



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:29 AM UTC

PDB ID : 7FST / pdb_00007fst
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z26968795
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 1.98 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

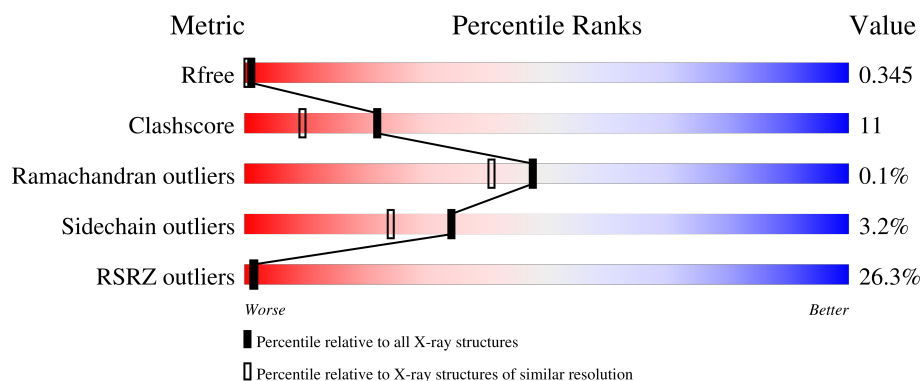
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	16% 82% 15% ..
1	B	195	15% 83% 16% ..
1	C	195	15% 82% 16% ..
1	D	195	56% 55% 41% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6376 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
			1514	953	270	282	9			
1	D	191	Total	C	N	O	S	0	1	0
			1481	935	262	275	9			

There are 8 discrepancies between the modelled and reference sequences:

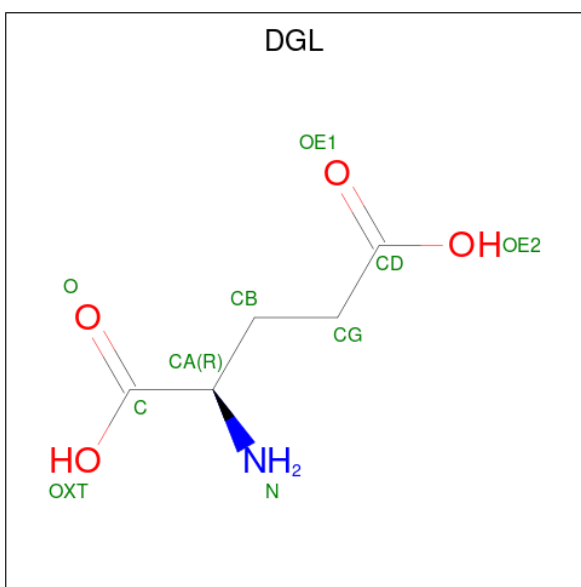
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



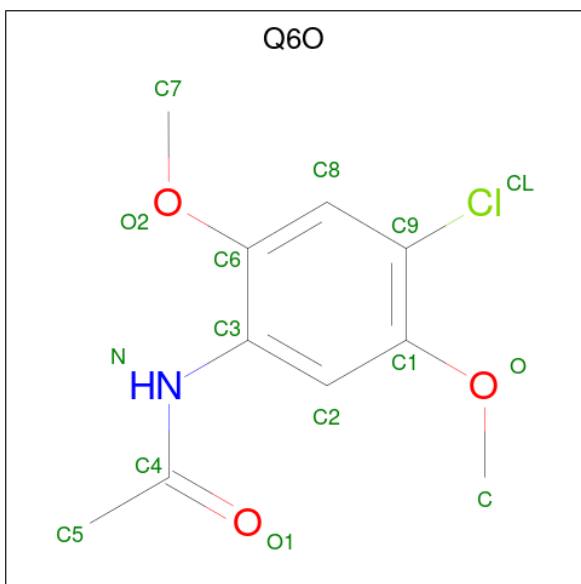
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



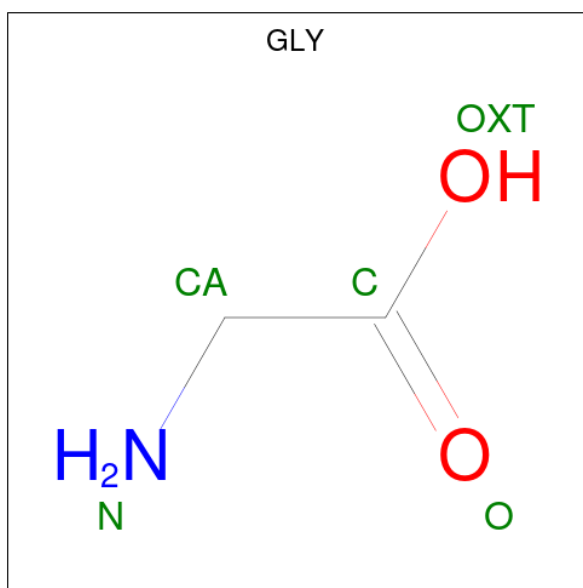
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is N-(4-chloro-2,5-dimethoxyphenyl)acetamide (CCD ID: Q6O) (formula: $C_{10}H_{12}ClNO_3$) (labeled as "Ligand of Interest" by depositor).



