



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:43 AM UTC

PDB ID : 5A1S / pdb_00005a1s
Title : Crystal structure of the sodium-dependent citrate symporter SeCitS form *Salmonella enterica*.
Authors : Woehlert, D.; Groetzinger, M.J.; Kuhlbrandt, W.; Yildiz, O.
Deposited on : 2015-05-05
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

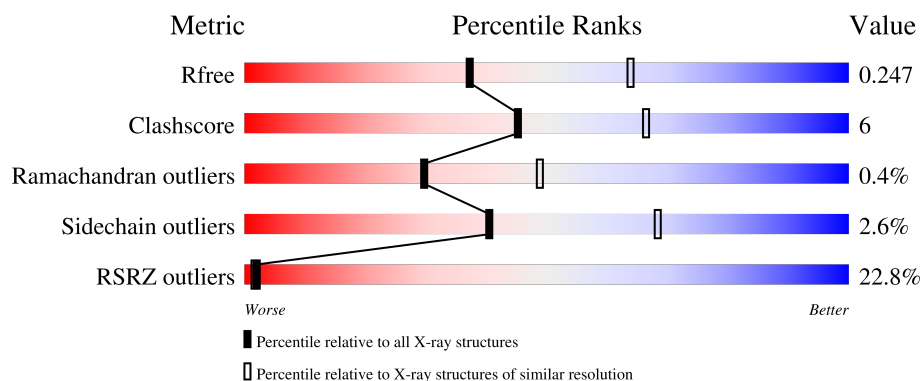
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	18% 84% 13% .
1	B	448	29% 78% 16% . 5%
1	C	448	21% 77% 18% . .
1	D	448	20% 82% 14% . .

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
7	PTY	A	1455	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13270 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 CITRATE-SODIUM SYMPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3256	2151	516	567	22			
1	B	426	Total	C	N	O	S	0	0	0
			3201	2117	508	554	22			
1	C	428	Total	C	N	O	S	0	0	0
			3206	2118	511	555	22			
1	D	434	Total	C	N	O	S	0	0	0
			3253	2147	517	567	22			

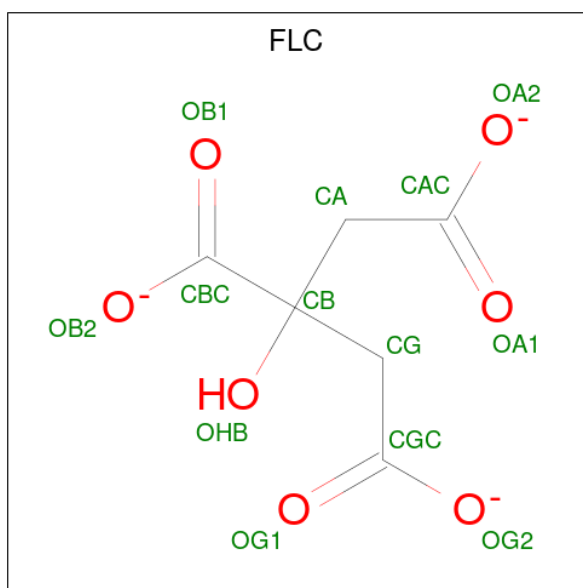
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	LEU	-	expression tag	UNP G4BX92
A	448	GLU	-	expression tag	UNP G4BX92
B	447	LEU	-	expression tag	UNP G4BX92
B	448	GLU	-	expression tag	UNP G4BX92
C	447	LEU	-	expression tag	UNP G4BX92
C	448	GLU	-	expression tag	UNP G4BX92
D	447	LEU	-	expression tag	UNP G4BX92
D	448	GLU	-	expression tag	UNP G4BX92

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

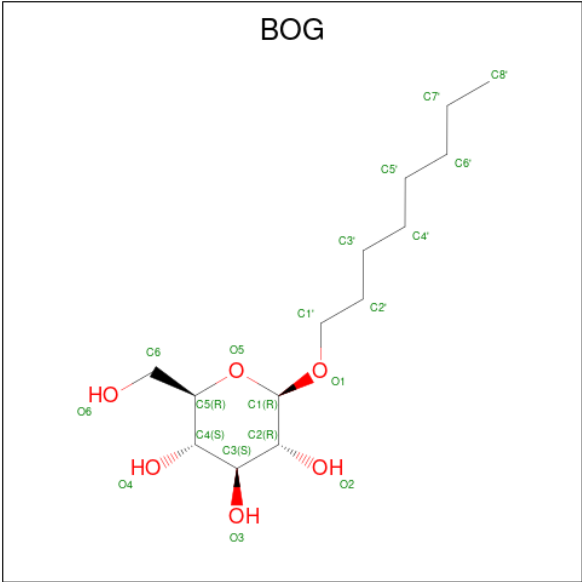
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	1	Total	Na	0	0
			1	1		
2	C	2	Total	Na	0	0
			2	2		
2	D	2	Total	Na	0	0
			2	2		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



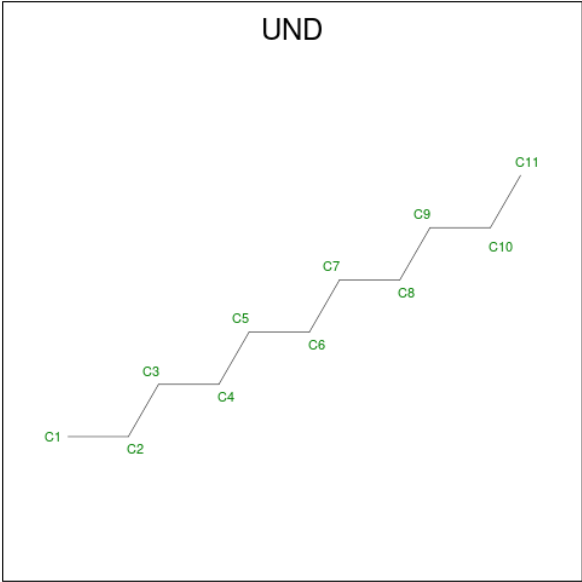
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄).

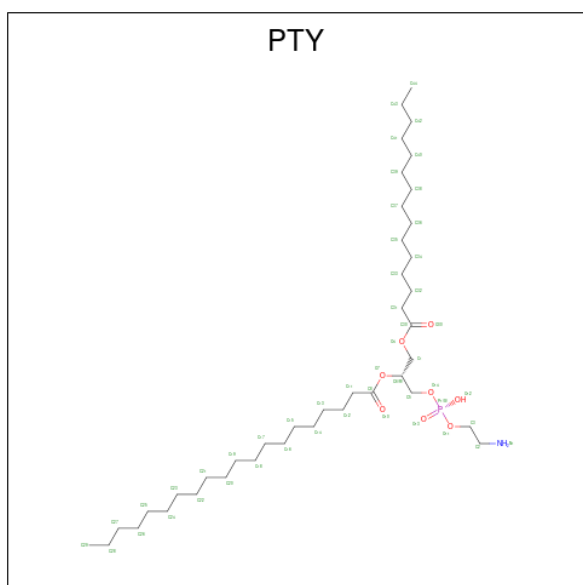


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 11 11	0	0
5	D	1	Total C 11 11	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	D	2	Total Cl 2 2	0	0

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

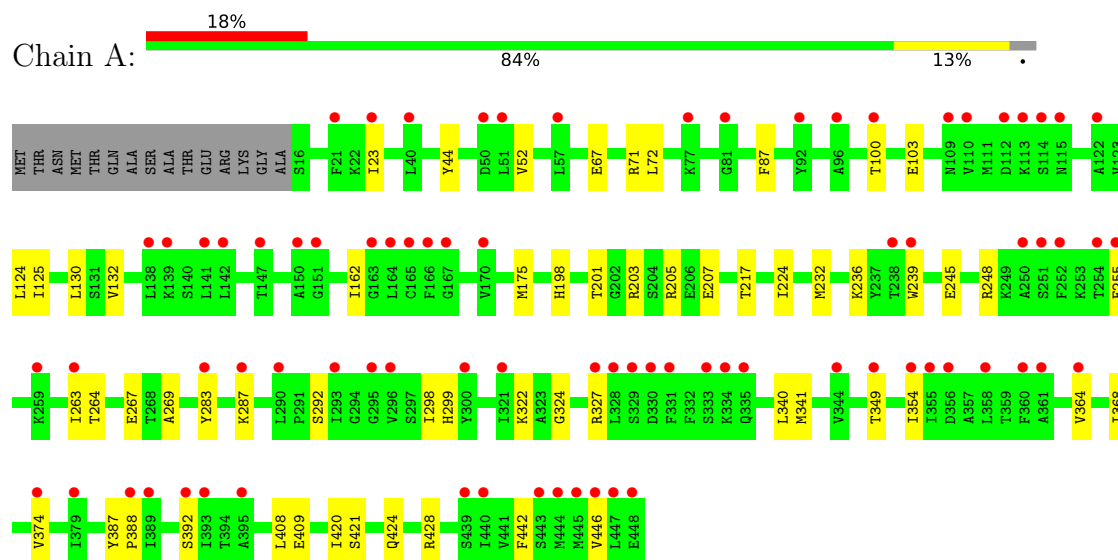
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total	O	0	0
			24	24		
9	B	14	Total	O	0	0
			14	14		
9	C	13	Total	O	0	0
			13	13		
9	D	18	Total	O	0	0
			18	18		

