



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:00 AM UTC

PDB ID : 7FSQ / pdb_00007fsq
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z1429867185
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.07 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

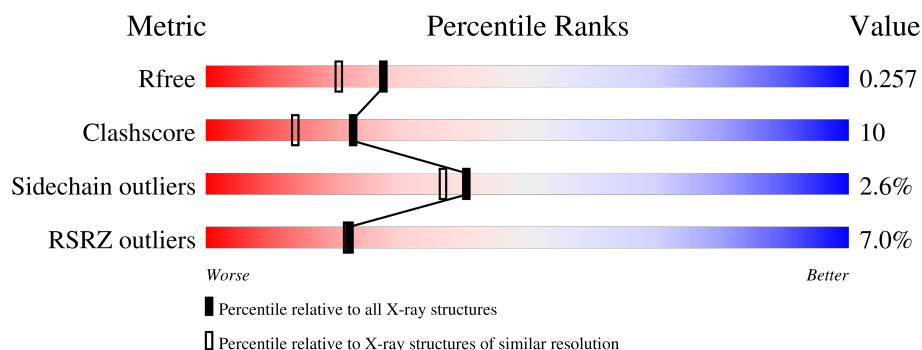
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	4% 79% 17% ..
1	B	195	2% 84% 15% .
1	C	195	5% 72% 26% ..
1	D	195	17% 68% 28% ..

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
2	VVP	A	401	-	X	-	-
6	SO4	D	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6381 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.

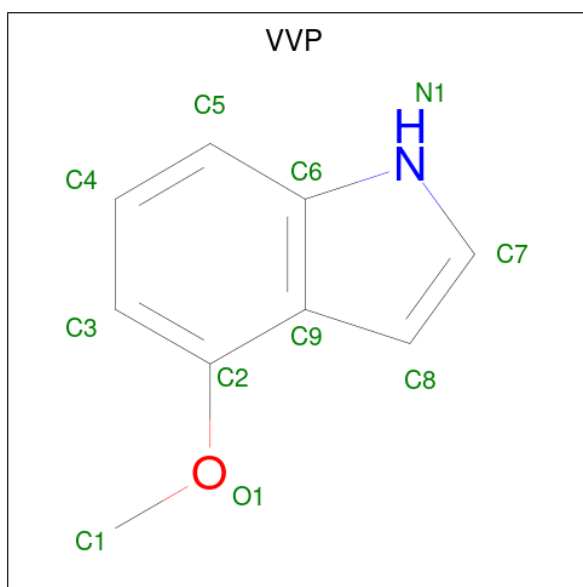
- Molecule 1 is a protein called Syntenin-1.

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:

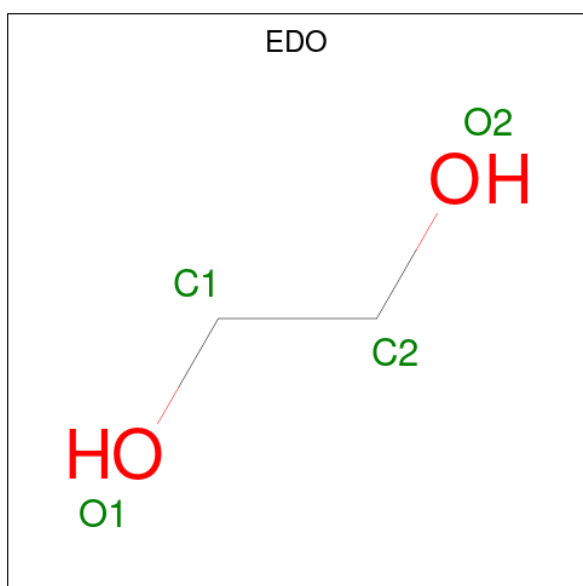
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

- Molecule 2 is 4-methoxy-1H-indole (CCD ID: VVP) (formula: C₉H₉NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



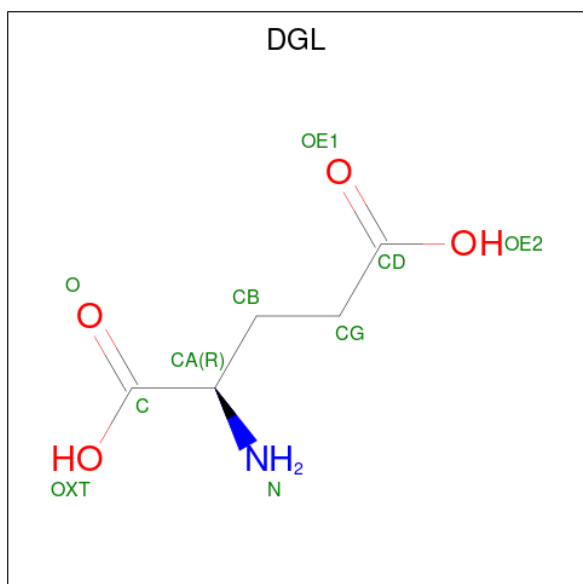
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

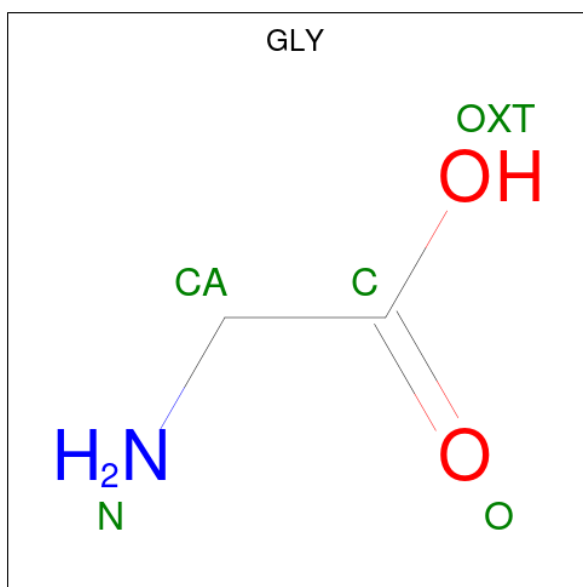
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