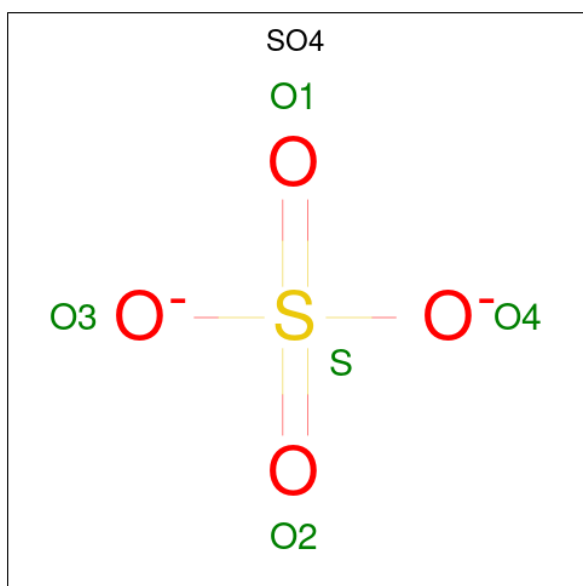
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Cl	N	O	0	0
			15	10	1	1	3		

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



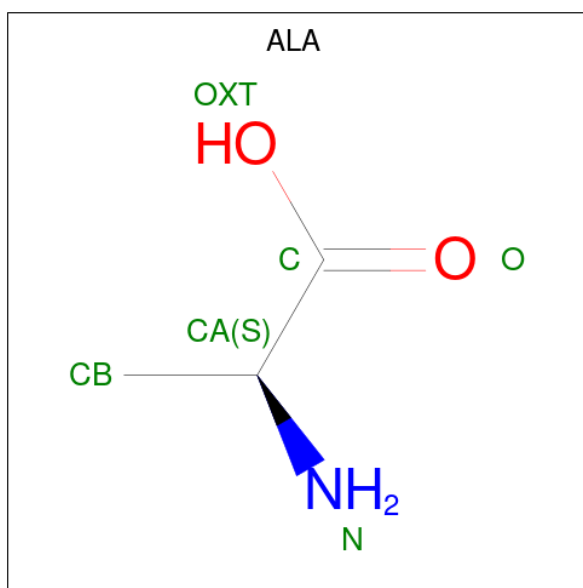
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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		

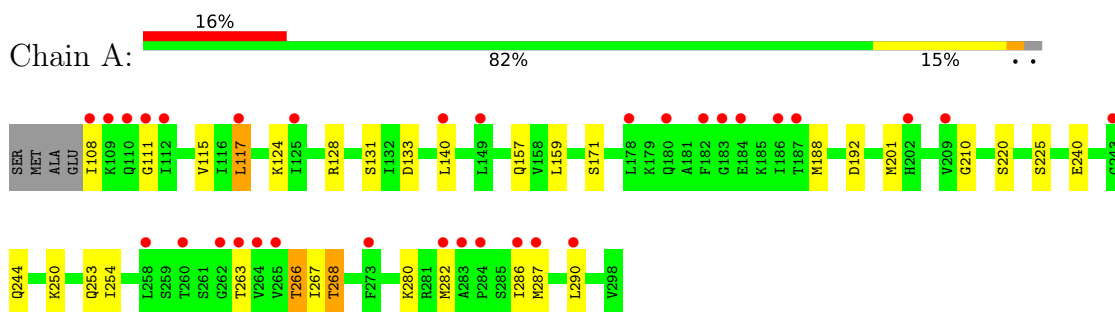
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	104	Total	O	0	0
			104	104		
8	C	81	Total	O	0	1
			82	82		
8	D	82	Total	O	0	0
			82	82		

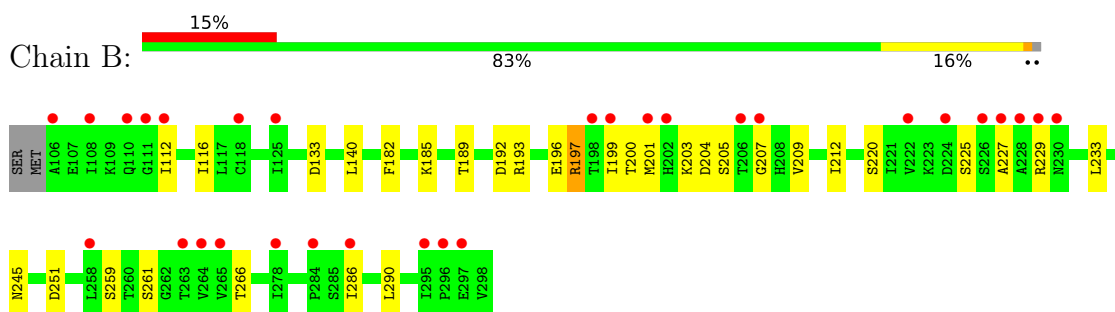
3 Residue-property plots [i](#)

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.

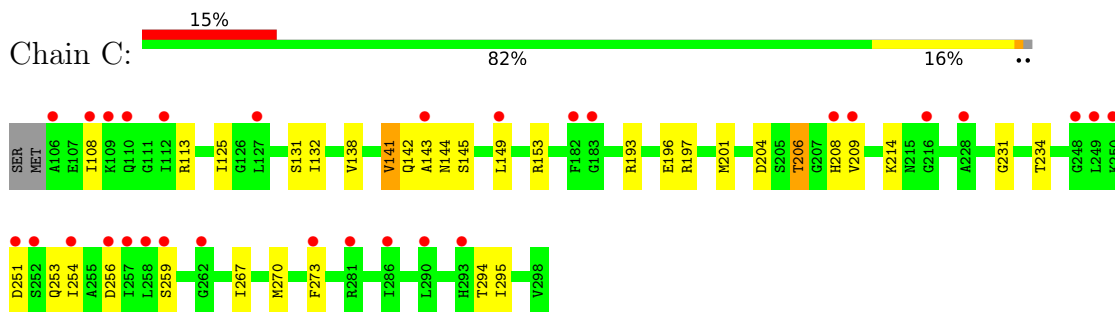
• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1