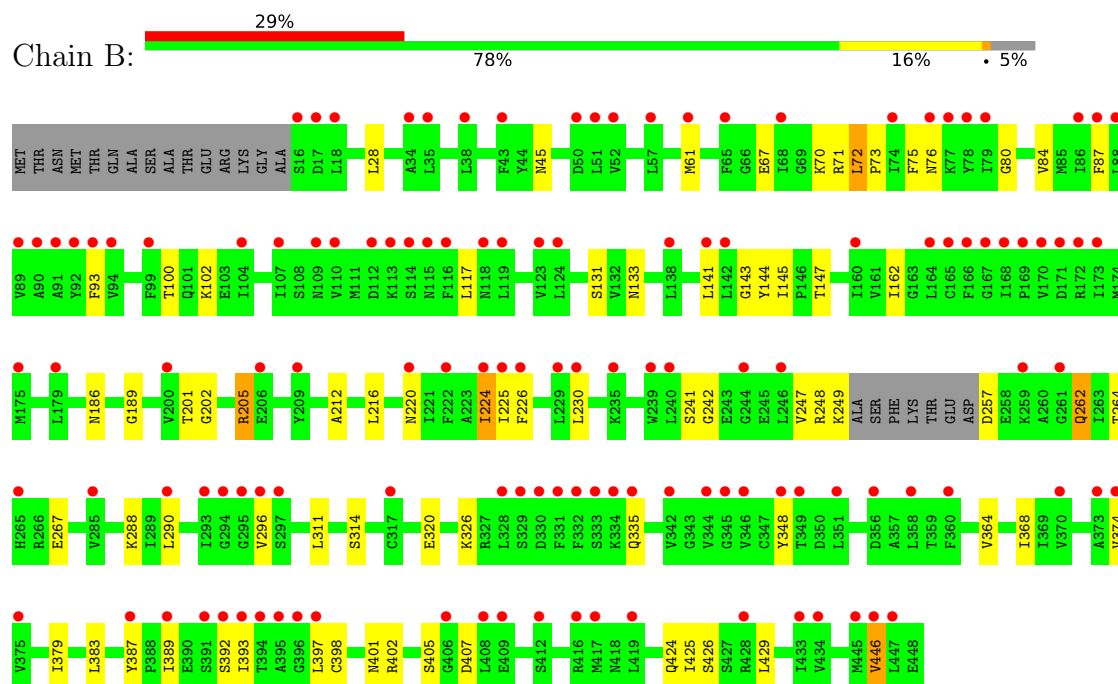
3 Residue-property plots [i](#)

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.

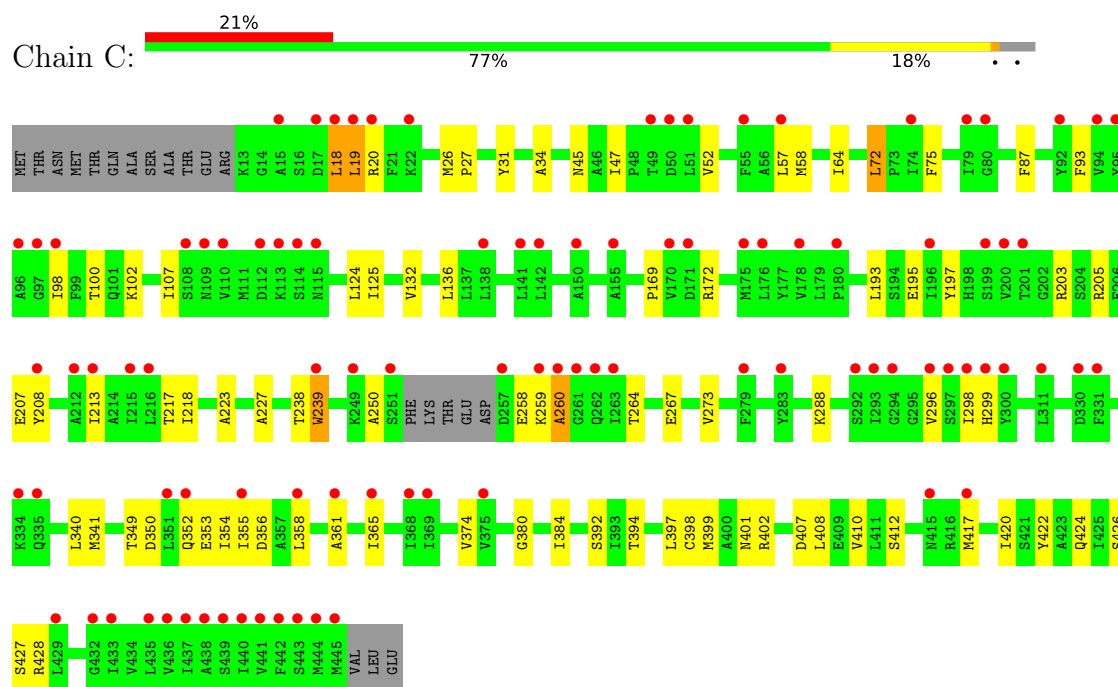
• Molecule 1: CITRATE-SODIUM SYMPORTER



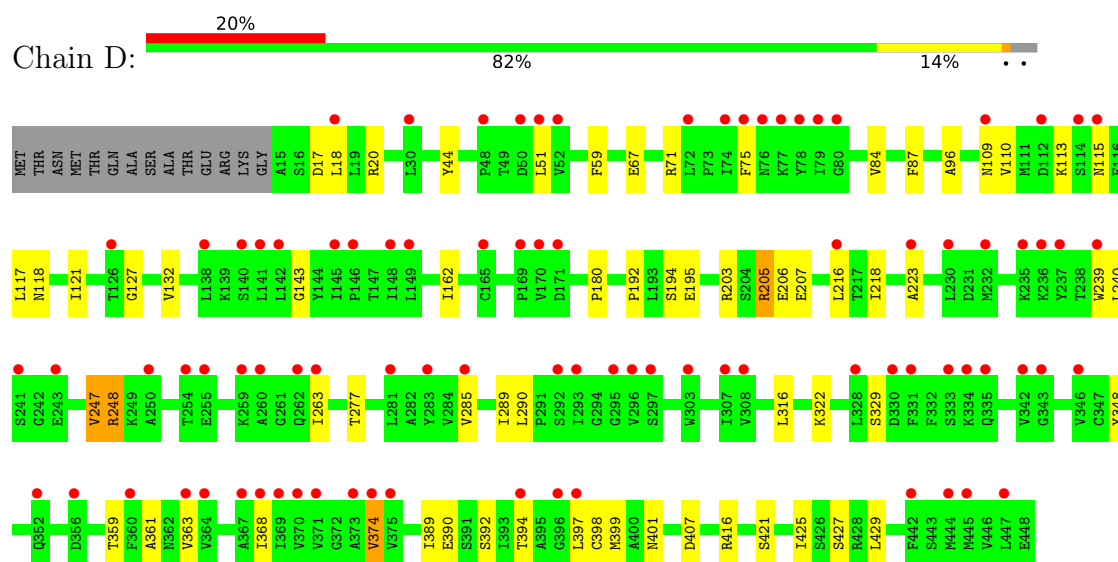
• Molecule 1: CITRATE-SODIUM SYMPORTER



• Molecule 1: CITRATE-SODIUM SYMPORTER



• Molecule 1: CITRATE-SODIUM SYMPORTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.38Å 89.94Å 91.84Å 90.44° 113.79° 99.55°	Depositor
Resolution (Å)	47.98 – 2.50 47.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.98-2.50) 98.7 (47.98-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.246 0.212 , 0.247	Depositor DCC
R_{free} test set	4200 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: MES, NA, BOG, FLC, CL, PTY, UND

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	0.32	0/3320	0.76	2/4503 (0.0%)
1	B	0.31	0/3263	0.80	3/4425 (0.1%)
1	C	0.31	0/3268	0.79	2/4430 (0.0%)
1	D	0.31	0/3316	0.77	1/4498 (0.0%)
All	All	0.31	0/13167	0.78	8/17856 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	VAL	N-CA-C	-6.31	106.04	113.42
1	B	387	TYR	CA-C-N	6.08	127.44	119.84
1	B	387	TYR	C-N-CA	6.08	127.44	119.84
1	C	72	LEU	CA-C-N	5.63	126.88	119.84
1	C	72	LEU	C-N-CA	5.63	126.88	119.84
1	D	399	MET	N-CA-C	-5.25	106.93	113.55
1	A	72	LEU	CA-C-N	5.19	126.33	119.84
1	A	72	LEU	C-N-CA	5.19	126.33	119.84

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	3256	0	3414	37	0
1	B	3201	0	3365	41	0
1	C	3206	0	3369	46	0
1	D	3253	0	3407	34	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	39	0	15	0	0
3	B	26	0	10	2	0
3	C	13	0	5	0	0
3	D	13	0	5	1	0
4	A	40	0	56	2	0
4	C	40	0	56	1	0
4	D	20	0	28	1	0
5	A	11	0	24	0	0
5	D	11	0	24	0	0
6	A	1	0	0	0	0
6	D	2	0	0	0	0
7	A	50	0	79	4	0
8	D	12	0	13	2	0
9	A	24	0	0	4	0
9	B	14	0	0	0	0
9	C	13	0	0	0	0
9	D	18	0	0	0	0
All	All	13270	0	13870	160	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 6.