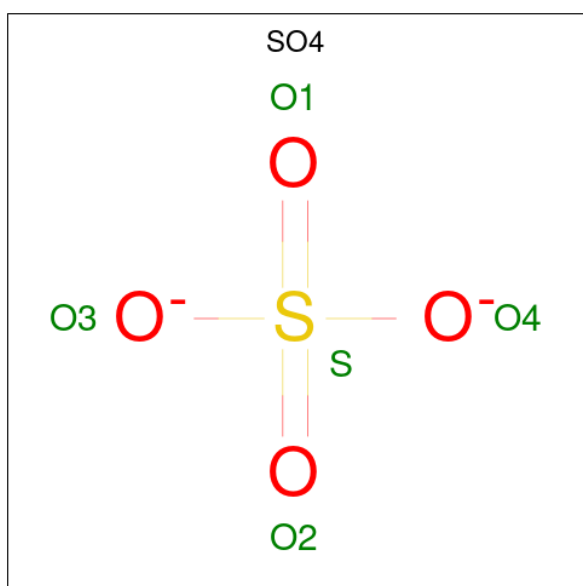
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

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



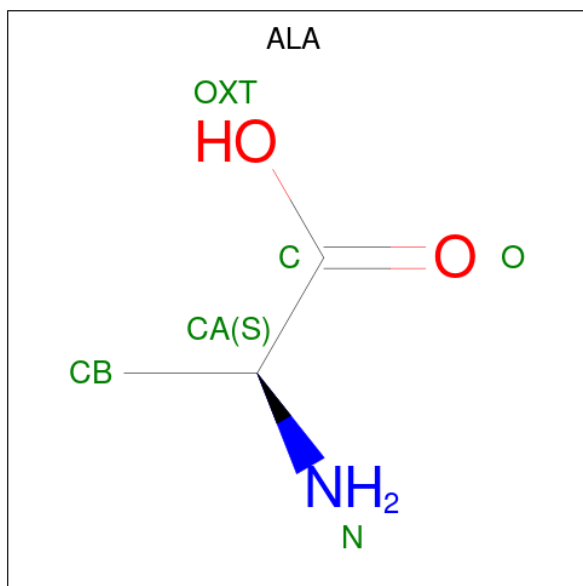
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- 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		

- 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		

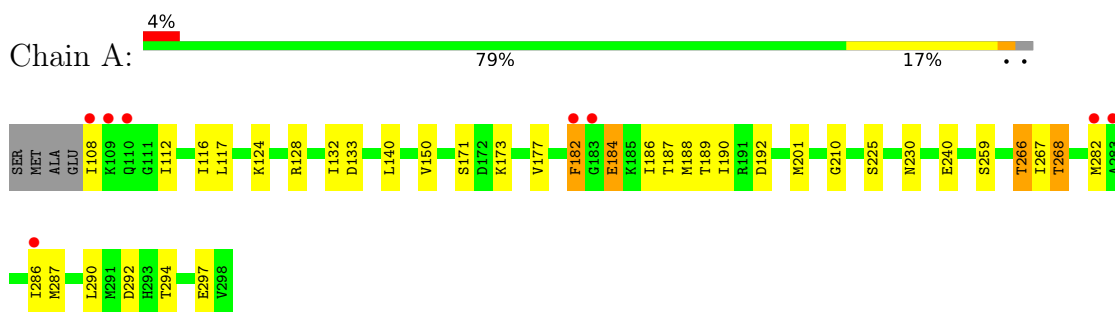
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	52	Total	O	0	0
			52	52		
8	B	100	Total	O	0	0
			100	100		
8	C	75	Total	O	0	1
			76	76		
8	D	82	Total	O	0	0
			82	82		

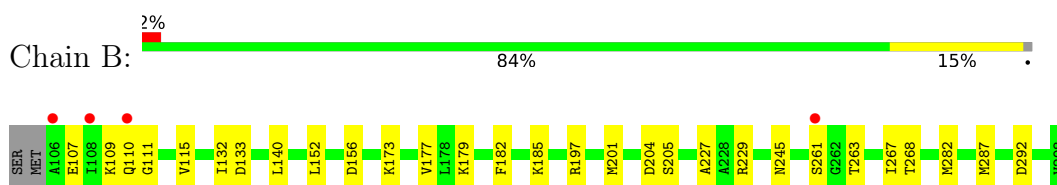
3 Residue-property plots [i](#)

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.

