



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:29 AM UTC

PDB ID : 7FT5 / pdb_00007ft5
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with POB0093
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 1.77 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

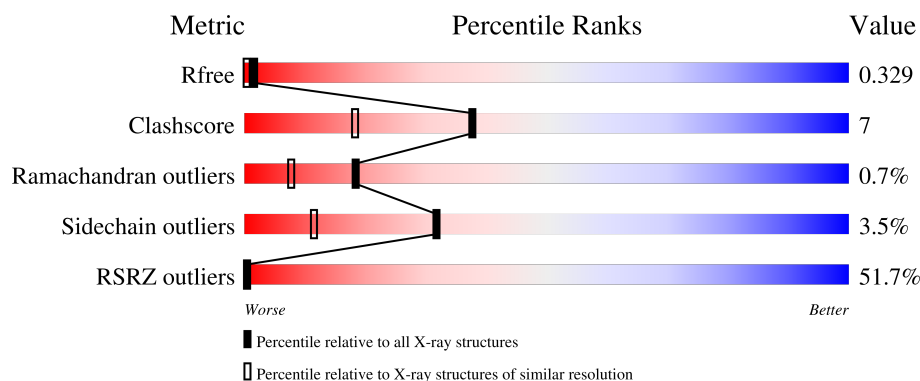
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	195	43% 77% 18% ...
1	B	195	38% 82% 16% ..
1	C	195	58% 73% 23% . ..
1	D	195	64% 74% 24% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6417 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.

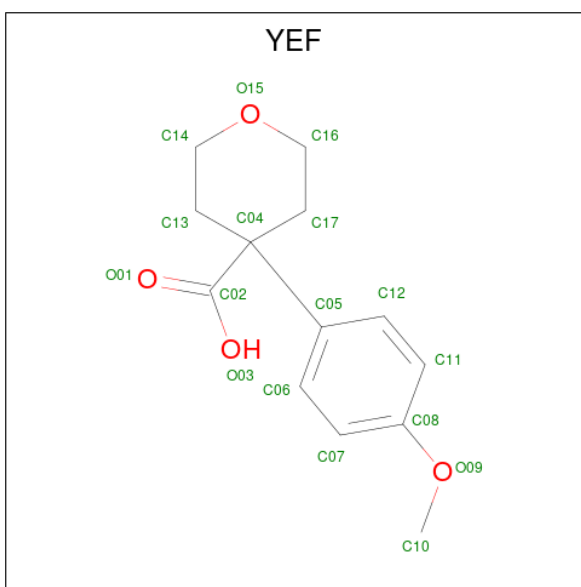
- Molecule 1 is a protein called Syntenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	1	0
			1481	935	262	275	9			
1	B	193	Total	C	N	O	S	0	1	0
			1495	943	264	279	9			
1	C	193	Total	C	N	O	S	0	3	0
			1517	955	272	281	9			
1	D	191	Total	C	N	O	S	0	2	0
			1489	939	263	278	9			

There are 8 discrepancies between the modelled and reference sequences:

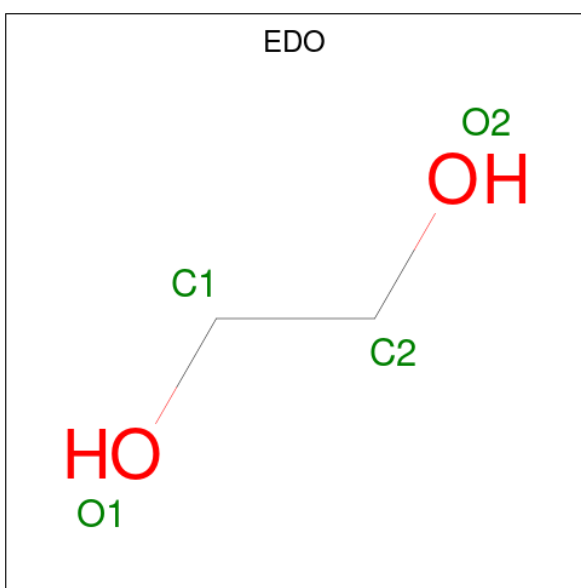
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag	UNP O00560
D	105	MET	-	expression tag	UNP O00560

- Molecule 2 is 4-(4-methoxyphenyl)oxane-4-carboxylic acid (CCD ID: YEF) (formula: $C_{13}H_{16}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	13	4		
2	C	1	Total	C	O	0	0
			17	13	4		

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



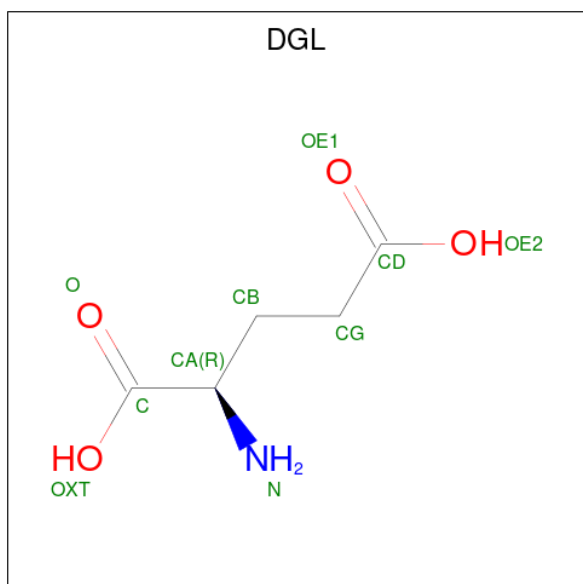
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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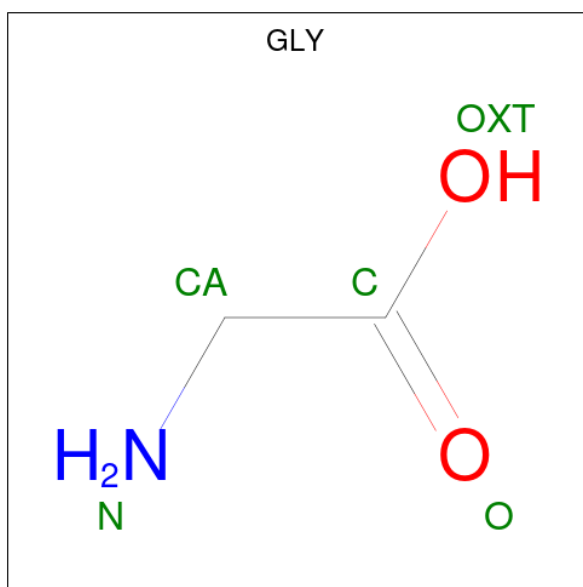
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



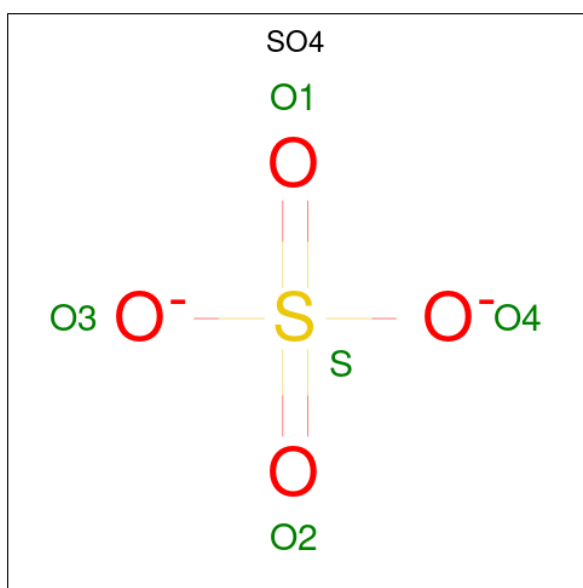
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