All (160) 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:136:LEU:HD21	1:C:250:ALA:HB1	1.65	0.78
1:A:340:LEU:HD21	1:A:408:LEU:HD13	1.66	0.77
1:C:340:LEU:HD21	1:C:408:LEU:HD13	1.71	0.73
1:A:67:GLU:HB3	1:A:71:ARG:HH21	1.55	0.72
1:C:288:LYS:NZ	1:D:44:TYR:O	2.26	0.69
1:B:424:GLN:OE1	3:B:1450:FLC:OHB	2.12	0.68
1:D:285:VAL:HA	1:D:289:ILE:HB	1.76	0.68
1:B:241:SER:HB2	1:B:389:ILE:HD12	1.77	0.65
1:C:124:LEU:HB3	1:C:420:ILE:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HB3	1:C:75:PHE:HB3	1.81	0.63
1:B:401:ASN:ND2	1:B:407:ASP:OD1	2.32	0.63
1:C:18:LEU:HD13	1:C:18:LEU:H	1.63	0.63
1:A:236:LYS:NZ	9:A:2017:HOH:O	2.30	0.63
1:A:205:ARG:NH1	9:A:2013:HOH:O	2.33	0.62
1:C:352:GLN:NE2	1:C:356:ASP:OD1	2.30	0.61
1:C:239:TRP:H	1:C:239:TRP:CD1	2.18	0.61
1:B:262:GLN:O	1:B:262:GLN:NE2	2.33	0.61
1:A:67:GLU:OE1	1:A:71:ARG:NH2	2.34	0.61
1:D:203:ARG:NH1	1:D:207:GLU:OE1	2.33	0.61
1:C:195:GLU:OE1	1:C:205:ARG:NH1	2.35	0.59
1:A:125:ILE:HD11	1:A:424:GLN:HG3	1.84	0.59
1:A:263:ILE:HD11	1:A:324:GLY:HA2	1.85	0.59
1:C:197:TYR:OH	1:C:207:GLU:OE2	2.21	0.58
1:D:194:SER:HB3	1:D:205:ARG:HB2	1.85	0.58
1:D:195:GLU:OE2	1:D:348:TYR:OH	2.17	0.57
3:D:1449:FLC:OA1	3:D:1449:FLC:OHB	2.21	0.57
1:D:359:THR:HG22	1:D:361:ALA:H	1.68	0.57
1:A:162:ILE:HD12	1:A:368:ILE:HG13	1.86	0.56
1:D:206:GLU:HG2	8:D:1453:MES:H22	1.87	0.56
1:D:127:GLY:HA3	1:D:329:SER:HB2	1.86	0.55
1:A:299:HIS:HB3	1:A:428:ARG:HB3	1.89	0.55
1:C:125:ILE:HD11	1:C:424:GLN:HG3	1.89	0.55
1:B:141:LEU:HD23	1:B:145:ILE:HD12	1.88	0.55
1:C:58:MET:HE3	1:C:107:ILE:HG23	1.88	0.54
1:C:399:MET:HG2	1:C:426:SER:HB3	1.90	0.54
1:B:425:ILE:HG23	1:B:429:LEU:HD12	1.90	0.54
1:A:203:ARG:NH2	9:A:2012:HOH:O	2.36	0.53
1:D:109:ASN:HA	1:D:113:LYS:HB3	1.91	0.53
1:C:361:ALA:O	1:C:365:ILE:HG12	2.09	0.53
1:B:67:GLU:O	1:B:71:ARG:HG2	2.09	0.53
1:C:218:ILE:HG12	1:C:354:ILE:HG23	1.91	0.53
1:A:245:GLU:OE2	4:A:1450:BOG:O4	2.16	0.52
1:D:425:ILE:HG23	1:D:429:LEU:HD12	1.91	0.52
1:C:374:VAL:HG13	1:C:392:SER:HB2	1.91	0.52
1:A:341:MET:HE1	1:A:409:GLU:HA	1.92	0.52
9:A:2018:HOH:O	1:B:102:LYS:NZ	2.39	0.51
1:D:374:VAL:HB	1:D:392:SER:HB2	1.92	0.51
1:A:87:PHE:CZ	1:A:349:THR:HG21	2.45	0.51
1:B:374:VAL:HG13	1:B:392:SER:HB3	1.91	0.51
1:C:169:PRO:HG2	1:C:172:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG13	1:A:392:SER:HB3	1.93	0.50
1:C:34:ALA:HA	1:D:277:THR:HG21	1.92	0.50
1:B:70:LYS:O	1:B:76:ASN:ND2	2.37	0.50
1:B:248:ARG:HG3	1:B:249:LYS:HG2	1.94	0.49
1:B:162:ILE:HG12	1:B:368:ILE:HG13	1.95	0.49
1:A:203:ARG:NH1	1:A:207:GLU:OE1	2.45	0.49
1:D:51:LEU:HD23	1:D:110:VAL:HG22	1.95	0.49
1:B:267:GLU:HG2	1:B:320:GLU:HB3	1.94	0.49
1:C:57:LEU:HD22	1:C:107:ILE:HD11	1.94	0.49
1:B:84:VAL:HA	1:B:87:PHE:CE2	2.48	0.49
1:B:241:SER:OG	1:B:242:GLY:O	2.27	0.48
1:A:292:SER:HA	1:A:298:ILE:HG12	1.95	0.48
1:A:23:ILE:HG23	1:A:67:GLU:HG3	1.96	0.48
1:A:264:THR:OG1	1:A:267:GLU:OE1	2.26	0.47
1:D:115:ASN:ND2	1:D:118:ASN:OD1	2.48	0.47
1:C:213:ILE:O	1:C:217:THR:OG1	2.25	0.47
1:A:248:ARG:HG2	1:A:387:TYR:CZ	2.50	0.47
1:B:398:CYS:HA	1:B:401:ASN:ND2	2.29	0.47
7:A:1455:PTY:H201	7:A:1455:PTY:H231	1.75	0.47
1:B:144:TYR:OH	1:B:426:SER:OG	2.28	0.47
1:B:144:TYR:HH	1:B:426:SER:HG	1.60	0.47
1:B:212:ALA:O	1:B:216:LEU:HB2	2.14	0.47
1:D:162:ILE:HG12	1:D:368:ILE:HD12	1.97	0.47
1:D:240:LEU:HB3	1:D:389:ILE:HG12	1.96	0.47
1:A:263:ILE:HD13	1:A:327:ARG:HD2	1.97	0.46
1:B:364:VAL:O	1:B:368:ILE:HG12	2.15	0.46
1:D:180:PRO:O	1:D:216:LEU:HD21	2.15	0.46
1:D:390:GLU:O	1:D:394:THR:HG22	2.15	0.46
1:A:255:GLU:OE1	1:A:255:GLU:N	2.39	0.46
1:A:239:TRP:H	1:A:239:TRP:CD1	2.34	0.46
1:B:402:ARG:NH1	1:B:405:SER:OG	2.48	0.46
1:B:61:MET:HE1	1:B:93:PHE:CE2	2.50	0.46
1:C:47:ILE:HG22	1:C:102:LYS:HG3	1.98	0.45
1:D:247:VAL:HG12	1:D:248:ARG:H	1.81	0.45
7:A:1455:PTY:H351	7:A:1455:PTY:H381	1.55	0.45
1:B:389:ILE:O	1:B:393:ILE:HG12	2.17	0.45
1:C:193:LEU:HB3	1:C:208:TYR:CE1	2.52	0.45
1:D:223:ALA:HA	1:D:397:LEU:HD22	1.98	0.45
1:A:175:MET:HG2	1:A:442:PHE:CE1	2.52	0.45
1:B:72:LEU:HB3	1:B:75:PHE:HB3	1.98	0.45
1:C:380:GLY:O	1:C:384:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HB3	1:C:208:TYR:HE1	1.82	0.45
1:C:355:ILE:HA	1:C:358:LEU:HB2	1.99	0.45
1:C:398:CYS:HA	1:C:401:ASN:ND2	2.32	0.45
1:D:84:VAL:HA	1:D:87:PHE:CE2	2.52	0.45
1:C:299:HIS:HB3	1:C:428:ARG:HB3	1.99	0.45
1:C:407:ASP:OD2	1:C:427:SER:OG	2.34	0.45
1:C:412:SER:HB3	1:C:417:MET:HE1	1.99	0.45
3:B:1449:FLC:OG1	3:B:1449:FLC:OHB	2.33	0.45
1:C:264:THR:OG1	1:C:267:GLU:OE2	2.34	0.44
1:B:379:ILE:O	1:B:383:LEU:HG	2.17	0.44
1:D:390:GLU:OE2	1:D:416:ARG:NE	2.41	0.44
1:A:283:TYR:O	1:A:287:LYS:HB2	2.17	0.44
1:A:87:PHE:HZ	1:A:349:THR:HG21	1.82	0.44
1:C:203:ARG:NH1	1:C:207:GLU:OE1	2.51	0.44
1:A:44:TYR:HB3	1:B:288:LYS:HG3	1.98	0.44
1:B:311:LEU:O	1:B:314:SER:OG	2.26	0.44
1:C:87:PHE:HB2	1:C:341:MET:HE3	1.99	0.44
1:C:349:THR:OG1	1:C:350:ASP:N	2.50	0.43
1:A:217:THR:HG22	1:A:354:ILE:HD11	1.99	0.43
1:D:218:ILE:HG21	1:D:363:VAL:HA	1.99	0.43
1:B:201:THR:OG1	1:B:202:GLY:N	2.51	0.43
1:C:223:ALA:HA	1:C:397:LEU:HD22	2.00	0.43
1:D:239:TRP:CD1	1:D:239:TRP:H	2.35	0.43
1:A:364:VAL:O	1:A:368:ILE:HG12	2.19	0.43
1:A:100:THR:HG23	1:A:103:GLU:H	1.83	0.43
1:A:130:LEU:O	1:A:322:LYS:HE3	2.19	0.43
1:A:387:TYR:HA	1:A:388:PRO:HD3	1.90	0.43
1:C:273:VAL:HG22	1:D:59:PHE:CG	2.54	0.43
1:B:133:ASN:HD21	1:B:257:ASP:HB3	1.84	0.43
1:C:258:GLU:O	1:C:260:ALA:N	2.53	0.42
1:A:201:THR:HG22	1:A:203:ARG:HG3	1.99	0.42
1:B:61:MET:HE2	1:B:61:MET:HB2	1.87	0.42
1:C:93:PHE:CD1	1:C:98:ILE:HD12	2.53	0.42
8:D:1453:MES:H82	8:D:1453:MES:H31	1.81	0.42
1:B:220:ASN:O	1:B:224:ILE:HG23	2.19	0.42
1:B:143:GLY:O	1:B:147:THR:OG1	2.35	0.42
1:C:26:MET:HA	1:C:27:PRO:HD2	1.91	0.42
1:A:124:LEU:HB3	1:A:420:ILE:HG21	2.02	0.42
1:D:203:ARG:HD3	1:D:207:GLU:OE2	2.20	0.42
7:A:1455:PTY:H352	7:A:1455:PTY:H322	1.68	0.42
1:B:224:ILE:HG13	1:B:225:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ALA:HB2	1:C:410:VAL:HG13	2.02	0.42
1:D:398:CYS:HA	1:D:401:ASN:ND2	2.34	0.42
1:C:19:LEU:HD23	1:C:20:ARG:H	1.84	0.41
1:B:162:ILE:HG12	1:B:368:ILE:HG21	2.03	0.41
1:B:201:THR:HG22	1:B:446:VAL:HG21	2.03	0.41
1:C:399:MET:HE3	1:C:399:MET:HB3	1.99	0.41
1:D:407:ASP:OD2	1:D:427:SER:OG	2.39	0.41
1:D:121:ILE:HD13	1:D:192:PRO:HB3	2.02	0.41
1:A:224:ILE:HD11	1:A:409:GLU:OE1	2.21	0.41
1:D:17:ASP:OD1	1:D:20:ARG:NH2	2.54	0.41
1:D:67:GLU:HG3	1:D:71:ARG:HH21	1.86	0.41
1:D:96:ALA:HA	4:D:1454:BOG:H61	2.03	0.41
1:A:198:HIS:ND1	1:A:203:ARG:O	2.54	0.41
1:A:269:ALA:HB2	1:B:335:GLN:HB3	2.03	0.41
1:B:45:ASN:OD1	1:B:100:THR:HG21	2.21	0.41
1:C:422:TYR:OH	4:C:1447:BOG:O6	2.38	0.40
7:A:1455:PTY:H251	7:A:1455:PTY:H222	1.78	0.40
1:B:205:ARG:HD2	1:B:348:TYR:CE2	2.56	0.40
1:D:132:VAL:O	1:D:322:LYS:NZ	2.55	0.40
1:B:131:SER:HB3	1:B:326:LYS:HD3	2.03	0.40
1:B:226:PHE:O	1:B:230:LEU:HG	2.22	0.40
1:C:31:TYR:OH	1:C:64:ILE:HB	2.21	0.40
1:C:45:ASN:OD1	1:C:100:THR:HG21	2.21	0.40
1:C:394:THR:O	1:C:398:CYS:HB2	2.21	0.40
1:D:421:SER:O	1:D:425:ILE:HG12	2.22	0.40
1:A:132:VAL:HG11	4:A:1450:BOG:H1	2.04	0.40
1:B:80:GLY:HA2	1:B:402:ARG:CZ	2.51	0.40
1:C:424:GLN:O	1:C:428:ARG:HG2	2.22	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	431/448 (96%)	412 (96%)	19 (4%)	0	100	100
1	B	422/448 (94%)	395 (94%)	24 (6%)	3 (1%)	18	34
1	C	424/448 (95%)	402 (95%)	20 (5%)	2 (0%)	24	43
1	D	432/448 (96%)	409 (95%)	22 (5%)	1 (0%)	43	63
All	All	1709/1792 (95%)	1618 (95%)	85 (5%)	6 (0%)	30	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	LYS
1	B	73	PRO
1	D	143	GLY
1	B	186	ASN
1	C	260	ALA
1	B	189	GLY

