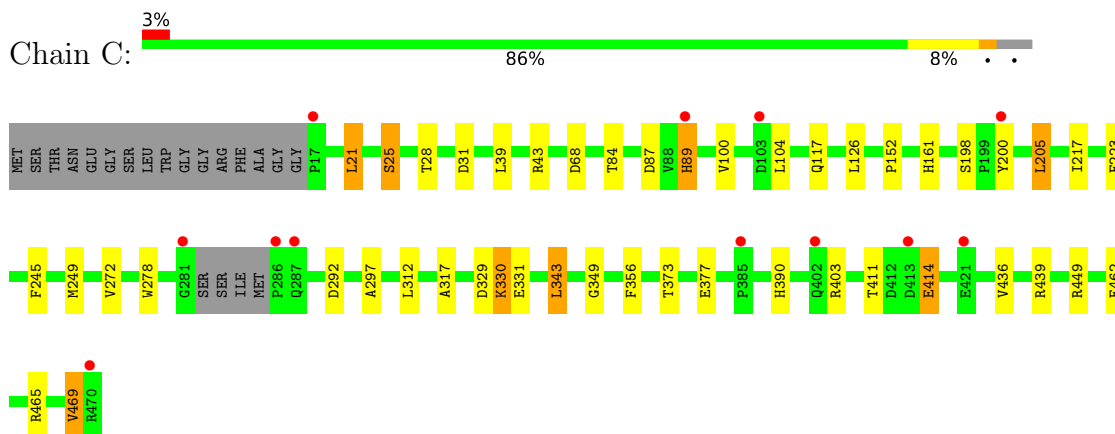
- Molecule 1: Argininosuccinate lyase



- Molecule 1: Argininosuccinate lyase

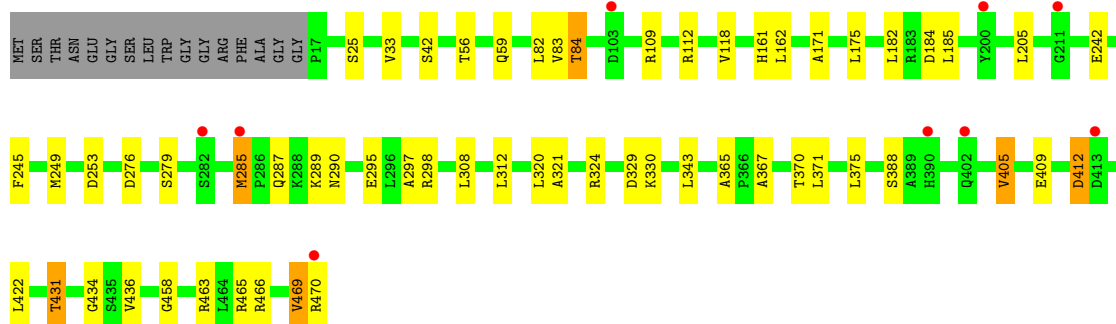


- Molecule 1: Argininosuccinate lyase



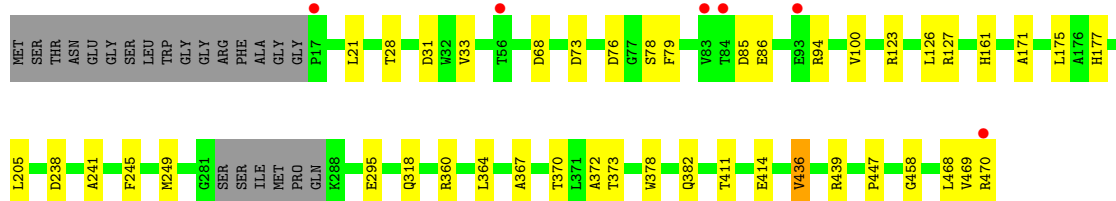
- Molecule 1: Argininosuccinate lyase

Chain D:  2% 84% 11% ..