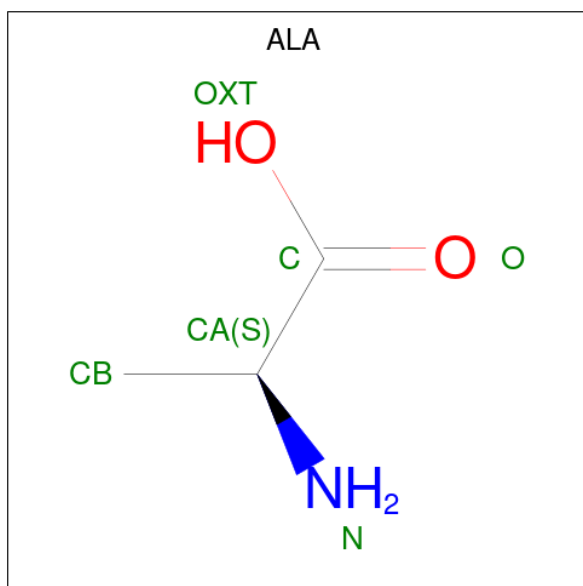
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			6	3	1	2		

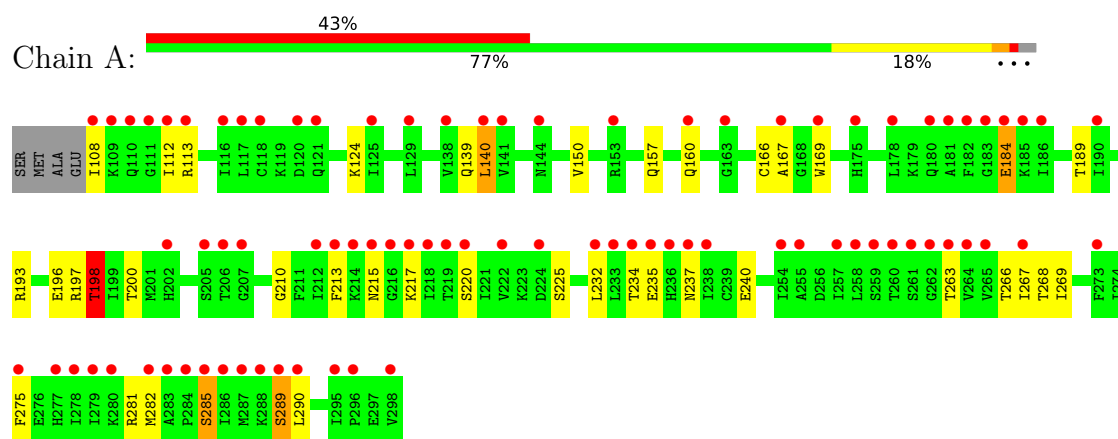
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	B	101	Total	O	0	1
			101	101		
8	C	74	Total	O	0	0
			74	74		
8	D	93	Total	O	0	1
			93	93		

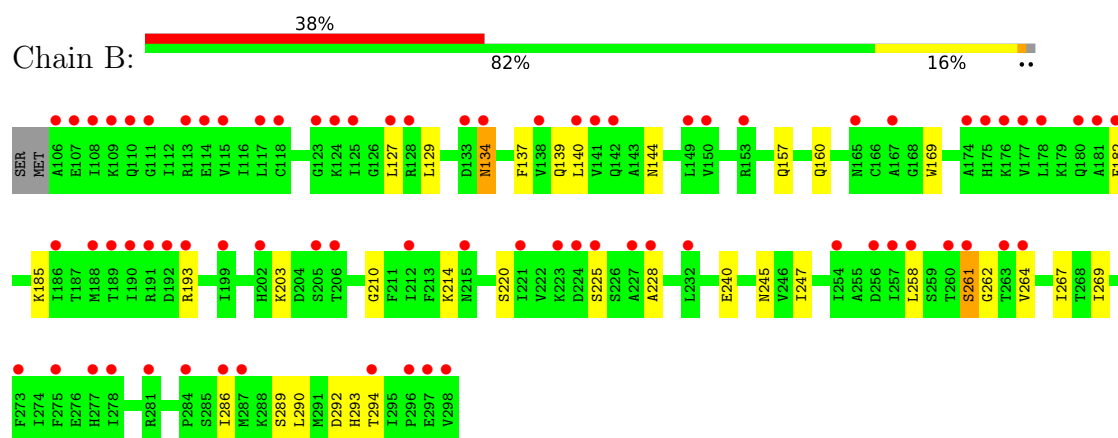
3 Residue-property plots [i](#)

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.