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	343/354 (97%)	339 (99%)	4 (1%)	63	83
1	B	337/354 (95%)	326 (97%)	11 (3%)	33	61
1	C	336/354 (95%)	326 (97%)	10 (3%)	36	64
1	D	341/354 (96%)	331 (97%)	10 (3%)	37	65
All	All	1357/1416 (96%)	1322 (97%)	35 (3%)	40	68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	232	MET
1	A	421	SER
1	A	446	VAL
1	B	28	LEU

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Mol	Chain	Res	Type
1	B	72	LEU
1	B	117	LEU
1	B	205	ARG
1	B	224	ILE
1	B	247	VAL
1	B	262	GLN
1	B	264	THR
1	B	290	LEU
1	B	296	VAL
1	B	397	LEU
1	C	18	LEU
1	C	19	LEU
1	C	52	VAL
1	C	132	VAL
1	C	238	THR
1	C	239	TRP
1	C	296	VAL
1	C	298	ILE
1	C	353	GLU
1	C	402	ARG
1	D	18	LEU
1	D	75	PHE
1	D	117	LEU
1	D	205	ARG
1	D	247	VAL
1	D	248	ARG
1	D	263	ILE
1	D	290	LEU
1	D	316	LEU
1	D	374	VAL

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	101	GLN
1	B	220	ASN
1	B	262	GLN
1	B	415	ASN
1	D	352	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 ⓘ

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FLC	C	1446	-	12,12,12	1.31	0	17,17,17	1.31	1 (5%)
4	BOG	A	1456	-	20,20,20	0.46	0	25,25,25	1.03	1 (4%)
7	PTY	A	1455	-	49,49,49	1.05	3 (6%)	52,54,54	1.10	3 (5%)
3	FLC	A	1454	-	12,12,12	1.32	0	17,17,17	1.38	1 (5%)
3	FLC	A	1453	-	12,12,12	1.24	0	17,17,17	1.34	1 (5%)
4	BOG	C	1447	-	20,20,20	0.52	0	25,25,25	0.88	1 (4%)
4	BOG	C	1448	-	20,20,20	0.49	0	25,25,25	0.88	1 (4%)
3	FLC	B	1449	-	12,12,12	1.25	0	17,17,17	1.38	2 (11%)
3	FLC	D	1449	-	12,12,12	1.29	0	17,17,17	1.39	1 (5%)
3	FLC	A	1449	-	12,12,12	1.32	0	17,17,17	1.27	1 (5%)
3	FLC	B	1450	-	12,12,12	1.27	0	17,17,17	1.35	1 (5%)
4	BOG	D	1454	-	20,20,20	0.41	0	25,25,25	1.37	2 (8%)
4	BOG	A	1450	-	20,20,20	0.56	0	25,25,25	1.00	1 (4%)
5	UND	D	1450	-	10,10,10	0.09	0	9,9,9	0.82	0
5	UND	A	1451	-	10,10,10	0.09	0	9,9,9	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MES	D	1453	-	12,12,12	1.31	2 (16%)	15,16,16	1.76	4 (26%)

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	FLC	C	1446	-	-	0/16/16/16	-
4	BOG	A	1456	-	-	7/11/31/31	0/1/1/1
7	PTY	A	1455	-	-	22/53/53/53	-
3	FLC	A	1454	-	-	5/16/16/16	-
3	FLC	A	1453	-	-	9/16/16/16	-
4	BOG	C	1447	-	-	4/11/31/31	0/1/1/1
4	BOG	C	1448	-	-	3/11/31/31	0/1/1/1
3	FLC	B	1449	-	-	8/16/16/16	-
3	FLC	D	1449	-	-	9/16/16/16	-
3	FLC	A	1449	-	-	0/16/16/16	-
3	FLC	B	1450	-	-	6/16/16/16	-
4	BOG	D	1454	-	-	2/11/31/31	0/1/1/1
4	BOG	A	1450	-	-	5/11/31/31	0/1/1/1
5	UND	D	1450	-	-	2/8/8/8	-
5	UND	A	1451	-	-	0/8/8/8	-
8	MES	D	1453	-	-	3/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1455	PTY	O4-C30	3.60	1.43	1.33
7	A	1455	PTY	O7-C8	3.22	1.43	1.34
8	D	1453	MES	O2S-S	2.48	1.52	1.45
7	A	1455	PTY	O7-C6	-2.36	1.41	1.46
8	D	1453	MES	O1S-S	2.09	1.51	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1454	BOG	O5-C5-C4	4.32	117.49	109.70
8	D	1453	MES	O3S-S-O2S	-4.27	100.72	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1455	PTY	O7-C8-C11	4.15	120.46	111.48
3	D	1449	FLC	OB2-CBC-CB	3.76	120.35	113.14
3	C	1446	FLC	OB2-CBC-CB	3.54	119.93	113.14
3	B	1450	FLC	OB2-CBC-CB	3.54	119.93	113.14
3	A	1454	FLC	OB2-CBC-CB	3.51	119.88	113.14
3	A	1449	FLC	OB2-CBC-CB	3.49	119.84	113.14
3	A	1453	FLC	OB2-CBC-CB	3.47	119.80	113.14
4	D	1454	BOG	C3-C4-C5	3.42	116.44	110.23
4	A	1450	BOG	C1-O5-C5	-3.42	107.05	113.72
3	B	1449	FLC	OB2-CBC-CB	3.32	119.52	113.14
4	A	1456	BOG	C1-O5-C5	-3.24	107.39	113.72
8	D	1453	MES	O2S-S-C8	3.21	111.58	106.73
4	C	1448	BOG	C1-O5-C5	-2.97	107.93	113.72
4	C	1447	BOG	C1-O5-C5	-2.91	108.03	113.72
8	D	1453	MES	O1S-S-C8	2.82	110.98	106.73
7	A	1455	PTY	O4-C30-O30	-2.41	117.59	123.63
8	D	1453	MES	O3S-S-C8	2.31	110.53	106.00
3	B	1449	FLC	OA2-CAC-CA	2.25	121.46	114.35
7	A	1455	PTY	O4-C30-C31	2.22	118.60	111.83