- Molecule 1: Argininosuccinate lyase

Chain E:  % 86% 9% 5%



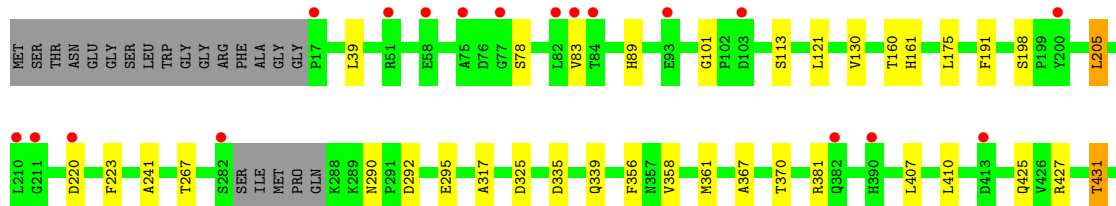
- Molecule 1: Argininosuccinate lyase

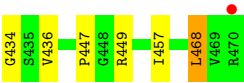
Chain F:  3% 84% 10% ..



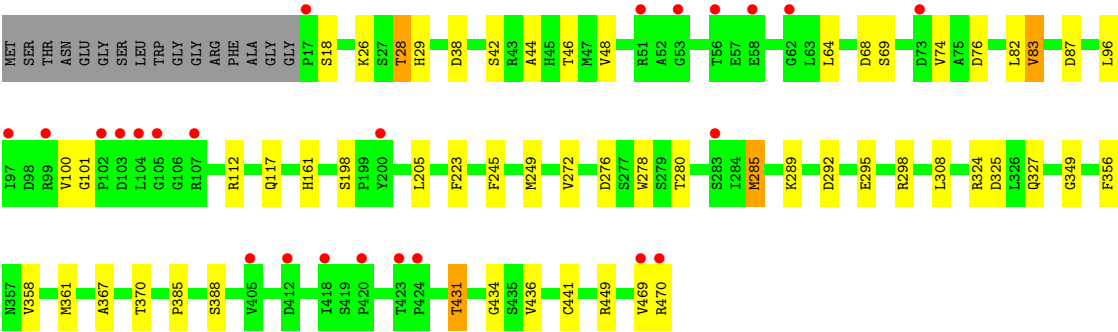
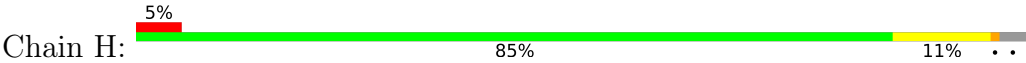
- Molecule 1: Argininosuccinate lyase

Chain G:  4% 87% 8% ..





● 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	127.55Å 183.82Å 190.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.48 – 2.20 40.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.48-2.20) 99.9 (40.48-2.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	11349 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 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	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.*

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: GOL, EDO, 2PE, PGE, P3G, PG4

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	0.67	0/3312	0.93	0/4517
1	B	0.70	0/3406	0.98	4/4645 (0.1%)
1	C	0.69	0/3337	0.92	1/4548 (0.0%)
1	D	0.68	0/3382	0.94	3/4607 (0.1%)
1	E	0.66	0/3324	0.93	0/4529
1	F	0.68	0/3331	0.93	4/4541 (0.1%)
1	G	0.62	0/3279	0.90	2/4476 (0.0%)
1	H	0.63	0/3328	0.93	4/4541 (0.1%)
All	All	0.67	0/26699	0.93	18/36404 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	344	LEU	CA-C-N	-6.18	112.64	119.19
1	F	344	LEU	C-N-CA	-6.18	112.64	119.19
1	B	365	ALA	CA-C-N	-6.13	113.95	120.94
1	B	365	ALA	C-N-CA	-6.13	113.95	120.94
1	H	101	GLY	CA-C-N	5.61	125.28	119.56
1	H	101	GLY	C-N-CA	5.61	125.28	119.56
1	F	101	GLY	CA-C-N	5.60	125.26	119.05
1	F	101	GLY	C-N-CA	5.60	125.26	119.05
1	C	292	ASP	N-CA-C	5.58	117.81	111.11
1	H	285	MET	CA-C-N	5.55	125.22	119.56
1	H	285	MET	C-N-CA	5.55	125.22	119.56
1	B	343	LEU	N-CA-C	5.32	117.16	111.36
1	D	365	ALA	CA-C-N	-5.18	115.00	121.00
1	D	365	ALA	C-N-CA	-5.18	115.00	121.00
1	G	101	GLY	CA-C-N	5.09	125.12	119.32
1	G	101	GLY	C-N-CA	5.09	125.12	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	LEU	N-CA-C	-5.04	103.39	110.50
1	D	469	VAL	N-CA-C	-5.01	105.71	110.52