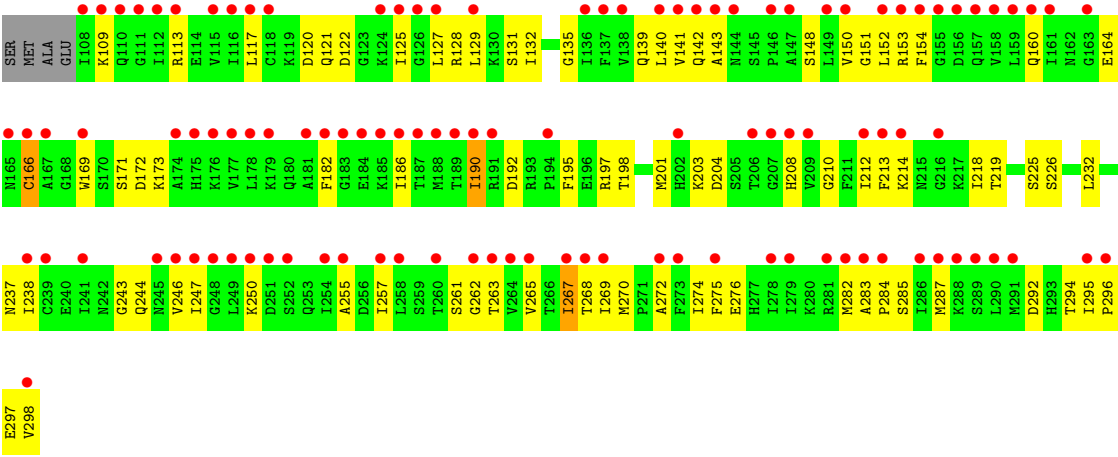


• Molecule 1: Syntenin-1



• 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	80.28Å 49.44Å 116.17Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	115.77 – 1.98 115.77 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.4 (115.77-1.98) 99.5 (115.77-1.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.268 , 0.343 0.275 , 0.345	Depositor DCC
R_{free} test set	3107 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6376	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.65 % 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 1.7756e-03. 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: EDO, DGL, SO4, Q6O

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	0.57	0/1502	1.08	3/2019 (0.1%)
1	B	0.58	0/1516	1.04	0/2038
1	C	0.57	0/1535	1.03	0/2063
1	D	0.63	0/1502	1.18	2/2019 (0.1%)
All	All	0.59	0/6055	1.08	5/8139 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	THR	CA-CB-OG1	-8.00	97.60	109.60
1	A	268	THR	CA-CB-OG1	-6.42	99.97	109.60
1	D	195	PHE	CB-CA-C	-5.96	100.50	110.81
1	A	266	THR	CA-CB-OG1	-5.51	101.33	109.60
1	D	182	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	GLY	Peptide
1	B	229	ARG	Sidechain
1	C	113	ARG	Sidechain
1	D	113	ARG	Sidechain
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	21	0
1	B	1495	0	1541	25	0
1	C	1514	0	1558	22	0
1	D	1481	0	1530	69	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	0	0
2	D	8	0	12	0	0
3	B	10	0	7	0	0
3	D	10	0	7	0	0
4	C	15	0	0	1	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	5	0	0	1	0
7	D	6	0	4	0	0
8	A	49	0	0	0	0
8	B	104	0	0	7	0
8	C	82	0	0	3	0
8	D	82	0	0	13	1
All	All	6376	0	6229	131	1

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 11.