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1453	FLC	CAC-CA-CB-CBC
3	A	1453	FLC	CAC-CA-CB-CG
3	A	1454	FLC	CAC-CA-CB-CBC
3	A	1454	FLC	CAC-CA-CB-OHB
3	B	1449	FLC	CG-CB-CBC-OB1
3	B	1449	FLC	CG-CB-CBC-OB2
3	B	1449	FLC	OHB-CB-CBC-OB1
3	B	1449	FLC	OHB-CB-CBC-OB2
3	B	1450	FLC	CG-CB-CBC-OB1
3	B	1450	FLC	CG-CB-CBC-OB2
3	B	1450	FLC	OHB-CB-CBC-OB1
3	B	1450	FLC	OHB-CB-CBC-OB2
3	D	1449	FLC	CAC-CA-CB-CBC
3	D	1449	FLC	CAC-CA-CB-CG
4	C	1448	BOG	O5-C1-O1-C1'
7	A	1455	PTY	C11-C8-O7-C6
8	D	1453	MES	C7-C8-S-O2S
7	A	1455	PTY	O30-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
7	A	1455	PTY	O10-C8-O7-C6
4	C	1447	BOG	O5-C5-C6-O6
7	A	1455	PTY	C31-C30-O4-C1
4	C	1447	BOG	C4-C5-C6-O6
4	A	1456	BOG	O5-C1-O1-C1'
4	A	1456	BOG	O5-C5-C6-O6
3	A	1454	FLC	CAC-CA-CB-CG
4	A	1456	BOG	C2-C1-O1-C1'
4	A	1456	BOG	O1-C1'-C2'-C3'
3	A	1453	FLC	CAC-CA-CB-OHB
3	A	1453	FLC	CA-CB-CBC-OB2
7	A	1455	PTY	C38-C39-C40-C41
7	A	1455	PTY	C19-C20-C21-C22
4	A	1450	BOG	C1'-C2'-C3'-C4'
7	A	1455	PTY	C40-C41-C42-C43
3	D	1449	FLC	CAC-CA-CB-OHB
4	A	1456	BOG	C4-C5-C6-O6
4	A	1450	BOG	C2'-C3'-C4'-C5'
7	A	1455	PTY	C25-C26-C27-C28
7	A	1455	PTY	C18-C19-C20-C21
7	A	1455	PTY	C34-C35-C36-C37
5	D	1450	UND	C2-C3-C4-C5
7	A	1455	PTY	C15-C16-C17-C18
7	A	1455	PTY	C23-C24-C25-C26
4	A	1450	BOG	C2'-C1'-O1-C1
4	C	1447	BOG	C2'-C1'-O1-C1
4	C	1448	BOG	C2-C1-O1-C1'
7	A	1455	PTY	C20-C21-C22-C23
7	A	1455	PTY	C32-C33-C34-C35
4	D	1454	BOG	C2-C1-O1-C1'
8	D	1453	MES	C7-C8-S-O1S
3	B	1449	FLC	CA-CB-CG-CGC
3	B	1449	FLC	CBC-CB-CG-CGC
3	D	1449	FLC	CA-CB-CG-CGC
3	A	1453	FLC	CG-CB-CBC-OB2
3	D	1449	FLC	CA-CB-CBC-OB2
3	D	1449	FLC	CG-CB-CBC-OB2
5	D	1450	UND	C1-C2-C3-C4
7	A	1455	PTY	C35-C36-C37-C38
3	D	1449	FLC	OHB-CB-CG-CGC
7	A	1455	PTY	C3-O11-P1-O12
7	A	1455	PTY	C5-O14-P1-O11

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Mol	Chain	Res	Type	Atoms
7	A	1455	PTY	C5-O14-P1-O13
7	A	1455	PTY	C6-C5-O14-P1
8	D	1453	MES	C7-C8-S-O3S
3	A	1453	FLC	OHB-CB-CBC-OB2
3	A	1453	FLC	CA-CB-CBC-OB1
3	A	1453	FLC	CG-CB-CBC-OB1
3	B	1450	FLC	CA-CB-CBC-OB1
3	B	1450	FLC	CA-CB-CBC-OB2
4	A	1456	BOG	C1'-C2'-C3'-C4'
4	D	1454	BOG	C1'-C2'-C3'-C4'
7	A	1455	PTY	C37-C38-C39-C40
7	A	1455	PTY	C16-C17-C18-C19
4	A	1456	BOG	C2'-C3'-C4'-C5'
4	C	1447	BOG	C5'-C6'-C7'-C8'
3	B	1449	FLC	CB-CA-CAC-OA1
3	A	1453	FLC	OHB-CB-CBC-OB1
3	D	1449	FLC	OHB-CB-CBC-OB2
3	A	1454	FLC	CB-CG-CGC-OG2
3	D	1449	FLC	CG-CB-CBC-OB1
3	A	1454	FLC	CB-CG-CGC-OG1
3	B	1449	FLC	CB-CA-CAC-OA2
4	A	1450	BOG	O5-C1-O1-C1'
4	A	1450	BOG	C2-C1-O1-C1'
7	A	1455	PTY	C36-C37-C38-C39
4	C	1448	BOG	C2'-C3'-C4'-C5'

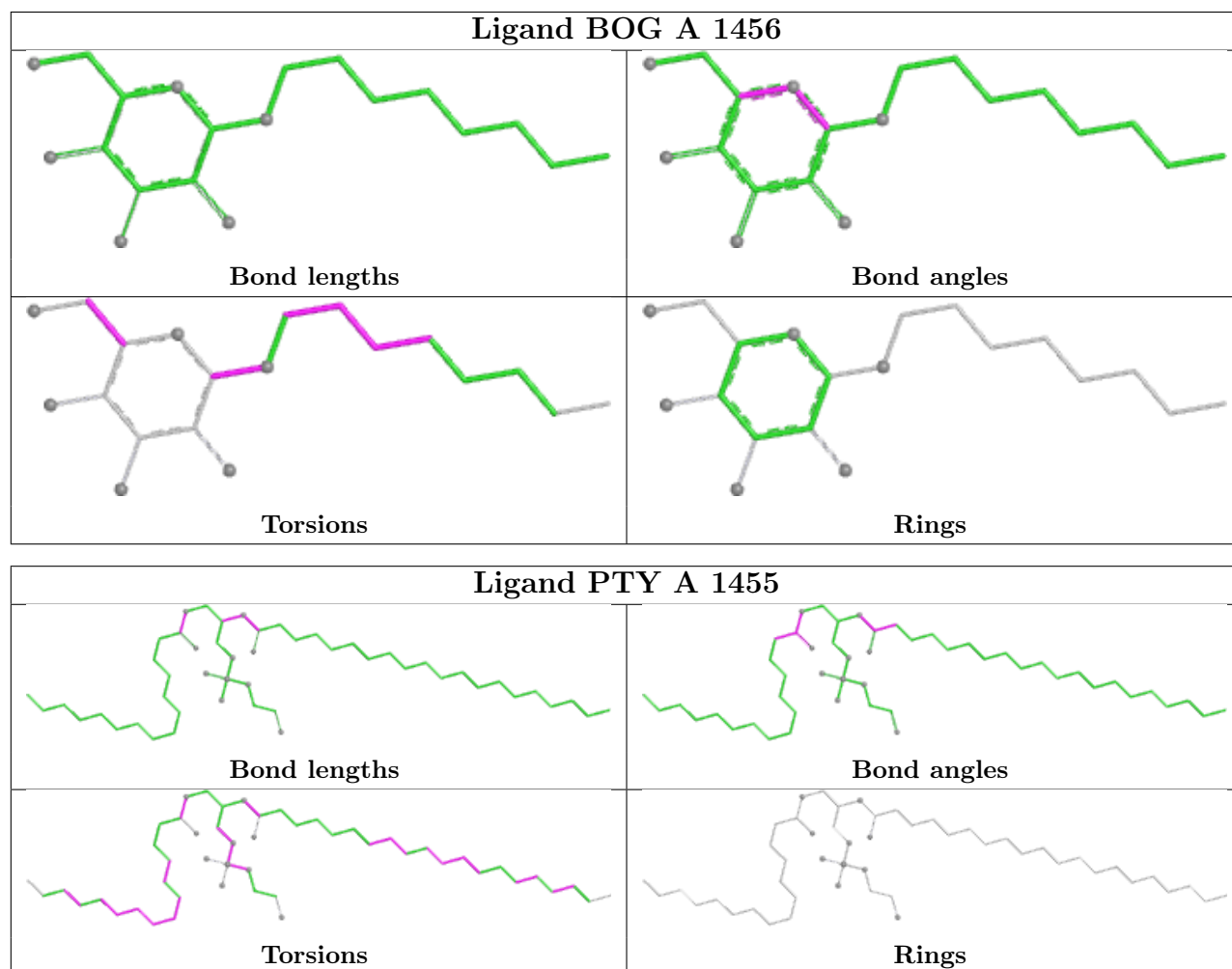
There are no ring outliers.