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	3255	0	3185	27	0
1	B	3343	0	3265	21	0
1	C	3280	0	3225	40	0
1	D	3325	0	3284	49	0
1	E	3269	0	3204	29	0
1	F	3274	0	3209	44	0
1	G	3224	0	3142	26	0
1	H	3269	0	3186	39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	67	0	0	1	0
8	H	71	0	0	0	0
All	All	27041	0	25872	230	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 (230) 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:C:312:LEU:HD21	1:D:249:MET:HE1	1.40	1.03
1:E:249:MET:HE1	1:F:241:ALA:HB3	1.42	1.01
1:C:87:ASP:OD2	1:C:89:HIS:HD2	1.54	0.89
1:E:249:MET:HE1	1:F:241:ALA:CB	2.06	0.85
1:C:249:MET:HE1	1:D:312:LEU:HD21	1.59	0.84
1:G:241:ALA:CB	1:H:249:MET:HE1	2.11	0.81
1:G:431:THR:HG22	1:G:434:GLY:N	2.01	0.74
1:C:312:LEU:CD2	1:D:249:MET:HE1	2.18	0.73
1:G:241:ALA:HB3	1:H:249:MET:HE1	1.70	0.72
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: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:C:245:PHE:CZ	1:C:249:MET:HE3	2.30	0.66
1:C:312:LEU:HD21	1:D:249:MET:CE	2.22	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:E:370:THR:HA	1:H:285:MET:HE2	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:245:PHE:CE1	1:C:249:MET:HE3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:THR:OG1	1:H:285:MET:HE1	2.00	0.61
1:D:458:GLY:HA3	5:D:503:P3G:H92	1.83	0.61
1:G:241:ALA:HB1	1:H:249:MET:HE1	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:F:245:PHE:CZ	1:F:249:MET:HE2	2.36	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: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: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:329:ASP:OD1	1:F:330:LYS:HG3	2.06	0.55
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:H:358:VAL:HA	1:H:361:MET:HE2	1.89	0.54
1:C:249:MET:CE	1:D:312:LEU:HD21	2.33	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:D:245:PHE:CE1	1:D:249:MET:HE3	2.43	0.53
1:E:73:ASP:HB3	1:E:79:PHE:HB2	1.90	0.53
1:D:245:PHE:CZ	1:D:249:MET:HE3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:ARG:CZ	1:E:364:LEU:HD11	2.40	0.52
1:E:241:ALA:HB3	1:F:249:MET:HE1	1.91	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:E:372:ALA:HB3	1:H:285:MET:HE3	1.93	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: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
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:E:238:ASP:HB2	1:F:249:MET:HE3	1.95	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:H:26:LYS:HZ2	1:H:83:VAL:HA	1.79	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:E:245:PHE:CZ	1:E:249:MET:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:PHE:CE1	1:H:249:MET:HE2	2.50	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: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: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:249:MET:CA	1:D:249:MET:HE2	2.47	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: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:82:LEU:C	1:D:84:THR:H	2.24	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:D:249:MET:HE2	1:D:249:MET:HA	1.99	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:D:82:LEU:C	1:D:84:THR:N	2.75	0.44
1:G:290:ASN:HB2	1:G:292:ASP:OD1	2.18	0.44
1:A:403:ARG:HH11	1:A:414:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:358:VAL:HA	1:G:361:MET:HE3	2.00	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:285:MET:HE2	1:D:285:MET:HB2	1.93	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:A:82:LEU:C	1:A:84:THR:N	2.75	0.42
1:G:356:PHE:HB3	1:G:361:MET:HE1	2.02	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
1:B:82:LEU:C	1:B:84:THR:H	2.27	0.42
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:H:82:LEU:O	1:H:83:VAL:C	2.63	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:F:385:PRO:O	1:F:386:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:245:PHE:HZ	1:F:249:MET:CE	2.33	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:C:249:MET:HE1	1:D:312:LEU:CD2	2.42	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:F:89:HIS:CD2	1:F:89:HIS:H	2.39	0.41
1:A:303:ARG:HH12	1:C:331:GLU:CD	2.27	0.41
1:C:465:ARG:HE	1:F:465:ARG:CZ	2.34	0.41
1:H:76:ASP:C	1:H:76:ASP:OD1	2.64	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: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: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
1:E:468:LEU:HD23	1:E:468:LEU:HA	1.96	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	446/470 (95%)	431 (97%)	14 (3%)	1 (0%)	43	51
1	B	459/470 (98%)	448 (98%)	9 (2%)	2 (0%)	30	34
1	C	446/470 (95%)	436 (98%)	9 (2%)	1 (0%)	43	51
1	D	452/470 (96%)	444 (98%)	7 (2%)	1 (0%)	43	51
1	E	444/470 (94%)	426 (96%)	16 (4%)	2 (0%)	24	27
1	F	446/470 (95%)	433 (97%)	12 (3%)	1 (0%)	43	51
1	G	445/470 (95%)	430 (97%)	13 (3%)	2 (0%)	30	34
1	H	453/470 (96%)	441 (97%)	10 (2%)	2 (0%)	30	34
All	All	3591/3760 (96%)	3489 (97%)	90 (2%)	12 (0%)	36	42