All (131) 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:D:197:ARG:NH1	8:D:401:HOH:O	2.01	0.93
1:A:140:LEU:HD22	1:B:182:PHE:CE1	2.13	0.84
1:D:197:ARG:NH2	8:D:404:HOH:O	2.13	0.80
1:B:201:MET:SD	1:B:227:ALA:HA	2.21	0.80
1:D:270:MET:SD	1:D:275:PHE:HA	2.23	0.77
1:D:237:ASN:OD1	8:D:402:HOH:O	2.02	0.75
1:D:125:ILE:HD11	1:D:186:ILE:HD13	1.67	0.75
1:D:226:SER:OG	6:D:303:SO4:O2	2.03	0.74
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.71	0.72
1:D:204:ASP:OD2	8:D:403:HOH:O	2.07	0.71
1:D:139:GLN:HG2	1:D:282:MET:CE	2.22	0.69
1:B:196:GLU:OE1	8:B:401:HOH:O	2.10	0.69
1:D:131:SER:O	1:D:132:ILE:HD13	1.95	0.66
1:B:251:ASP:OD1	8:B:402:HOH:O	2.14	0.66
1:D:261:SER:OG	1:D:265:VAL:HG22	1.98	0.63
1:D:244:GLN:HE22	1:D:257:ILE:HD13	1.63	0.62
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.81	0.61
1:C:142:GLN:O	1:C:145:SER:OG	2.11	0.61
1:B:197:ARG:HH22	1:B:233:LEU:HD12	1.65	0.61
1:D:139:GLN:HG2	1:D:282:MET:HE2	1.83	0.61
1:D:287:MET:CE	8:D:481:HOH:O	2.48	0.61
1:D:152:LEU:CD2	1:D:190:ILE:HD12	2.31	0.59
1:B:203:LYS:NZ	1:B:259:SER:O	2.36	0.59
1:C:253:GLN:O	1:C:254:ILE:C	2.46	0.58
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.86	0.58
1:A:128:ARG:HG2	1:B:182:PHE:CZ	2.40	0.57
1:D:237:ASN:O	1:D:269:ILE:HA	2.05	0.56
1:A:210:GLY:HA3	1:A:225:SER:CB	2.36	0.56
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.87	0.56
1:B:204:ASP:HB2	8:B:453:HOH:O	2.04	0.56
1:D:203:LYS:NZ	1:D:261:SER:O	2.36	0.56
1:D:139:GLN:HG2	1:D:282:MET:HE1	1.88	0.55
1:D:203:LYS:HG3	1:D:263:THR:O	2.06	0.55
1:D:140:LEU:C	1:D:140:LEU:HD23	2.33	0.54
1:D:287:MET:HE1	8:D:481:HOH:O	2.08	0.54
1:D:255:ALA:O	8:D:405:HOH:O	2.18	0.54
1:D:140:LEU:HD23	1:D:141:VAL:C	2.34	0.53
1:D:212:ILE:O	1:D:219:THR:OG1	2.27	0.52
1:D:270:MET:SD	1:D:275:PHE:CA	2.96	0.52
1:D:218:ILE:HD13	1:D:232:LEU:HD11	1.90	0.52
1:D:250:LYS:HE2	8:D:456:HOH:O	2.09	0.52
1:D:143:ALA:HB2	1:D:292:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:MET:HE3	8:D:481:HOH:O	2.10	0.52
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.41	0.52
1:D:120:ASP:OD1	1:D:120:ASP:C	2.53	0.52
1:A:133:ASP:HB3	1:C:234:THR:O	2.10	0.51
1:A:117:LEU:CD1	1:A:188:MET:HE3	2.41	0.51
1:C:253:GLN:O	1:C:256:ASP:N	2.40	0.51
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.11	0.51
1:A:159:LEU:HD22	1:C:231:GLY:HA3	1.93	0.51
1:B:203:LYS:HB3	1:B:207:GLY:HA2	1.91	0.51
1:D:125:ILE:HD11	1:D:186:ILE:CD1	2.39	0.51
1:D:204:ASP:N	1:D:208:HIS:O	2.41	0.50
1:C:145:SER:O	1:C:149:LEU:HG	2.10	0.50
1:D:172:ASP:O	1:D:173:LYS:C	2.54	0.50
1:D:283:ALA:O	1:D:284:PRO:C	2.53	0.50
1:C:193:ARG:HB3	1:C:196:GLU:CG	2.42	0.49
1:D:204:ASP:OD1	1:D:204:ASP:C	2.56	0.49
1:B:261:SER:HB2	8:B:477:HOH:O	2.12	0.49
1:D:197:ARG:O	1:D:268:THR:HA	2.13	0.49
1:A:240:GLU:HB2	1:A:268:THR:HB	1.94	0.48
1:B:116:ILE:HG23	1:B:185:LYS:HG3	1.93	0.48
1:A:128:ARG:HG2	1:B:182:PHE:CE1	2.48	0.48
1:C:153:ARG:HD3	8:C:401:HOH:O	2.13	0.48
1:D:218:ILE:CD1	1:D:232:LEU:HD11	2.44	0.48
1:D:272:ALA:O	1:D:276:GLU:HG2	2.14	0.48
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.94	0.48
1:D:295:ILE:HD11	1:D:298:VAL:HG12	1.96	0.48
1:D:197:ARG:HB3	8:D:434:HOH:O	2.14	0.48
1:B:204:ASP:O	1:B:207:GLY:N	2.45	0.48
1:B:192:ASP:O	1:B:193:ARG:C	2.57	0.47
1:C:108:ILE:HD13	1:C:197[B]:ARG:HA	1.97	0.47
1:D:152:LEU:HD22	1:D:190:ILE:HD12	1.96	0.47
1:D:203:LYS:HD2	1:D:262:GLY:O	2.13	0.47
1:A:117:LEU:HD13	1:A:188:MET:HE3	1.96	0.47
1:D:139:GLN:CG	1:D:282:MET:HE2	2.43	0.47
1:D:274:ILE:O	1:D:275:PHE:C	2.56	0.47
1:A:250:LYS:HB2	1:A:253:GLN:HG3	1.97	0.47
1:B:133:ASP:OD1	8:B:405:HOH:O	2.20	0.47
1:D:164:GLU:HB2	8:D:409:HOH:O	2.14	0.46
1:D:117:LEU:HD12	1:D:117:LEU:N	2.30	0.46
1:C:201:MET:HE1	1:C:267:ILE:HG12	1.97	0.46
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:MET:HE3	1:D:201:MET:HB2	1.88	0.46
1:B:209:VAL:O	1:B:225:SER:HB2	2.15	0.46
1:C:214:LYS:HA	1:C:251:ASP:OD2	2.17	0.45
1:A:282:MET:HE3	1:A:287:MET:SD	2.57	0.45
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.46	0.44
1:C:138:VAL:HG11	1:C:141:VAL:HG22	1.99	0.44
1:D:150:VAL:HG12	8:D:478:HOH:O	2.16	0.44
1:D:213:PHE:C	8:D:417:HOH:O	2.59	0.44
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.98	0.44
1:A:115:VAL:HG22	1:A:188:MET:HB2	1.99	0.44
1:C:253:GLN:NE2	4:C:301:Q6O:CL	2.87	0.44
1:A:250:LYS:O	1:A:254:ILE:HG13	2.17	0.44
1:B:245:ASN:OD1	1:B:245:ASN:C	2.60	0.44
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.98	0.44
1:C:143:ALA:O	1:C:144[A]:ASN:HB2	2.18	0.43
1:D:203:LYS:HA	1:D:208:HIS:O	2.18	0.43
1:D:218:ILE:HD13	1:D:232:LEU:HD21	2.00	0.43
1:D:127:LEU:HD21	1:D:152:LEU:CD1	2.48	0.43
1:D:244:GLN:O	1:D:246:VAL:HG13	2.19	0.43
1:B:200:THR:N	8:B:404:HOH:O	2.18	0.43
1:B:212:ILE:HB	1:B:220:SER:HB3	2.01	0.43
1:C:131:SER:C	1:C:132:ILE:HG12	2.44	0.43
1:C:294:THR:HG22	1:C:295:ILE:N	2.34	0.43
1:C:125:ILE:O	1:C:145:SER:HB2	2.19	0.43
1:C:153:ARG:CD	8:C:401:HOH:O	2.65	0.42
1:A:157:GLN:HG2	1:A:159:LEU:HD23	2.01	0.42
1:D:121:GLN:HE21	1:D:122:ASP:CG	2.27	0.42
1:A:240:GLU:HA	1:A:244:GLN:O	2.19	0.42
1:C:294:THR:CG2	1:C:295:ILE:N	2.82	0.42
1:D:198:THR:HG22	1:D:268:THR:OG1	2.20	0.42
1:D:238:ILE:HG12	1:D:267:ILE:HD12	2.02	0.42
1:B:261:SER:CB	8:B:477:HOH:O	2.66	0.42
1:C:273[A]:PHE:HD1	8:C:454:HOH:O	2.01	0.42
1:B:204:ASP:O	1:B:205:SER:C	2.63	0.42
1:D:128:ARG:O	1:D:129:LEU:HD23	2.20	0.42
1:D:166:CYS:HA	1:D:169:TRP:CE2	2.55	0.42
1:D:121:GLN:NE2	1:D:122:ASP:OD2	2.53	0.41
1:C:201:MET:CE	1:C:267:ILE:HG12	2.49	0.41
1:D:153:ARG:NH1	1:D:243:GLY:O	2.54	0.41
1:A:115:VAL:CG2	1:A:188:MET:HB2	2.51	0.41
1:D:131:SER:HA	1:D:135:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLN:HG2	1:D:143:ALA:O	2.21	0.41
1:A:108:ILE:HA	1:A:192:ASP:OD2	2.21	0.41
1:B:199:ILE:O	1:B:266:THR:HA	2.21	0.41
1:D:109:LYS:N	1:D:192:ASP:OD2	2.49	0.40
1:D:261:SER:CB	1:D:265:VAL:HG22	2.50	0.40
1:D:148:SER:O	1:D:151:GLY:N	2.49	0.40
1:D:117:LEU:HG	1:D:150:VAL:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:472:HOH:O	8:D:479:HOH:O[2_555]	2.08	0.12