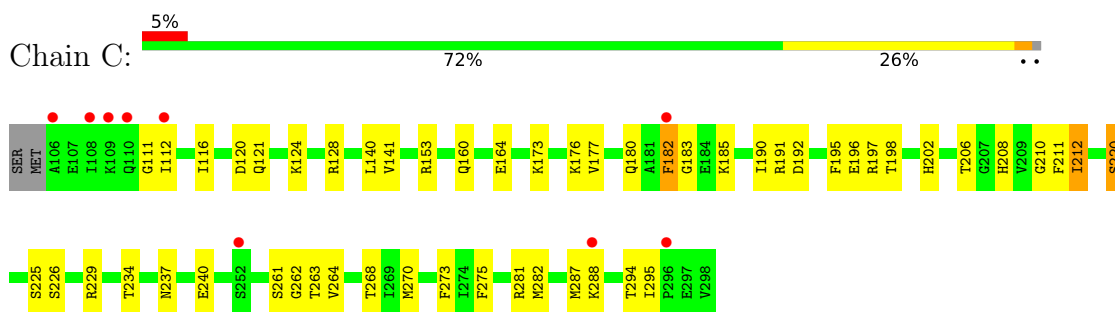
• Molecule 1: Syntenin-1



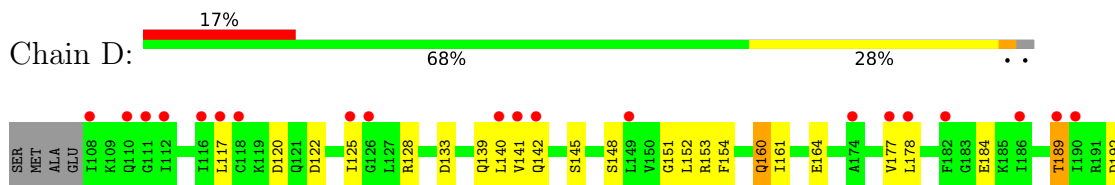
• Molecule 1: Syntenin-1

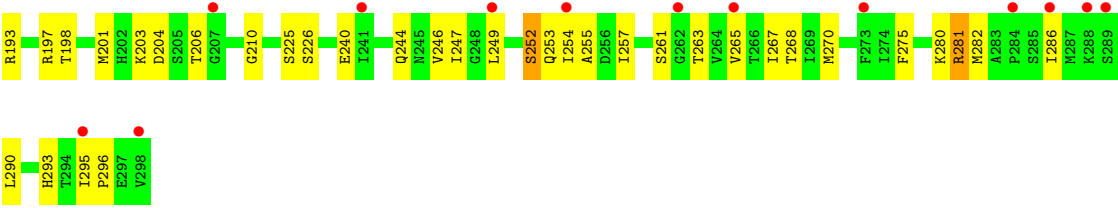


• Molecule 1: Syntenin-1



• 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	80.33Å 49.62Å 115.94Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	68.58 – 2.07 68.58 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.58-2.07) 99.8 (68.58-2.07)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.229 , 0.301 (Not available) , 0.257	Depositor DCC
R_{free} test set	2659 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6381	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 29.39 % 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 1.5627e-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: DGL, SO4, VVP, EDO

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	0.61	0/1502	1.15	4/2019 (0.2%)
1	B	0.62	0/1516	1.12	4/2038 (0.2%)
1	C	0.61	0/1535	1.09	1/2063 (0.0%)
1	D	0.64	0/1502	1.19	1/2019 (0.0%)
All	All	0.62	0/6055	1.14	10/8139 (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	B	0	1
1	C	0	2
1	D	0	3
All	All	0	6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	THR	CA-CB-OG1	-10.19	94.32	109.60
1	A	268	THR	CA-CB-OG1	-7.39	98.51	109.60
1	B	292	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	189	THR	CA-CB-OG1	-7.06	99.01	109.60
1	B	156	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	204	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	184	GLU	CB-CG-CD	5.19	121.42	112.60
1	C	182	PHE	CB-CA-C	5.17	119.83	111.26
1	B	263	THR	CA-CB-OG1	-5.12	101.93	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	THR	CB-CA-C	5.07	118.10	109.53

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	GLY	Peptide
1	C	111	GLY	Peptide
1	C	281	ARG	Sidechain
1	D	128	ARG	Sidechain
1	D	160	GLN	Peptide
1	D	281	ARG	Sidechain

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	24	0
1	B	1495	0	1541	17	0
1	C	1514	0	1558	36	0
1	D	1481	0	1530	56	0
2	A	11	0	0	0	0
2	B	11	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	1	0
6	D	10	0	0	2	0
7	D	6	0	4	0	0
8	A	52	0	0	1	0
8	B	100	0	0	4	0
8	C	76	0	0	6	0
8	D	82	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6381	0	6229	128	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 10.