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
1	H	83	VAL
1	E	100	VAL
1	G	83	VAL

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	312/352 (89%)	303 (97%)	9 (3%)	37	51
1	B	320/352 (91%)	306 (96%)	14 (4%)	25	34
1	C	317/352 (90%)	304 (96%)	13 (4%)	27	37
1	D	324/352 (92%)	312 (96%)	12 (4%)	30	41
1	E	316/352 (90%)	308 (98%)	8 (2%)	42	56
1	F	317/352 (90%)	305 (96%)	12 (4%)	29	40
1	G	305/352 (87%)	294 (96%)	11 (4%)	31	42
1	H	311/352 (88%)	302 (97%)	9 (3%)	37	51
All	All	2522/2816 (90%)	2434 (96%)	88 (4%)	32	43

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	83	VAL
1	A	117	GLN
1	A	121	LEU
1	A	126	LEU
1	A	205	LEU
1	A	289	LYS
1	A	325	ASP
1	A	436	VAL
1	B	83	VAL
1	B	84	THR
1	B	100	VAL
1	B	112	ARG
1	B	118	VAL
1	B	121	LEU
1	B	162	LEU
1	B	205	LEU
1	B	212	LEU
1	B	325	ASP
1	B	358	VAL
1	B	436	VAL
1	B	449	ARG
1	B	468	LEU

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Mol	Chain	Res	Type
1	C	21	LEU
1	C	25	SER
1	C	84	THR
1	C	89	HIS
1	C	117	GLN
1	C	126	LEU
1	C	205	LEU
1	C	330	LYS
1	C	343	LEU
1	C	390	HIS
1	C	414	GLU
1	C	436	VAL
1	C	469	VAL
1	D	33	VAL
1	D	84	THR
1	D	118	VAL
1	D	162	LEU
1	D	285	MET
1	D	308	LEU
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	436	VAL
1	F	89	HIS
1	F	93	GLU
1	F	256	ARG
1	F	267	THR
1	F	320	LEU
1	F	371	LEU
1	F	408	GLN
1	F	412	ASP
1	F	431	THR

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Mol	Chain	Res	Type
1	F	449	ARG
1	F	463	ARG
1	F	465	ARG
1	G	78	SER
1	G	113	SER
1	G	121	LEU
1	G	205	LEU
1	G	220	ASP
1	G	267	THR
1	G	325	ASP
1	G	407	LEU
1	G	425	GLN
1	G	431	THR
1	G	468	LEU
1	H	28	THR
1	H	68	ASP
1	H	69	SER
1	H	74	VAL
1	H	325	ASP
1	H	431	THR
1	H	436	VAL
1	H	469	VAL
1	H	470	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	318	GLN
1	A	323	ASN
1	B	151	HIS
1	B	318	GLN
1	B	323	ASN
1	B	467	GLN
1	C	89	HIS
1	C	117	GLN
1	C	323	ASN
1	C	357	ASN
1	C	425	GLN
1	D	166	GLN
1	D	287	GLN
1	D	290	ASN