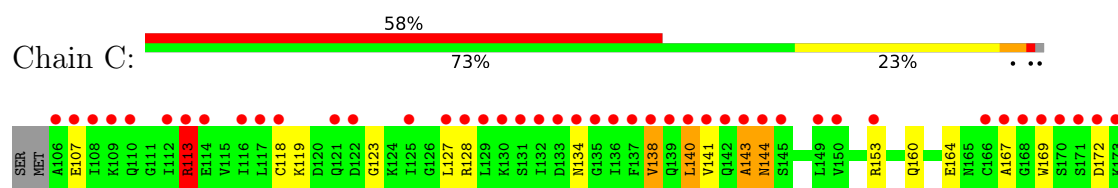
• Molecule 1: Syntenin-1

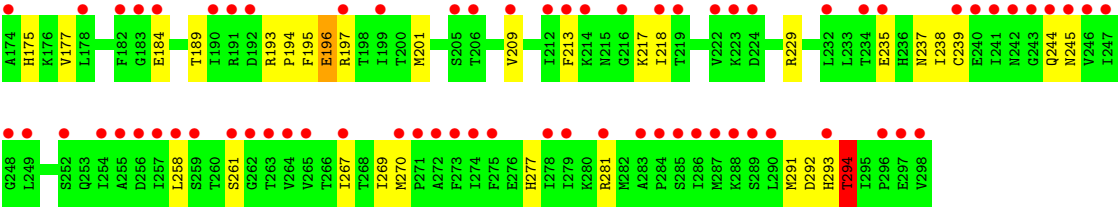


• Molecule 1: Syntenin-1

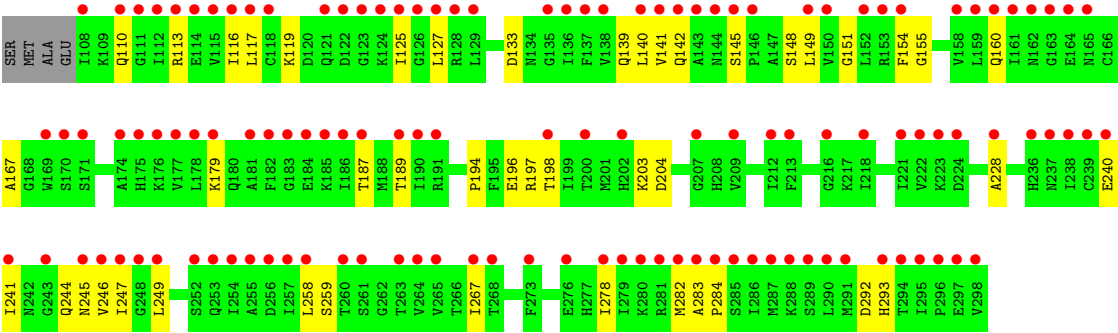


• Molecule 1: Syntenin-1





● Molecule 1: Syntenin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.34Å 49.17Å 116.22Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	80.04 – 1.77 80.04 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.04-1.77) 96.9 (80.04-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.256 , 0.299 0.291 , 0.329	Depositor DCC
R_{free} test set	4355 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6417	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9723e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGL, YEF, EDO, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.41	10/1502 (0.7%)	1.45	7/2019 (0.3%)
1	B	1.20	4/1516 (0.3%)	1.39	2/2038 (0.1%)
1	C	1.58	22/1538 (1.4%)	1.43	9/2066 (0.4%)
1	D	1.25	2/1510 (0.1%)	1.46	3/2030 (0.1%)
All	All	1.37	38/6066 (0.6%)	1.43	21/8153 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	270	MET	CG-SD	13.07	2.13	1.80
1	C	239	CYS	CB-SG	12.12	2.21	1.81
1	A	235	GLU	CD-OE2	12.02	1.48	1.25
1	A	213	PHE	C-O	11.28	1.37	1.23
1	C	238	ILE	C-O	11.06	1.35	1.23
1	A	235	GLU	CD-OE1	10.71	1.45	1.25
1	A	217	LYS	C-O	10.01	1.36	1.24
1	A	234	THR	C-O	9.91	1.34	1.23
1	C	169	TRP	C-O	9.30	1.34	1.23
1	C	196	GLU	CD-OE2	9.22	1.42	1.25
1	A	232	LEU	C-O	8.57	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	VAL	C-O	8.20	1.33	1.24
1	B	134	ASN	C-O	7.96	1.34	1.23
1	C	218	ILE	C-O	7.71	1.31	1.24
1	C	291	MET	C-O	7.61	1.33	1.23
1	A	157	GLN	C-N	7.41	1.40	1.33
1	C	172	ASP	CG-OD2	7.41	1.39	1.25
1	C	277	HIS	C-O	7.30	1.32	1.24
1	C	244	GLN	C-N	7.13	1.43	1.33
1	C	143	ALA	C-O	6.95	1.32	1.24
1	D	228	ALA	C-O	6.88	1.32	1.24
1	C	167	ALA	C-O	6.58	1.31	1.23
1	B	169	TRP	C-O	6.54	1.31	1.23
1	C	127	LEU	C-O	6.43	1.32	1.23
1	C	175	HIS	C-O	6.23	1.31	1.24
1	C	235	GLU	C-N	6.06	1.41	1.33
1	C	237	ASN	C-O	5.80	1.31	1.23
1	A	169	TRP	C-O	5.77	1.31	1.23
1	B	140	LEU	C-O	5.75	1.30	1.23
1	C	195	PHE	C-N	5.72	1.41	1.33
1	C	138	VAL	C-N	5.68	1.42	1.33
1	D	196	GLU	C-O	5.59	1.31	1.23
1	C	140	LEU	C-O	5.49	1.30	1.23
1	C	235	GLU	CD-OE2	5.16	1.35	1.25
1	B	134	ASN	C-N	5.13	1.42	1.34
1	A	237	ASN	C-O	5.12	1.30	1.23
1	C	196	GLU	C-O	5.11	1.30	1.23
1	A	275	PHE	C-O	5.09	1.30	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLU	OE1-CD-OE2	9.59	145.92	122.90
1	C	244	GLN	O-C-N	7.86	132.18	123.22
1	A	198	THR	CA-CB-OG1	-7.38	98.53	109.60
1	C	293	HIS	CA-C-N	6.99	130.76	120.90
1	C	293	HIS	C-N-CA	6.99	130.76	120.90
1	D	189	THR	CB-CA-C	6.93	121.18	109.75
1	C	189	THR	CB-CA-C	6.91	121.81	109.38
1	A	235	GLU	CG-CD-OE2	-6.50	103.44	118.40
1	A	215	ASN	O-C-N	6.48	130.59	122.55
1	C	270	MET	CG-SD-CE	-6.20	87.26	100.90
1	B	294	THR	CA-CB-OG1	-6.11	100.44	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	ARG	N-CA-C	-5.83	105.47	112.58
1	C	294	THR	CA-CB-OG1	-5.76	100.96	109.60
1	A	150	VAL	N-CA-C	-5.67	107.22	112.83
1	C	189	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	200	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	139	GLN	N-CA-C	-5.44	107.19	113.88
1	C	134	ASN	N-CA-C	-5.35	106.70	113.23
1	D	292	ASP	CA-CB-CG	5.33	117.92	112.60
1	D	245	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	139	GLN	N-CA-C	-5.17	107.00	113.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	ASN	Mainchain
1	C	113[A]	ARG	Mainchain
1	D	160	GLN	Peptide

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	1481	0	1530	20	0
1	B	1495	0	1541	16	0
1	C	1517	0	1565	27	0
1	D	1489	0	1533	28	0
2	A	17	0	0	0	0
2	C	17	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	12	0	18	0	0
3	D	8	0	12	1	0
4	B	10	0	7	0	0
4	D	10	0	7	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	15	0	0	0	0
7	D	6	0	4	0	0
8	A	50	0	0	1	0
8	B	101	0	0	3	0
8	C	74	0	0	3	0
8	D	93	0	0	6	0
All	All	6417	0	6239	87	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 7.

