



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 AM UTC

PDB ID : 7FSS / pdb_00007fss
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z839706072
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.11 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

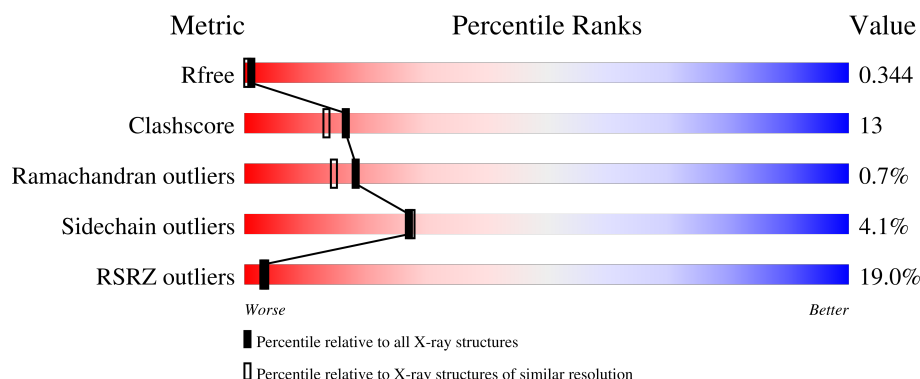
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	9% 82% 16% ..
1	B	195	5% 81% 17% ..
1	C	195	15% 75% 23% ..
1	D	195	45% 51% 44% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6365 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:

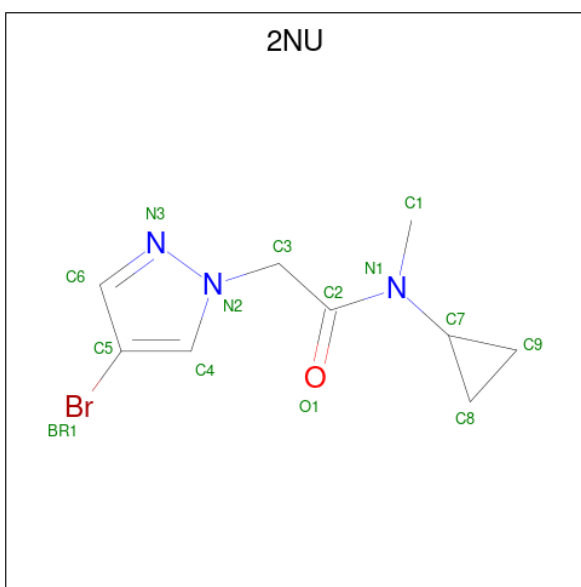
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



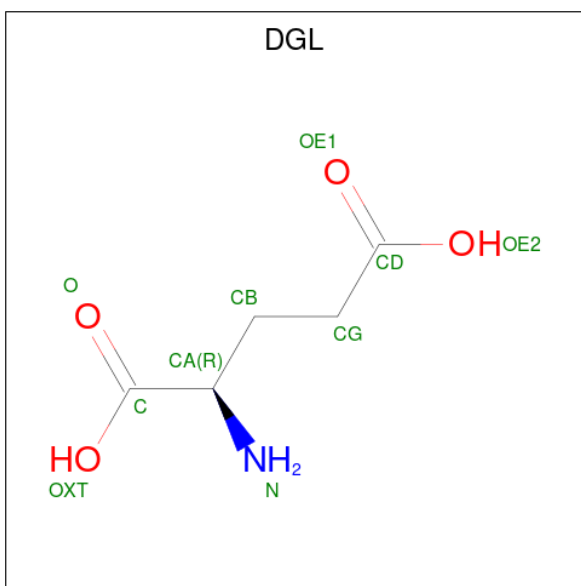
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 2-(4-bromanylpyrazol-1-yl)- {N}-cyclopropyl- {N}-methyl-ethanamide (CCD ID: 2NU) (formula: C₉H₁₂BrN₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	0	0
			14	1	9	3	1		

- 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: $C_2H_5NO_2$).