All (128) 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:A:286:ILE:HG23	1:A:290:LEU:HD12	1.48	0.94
1:C:182:PHE:O	1:C:183:GLY:O	2.00	0.79
1:D:197:ARG:NH2	8:D:404:HOH:O	2.16	0.78
1:D:197:ARG:NH1	8:D:405:HOH:O	2.18	0.76
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.18	0.75
1:D:255:ALA:O	8:D:401:HOH:O	2.04	0.75
1:D:203:LYS:HD2	1:D:263:THR:HA	1.70	0.74
1:D:206:THR:HG22	1:D:206:THR:O	1.88	0.72
1:A:140:LEU:HD22	1:B:182:PHE:CE1	2.27	0.70
1:D:198:THR:HG22	1:D:268:THR:OG1	1.92	0.69
1:D:152:LEU:O	8:D:402:HOH:O	2.11	0.69
1:A:173:LYS:O	1:A:177:VAL:HG23	1.92	0.67
1:D:293:HIS:NE2	8:D:407:HOH:O	2.27	0.67
1:C:192:ASP:OD1	8:C:402:HOH:O	2.14	0.65
1:B:177:VAL:O	8:B:401:HOH:O	2.14	0.65
1:C:211:PHE:C	1:C:212:ILE:HD12	2.21	0.65
1:D:204:ASP:OD2	8:D:403:HOH:O	2.14	0.65
1:C:212:ILE:HD12	1:C:212:ILE:N	2.12	0.64
1:D:226:SER:OG	6:D:303:SO4:O2	2.15	0.64
1:C:121:GLN:CD	1:C:121:GLN:H	2.05	0.64
1:A:116:ILE:CD1	1:A:187:THR:HG22	2.29	0.63
1:A:240:GLU:HB2	1:A:268:THR:HB	1.81	0.62
1:A:282:MET:HE3	1:A:287:MET:CG	2.31	0.61
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.82	0.60
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.37	0.60
1:D:139:GLN:O	1:D:282:MET:HE1	2.04	0.58
1:A:117:LEU:HD22	1:A:188:MET:HE3	1.85	0.58
1:D:203:LYS:NZ	1:D:261:SER:O	2.33	0.57
1:C:198:THR:HG22	1:C:268:THR:OG1	2.05	0.57
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.88	0.57
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.22	0.57
1:B:173:LYS:O	1:B:177:VAL:HG23	2.05	0.56
1:D:161:ILE:O	1:D:164:GLU:N	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HA	1:A:192:ASP:OD2	2.06	0.55
1:D:244:GLN:O	1:D:246:VAL:HG13	2.07	0.55
1:C:116:ILE:HG23	1:C:185:LYS:HD2	1.88	0.54
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.07	0.54
1:D:140:LEU:C	1:D:140:LEU:HD23	2.33	0.54
1:D:133:ASP:OD1	3:D:302:EDO:O1	2.26	0.54
1:D:153:ARG:HG2	8:D:437:HOH:O	2.08	0.53
1:D:261:SER:CB	1:D:265:VAL:HG22	2.38	0.53
1:D:253:GLN:O	1:D:257:ILE:HG13	2.08	0.53
1:A:116:ILE:HD12	1:A:187:THR:HG22	1.90	0.52
1:C:202:HIS:CD2	1:C:264:VAL:HG22	2.43	0.52
1:C:273[A]:PHE:HD1	8:C:445:HOH:O	1.91	0.52
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.91	0.52
1:D:140:LEU:HD23	1:D:141:VAL:C	2.35	0.52
1:C:240:GLU:HB2	1:C:268:THR:HB	1.92	0.51
1:D:198:THR:HA	1:D:267:ILE:O	2.09	0.51
1:C:120:ASP:OD2	8:C:403:HOH:O	2.19	0.51
1:C:282:MET:HE3	1:C:287:MET:HB2	1.92	0.51
1:B:115:VAL:HG21	1:B:152:LEU:HD21	1.91	0.51
1:D:252:SER:O	1:D:255:ALA:HB3	2.10	0.51
1:D:206:THR:O	1:D:206:THR:CG2	2.56	0.50
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.93	0.49
1:D:140:LEU:HD23	1:D:141:VAL:N	2.27	0.49
1:D:154:PHE:CE1	1:D:247:ILE:CD1	2.95	0.49
1:D:240:GLU:HB2	1:D:268:THR:HB	1.94	0.49
1:C:153:ARG:HD3	8:C:409:HOH:O	2.13	0.49
1:B:110:GLN:NE2	8:B:414:HOH:O	2.46	0.49
1:D:226:SER:CB	6:D:303:SO4:O2	2.61	0.49
1:C:176:LYS:O	1:C:180:GLN:HG3	2.13	0.48
1:C:212:ILE:N	1:C:212:ILE:CD1	2.77	0.48
1:D:261:SER:HB3	1:D:265:VAL:HG22	1.96	0.48
1:A:282:MET:HE3	1:A:287:MET:HG3	1.96	0.47
1:A:133:ASP:HB3	1:C:234:THR:O	2.15	0.47
1:A:117:LEU:HD13	1:A:150:VAL:HG21	1.97	0.47
1:D:249:LEU:HD21	1:D:293:HIS:CD2	2.50	0.47
1:D:203:LYS:HG3	1:D:263:THR:O	2.16	0.46
1:B:229:ARG:NH1	8:B:405:HOH:O	2.34	0.46
1:B:282:MET:HE3	1:B:287:MET:HB2	1.97	0.46
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.97	0.46
1:D:192:ASP:O	1:D:193:ARG:C	2.58	0.46
1:C:195:PHE:HB2	1:C:270:MET:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LYS:O	1:C:177:VAL:HG23	2.16	0.46
1:D:192:ASP:CG	1:D:193:ARG:HH21	2.23	0.46
5:D:307:GLY:N	8:D:418:HOH:O	2.49	0.45
1:C:206:THR:HG1	1:C:208:HIS:CE1	2.34	0.45
1:C:206:THR:OG1	1:C:208:HIS:CE1	2.69	0.45
1:C:212:ILE:HD13	1:C:220:SER:HB2	1.99	0.45
1:D:151:GLY:C	8:D:402:HOH:O	2.59	0.44
1:D:151:GLY:HA2	8:D:402:HOH:O	2.16	0.44
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.52	0.44
1:D:117:LEU:HD22	1:D:125:ILE:HB	1.99	0.44
1:A:182:PHE:CD1	1:A:182:PHE:N	2.85	0.44
1:A:116:ILE:HD13	1:A:187:THR:HG22	1.98	0.43
1:A:124:LYS:HD3	1:B:185:LYS:HB3	2.00	0.43
1:D:139:GLN:HG2	1:D:282:MET:CE	2.48	0.43
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.99	0.43
1:D:286:ILE:HG23	1:D:290:LEU:HD12	1.99	0.43
1:C:128:ARG:HD3	1:C:140:LEU:HD22	2.01	0.43
1:D:148:SER:O	1:D:151:GLY:N	2.43	0.43
1:C:182:PHE:O	1:C:183:GLY:C	2.61	0.42
1:C:210:GLY:HA3	1:C:225:SER:CB	2.49	0.42
1:C:261:SER:OG	1:C:262:GLY:N	2.51	0.42
1:B:201:MET:SD	1:B:227:ALA:HA	2.60	0.42
1:C:202:HIS:HA	1:C:263:THR:O	2.19	0.42
1:D:254:ILE:O	1:D:255:ALA:C	2.63	0.42
1:B:197:ARG:O	1:B:268:THR:HA	2.20	0.42
1:D:270:MET:SD	1:D:275:PHE:HA	2.59	0.42
1:D:280:LYS:O	1:D:281:ARG:HB2	2.19	0.42
1:A:210:GLY:HA3	1:A:225:SER:CB	2.49	0.42
1:C:124:LYS:HB3	8:C:459:HOH:O	2.19	0.42
1:C:229:ARG:NH2	8:C:407:HOH:O	2.53	0.42
1:D:142:GLN:O	1:D:145:SER:OG	2.37	0.41
1:D:201:MET:HE3	1:D:201:MET:HB2	1.96	0.41
1:A:128:ARG:HG2	1:B:182:PHE:CZ	2.55	0.41
1:C:226:SER:HA	1:C:229:ARG:NH2	2.35	0.41
1:C:294:THR:HG22	1:C:295:ILE:C	2.46	0.41
1:D:203:LYS:HE3	1:D:265:VAL:CG2	2.50	0.41
1:D:244:GLN:NE2	1:D:257:ILE:HD13	2.35	0.41
1:C:160:GLN:HA	1:C:164:GLU:O	2.20	0.41
1:B:109:LYS:HD2	1:B:109:LYS:HA	1.91	0.41
1:B:179:LYS:HE3	1:B:179:LYS:HB2	1.90	0.41
1:C:112:ILE:HA	1:C:190:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASN:CG	1:C:275:PHE:CD2	2.99	0.41
1:D:160:GLN:OE1	1:D:189:THR:HB	2.21	0.41
1:D:184:GLU:H	1:D:184:GLU:CD	2.29	0.41
1:A:230:ASN:O	1:C:191:ARG:NH2	2.47	0.41
1:B:132:ILE:O	1:B:133:ASP:C	2.63	0.41
1:A:112:ILE:HA	1:A:190:ILE:O	2.21	0.40
1:A:132:ILE:O	1:A:133:ASP:C	2.65	0.40
1:A:184:GLU:HG2	8:A:549:HOH:O	2.21	0.40
1:B:261:SER:HB2	8:B:474:HOH:O	2.21	0.40
1:D:120:ASP:OD1	1:D:120:ASP:C	2.64	0.40
1:D:210:GLY:HA3	1:D:225:SER:CB	2.52	0.40
1:B:245:ASN:OD1	1:B:245:ASN:C	2.65	0.40
1:D:192:ASP:O	8:D:406:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/168 (99%)	160 (96%)	6 (4%)	31	25
1	B	167/168 (99%)	163 (98%)	4 (2%)	43	40
1	C	169/168 (101%)	165 (98%)	4 (2%)	43	40
1	D	166/168 (99%)	163 (98%)	3 (2%)	51	51
All	All	668/672 (99%)	651 (98%)	17 (2%)	40	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	182	PHE
1	A	186	ILE
1	A	259	SER
1	A	266	THR
1	A	297	GLU
1	B	107	GLU
1	B	140	LEU
1	B	205	SER
1	B	267	ILE
1	C	141	VAL
1	C	212	ILE
1	C	220	SER
1	C	288	LYS
1	D	122	ASP
1	D	177	VAL
1	D	252	SER