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%)	183 (96%)	7 (4%)	0	100	100
1	B	192/195 (98%)	181 (94%)	11 (6%)	0	100	100
1	C	194/195 (100%)	183 (94%)	10 (5%)	1 (0%)	24	14
1	D	190/195 (97%)	176 (93%)	14 (7%)	0	100	100
All	All	766/780 (98%)	723 (94%)	42 (6%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	204	ASP

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%)	159 (96%)	7 (4%)	26	15
1	B	167/168 (99%)	165 (99%)	2 (1%)	63	58
1	C	169/168 (101%)	164 (97%)	5 (3%)	36	27
1	D	166/168 (99%)	159 (96%)	7 (4%)	26	15
All	All	668/672 (99%)	647 (97%)	21 (3%)	34	26

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	124	LYS
1	A	131	SER
1	A	171	SER
1	A	220	SER
1	A	266	THR
1	A	280	LYS
1	B	140	LEU
1	B	197	ARG
1	C	141	VAL
1	C	206	THR
1	C	209	VAL
1	C	259	SER
1	C	270	MET
1	D	166	CYS
1	D	171	SER
1	D	190	ILE
1	D	214	LYS
1	D	267	ILE
1	D	285	SER
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	B	157	GLN
1	B	160	GLN
1	B	165	ASN
1	B	202	HIS
1	B	215	ASN
1	C	215	ASN
1	D	121	GLN
1	D	134	ASN
1	D	215	ASN
1	D	244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	D	302	-	3,3,3	0.09	0	2,2,2	0.13	0
4	Q6O	C	301	-	15,15,15	2.12	4 (26%)	20,20,20	1.42	4 (20%)
2	EDO	C	304	-	3,3,3	0.27	0	2,2,2	0.50	0
5	GLY	D	306	-	4,4,4	1.08	0	3,4,4	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ALA	D	304	-	5,5,5	0.91	0	6,6,6	0.92	0
2	EDO	B	301	-	3,3,3	0.38	0	2,2,2	0.03	0
2	EDO	D	301	-	3,3,3	0.25	0	2,2,2	0.27	0
6	SO4	D	303	-	4,4,4	0.25	0	6,6,6	0.09	0
2	EDO	C	302	-	3,3,3	0.37	0	2,2,2	0.16	0
2	EDO	A	301	-	3,3,3	0.12	0	2,2,2	0.03	0
3	DGL	B	303	-	8,9,9	0.97	0	8,11,11	1.04	0
2	EDO	B	302	-	3,3,3	0.30	0	2,2,2	0.52	0
2	EDO	C	303	-	3,3,3	0.23	0	2,2,2	0.13	0
3	DGL	D	305	-	8,9,9	0.99	0	8,11,11	0.92	0
5	GLY	C	305	-	4,4,4	0.92	0	3,4,4	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	302	-	-	1/1/1/1	-
4	Q6O	C	301	-	-	0/8/8/8	0/1/1/1
2	EDO	C	304	-	-	1/1/1/1	-
5	GLY	D	306	-	-	2/2/2/2	-
7	ALA	D	304	-	-	4/4/4/4	-
2	EDO	B	301	-	-	1/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
3	DGL	B	303	-	-	0/9/9/9	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
3	DGL	D	305	-	-	1/9/9/9	-
5	GLY	C	305	-	-	2/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	Q6O	C4-N	5.33	1.46	1.36
4	C	301	Q6O	O2-C6	3.16	1.42	1.37
4	C	301	Q6O	C9-CL	2.99	1.80	1.73
4	C	301	Q6O	C3-N	2.42	1.46	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	Q6O	O2-C6-C3	3.84	119.59	114.81
4	C	301	Q6O	C1-C9-CL	2.38	122.16	119.44
4	C	301	Q6O	C7-O2-C6	2.37	120.98	117.51
4	C	301	Q6O	O2-C6-C8	-2.00	120.63	124.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	GLY	OXT-C-CA-N
5	C	305	GLY	O-C-CA-N
5	D	306	GLY	O-C-CA-N
5	D	306	GLY	OXT-C-CA-N
7	D	304	ALA	O-C-CA-CB
7	D	304	ALA	OXT-C-CA-CB
2	B	301	EDO	O1-C1-C2-O2
7	D	304	ALA	O-C-CA-N
7	D	304	ALA	OXT-C-CA-N
2	C	303	EDO	O1-C1-C2-O2
2	C	304	EDO	O1-C1-C2-O2
3	D	305	DGL	O-C-CA-N
2	C	302	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2