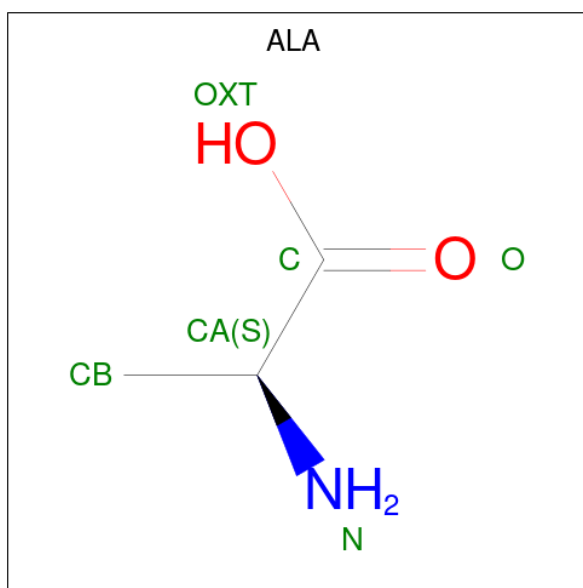
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- 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		

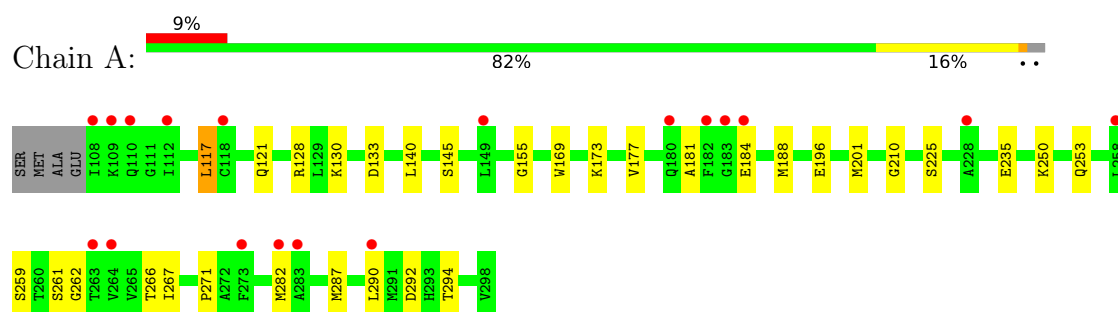
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	B	98	Total	O	0	0
			98	98		
8	C	69	Total	O	0	1
			70	70		
8	D	84	Total	O	0	1
			84	84		

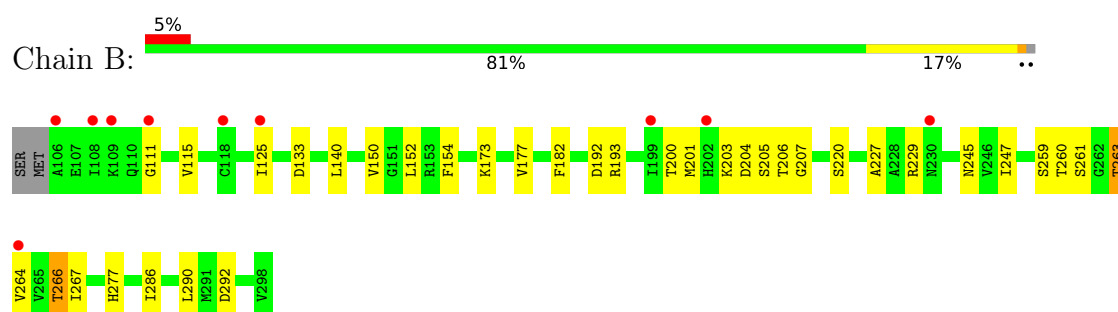
3 Residue-property plots [i](#)

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.