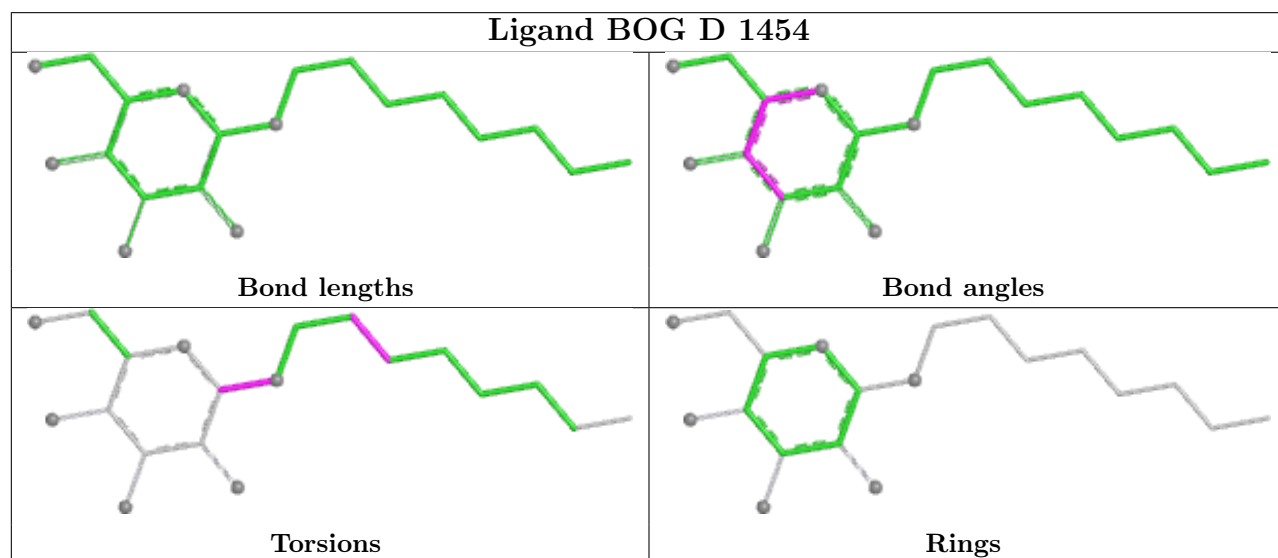
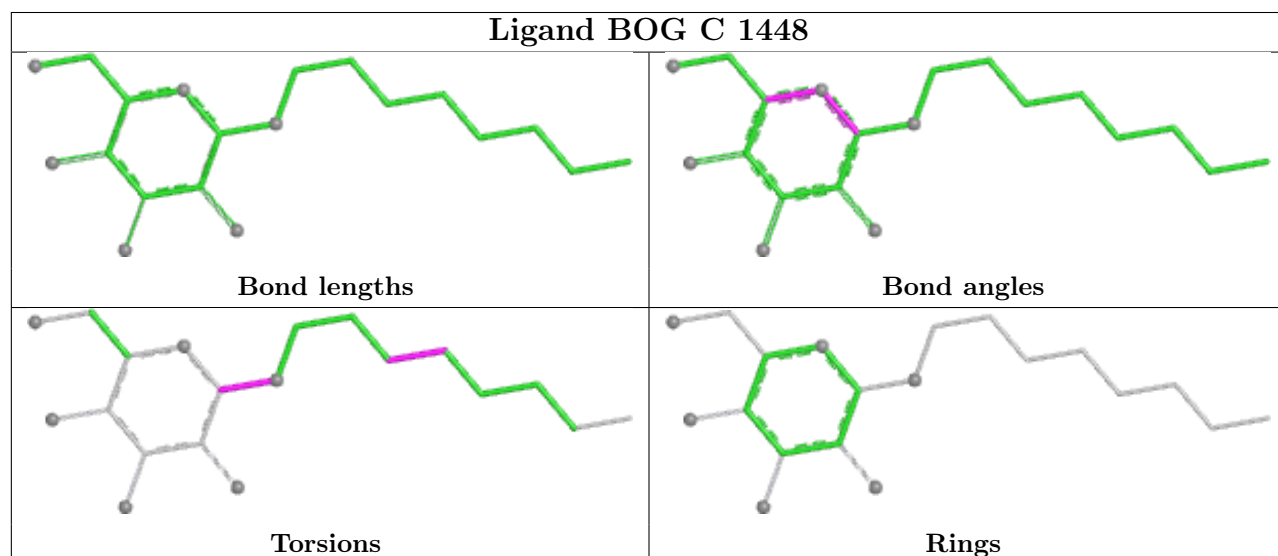
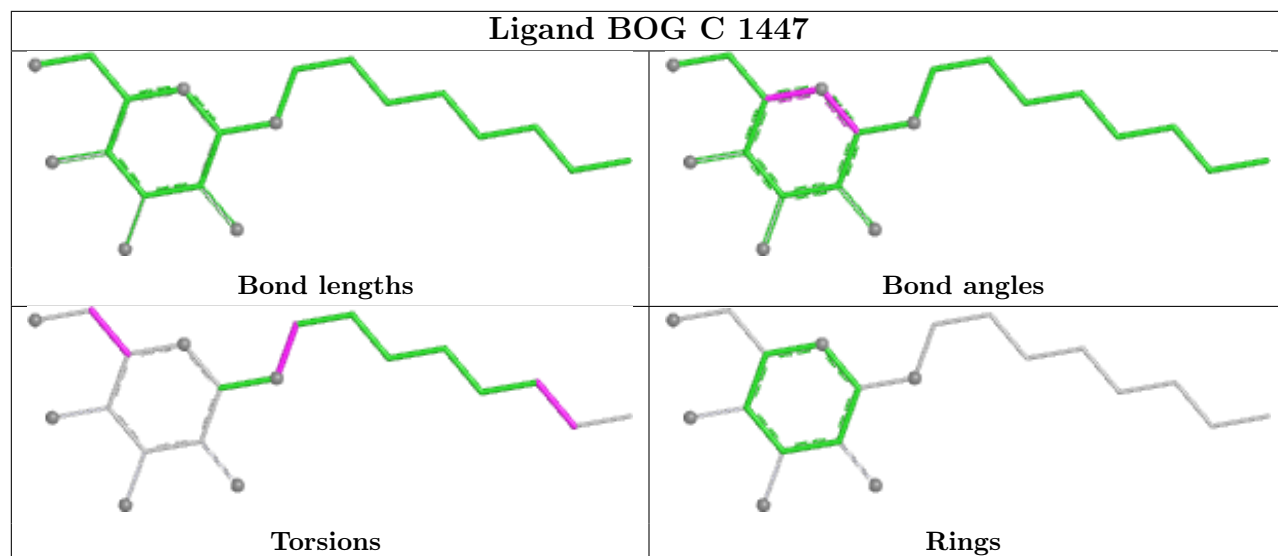
8 monomers are involved in 13 short contacts:

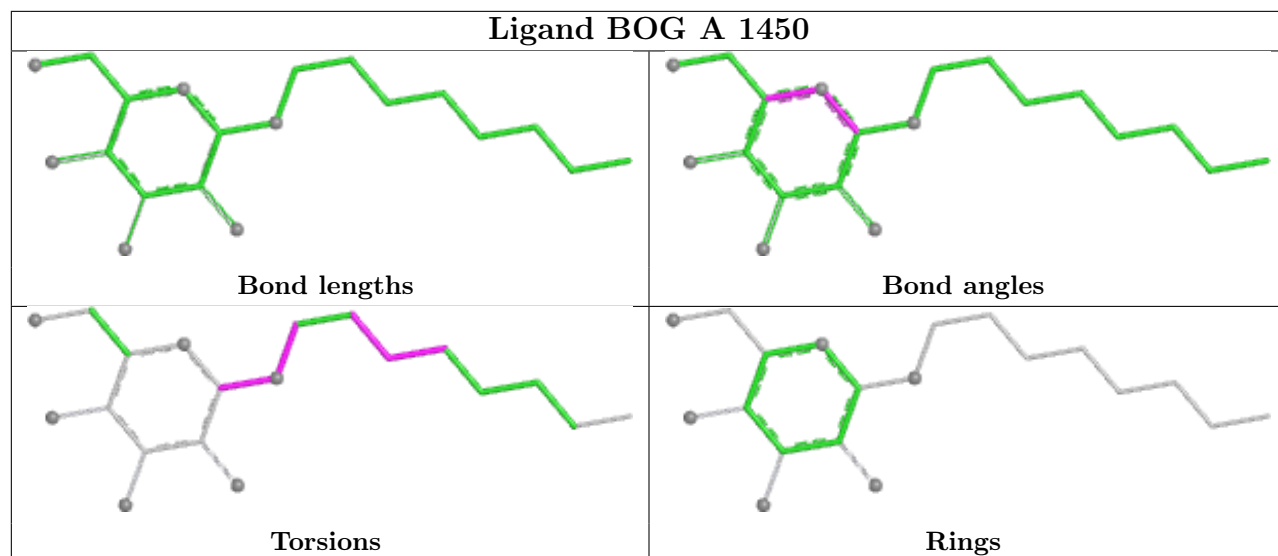
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1455	PTY	4	0
4	C	1447	BOG	1	0
3	B	1449	FLC	1	0
3	D	1449	FLC	1	0
3	B	1450	FLC	1	0
4	D	1454	BOG	1	0
4	A	1450	BOG	2	0
8	D	1453	MES	2	0