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Mol	Chain	Res	Type
1	D	318	GLN
1	D	323	ASN
1	D	382	GLN
1	E	163	GLN
1	E	166	GLN
1	E	290	ASN
1	E	318	GLN
1	E	323	ASN
1	E	390	HIS
1	E	467	GLN
1	F	357	ASN
1	F	382	GLN
1	F	455	ASN
1	F	467	GLN
1	G	318	GLN
1	G	323	ASN
1	H	151	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	502	-	3,3,3	0.52	0	2,2,2	0.48	0
3	EDO	F	502	-	3,3,3	0.64	0	2,2,2	0.23	0
5	P3G	D	503	-	16,16,16	0.59	0	15,15,15	0.23	0
6	2PE	E	501	-	27,27,27	0.56	0	26,26,26	0.34	0
3	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	B	503	-	3,3,3	0.52	0	2,2,2	0.19	0
3	EDO	A	502	-	3,3,3	0.63	0	2,2,2	0.08	0
4	PG4	B	501	-	12,12,12	0.46	0	11,11,11	0.61	0
4	PG4	C	501	-	12,12,12	0.49	0	11,11,11	0.32	0
7	PGE	F	501	-	9,9,9	0.50	0	8,8,8	0.35	0
3	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.55	0
2	GOL	B	502	-	5,5,5	0.41	0	5,5,5	0.40	0
2	GOL	A	501	-	5,5,5	0.41	0	5,5,5	1.07	0
3	EDO	D	501	-	3,3,3	0.46	0	2,2,2	0.40	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	E	502	-	-	1/1/1/1	-
3	EDO	F	502	-	-	0/1/1/1	-
5	P3G	D	503	-	-	6/14/14/14	-
6	2PE	E	501	-	-	16/25/25/25	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
4	PG4	B	501	-	-	6/10/10/10	-
4	PG4	C	501	-	-	8/10/10/10	-
7	PGE	F	501	-	-	5/7/7/7	-
3	EDO	D	502	-	-	1/1/1/1	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	501	-	-	3/4/4/4	-
3	EDO	D	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (52) 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	O6-C13-C14-O7
5	D	503	P3G	O5-C11-C12-O6
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
6	E	501	2PE	O19-C20-C21-O22
4	B	501	PG4	O1-C1-C2-O2
4	B	501	PG4	O4-C7-C8-O5
2	A	501	GOL	O1-C1-C2-C3
2	A	501	GOL	C1-C2-C3-O3
4	B	501	PG4	O3-C5-C6-O4
6	E	501	2PE	O25-C26-C27-O28
3	E	502	EDO	O1-C1-C2-O2
6	E	501	2PE	O22-C23-C24-O25
4	C	501	PG4	O4-C7-C8-O5
7	F	501	PGE	O1-C1-C2-O2
7	F	501	PGE	O3-C5-C6-O4
2	B	502	GOL	O2-C2-C3-O3
3	C	502	EDO	O1-C1-C2-O2
5	D	503	P3G	O5-C10-C9-O4
2	A	501	GOL	O1-C1-C2-O2
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
4	C	501	PG4	O3-C5-C6-O4
6	E	501	2PE	C12-C11-O10-C9
6	E	501	2PE	C21-C20-O19-C18
6	E	501	2PE	C27-C26-O25-C24
4	C	501	PG4	C3-C4-O3-C5
6	E	501	2PE	C14-C15-O16-C17
4	C	501	PG4	C4-C3-O2-C2
7	F	501	PGE	C1-C2-O2-C3
6	E	501	2PE	C11-C12-O13-C14
6	E	501	2PE	C17-C18-O19-C20
4	B	501	PG4	C6-C5-O3-C4
6	E	501	2PE	O10-C11-C12-O13
4	C	501	PG4	C5-C6-O4-C7
6	E	501	2PE	C24-C23-O22-C21