All (87) 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:113[A]:ARG:CB	1:C:113[A]:ARG:CA	1.91	1.45
1:C:113[A]:ARG:CA	1:C:113[A]:ARG:C	1.90	1.42
1:C:113[A]:ARG:CB	1:C:113[A]:ARG:HA	1.96	0.95
1:D:187:THR:HG22	8:D:467:HOH:O	1.73	0.89
1:C:113[A]:ARG:CA	1:C:113[A]:ARG:O	2.24	0.84
1:C:267:ILE:HG22	1:C:269:ILE:HG23	1.64	0.79
1:C:261:SER:HB2	8:C:416:HOH:O	1.86	0.76
1:C:118:CYS:SG	1:C:184:GLU:O	2.44	0.75
1:D:197:ARG:NH2	8:D:401:HOH:O	2.07	0.75
1:C:292:ASP:OD1	1:C:294:THR:HB	1.87	0.73
1:A:198:THR:HG23	1:A:266:THR:HG23	1.76	0.68
1:A:160:GLN:OE1	1:A:189:THR:HB	1.95	0.66
1:C:143:ALA:O	1:C:144:ASN:HB2	1.95	0.66
1:A:140:LEU:HG	1:A:282:MET:SD	2.36	0.66
1:A:196:GLU:OE1	8:A:501:HOH:O	2.14	0.65
1:B:228:ALA:O	8:B:401:HOH:O	2.16	0.63
1:B:214:LYS:NZ	8:B:402:HOH:O	2.32	0.59
1:D:204:ASP:OD2	8:D:402:HOH:O	2.16	0.59
1:D:197:ARG:NH1	8:D:403:HOH:O	2.27	0.58
1:C:138:VAL:HG11	1:C:141:VAL:CG2	2.34	0.58
1:A:112:ILE:CG2	1:A:189:THR:CG2	2.82	0.57
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.40	0.57
1:D:139:GLN:HG2	1:D:282:MET:CE	2.35	0.56
1:C:128:ARG:HB2	1:C:140:LEU:HB3	1.88	0.56
1:C:119:LYS:HD3	1:C:123:GLY:O	2.08	0.54
1:D:119:LYS:NZ	8:D:407:HOH:O	2.38	0.54
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:SER:OG	1:B:262:GLY:N	2.40	0.52
1:A:285:SER:O	1:A:289:SER:HB2	2.10	0.52
1:D:113:ARG:O	1:D:113:ARG:HG3	2.09	0.51
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.10	0.51
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.46	0.51
1:C:213:PHE:HA	1:C:217:LYS:O	2.11	0.50
1:D:283:ALA:O	1:D:284:PRO:C	2.53	0.50
1:C:153:ARG:HD3	8:C:408:HOH:O	2.12	0.49
1:C:113[A]:ARG:C	1:C:113[A]:ARG:HA	2.19	0.49
1:D:155:GLY:O	1:D:194:PRO:HD2	2.12	0.49
1:D:133:ASP:OD1	3:D:302:EDO:O1	2.31	0.49
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.94	0.48
1:B:210:GLY:HA3	1:B:225:SER:HB2	1.95	0.48
1:C:201:MET:SD	1:C:209:VAL:CG1	3.03	0.47
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.97	0.46
1:D:203:LYS:NZ	1:D:259:SER:O	2.47	0.46
1:A:140:LEU:HD22	1:B:182:PHE:HE1	1.81	0.46
1:B:267:ILE:HG22	1:B:269:ILE:HG23	1.98	0.45
1:D:140:LEU:HD23	1:D:141:VAL:C	2.41	0.45
1:D:240:GLU:HA	1:D:244:GLN:O	2.17	0.45
1:D:249:LEU:HD21	1:D:293:HIS:CD2	2.52	0.45
1:C:138:VAL:HG11	1:C:141:VAL:HG23	1.99	0.45
1:A:112:ILE:CG2	1:A:189:THR:HG22	2.46	0.45
1:A:112:ILE:HG23	1:A:189:THR:HG22	1.99	0.45
1:C:113[A]:ARG:O	1:C:113[A]:ARG:N	2.49	0.44
1:D:139:GLN:O	1:D:282:MET:HE1	2.18	0.44
1:A:210:GLY:HA3	1:A:225:SER:CB	2.48	0.44
1:A:267:ILE:HG22	1:A:269:ILE:HG23	2.00	0.44
1:C:153:ARG:NH2	1:C:193:ARG:CZ	2.81	0.44
1:C:160:GLN:HA	1:C:164:GLU:O	2.18	0.44
1:C:258:LEU:HD21	1:C:267:ILE:HD11	2.00	0.44
1:D:149:LEU:N	8:D:410:HOH:O	2.51	0.44
1:D:246:VAL:O	1:D:249:LEU:HG	2.18	0.44
1:C:138:VAL:CG1	1:C:141:VAL:HG23	2.48	0.44
1:C:143:ALA:HB2	1:C:292:ASP:HA	2.00	0.44
1:D:198:THR:HA	1:D:267:ILE:O	2.18	0.44
1:A:124:LYS:HE2	1:B:185:LYS:HD3	1.99	0.43
1:D:154:PHE:CE1	1:D:247:ILE:CD1	3.01	0.43
1:A:166:CYS:O	1:A:167:ALA:C	2.62	0.43
1:D:154:PHE:C	1:D:154:PHE:CD1	2.96	0.43
1:C:229:ARG:NH2	8:C:401:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ILE:O	1:B:293:HIS:HE1	2.01	0.43
1:A:193:ARG:NH1	1:A:240:GLU:OE1	2.52	0.43
1:D:154:PHE:CE2	1:D:247:ILE:HD13	2.54	0.43
1:D:148:SER:O	1:D:151:GLY:N	2.42	0.42
1:B:245:ASN:HB3	1:B:292:ASP:O	2.20	0.42
1:D:140:LEU:HD23	1:D:141:VAL:N	2.34	0.42
1:A:160:GLN:OE1	1:A:189:THR:CB	2.65	0.42
1:D:241:ILE:HD13	1:D:258:LEU:HG	2.02	0.42
1:A:290:LEU:HD13	1:B:182:PHE:HB2	2.01	0.41
1:B:261:SER:HB2	8:B:478:HOH:O	2.19	0.41
1:D:125:ILE:HD11	1:D:127:LEU:HD12	2.03	0.41
1:A:240:GLU:HB2	1:A:268:THR:HB	2.03	0.41
1:B:127:LEU:HD13	1:B:129:LEU:HD21	2.03	0.41
1:C:213:PHE:HB2	1:C:217:LYS:O	2.21	0.40
1:B:203:LYS:CE	1:B:258:LEU:O	2.69	0.40
1:B:193:ARG:NH1	1:B:240:GLU:OE1	2.54	0.40
1:A:112:ILE:HG22	1:A:189:THR:CG2	2.51	0.40
1:A:197:ARG:HD3	1:C:194:PRO:O	2.22	0.40
1:B:137:PHE:CE2	1:B:157:GLN:HB2	2.56	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	190/195 (97%)	179 (94%)	9 (5%)	2 (1%)	11	3
1	B	192/195 (98%)	186 (97%)	5 (3%)	1 (0%)	24	11
1	C	194/195 (100%)	185 (95%)	8 (4%)	1 (0%)	24	11
1	D	191/195 (98%)	183 (96%)	7 (4%)	1 (0%)	24	11
All	All	767/780 (98%)	733 (96%)	29 (4%)	5 (1%)	18	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	281	ARG
1	D	167	ALA
1	B	261	SER
1	C	144	ASN

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	166/168 (99%)	157 (95%)	9 (5%)	20	4
1	B	167/168 (99%)	162 (97%)	5 (3%)	36	15
1	C	169/168 (101%)	164 (97%)	5 (3%)	36	15
1	D	167/168 (99%)	162 (97%)	5 (3%)	36	15
All	All	669/672 (100%)	645 (96%)	24 (4%)	32	10

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	113	ARG
1	A	140	LEU
1	A	184	GLU
1	A	198	THR
1	A	220	SER
1	A	263	THR
1	A	285	SER
1	A	289	SER
1	B	144	ASN
1	B	160	GLN
1	B	220	SER
1	B	264	VAL
1	B	289	SER
1	C	107	GLU

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Mol	Chain	Res	Type
1	C	113[A]	ARG
1	C	113[B]	ARG
1	C	245	ASN
1	C	294	THR
1	D	110	GLN
1	D	116	ILE
1	D	117	LEU
1	D	179	LYS
1	D	278	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	215	ASN
1	B	121	GLN
1	B	142	GLN
1	B	208	HIS
1	B	215	ASN
1	C	142	GLN
1	C	230	ASN

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](#)