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	215	ASN
1	A	230	ASN
1	B	139	GLN
1	B	142	GLN
1	B	215	ASN
1	C	139	GLN
1	C	160	GLN
1	C	215	ASN
1	D	157	GLN
1	D	215	ASN
1	D	244	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	C	301	-	3,3,3	0.12	0	2,2,2	0.07	0
4	DGL	B	304	-	8,9,9	1.15	0	8,11,11	1.28	1 (12%)
4	DGL	D	306	-	8,9,9	1.23	1 (12%)	8,11,11	0.89	0
3	EDO	B	303	-	3,3,3	0.24	0	2,2,2	0.12	0
3	EDO	A	402	-	3,3,3	0.08	0	2,2,2	0.21	0
6	SO4	D	304	-	4,4,4	0.35	0	6,6,6	0.15	0
3	EDO	D	301	-	3,3,3	0.39	0	2,2,2	0.48	0
3	EDO	B	302	-	3,3,3	0.39	0	2,2,2	0.29	0
6	SO4	D	303	-	4,4,4	0.26	0	6,6,6	0.12	0
5	GLY	D	307	-	4,4,4	1.21	1 (25%)	3,4,4	1.08	0
2	VVP	A	401	-	12,12,12	1.86	4 (33%)	15,16,16	2.42	9 (60%)
3	EDO	C	303	-	3,3,3	0.67	0	2,2,2	0.84	0
5	GLY	C	304	-	4,4,4	0.85	0	3,4,4	1.09	0
7	ALA	D	305	-	5,5,5	0.91	0	6,6,6	0.91	0
3	EDO	C	302	-	3,3,3	0.16	0	2,2,2	0.43	0
3	EDO	D	302	-	3,3,3	0.16	0	2,2,2	0.44	0
2	VVP	B	301	-	12,12,12	1.80	4 (33%)	15,16,16	1.72	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	EDO	C	301	-	-	1/1/1/1	-
4	DGL	B	304	-	-	1/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DGL	D	306	-	-	1/9/9/9	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
5	GLY	D	307	-	-	0/2/2/2	-
2	VVP	A	401	-	-	2/2/2/2	0/2/2/2
3	EDO	C	303	-	-	1/1/1/1	-
5	GLY	C	304	-	-	0/2/2/2	-
7	ALA	D	305	-	-	0/4/4/4	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
2	VVP	B	301	-	-	2/2/2/2	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	VVP	C9-C6	-4.00	1.37	1.41
2	B	301	VVP	C9-C6	-2.99	1.38	1.41
2	A	401	VVP	O1-C2	2.91	1.41	1.37
2	B	301	VVP	O1-C2	2.83	1.41	1.37
4	D	306	DGL	O-C	2.64	1.29	1.22
2	B	301	VVP	C7-N1	-2.59	1.33	1.38
2	A	401	VVP	C7-N1	-2.38	1.33	1.38
2	B	301	VVP	C5-C6	2.22	1.43	1.39
2	A	401	VVP	C9-C2	2.09	1.44	1.41
5	D	307	GLY	OXT-C	-2.04	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	VVP	C5-C6-C9	-4.50	119.09	122.66
2	B	301	VVP	C5-C6-C9	-3.68	119.74	122.66
2	A	401	VVP	C6-C9-C8	-3.36	104.57	107.02
2	A	401	VVP	C8-C7-N1	-3.17	106.59	110.25
2	A	401	VVP	C9-C6-N1	2.98	108.79	107.09
2	A	401	VVP	O1-C2-C9	2.95	120.48	115.23
2	A	401	VVP	O1-C2-C3	-2.66	119.82	124.30
2	A	401	VVP	C9-C8-C7	2.65	109.38	106.64
2	B	301	VVP	O1-C2-C9	2.45	119.59	115.23
2	A	401	VVP	C6-N1-C7	2.41	110.67	108.91
2	B	301	VVP	C1-O1-C2	2.35	120.95	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	DGL	CB-CG-CD	2.30	118.62	112.49
2	A	401	VVP	C1-O1-C2	2.09	120.58	117.51
2	B	301	VVP	C9-C6-N1	2.02	108.24	107.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