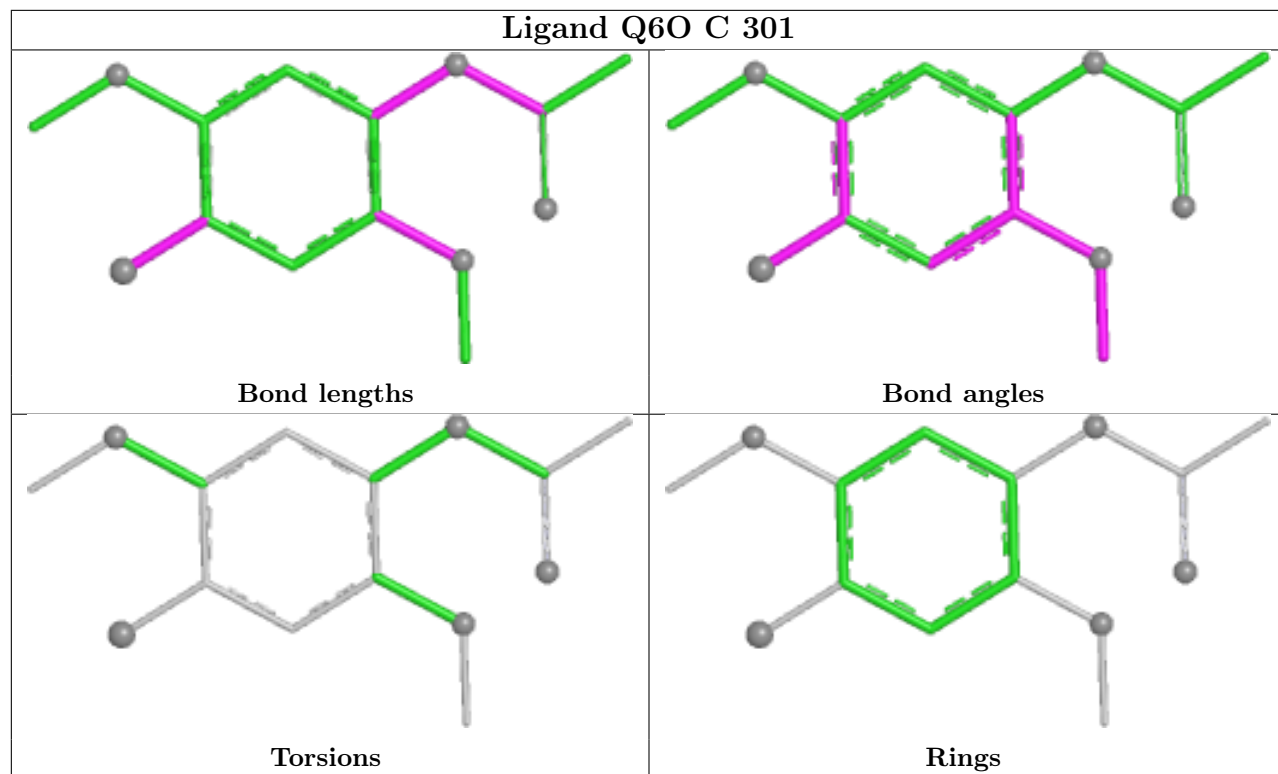
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	Q6O	1	0
6	D	303	SO4	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 [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	191/195 (97%)	1.09	32 (16%) 4 5	13, 42, 69, 96	1 (0%)
1	B	193/195 (98%)	1.05	30 (15%) 5 6	14, 42, 62, 71	1 (0%)
1	C	193/195 (98%)	1.16	30 (15%) 5 6	15, 42, 65, 78	3 (1%)
1	D	191/195 (97%)	2.41	110 (57%) 0 0	18, 48, 72, 104	1 (0%)
All	All	768/780 (98%)	1.43	202 (26%) 1 1	13, 44, 66, 104	6 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	PHE	8.0
1	D	125	ILE	6.9
1	D	117	LEU	6.5
1	D	116	ILE	6.4
1	A	182	PHE	6.3
1	D	238	ILE	5.9
1	B	106	ALA	5.4
1	B	264	VAL	5.4
1	D	108	ILE	5.0
1	D	138	VAL	4.9
1	D	177	VAL	4.8
1	D	190	ILE	4.8
1	D	178	LEU	4.8
1	D	189	THR	4.8
1	C	110	GLN	4.7
1	C	106	ALA	4.6
1	D	265	VAL	4.6
1	C	109	LYS	4.6
1	D	254	ILE	4.6
1	A	282	MET	4.6
1	D	273[A]	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	267	ILE	4.5
1	D	141	VAL	4.4
1	D	241	ILE	4.4
1	D	268	THR	4.3
1	D	150	VAL	4.3
1	D	284	PRO	4.3
1	B	199	ILE	4.2
1	D	161	ILE	4.2
1	D	152	LEU	4.1
1	D	112	ILE	4.1
1	A	108	ILE	4.0
1	D	216	GLY	4.0
1	A	263	THR	4.0
1	A	109	LYS	3.9
1	D	127	LEU	3.9
1	D	111	GLY	3.9
1	D	269	ILE	3.9
1	D	149	LEU	3.8
1	D	263	THR	3.8
1	C	249	LEU	3.8
1	D	158	VAL	3.8
1	D	248	GLY	3.7
1	D	288	LYS	3.7
1	D	286	ILE	3.7
1	B	202	HIS	3.7
1	D	186	ILE	3.7
1	B	230	ASN	3.6
1	D	249	LEU	3.6
1	C	108	ILE	3.6
1	D	159	LEU	3.6
1	A	264	VAL	3.6
1	D	115	VAL	3.6
1	D	143	ALA	3.5
1	D	118	CYS	3.5
1	D	154	PHE	3.5
1	C	112	ILE	3.5
1	D	279	ILE	3.5
1	D	147	ALA	3.4
1	D	283	ALA	3.4
1	D	169	TRP	3.4
1	D	298	VAL	3.4
1	A	290	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	209	VAL	3.3
1	D	155	GLY	3.3
1	D	174	ALA	3.3
1	D	179	LYS	3.3
1	D	140	LEU	3.3
1	A	186	ILE	3.3
1	D	255	ALA	3.2
1	A	286	ILE	3.2
1	D	181	ALA	3.2
1	D	142	GLN	3.2
1	D	163	GLY	3.2
1	B	118	CYS	3.2
1	D	144	ASN	3.1
1	C	258	LEU	3.1
1	D	187	THR	3.1
1	B	108	ILE	3.1
1	D	295	ILE	3.1
1	D	290	LEU	3.0
1	B	265	VAL	3.0
1	D	213	PHE	3.0
1	D	194	PRO	3.0
1	A	283	ALA	3.0
1	B	295	ILE	3.0
1	D	165	ASN	3.0
1	D	258	LEU	2.9
1	D	239	CYS	2.9
1	B	111	GLY	2.9
1	D	109	LYS	2.9
1	D	207	GLY	2.9
1	B	227	ALA	2.8
1	B	226	SER	2.8
1	D	160	GLN	2.8
1	C	257	ILE	2.8
1	A	284	PRO	2.8
1	C	281	ARG	2.7
1	D	137	PHE	2.7