18 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	B	302	-	3,3,3	0.12	0	2,2,2	0.11	0
6	SO4	D	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	DGL	D	307	-	8,9,9	1.05	0	8,11,11	1.11	1 (12%)
6	SO4	D	303	-	4,4,4	0.32	0	6,6,6	0.09	0
2	YEF	A	401	-	18,18,18	2.22	4 (22%)	24,25,25	0.94	0
3	EDO	D	302	-	3,3,3	0.08	0	2,2,2	0.25	0
5	GLY	D	308	-	4,4,4	1.15	1 (25%)	3,4,4	1.50	0
4	DGL	B	303	-	8,9,9	1.02	0	8,11,11	1.26	1 (12%)
3	EDO	C	304	-	3,3,3	0.33	0	2,2,2	0.38	0
2	YEF	C	301	-	18,18,18	2.19	3 (16%)	24,25,25	1.35	3 (12%)
5	GLY	C	305	-	4,4,4	0.99	0	3,4,4	1.40	0
3	EDO	A	402	-	3,3,3	0.09	0	2,2,2	0.16	0
6	SO4	D	305	-	4,4,4	0.31	0	6,6,6	0.10	0
3	EDO	C	302	-	3,3,3	0.15	0	2,2,2	0.27	0
3	EDO	C	303	-	3,3,3	0.10	0	2,2,2	0.19	0
3	EDO	B	301	-	3,3,3	0.16	0	2,2,2	0.13	0
3	EDO	D	301	-	3,3,3	0.12	0	2,2,2	0.25	0
7	ALA	D	306	-	5,5,5	1.07	1 (20%)	6,6,6	1.39	1 (16%)

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	B	302	-	-	0/1/1/1	-
4	DGL	D	307	-	-	2/9/9/9	-
2	YEF	A	401	-	-	0/14/24/24	0/2/2/2
3	EDO	D	302	-	-	0/1/1/1	-
5	GLY	D	308	-	-	2/2/2/2	-
4	DGL	B	303	-	-	2/9/9/9	-
3	EDO	C	304	-	-	1/1/1/1	-
2	YEF	C	301	-	-	0/14/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLY	C	305	-	-	2/2/2/2	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
7	ALA	D	306	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	YEF	C04-C05	5.98	1.62	1.53
2	A	401	YEF	C04-C05	5.62	1.62	1.53
2	A	401	YEF	C13-C04	-5.14	1.48	1.54
2	C	301	YEF	C13-C04	-4.90	1.48	1.54
2	A	401	YEF	C17-C04	-3.99	1.49	1.54
2	C	301	YEF	C17-C04	-3.06	1.50	1.54
5	D	308	GLY	OXT-C	-2.21	1.23	1.30
7	D	306	ALA	OXT-C	-2.21	1.23	1.30
2	A	401	YEF	O01-C02	2.03	1.28	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	306	ALA	OXT-C-O	-2.75	117.83	124.08
2	C	301	YEF	C16-C17-C04	2.75	115.19	111.77
2	C	301	YEF	O15-C16-C17	2.73	114.22	111.50
4	B	303	DGL	OXT-C-O	-2.61	118.16	124.08
2	C	301	YEF	C17-C04-C13	2.49	110.54	107.82
4	D	307	DGL	OXT-C-O	-2.16	119.17	124.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	GLY	O-C-CA-N
5	D	308	GLY	OXT-C-CA-N
5	D	308	GLY	O-C-CA-N
5	C	305	GLY	OXT-C-CA-N
3	C	303	EDO	O1-C1-C2-O2
3	C	304	EDO	O1-C1-C2-O2

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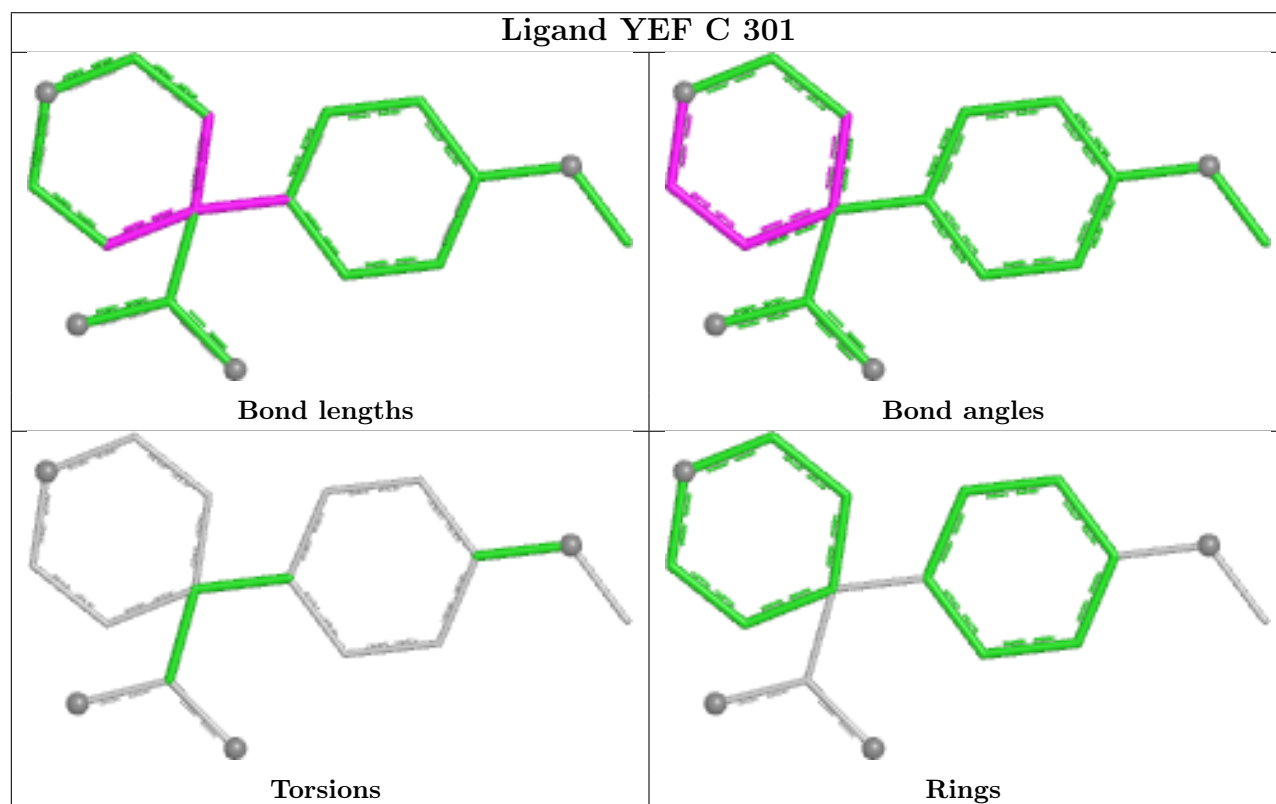
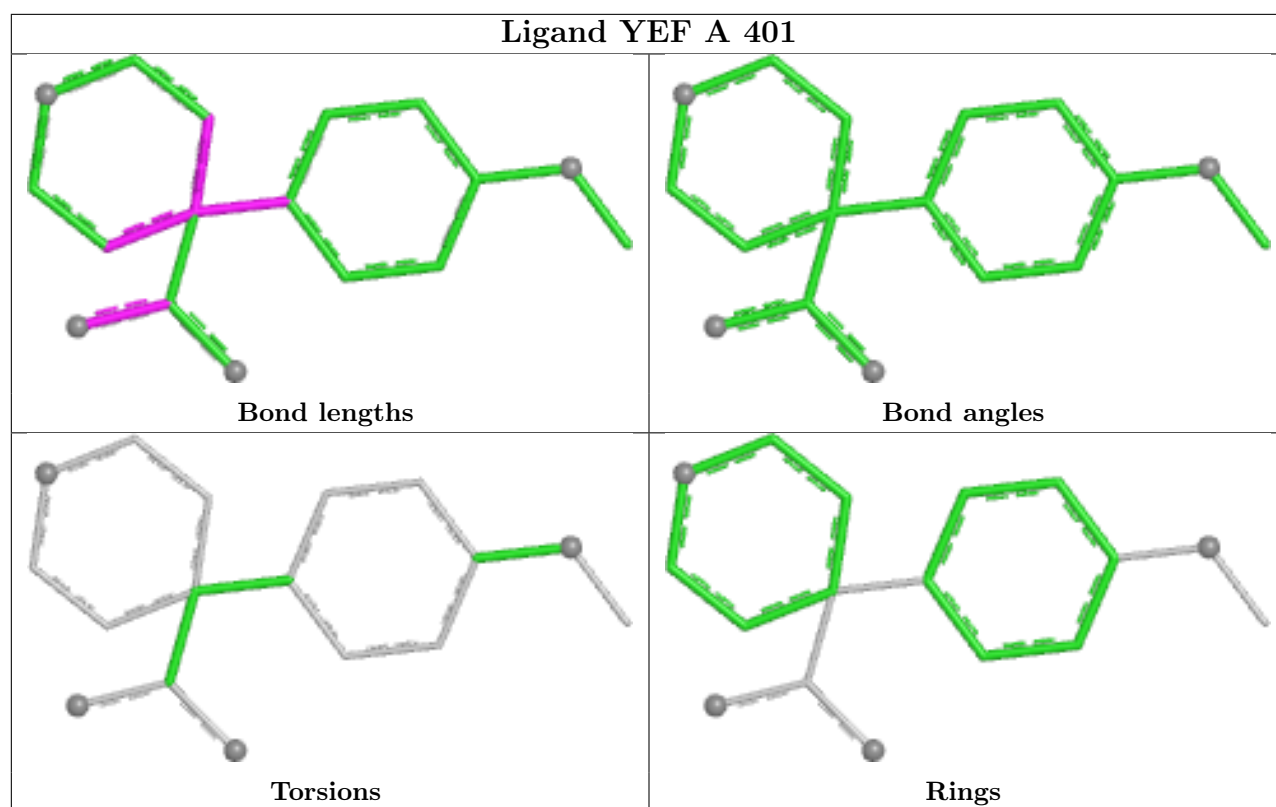
Mol	Chain	Res	Type	Atoms
3	A	402	EDO	O1-C1-C2-O2
4	D	307	DGL	O-C-CA-CB
4	D	307	DGL	OXT-C-CA-CB
4	B	303	DGL	OE2-CD-CG-CB
4	B	303	DGL	OE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/195 (97%)	2.64	84 (43%) 0 0	12, 46, 75, 85	23 (12%)
1	B	193/195 (98%)	2.17	75 (38%) 1 1	13, 46, 64, 70	18 (9%)
1	C	193/195 (98%)	3.84	114 (59%) 0 0	12, 46, 68, 89	55 (28%)
1	D	191/195 (97%)	3.07	124 (64%) 0 0	14, 48, 71, 80	20 (10%)
All	All	768/780 (98%)	2.93	397 (51%) 0 0	12, 47, 68, 89	116 (15%)