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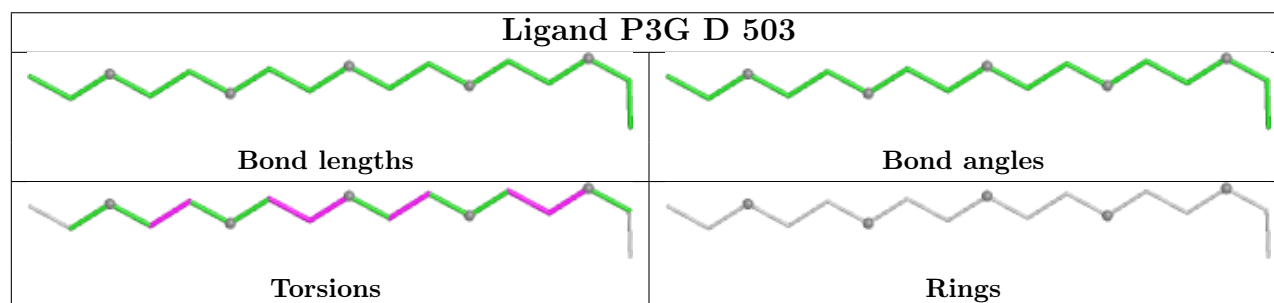
Mol	Chain	Res	Type	Atoms
6	E	501	2PE	C23-C24-O25-C26
6	E	501	2PE	C18-C17-O16-C15
3	B	503	EDO	O1-C1-C2-O2
3	D	501	EDO	O1-C1-C2-O2
4	B	501	PG4	C8-C7-O4-C6
3	A	502	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
6	E	501	2PE	C2-C3-O4-C5
7	F	501	PGE	C3-C4-O3-C5