1	D	262	GLY	2.7
1	D	136	ILE	2.7
1	D	247	ILE	2.7
1	D	246	VAL	2.7
1	D	250	LYS	2.7
1	A	243	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	PHE	2.7
1	C	209	VAL	2.7
1	D	202	HIS	2.7
1	A	183	GLY	2.7
1	D	126	GLY	2.7
1	D	206	THR	2.7
1	A	209	VAL	2.7
1	D	264	VAL	2.7
1	D	287	MET	2.6
1	D	146	PRO	2.6
1	B	125	ILE	2.6
1	D	212	ILE	2.6
1	C	252	SER	2.6
1	C	208	HIS	2.6
1	D	175	HIS	2.6
1	A	184	GLU	2.6
1	B	286	ILE	2.6
1	A	202	HIS	2.5
1	A	273[A]	PHE	2.5
1	D	110	GLN	2.5
1	C	254	ILE	2.5
1	D	257	ILE	2.5
1	D	282	MET	2.5
1	C	149	LEU	2.5
1	B	112	ILE	2.5
1	D	167	ALA	2.5
1	D	157	GLN	2.5
1	D	153	ARG	2.5
1	C	228	ALA	2.5
1	C	262	GLY	2.4
1	D	281	ARG	2.4
1	A	117	LEU	2.4
1	B	258	LEU	2.4
1	D	275	PHE	2.4
1	D	260	THR	2.4
1	D	183	GLY	2.4
1	B	201	MET	2.4
1	C	273[A]	PHE	2.4
1	A	125	ILE	2.4
1	A	262	GLY	2.4
1	C	183	GLY	2.4
1	A	149	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	251	ASP	2.4
1	B	297	GLU	2.4
1	D	208	HIS	2.4
1	D	113	ARG	2.3
1	B	198	THR	2.3
1	A	180	GLN	2.3
1	B	296	PRO	2.3
1	B	222	VAL	2.3
1	D	252	SER	2.3
1	D	245	ASN	2.3
1	C	286	ILE	2.3
1	C	248	GLY	2.3
1	D	191	ARG	2.3
1	A	110	GLN	2.3
1	A	178	LEU	2.3
1	A	258	LEU	2.3
1	D	251	ASP	2.2
1	D	214	LYS	2.2
1	D	291	MET	2.2
1	A	140	LEU	2.2
1	C	250	LYS	2.2
1	D	185	LYS	2.2
1	B	229	ARG	2.2
1	A	265	VAL	2.2
1	D	184	GLU	2.2
1	D	166	CYS	2.2
1	D	129	LEU	2.2
1	C	259	SER	2.2
1	B	206	THR	2.2
1	B	224	ASP	2.2
1	D	156	ASP	2.2
1	D	296	PRO	2.2
1	B	228	ALA	2.2
1	D	176	LYS	2.2
1	D	188	MET	2.1
1	D	278	ILE	2.1
1	A	260	THR	2.1
1	B	284	PRO	2.1
1	D	124	LYS	2.1
1	A	112	ILE	2.1
1	A	187	THR	2.1
1	B	263	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	2.1
1	C	290	LEU	2.1
1	B	110	GLN	2.1
1	B	278	ILE	2.1
1	D	289	SER	2.1
1	C	127	LEU	2.1
1	C	143	ALA	2.1
1	A	287	MET	2.0
1	D	272	ALA	2.0
1	C	256	ASP	2.0
1	C	293	HIS	2.0
1	A	111	GLY	2.0
1	C	216	GLY	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(Å ²)	Q<0.9
3	DGL	D	305	10/10	0.66	0.21	53,76,86,87	0
2	EDO	C	302	4/4	0.69	0.18	39,40,40,44	0
7	ALA	D	304	6/6	0.72	0.22	68,79,82,85	0
3	DGL	B	303	10/10	0.78	0.14	45,57,63,66	0
5	GLY	C	305	5/5	0.79	0.15	52,60,68,76	0
6	SO4	D	303	5/5	0.80	0.12	59,67,70,73	0
4	Q6O	C	301	15/15	0.82	0.14	47,53,61,66	0
5	GLY	D	306	5/5	0.82	0.14	53,54,57,59	0
2	EDO	C	304	4/4	0.85	0.22	53,53,54,55	0
2	EDO	D	302	4/4	0.89	0.12	40,45,48,49	0