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	295	ILE	14.4
1	C	167	ALA	13.5
1	D	298	VAL	13.4
1	A	216	GLY	12.5
1	B	189	THR	12.3
1	C	169	TRP	12.2
1	D	238	ILE	12.0
1	A	212	ILE	11.8
1	C	247	ILE	11.7
1	C	174	ALA	11.7
1	D	296	PRO	11.7
1	A	213	PHE	11.7
1	C	274	ILE	11.5
1	C	249	LEU	11.4
1	A	218	ILE	11.4
1	C	132	ILE	11.3
1	A	232	LEU	11.2
1	C	275	PHE	11.2
1	C	136	ILE	11.2
1	B	190	ILE	11.1
1	A	238	ILE	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	11.0
1	D	239	CYS	10.8
1	C	271	PRO	10.7
1	D	294	THR	10.6
1	C	138	VAL	10.4
1	C	246	VAL	10.4
1	D	115	VAL	10.4
1	A	219	THR	10.4
1	C	113[A]	ARG	10.4
1	D	297	GLU	10.3
1	A	234	THR	10.3
1	C	241	ILE	10.2
1	C	168	GLY	10.2
1	A	215	ASN	10.1
1	C	272	ALA	10.0
1	C	248	GLY	9.9
1	D	237	ASN	9.8
1	C	171	SER	9.6
1	C	170	SER	9.4
1	B	118	CYS	9.3
1	C	137	PHE	9.2
1	B	192	ASP	9.2
1	C	135	GLY	9.1
1	C	243	GLY	9.0
1	D	240	GLU	8.8
1	C	166	CYS	8.8
1	C	245	ASN	8.8
1	D	236	HIS	8.7
1	A	217	LYS	8.6
1	A	236	HIS	8.6
1	C	173	LYS	8.6
1	C	190	ILE	8.6
1	B	174	ALA	8.5
1	A	214	LYS	8.4
1	C	131	SER	8.4
1	C	239	CYS	8.4
1	C	172	ASP	8.4
1	D	112	ILE	8.2
1	A	235	GLU	8.1
1	A	260	THR	8.1
1	D	256[A]	ASP	8.1
1	C	133	ASP	8.0