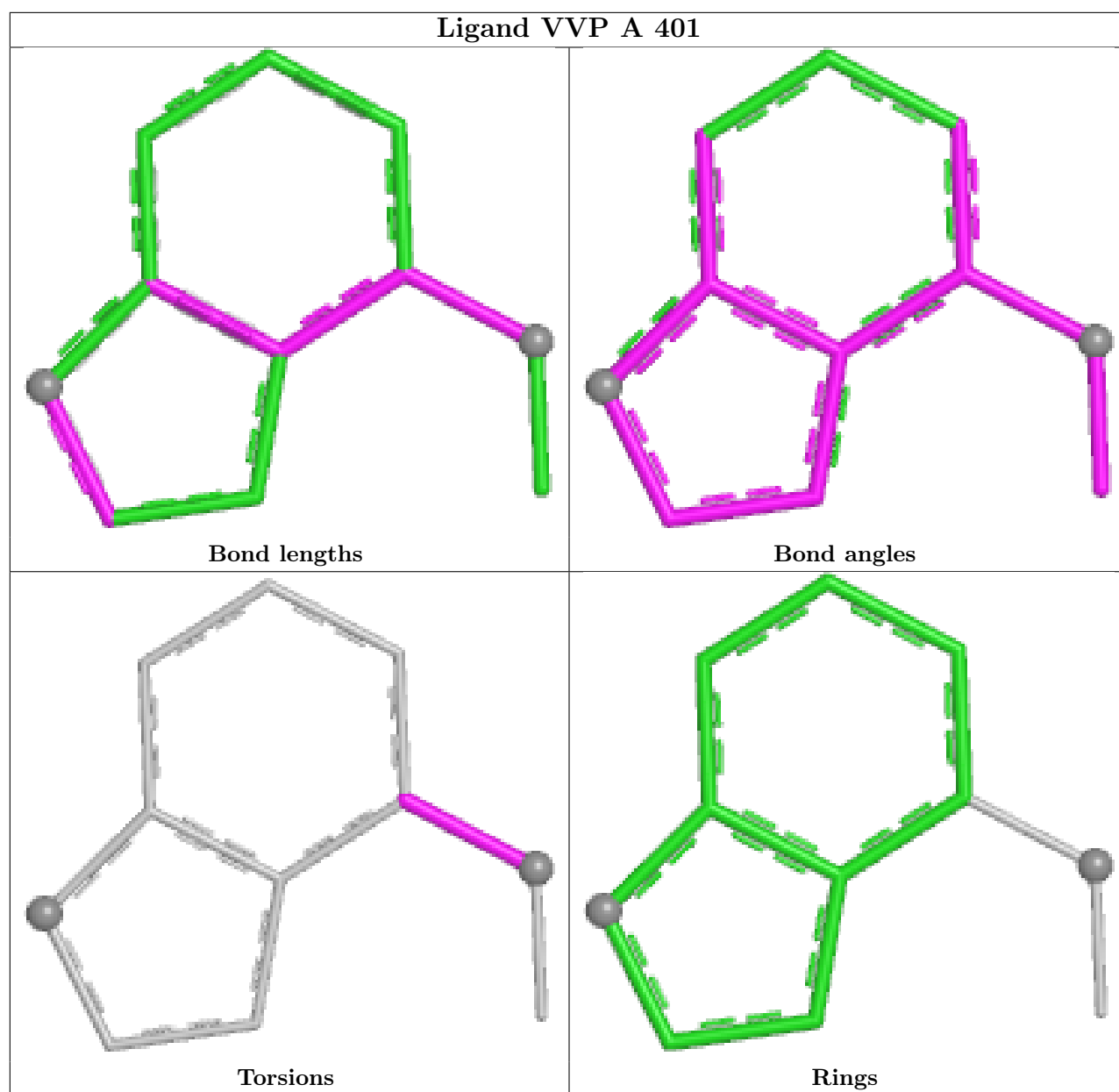
Mol	Chain	Res	Type	Atoms
2	B	301	VVP	C3-C2-O1-C1
2	B	301	VVP	C9-C2-O1-C1
3	C	303	EDO	O1-C1-C2-O2
2	A	401	VVP	C3-C2-O1-C1
2	A	401	VVP	C9-C2-O1-C1
3	A	402	EDO	O1-C1-C2-O2
3	C	301	EDO	O1-C1-C2-O2
4	D	306	DGL	O-C-CA-CB
4	B	304	DGL	OE2-CD-CG-CB