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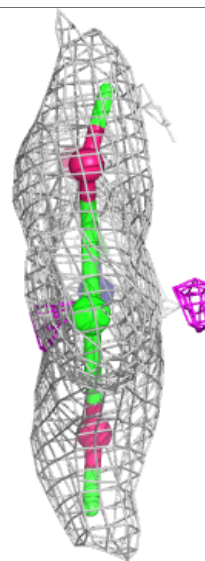
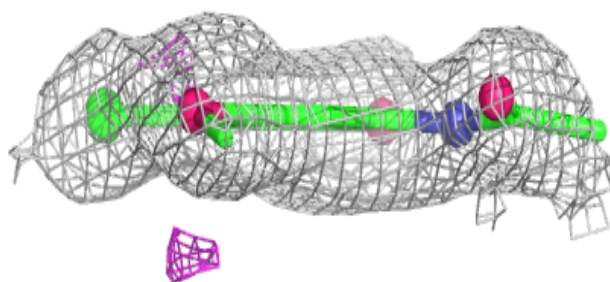
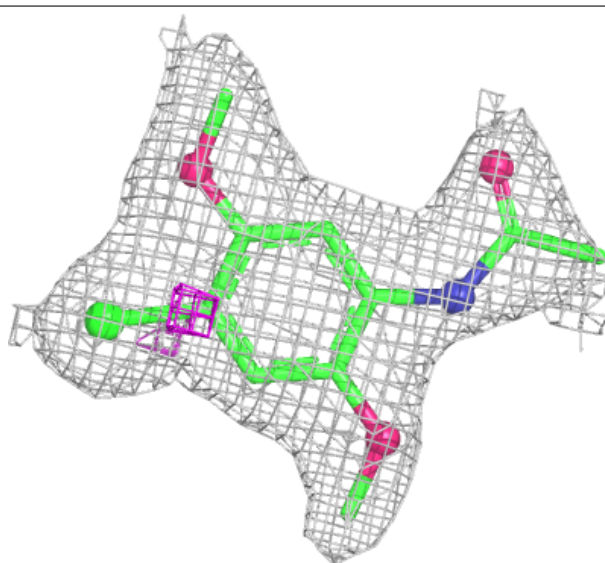
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	301	4/4	0.90	0.11	32,33,34,36	0
2	EDO	C	303	4/4	0.91	0.11	35,38,42,42	0
2	EDO	D	301	4/4	0.91	0.11	32,35,37,41	0
2	EDO	A	301	4/4	0.93	0.10	36,37,38,40	0
2	EDO	B	302	4/4	0.94	0.08	33,36,39,40	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 Q6O 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 [i](#)

There are no such residues in this entry.