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Mol	Chain	Res	Type	RSRZ
1	D	273[A]	PHE	8.0
1	A	273[A]	PHE	7.9
1	C	134	ASN	7.9
1	B	191	ARG	7.9
1	B	193	ARG	7.8
1	A	237	ASN	7.7
1	B	298	VAL	7.7
1	C	112	ILE	7.6
1	C	242	ASN	7.4
1	C	270	MET	7.4
1	B	188	MET	7.4
1	C	273[A]	PHE	7.2
1	B	296	PRO	7.0
1	C	130	LYS	6.9
1	D	116	ILE	6.8
1	D	182	PHE	6.8
1	D	254	ILE	6.7
1	C	139	GLN	6.6
1	C	298	VAL	6.6
1	A	117	LEU	6.5
1	C	143	ALA	6.3
1	D	190	ILE	6.3
1	A	220	SER	6.2
1	C	244	GLN	6.2
1	D	113	ARG	6.2
1	A	290	LEU	6.1
1	C	191	ARG	6.1
1	C	182	PHE	6.0
1	D	191	ARG	6.0
1	C	256	ASP	6.0
1	A	282	MET	5.9
1	C	141	VAL	5.9
1	A	259	SER	5.9
1	C	288	LYS	5.9
1	C	117	LEU	5.9
1	B	273[A]	PHE	5.9
1	A	118	CYS	5.8
1	A	182	PHE	5.8
1	D	286	ILE	5.7
1	C	106	ALA	5.7
1	A	140	LEU	5.6
1	B	109	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLN	5.6
1	D	177	VAL	5.5
1	A	153	ARG	5.4
1	C	240	GLU	5.3
1	C	108	ILE	5.3
1	A	206	THR	5.2
1	D	149	LEU	5.1
1	C	121	GLN	5.0
1	C	110	GLN	5.0
1	B	175	HIS	5.0
1	D	141	VAL	5.0
1	D	153	ARG	4.9
1	C	107	GLU	4.9
1	C	262	GLY	4.9
1	B	297	GLU	4.8
1	A	298	VAL	4.8
1	B	205	SER	4.8
1	C	286	ILE	4.7
1	A	202	HIS	4.7
1	C	296	PRO	4.7
1	B	223	LYS	4.6
1	B	106	ALA	4.6
1	C	283	ALA	4.6
1	C	297	GLU	4.5
1	D	144	ASN	4.5
1	B	125	ILE	4.5
1	D	165	ASN	4.5
1	A	284	PRO	4.5
1	D	117	LEU	4.5
1	D	143	ALA	4.5
1	D	114	GLU	4.4
1	C	128	ARG	4.4
1	A	286	ILE	4.4
1	D	284	PRO	4.3
1	B	114	GLU	4.3
1	A	263	THR	4.3
1	A	116	ILE	4.3
1	C	252	SER	4.2
1	D	178	LEU	4.2
1	D	290	LEU	4.2
1	A	283	ALA	4.2
1	B	202	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	224	ASP	4.2
1	C	209	VAL	4.2
1	C	114	GLU	4.1
1	B	224	ASP	4.1
1	D	140	LEU	4.1
1	D	248	GLY	4.1
1	D	265	VAL	4.1
1	A	287	MET	4.0
1	B	264	VAL	4.0
1	D	255	ALA	4.0
1	C	267	ILE	4.0
1	D	125	ILE	3.9
1	C	290	LEU	3.9
1	D	129	LEU	3.9
1	C	197[A]	ARG	3.9
1	A	108	ILE	3.8
1	D	279	ILE	3.8
1	C	145	SER	3.8
1	C	281	ARG	3.8
1	D	136	ILE	3.8
1	C	265	VAL	3.8
1	B	176	LYS	3.8
1	B	110	GLN	3.8
1	C	192	ASP	3.8
1	D	163	GLY	3.7
1	A	184	GLU	3.7
1	A	169	TRP	3.7
1	B	286	ILE	3.7
1	C	235	GLU	3.7
1	D	186	ILE	3.7
1	D	108	ILE	3.6
1	D	212	ILE	3.6
1	D	241	ILE	3.6
1	D	150	VAL	3.6
1	C	118	CYS	3.6
1	D	161	ILE	3.6
1	D	278	ILE	3.6
1	A	111	GLY	3.6
1	D	246	VAL	3.6
1	C	142	GLN	3.5
1	C	183	GLY	3.5
1	C	109	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLN	3.5
1	D	187	THR	3.5
1	D	126	GLY	3.5
1	D	261	SER	3.5
1	C	234	THR	3.5
1	B	281	ARG	3.4
1	B	263	THR	3.4
1	C	284	PRO	3.4
1	D	247	ILE	3.4
1	D	164	GLU	3.4
1	D	263	THR	3.4
1	C	264	VAL	3.4
1	A	175	HIS	3.3
1	C	254	ILE	3.3
1	B	117	LEU	3.3
1	C	149	LEU	3.3
1	A	288	LYS	3.3
1	C	153	ARG	3.3
1	C	263	THR	3.3
1	C	140	LEU	3.3
1	C	122	ASP	3.3
1	A	125	ILE	3.2
1	D	175	HIS	3.2
1	C	287	MET	3.2
1	D	138	VAL	3.2
1	C	144	ASN	3.2
1	D	288	LYS	3.2
1	A	265	VAL	3.2
1	A	186	ILE	3.2
1	B	108	ILE	3.2
1	D	174	ALA	3.2
1	D	258	LEU	3.1
1	C	255	ALA	3.1
1	A	113	ARG	3.1
1	D	289	SER	3.1
1	D	267	ILE	3.1
1	B	153	ARG	3.1
1	D	137	PHE	3.1
1	C	223	LYS	3.0
1	C	278	ILE	3.0
1	D	249	LEU	3.0
1	C	206	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	127	LEU	3.0
1	D	159	LEU	3.0
1	D	142	GLN	3.0
1	A	255	ALA	3.0
1	A	279	ILE	3.0
1	B	182	PHE	3.0
1	D	213	PHE	3.0
1	D	110	GLN	2.9
1	B	128	ARG	2.9
1	B	232	LEU	2.9
1	D	118	CYS	2.9
1	C	259	SER	2.9
1	D	264	VAL	2.8
1	B	133	ASP	2.8
1	D	111	GLY	2.8
1	C	213	PHE	2.8
1	B	260	THR	2.8
1	D	287	MET	2.8
1	A	224	ASP	2.8
1	D	207	GLY	2.8
1	A	181	ALA	2.8
1	C	150	VAL	2.8
1	C	222	VAL	2.8
1	D	146	PRO	2.8
1	B	258	LEU	2.8
1	C	232	LEU	2.7
1	B	278	ILE	2.7
1	C	116	ILE	2.7
1	D	121	GLN	2.7
1	A	296	PRO	2.7
1	B	177	VAL	2.7
1	B	294	THR	2.7
1	B	199	ILE	2.7
1	C	212	ILE	2.7
1	A	180	GLN	2.7
1	C	127	LEU	2.7
1	B	134	ASN	2.7
1	D	216	GLY	2.7
1	D	202	HIS	2.6
1	C	178	LEU	2.6
1	C	258	LEU	2.6
1	D	282	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	2.6
1	C	125	ILE	2.6
1	B	107	GLU	2.6
1	A	205	SER	2.6
1	C	285	SER	2.6
1	C	289	SER	2.6
1	B	123	GLY	2.6
1	D	154	PHE	2.6
1	D	200	THR	2.6
1	B	178	LEU	2.6
1	A	160	GLN	2.6
1	A	295	ILE	2.6
1	D	257	ILE	2.6
1	D	145	SER	2.6
1	A	190	ILE	2.6
1	B	257	ILE	2.6
1	B	111	GLY	2.5
1	D	189	THR	2.5
1	A	185	LYS	2.5
1	A	285	SER	2.5
1	A	258	LEU	2.5
1	A	112	ILE	2.5
1	B	181	ALA	2.5
1	D	209	VAL	2.5
1	B	227	ALA	2.5
1	B	150	VAL	2.5
1	D	176	LYS	2.5
1	D	183	GLY	2.5
1	B	261	SER	2.5
1	D	252	SER	2.5
1	A	275	PHE	2.4
1	D	281	ARG	2.4
1	A	264	VAL	2.4
1	D	245	ASN	2.4
1	D	122	ASP	2.4
1	D	291	MET	2.4
1	D	293	HIS	2.4
1	B	149	LEU	2.4
1	D	123	GLY	2.4
1	D	135	GLY	2.4
1	D	170	SER	2.4
1	C	219	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	260	THR	2.4
1	B	141	VAL	2.4
1	C	257	ILE	2.4
1	A	121	GLN	2.4
1	B	284	PRO	2.4
1	C	205	SER	2.4
1	B	127	LEU	2.4
1	C	184	GLU	2.4
1	B	277	HIS	2.4
1	D	253	GLN	2.3
1	B	167	ALA	2.3
1	A	254	ILE	2.3
1	B	115	VAL	2.3
1	B	138	VAL	2.3
1	D	162	ASN	2.3
1	D	171	SER	2.3
1	B	256	ASP	2.3
1	D	179	LYS	2.3
1	B	206	THR	2.3
1	D	181	ALA	2.3
1	C	261	SER	2.3
1	A	141	VAL	2.3
1	A	120	ASP	2.3
1	A	144	ASN	2.3
1	A	280	LYS	2.3
1	D	223	LYS	2.3
1	A	278	ILE	2.3
1	B	186	ILE	2.3
1	B	287	MET	2.3
1	A	178	LEU	2.2
1	D	276	GLU	2.2
1	A	167	ALA	2.2
1	B	254	ILE	2.2
1	D	218	ILE	2.2
1	D	124	LYS	2.2
1	D	158	VAL	2.2
1	B	228	ALA	2.2
1	D	283	ALA	2.2
1	D	169	TRP	2.2
1	B	140	LEU	2.2
1	C	216	GLY	2.2
1	B	113	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	280	LYS	2.2
1	B	212	ILE	2.2
1	C	218	ILE	2.2
1	A	261	SER	2.2
1	D	228	ALA	2.1
1	A	129	LEU	2.1
1	A	289	SER	2.1
1	B	225	SER	2.1
1	B	275	PHE	2.1
1	D	198	THR	2.1
1	B	142	GLN	2.1
1	C	279	ILE	2.1
1	A	138	VAL	2.1
1	A	207	GLY	2.1
1	B	124	LYS	2.1
1	C	129	LEU	2.1
1	D	152	LEU	2.1
1	D	160	GLN	2.1
1	A	257	ILE	2.1
1	A	267	ILE	2.1
1	C	199	ILE	2.1
1	A	109	LYS	2.1
1	A	163	GLY	2.1
1	A	262	GLY	2.1
1	B	165	ASN	2.1
1	D	184	GLU	2.1
1	D	224	ASP	2.1
1	A	277	HIS	2.1
1	B	221	ILE	2.1
1	D	221	ILE	2.1
1	A	183	GLY	2.0
1	D	128	ARG	2.0
1	C	293	HIS	2.0
1	D	268	THR	2.0
1	C	214	LYS	2.0
1	D	185	LYS	2.0
1	B	215	ASN	2.0
1	D	243	GLY	2.0
1	D	285	SER	2.0
1	D	222	VAL	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](#)