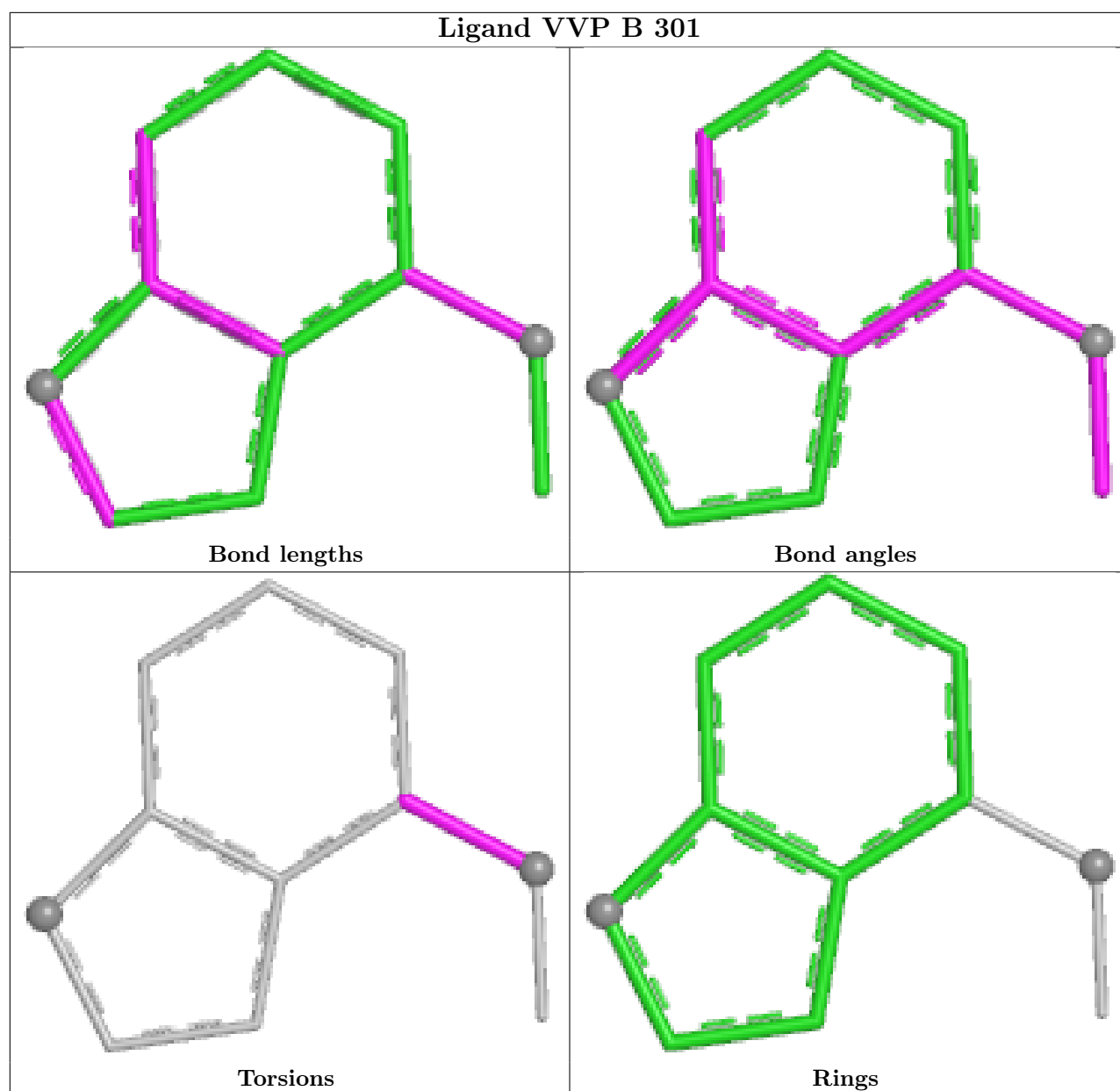
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	SO4	2	0
5	D	307	GLY	1	0
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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/195 (97%)	0.42	8 (4%) 40 41	16, 47, 78, 108	1 (0%)
1	B	193/195 (98%)	0.19	4 (2%) 63 66	16, 43, 66, 84	1 (0%)
1	C	193/195 (98%)	0.51	9 (4%) 36 36	17, 48, 81, 105	3 (1%)
1	D	191/195 (97%)	1.06	33 (17%) 4 4	17, 52, 75, 126	1 (0%)
All	All	768/780 (98%)	0.54	54 (7%) 22 22	16, 48, 76, 126	6 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	PHE	5.0
1	A	182	PHE	4.9
1	C	108	ILE	4.3
1	C	110	GLN	4.0
1	C	106	ALA	3.8
1	A	108	ILE	3.8
1	D	108	ILE	3.5
1	D	186	ILE	3.3
1	D	125	ILE	3.3
1	C	182	PHE	3.2
1	D	241	ILE	3.2
1	D	254	ILE	3.2
1	C	109	LYS	2.9
1	D	295	ILE	2.9
1	B	106	ALA	2.9
1	D	117	LEU	2.8
1	D	284	PRO	2.8
1	A	282	MET	2.8
1	A	286	ILE	2.8
1	C	112	ILE	2.8
1	D	273[A]	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	VAL	2.6
1	D	126	GLY	2.6
1	D	149	LEU	2.6
1	A	110	GLN	2.6
1	D	265	VAL	2.6
1	D	298	VAL	2.5
1	A	283	ALA	2.5
1	B	110	GLN	2.5
1	D	189	THR	2.4
1	A	109	LYS	2.4
1	D	116	ILE	2.4
1	D	177	VAL	2.4
1	C	252	SER	2.4
1	D	289	SER	2.4
1	A	183	GLY	2.3
1	D	112	ILE	2.3
1	D	142	GLN	2.3
1	D	190	ILE	2.3
1	D	286	ILE	2.3
1	D	174	ALA	2.3
1	D	140	LEU	2.3
1	B	108	ILE	2.2
1	D	110	GLN	2.2
1	D	288	LYS	2.2
1	D	262	GLY	2.2
1	D	249	LEU	2.2
1	D	111	GLY	2.1
1	D	118	CYS	2.1
1	C	296	PRO	2.1
1	D	178	LEU	2.1
1	D	207	GLY	2.1
1	C	288	LYS	2.0
1	B	261	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 ⓘ