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	433/448 (96%)	1.05	80 (18%) 3 2	34, 56, 99, 136	0
1	B	426/448 (95%)	1.61	128 (30%) 1 1	46, 80, 120, 132	0
1	C	428/448 (95%)	1.27	96 (22%) 2 2	38, 62, 109, 143	0
1	D	434/448 (96%)	1.02	88 (20%) 3 2	38, 59, 101, 142	0
All	All	1721/1792 (96%)	1.24	392 (22%) 2 2	34, 63, 110, 143	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	SER	10.5
1	C	296	VAL	10.2
1	A	444	MET	10.1
1	C	109	ASN	10.0
1	B	78	TYR	9.0
1	C	262	GLN	8.8
1	A	360	PHE	8.6
1	D	114	SER	8.1
1	B	51	LEU	8.1
1	C	114	SER	8.0
1	C	96	ALA	7.8
1	B	74	ILE	7.7
1	B	114	SER	7.6
1	C	355	ILE	7.2
1	D	237	TYR	7.1
1	B	52	VAL	6.9
1	A	296	VAL	6.8
1	C	261	GLY	6.7
1	B	77	LYS	6.7
1	D	236	LYS	6.6
1	C	239	TRP	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASN	6.6
1	C	18	LEU	6.5
1	A	440	ILE	6.5
1	B	171	ASP	6.4
1	C	51	LEU	6.2
1	C	297	SER	6.1
1	C	95	TYR	5.8
1	C	97	GLY	5.7
1	D	74	ILE	5.6
1	C	80	GLY	5.6
1	D	50	ASP	5.5
1	C	115	ASN	5.5
1	C	50	ASP	5.5
1	B	115	ASN	5.5
1	C	442	PHE	5.4
1	A	165	CYS	5.3
1	B	113	LYS	5.3
1	C	260	ALA	5.3
1	A	251	SER	5.3
1	B	235	LYS	5.2
1	C	441	VAL	5.1
1	C	142	LEU	5.1
1	C	113	LYS	5.1
1	A	51	LEU	5.1
1	D	149	LEU	5.1
1	C	352	GLN	5.0
1	B	50	ASP	5.0
1	D	371	VAL	4.9
1	D	78	TYR	4.9
1	C	292	SER	4.9
1	C	49	THR	4.9
1	D	444	MET	4.9
1	B	110	VAL	4.8
1	B	332	PHE	4.8
1	B	138	LEU	4.7
1	C	110	VAL	4.7
1	A	142	LEU	4.7
1	B	169	PRO	4.6
1	D	360	PHE	4.6
1	B	342	VAL	4.6
1	B	116	PHE	4.5
1	A	358	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	LYS	4.5
1	C	331	PHE	4.4
1	C	138	LEU	4.4
1	B	76	ASN	4.4
1	B	57	LEU	4.4
1	B	164	LEU	4.4
1	D	72	LEU	4.4
1	C	293	ILE	4.4
1	A	167	GLY	4.3
1	D	374	VAL	4.3
1	C	92	TYR	4.3
1	B	166	PHE	4.3
1	B	141	LEU	4.3
1	C	19	LEU	4.3
1	D	115	ASN	4.3
1	A	112	ASP	4.3
1	D	75	PHE	4.3
1	C	436	VAL	4.2
1	B	90	ALA	4.2
1	B	293	ILE	4.2
1	A	252	PHE	4.2
1	A	443	SER	4.2
1	B	112	ASP	4.2
1	A	115	ASN	4.1
1	C	298	ILE	4.1
1	A	293	ILE	4.1
1	B	393	ILE	4.1
1	C	300	TYR	4.1
1	B	17	ASP	4.0
1	A	447	LEU	4.0
1	A	330	ASP	4.0
1	C	351	LEU	4.0
1	B	167	GLY	4.0
1	B	333	SER	4.0
1	B	87	PHE	4.0
1	C	415	ASN	3.9
1	B	168	ILE	3.9
1	A	295	GLY	3.9
1	D	296	VAL	3.9
1	A	254	THR	3.9
1	C	358	LEU	3.9
1	D	51	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	239	TRP	3.8
1	B	356	ASP	3.8
1	B	346	VAL	3.8
1	C	15	ALA	3.8
1	A	300	TYR	3.8
1	D	142	LEU	3.8
1	D	140	SER	3.7
1	D	235	LYS	3.7
1	B	244	GLY	3.7
1	C	20	ARG	3.7
1	D	79	ILE	3.7
1	A	333	SER	3.7
1	A	445	MET	3.7
1	A	163	GLY	3.6
1	B	295	GLY	3.6
1	B	447	LEU	3.6
1	D	445	MET	3.6
1	C	216	LEU	3.6
1	A	355	ILE	3.5
1	B	142	LEU	3.5
1	C	365	ILE	3.5
1	A	21	PHE	3.5
1	A	166	PHE	3.5
1	B	345	GLY	3.5
1	A	354	ILE	3.5
1	D	48	PRO	3.5
1	A	349	THR	3.4
1	C	94	VAL	3.4
1	C	443	SER	3.4
1	D	307	ILE	3.4
1	D	171	ASP	3.4
1	A	374	VAL	3.4
1	C	170	VAL	3.4
1	B	397	LEU	3.4
1	A	170	VAL	3.4
1	B	123	VAL	3.4
1	A	138	LEU	3.4
1	B	179	LEU	3.4
1	B	334	LYS	3.4
1	B	387	TYR	3.4
1	D	77	LYS	3.4
1	C	155	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	3.3
1	B	428	ARG	3.3
1	B	175	MET	3.3
1	D	356	ASP	3.3
1	C	435	LEU	3.3
1	B	173	ILE	3.3
1	C	79	ILE	3.3
1	C	369	ILE	3.3
1	B	16	SER	3.3
1	B	172	ARG	3.3
1	C	429	LEU	3.3
1	B	170	VAL	3.3
1	B	296	VAL	3.3
1	D	364	VAL	3.3
1	D	239	TRP	3.3
1	B	86	ILE	3.3
1	D	373	ALA	3.3
1	D	223	ALA	3.2
1	C	215	ILE	3.2
1	D	295	GLY	3.2
1	B	91	ALA	3.2
1	C	251	SER	3.2
1	A	356	ASP	3.2
1	C	330	ASP	3.2
1	A	259	LYS	3.2
1	B	94	VAL	3.2
1	D	262	GLN	3.1
1	A	57	LEU	3.1
1	B	119	LEU	3.1
1	D	346	VAL	3.1
1	A	361	ALA	3.1
1	A	109	ASN	3.1
1	A	92	TYR	3.1
1	C	212	ALA	3.1
1	C	439	SER	3.1
1	D	308	VAL	3.1
1	B	259	LYS	3.0
1	A	328	LEU	3.0
1	B	331	PHE	3.0
1	D	397	LEU	3.0
1	D	370	VAL	3.0
1	D	335	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	349	THR	3.0
1	B	88	LEU	3.0
1	D	333	SER	3.0
1	C	361	ALA	3.0
1	B	394	THR	3.0
1	D	250	ALA	3.0
1	D	169	PRO	3.0
1	B	165	CYS	3.0
1	C	108	SER	3.0
1	A	77	LYS	2.9
1	C	171	ASP	2.9
1	A	393	ILE	2.9
1	B	89	VAL	2.9
1	B	412	SER	2.9
1	D	297	SER	2.9
1	B	409	GLU	2.9
1	B	222	PHE	2.9
1	B	389	ILE	2.9
1	B	374	VAL	2.9
1	D	170	VAL	2.9
1	D	146	PRO	2.9
1	B	43	PHE	2.9
1	D	232	MET	2.9
1	B	416	ARG	2.8
1	C	196	ILE	2.8
1	D	145	ILE	2.8
1	D	259	LYS	2.8
1	A	110	VAL	2.8
1	B	294	GLY	2.8
1	C	294	GLY	2.8
1	B	79	ILE	2.8
1	C	437	ILE	2.8
1	B	344	VAL	2.8
1	C	208	TYR	2.8
1	A	23	ILE	2.8
1	A	389	ILE	2.8
1	C	440	ILE	2.8
1	D	263	ILE	2.8
1	C	112	ASP	2.8
1	D	112	ASP	2.8
1	C	283	TYR	2.8
1	C	200	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	2.7
1	B	240	LEU	2.7
1	B	395	ALA	2.7
1	B	317	CYS	2.7
1	B	160	ILE	2.7
1	C	433	ILE	2.7
1	D	76	ASN	2.7
1	D	285	VAL	2.7
1	D	375	VAL	2.7
1	A	164	LEU	2.7
1	B	246	LEU	2.7
1	B	408	LEU	2.7
1	C	176	LEU	2.7
1	B	34	ALA	2.7
1	C	444	MET	2.7
1	A	283	TYR	2.7
1	B	209	TYR	2.7
1	C	311	LEU	2.7
1	A	150	ALA	2.7
1	C	438	ALA	2.7
1	C	201	THR	2.7
1	A	50	ASP	2.6
1	B	396	GLY	2.6
1	C	257	ASP	2.6
1	A	388	PRO	2.6
1	D	442	PHE	2.6
1	C	175	MET	2.6
1	C	178	VAL	2.6
1	B	392	SER	2.6
1	B	65	PHE	2.6
1	A	392	SER	2.6
1	B	373	ALA	2.6
1	D	254	THR	2.6
1	D	369	ILE	2.6
1	A	395	ALA	2.6
1	B	93	PHE	2.5
1	D	281	LEU	2.5
1	C	299	HIS	2.5
1	A	287	LYS	2.5
1	A	379	ILE	2.5
1	B	38	LEU	2.5
1	B	358	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	55	PHE	2.5
1	A	329	SER	2.5
1	B	61	MET	2.5
1	B	330	ASP	2.5
1	A	139	LYS	2.5
1	A	141	LEU	2.5
1	B	265	HIS	2.5
1	C	432	GLY	2.4
1	C	22	LYS	2.4
1	B	360	PHE	2.4
1	B	445	MET	2.4
1	B	391	SER	2.4
1	C	180	PRO	2.4
1	A	334	LYS	2.4
1	B	406	GLY	2.4
1	D	330	ASP	2.4
1	A	40	LEU	2.4
1	C	57	LEU	2.4
1	A	331	PHE	2.4
1	B	99	PHE	2.4
1	A	96	ALA	2.4
1	C	259	LYS	2.4
1	B	261	GLY	2.4
1	D	396	GLY	2.4
1	D	138	LEU	2.4
1	D	141	LEU	2.4
1	A	364	VAL	2.4
1	A	290	LEU	2.4
1	B	285	VAL	2.4
1	D	363	VAL	2.4
1	B	239	TRP	2.4
1	B	35	LEU	2.3
1	B	230	LEU	2.3
1	B	433	ILE	2.3
1	C	249	LYS	2.3
1	D	260	ALA	2.3
1	A	100	THR	2.3
1	B	107	ILE	2.3
1	D	328	LEU	2.3
1	D	447	LEU	2.3
1	C	334	LYS	2.3
1	D	343	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	2.3
1	C	368	ILE	2.3
1	D	18	LEU	2.3
1	C	17	ASP	2.3
1	A	255	GLU	2.3
1	A	344	VAL	2.3
1	D	342	VAL	2.3
1	D	394	THR	2.3
1	B	329	SER	2.3
1	D	241	SER	2.3
1	D	30	LEU	2.3
1	D	368	ILE	2.3
1	B	417	MET	2.3
1	D	243	GLU	2.3
1	C	150	ALA	2.2
1	D	352	GLN	2.2
1	A	263	ILE	2.2
1	B	224	ILE	2.2
1	C	74	ILE	2.2
1	C	213	ILE	2.2
1	D	230	LEU	2.2
1	A	448	GLU	2.2
1	D	283	TYR	2.2
1	A	335	GLN	2.2
1	B	419	LEU	2.2
1	B	225	ILE	2.2
1	B	118	ASN	2.2
1	D	334	LYS	2.2
1	C	417	MET	2.2
1	B	229	LEU	2.2
1	D	216	LEU	2.2
1	C	98	ILE	2.2
1	A	439	SER	2.2
1	B	446	VAL	2.2
1	D	52	VAL	2.2
1	A	250	ALA	2.2
1	C	335	GLN	2.2
1	B	351	LEU	2.2
1	C	263	ILE	2.2
1	D	148	ILE	2.2
1	A	327	ARG	2.2
1	B	220	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	ASN	2.1
1	D	367	ALA	2.1
1	D	165	CYS	2.1
1	D	255	GLU	2.1
1	B	370	VAL	2.1
1	A	122	ALA	2.1
1	A	238	THR	2.1
1	B	104	ILE	2.1
1	C	445	MET	2.1
1	D	331	PHE	2.1
1	B	200	VAL	2.1
1	B	375	VAL	2.1
1	B	434	VAL	2.1
1	B	18	LEU	2.1
1	C	141	LEU	2.1
1	B	92	TYR	2.1
1	B	348	TYR	2.1
1	B	226	PHE	2.1
1	C	375	VAL	2.1
1	A	81	GLY	2.1
1	D	293	ILE	2.1
1	B	335	GLN	2.0
1	B	290	LEU	2.0
1	D	303	TRP	2.0
1	A	321	ILE	2.0
1	A	446	VAL	2.0
1	C	279	PHE	2.0
1	B	206	GLU	2.0
1	A	151	GLY	2.0
1	D	80	GLY	2.0
1	A	147	THR	2.0
1	D	126	THR	2.0
1	B	297	SER	2.0
1	C	199	SER	2.0
1	D	292	SER	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