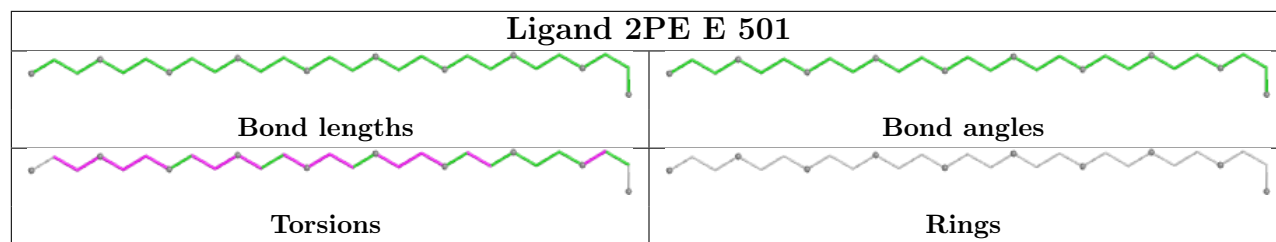
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	503	P3G	1	0
6	E	501	2PE	1	0
3	B	503	EDO	1	0
2	A	501	GOL	2	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 [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	450/470 (95%)	0.05	15 (3%)	49	46	15, 32, 63, 76	0
1	B	462/470 (98%)	-0.08	22 (4%)	35	32	13, 28, 60, 78	1 (0%)
1	C	450/470 (95%)	-0.18	12 (2%)	56	53	14, 28, 56, 80	0
1	D	454/470 (96%)	-0.17	9 (1%)	65	62	16, 29, 54, 65	1 (0%)
1	E	448/470 (95%)	-0.08	6 (1%)	75	73	14, 29, 62, 83	1 (0%)
1	F	450/470 (95%)	-0.09	12 (2%)	56	53	14, 30, 58, 74	0
1	G	449/470 (95%)	0.16	19 (4%)	40	37	17, 37, 65, 76	0
1	H	454/470 (96%)	0.21	24 (5%)	32	29	16, 36, 65, 76	1 (0%)
All	All	3617/3760 (96%)	-0.02	119 (3%)	49	46	13, 31, 62, 83	4 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	GLN	6.2
1	A	286	PRO	5.1
1	G	282	SER	5.1
1	C	470	ARG	4.9
1	F	286	PRO	4.7
1	B	285	MET	4.7
1	H	17	PRO	4.6
1	E	470[A]	ARG	4.4
1	C	286	PRO	4.2
1	F	281	GLY	4.1
1	B	103	ASP	3.8
1	A	146	GLU	3.6
1	B	409	GLU	3.6
1	D	470[A]	ARG	3.5
1	B	210	LEU	3.5
1	H	423	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	105	GLY	3.5
1	A	287	GLN	3.5
1	A	103	ASP	3.4
1	B	287	GLN	3.4
1	A	200	TYR	3.4
1	H	107	ARG	3.4
1	G	413	ASP	3.2
1	G	382	GLN	3.2
1	G	51	ARG	3.2
1	F	287	GLN	3.2
1	H	405	VAL	3.2
1	B	110	ALA	3.1
1	B	284	ILE	3.0
1	A	281	GLY	3.0
1	F	17	PRO	3.0
1	A	402	GLN	2.9
1	G	82	LEU	2.9
1	G	220	ASP	2.9
1	F	418	ILE	2.8
1	C	17	PRO	2.8
1	D	200	TYR	2.8
1	A	413	ASP	2.8
1	B	286	PRO	2.8
1	H	470	ARG	2.8
1	G	17	PRO	2.7
1	E	84	THR	2.7
1	G	84	THR	2.7
1	G	211	GLY	2.7
1	D	413	ASP	2.7
1	H	103	ASP	2.7
1	B	109	ARG	2.6
1	B	470	ARG	2.6
1	F	405	VAL	2.6
1	F	423	THR	2.6
1	F	424	PRO	2.6
1	G	83	VAL	2.5
1	H	283	SER	2.5
1	B	423	THR	2.4
1	G	200	TYR	2.4
1	B	281	GLY	2.4
1	E	93	GLU	2.4
1	B	418	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	2.4
1	F	288	LYS	2.4
1	D	390	HIS	2.4
1	H	58	GLU	2.4
1	H	56	THR	2.4
1	C	200	TYR	2.4
1	C	103	ASP	2.4
1	A	420	PRO	2.4
1	B	390	HIS	2.4
1	C	89	HIS	2.4
1	G	103	ASP	2.3
1	B	416	ALA	2.3
1	G	210	LEU	2.3
1	H	104	LEU	2.3
1	B	413	ASP	2.3
1	A	405	VAL	2.3
1	D	402	GLN	2.3
1	H	420	PRO	2.3
1	G	75	ALA	2.3
1	G	93	GLU	2.3
1	A	385	PRO	2.3
1	C	281	GLY	2.3
1	C	421	GLU	2.3
1	H	97	ILE	2.3
1	B	48	VAL	2.3
1	H	469	VAL	2.3
1	C	385	PRO	2.2
1	G	470	ARG	2.2
1	B	402	GLN	2.2
1	D	285	MET	2.2
1	F	421	GLU	2.2
1	A	210	LEU	2.2
1	A	83	VAL	2.2
1	A	98	ASP	2.2
1	H	53	GLY	2.2
1	H	51	ARG	2.1
1	G	58	GLU	2.1
1	E	56	THR	2.1
1	B	410	LEU	2.1
1	A	58	GLU	2.1
1	C	413	ASP	2.1
1	H	73	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	62	GLY	2.1
1	D	282	SER	2.1
1	C	402	GLN	2.1
1	E	17	PRO	2.1
1	B	111	GLY	2.1
1	D	211	GLY	2.1
1	D	103	ASP	2.1
1	F	413	ASP	2.1
1	H	412	ASP	2.1
1	H	200	TYR	2.1
1	G	390	HIS	2.0
1	H	418	ILE	2.0
1	H	424	PRO	2.0
1	H	99	ARG	2.0
1	G	77	GLY	2.0
1	B	220	ASP	2.0
1	F	422	LEU	2.0
1	B	420	PRO	2.0
1	H	102	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	502	4/4	0.79	0.23	59,61,65,65	0
3	EDO	F	502	4/4	0.82	0.18	40,44,47,47	0
5	P3G	D	503	17/17	0.83	0.19	51,59,67,69	0
3	EDO	D	501	4/4	0.86	0.20	52,56,57,58	0