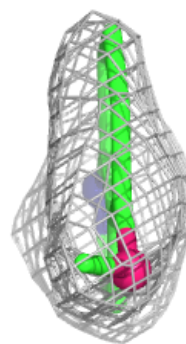
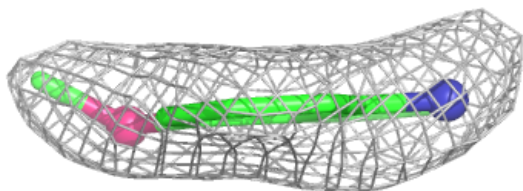
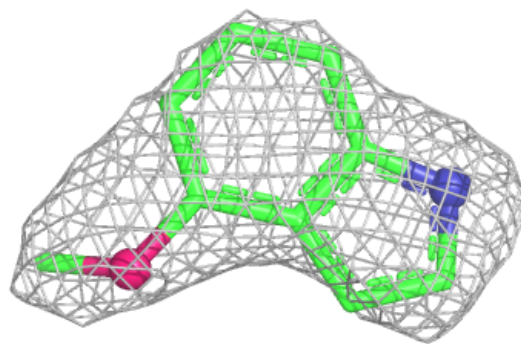
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	304	5/5	0.61	0.14	101,106,110,118	0
5	GLY	C	304	5/5	0.83	0.12	54,60,68,75	0
5	GLY	D	307	5/5	0.83	0.15	59,60,66,68	0
4	DGL	D	306	10/10	0.83	0.13	50,70,75,75	0
6	SO4	D	303	5/5	0.86	0.10	74,75,86,93	0
4	DGL	B	304	10/10	0.86	0.12	42,64,70,71	0
2	VVP	A	401	11/11	0.87	0.16	66,69,74,75	0
2	VVP	B	301	11/11	0.87	0.16	65,73,78,79	0
3	EDO	C	301	4/4	0.90	0.12	46,50,51,55	0
3	EDO	C	303	4/4	0.91	0.17	52,57,64,65	0
7	ALA	D	305	6/6	0.93	0.11	66,74,85,88	0
3	EDO	D	302	4/4	0.95	0.09	39,45,46,49	0
3	EDO	C	302	4/4	0.95	0.07	37,38,39,43	0
3	EDO	B	302	4/4	0.95	0.09	33,41,42,49	0
3	EDO	D	301	4/4	0.95	0.08	31,33,33,37	0
3	EDO	A	402	4/4	0.97	0.06	35,38,40,42	0
3	EDO	B	303	4/4	0.98	0.05	34,35,36,36	0

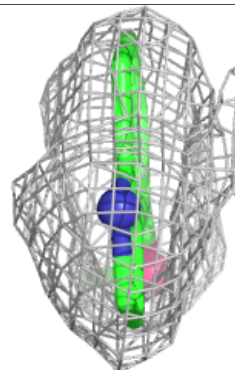
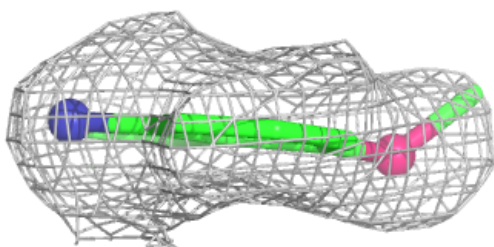
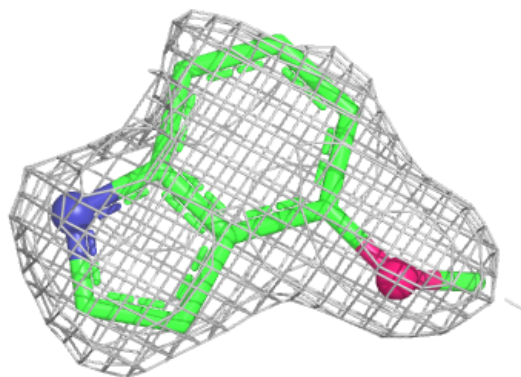
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VVP 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 VVP B 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.