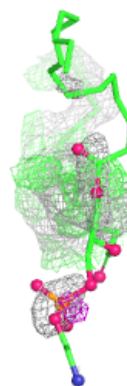
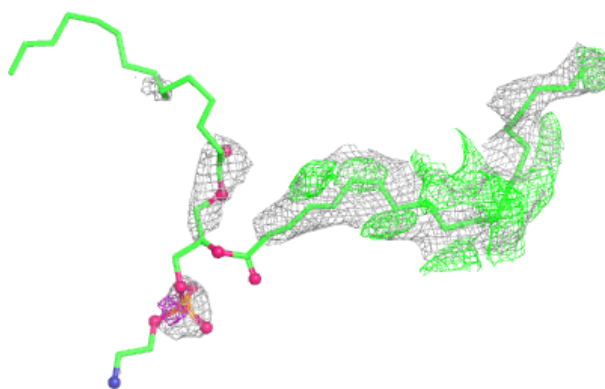
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSR	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PTY	A	1455	50/50	0.52	0.46	66,90,101,110	50
8	MES	D	1453	12/12	0.55	0.29	75,103,106,113	0
3	FLC	B	1449	13/13	0.57	0.19	76,87,98,105	0
3	FLC	A	1454	13/13	0.58	0.12	98,120,125,128	0
4	BOG	C	1448	20/20	0.59	0.16	80,99,115,118	0
4	BOG	D	1454	20/20	0.60	0.20	84,105,112,113	0
3	FLC	A	1453	13/13	0.66	0.18	79,108,121,121	0
3	FLC	B	1450	13/13	0.66	0.16	98,108,114,116	0
4	BOG	A	1456	20/20	0.67	0.17	71,113,125,131	0
6	CL	A	1452	1/1	0.79	0.22	108,108,108,108	0
3	FLC	D	1449	13/13	0.82	0.15	68,82,91,93	0
5	UND	D	1450	11/11	0.85	0.22	55,61,81,83	0
2	NA	C	501	1/1	0.86	0.11	54,54,54,54	0
5	UND	A	1451	11/11	0.87	0.20	55,62,68,75	0
3	FLC	C	1446	13/13	0.92	0.08	44,57,65,66	0
4	BOG	A	1450	20/20	0.92	0.11	44,57,70,77	0
3	FLC	A	1449	13/13	0.93	0.07	38,43,52,54	0
2	NA	B	502	1/1	0.93	0.06	72,72,72,72	0
2	NA	D	502	1/1	0.94	0.07	50,50,50,50	0
4	BOG	C	1447	20/20	0.95	0.08	57,63,76,76	0
2	NA	A	501	1/1	0.96	0.04	39,39,39,39	0
6	CL	D	1451	1/1	0.96	0.07	62,62,62,62	0
2	NA	D	501	1/1	0.97	0.04	54,54,54,54	0
6	CL	D	1452	1/1	0.98	0.20	56,56,56,56	0
2	NA	A	502	1/1	0.98	0.03	42,42,42,42	0
2	NA	C	502	1/1	0.98	0.05	56,56,56,56	0

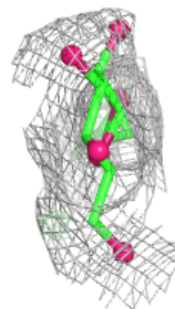
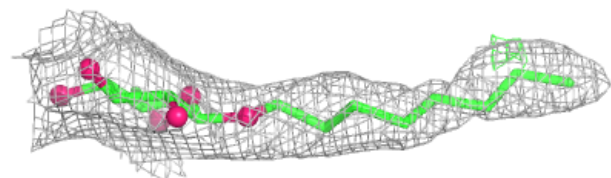
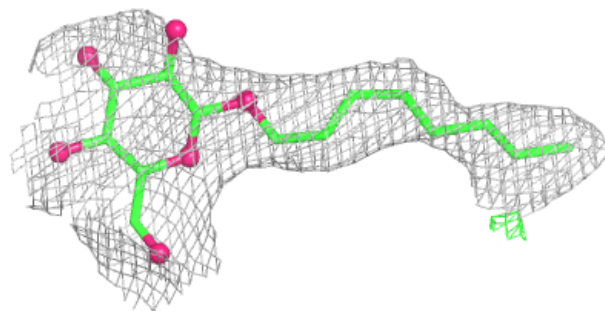
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY A 1455:

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

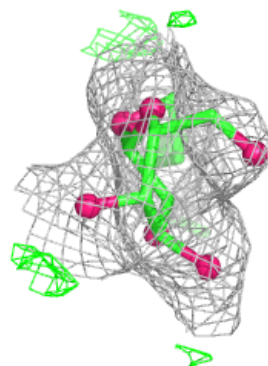
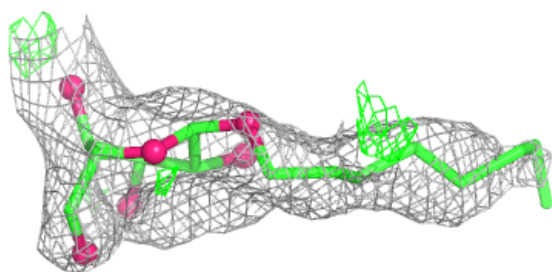
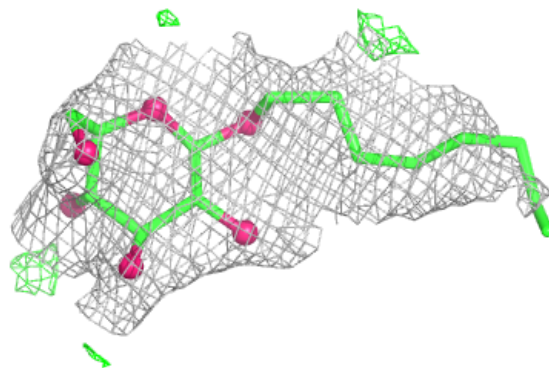
**Electron density around BOG C 1448:**

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

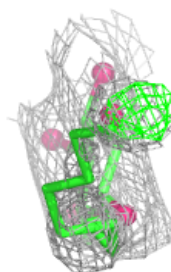
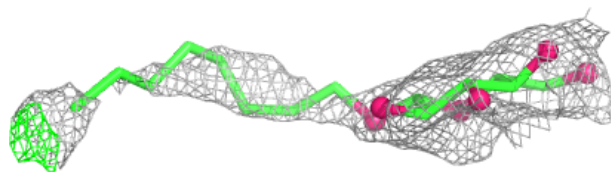
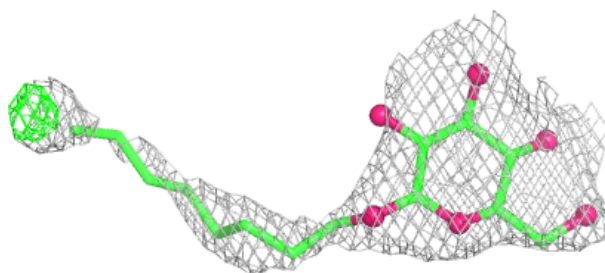


Electron density around BOG D 1454:

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

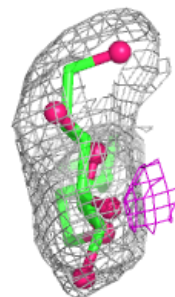
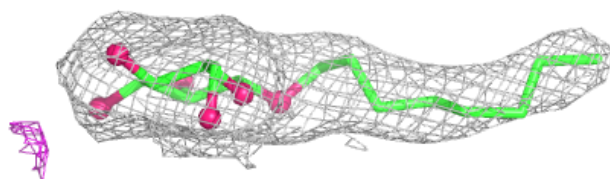
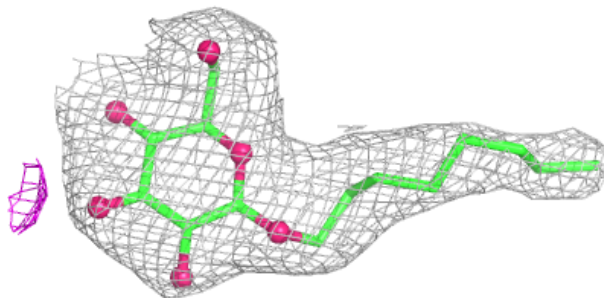
**Electron density around BOG A 1456:**

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

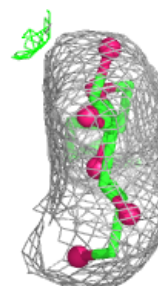
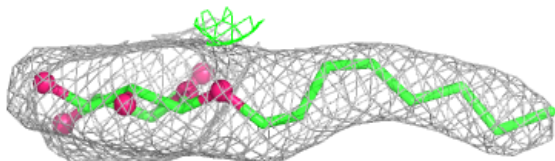
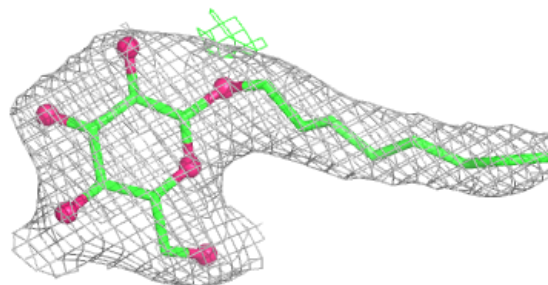


Electron density around BOG A 1450:

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

**Electron density around BOG C 1447:**

$2mF_o-DF_c$ (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.