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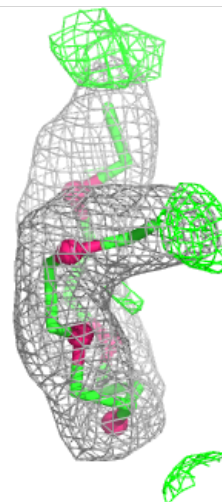
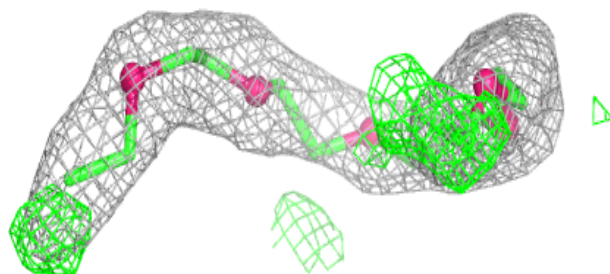
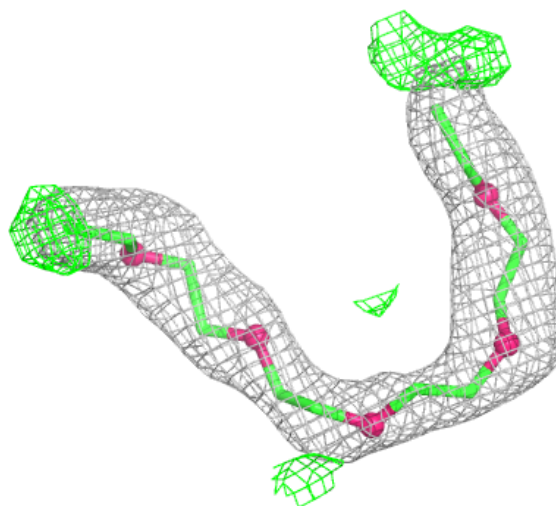
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	2PE	E	501	28/28	0.87	0.16	46,56,65,67	0
4	PG4	B	501	13/13	0.89	0.12	41,47,52,52	0
4	PG4	C	501	13/13	0.90	0.13	48,55,62,64	0
3	EDO	C	502	4/4	0.90	0.17	57,60,60,61	0
3	EDO	E	502	4/4	0.90	0.11	37,41,42,46	0
3	EDO	B	503	4/4	0.91	0.15	41,43,43,44	0
3	EDO	A	502	4/4	0.91	0.12	33,38,39,40	0
7	PGE	F	501	10/10	0.91	0.12	43,52,54,57	0
2	GOL	A	501	6/6	0.92	0.12	37,44,47,47	0
2	GOL	B	502	6/6	0.94	0.10	36,37,41,44	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.

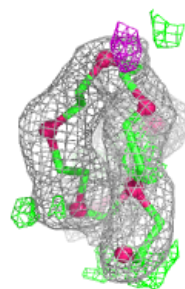
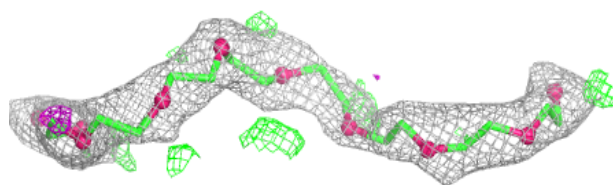
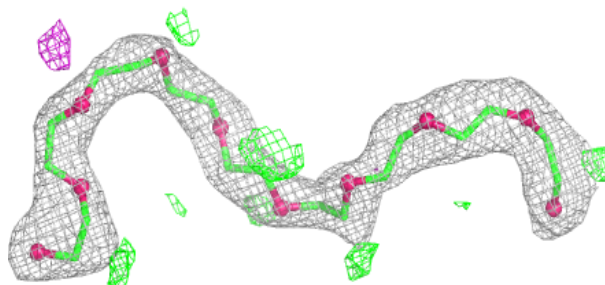
Electron density around P3G D 503:

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.