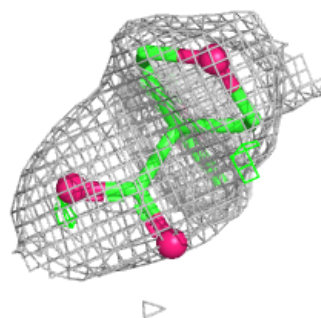
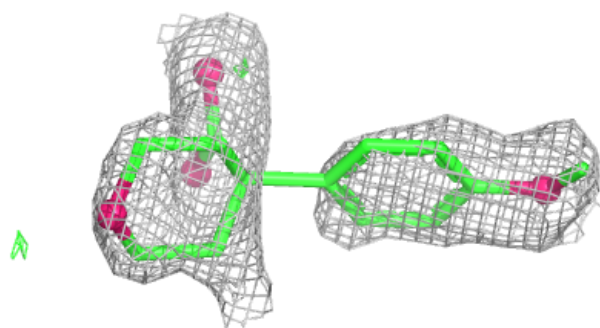
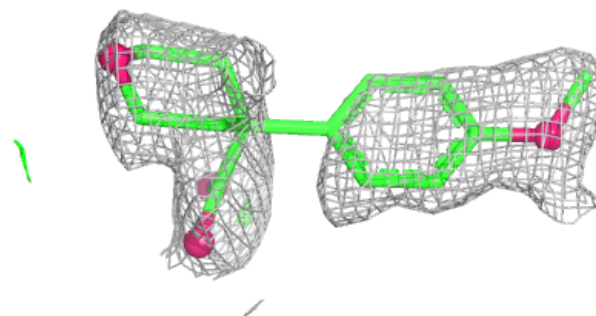
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	SO4	D	305	5/5	0.42	0.25	103,106,108,116	0
4	DGL	D	307	10/10	0.47	0.30	85,99,106,107	0
5	GLY	C	305	5/5	0.66	0.19	50,58,64,67	0
3	EDO	C	304	4/4	0.68	0.25	47,54,54,55	0
6	SO4	D	303	5/5	0.70	0.17	69,77,84,84	0
6	SO4	D	304	5/5	0.72	0.16	114,115,117,120	0
7	ALA	D	306	6/6	0.73	0.21	75,79,80,81	0
5	GLY	D	308	5/5	0.75	0.18	69,72,74,75	0
4	DGL	B	303	10/10	0.76	0.17	52,68,81,84	0
2	YEF	A	401	17/17	0.79	0.20	48,50,52,52	17
3	EDO	A	402	4/4	0.81	0.20	56,60,61,63	0
2	YEF	C	301	17/17	0.83	0.18	73,75,78,78	0
3	EDO	B	301	4/4	0.84	0.17	52,55,57,58	0
3	EDO	C	302	4/4	0.84	0.14	29,31,32,35	0
3	EDO	C	303	4/4	0.84	0.15	50,58,59,61	0
3	EDO	D	302	4/4	0.85	0.16	48,54,58,61	0
3	EDO	D	301	4/4	0.89	0.15	31,34,35,41	0
3	EDO	B	302	4/4	0.94	0.11	37,37,38,38	0

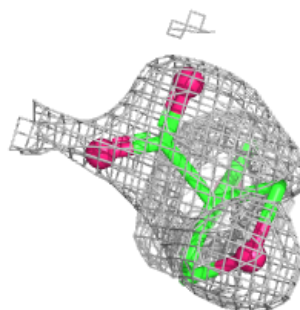
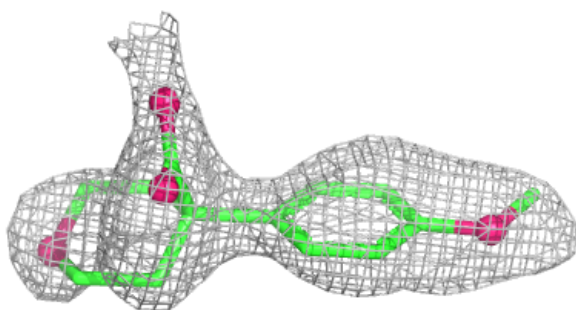
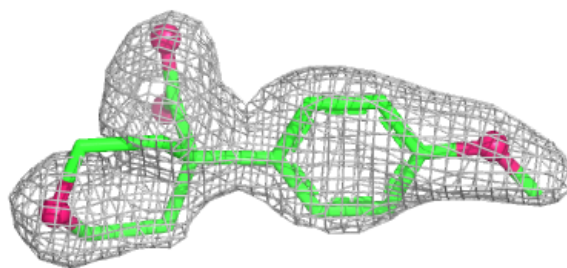
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YEF A 401:

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

**Electron density around YEF C 301:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.