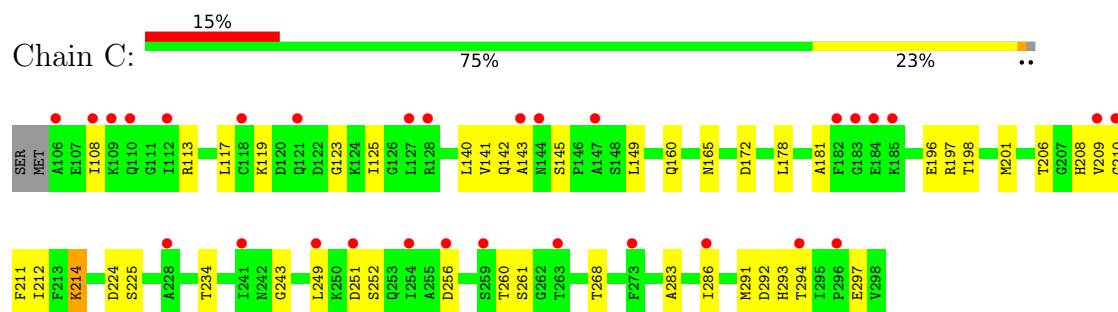
• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1

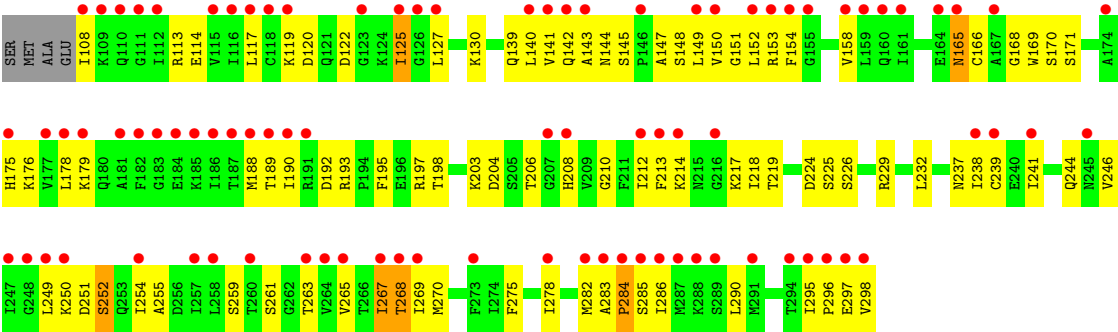


• Molecule 1: Syntenin-1



• 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	80.13Å 49.38Å 116.28Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	115.87 – 2.11 115.87 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (115.87-2.11) 99.7 (115.87-2.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.257 , 0.343 0.263 , 0.344	Depositor DCC
R_{free} test set	2583 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	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	0.94	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 28.60 % 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 1.7909e-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, EDO, 2NU, 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	0.55	1/1502 (0.1%)	1.02	0/2019
1	B	0.56	0/1516	1.06	2/2038 (0.1%)
1	C	0.55	0/1535	1.01	1/2063 (0.0%)
1	D	0.61	0/1502	1.10	1/2019 (0.0%)
All	All	0.57	1/6055 (0.0%)	1.05	4/8139 (0.0%)

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
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	SER	CA-CB	-5.07	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CA-CB-CG	6.28	118.88	112.60
1	D	213	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	277	HIS	CA-CB-CG	5.16	118.96	113.80
1	C	172	ASP	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	GLY	Peptide
1	C	113	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	20	0
1	B	1495	0	1541	23	0
1	C	1514	0	1558	32	0
1	D	1481	0	1530	88	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	1	0
2	D	8	0	12	0	0
3	B	14	0	0	2	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
6	D	10	0	0	1	0
7	D	6	0	4	0	0
8	A	50	0	0	2	0
8	B	98	0	0	5	0
8	C	70	0	0	3	0
8	D	84	0	0	23	0
All	All	6365	0	6229	158	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 13.

All (158) 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:152:LEU:O	8:D:401:HOH:O	1.75	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:NH2	8:D:402:HOH:O	1.99	0.94
1:B:133:ASP:OD1	8:B:401:HOH:O	1.87	0.90
1:D:197:ARG:NH1	8:D:406:HOH:O	2.12	0.82
1:C:108:ILE:HD12	1:C:198:THR:HG23	1.63	0.80
1:C:211:PHE:C	1:C:212:ILE:HD12	2.10	0.77
1:D:198:THR:HG22	1:D:268:THR:OG1	1.83	0.77
1:D:270:MET:SD	1:D:275:PHE:HA	2.26	0.74
1:D:139:GLN:HG2	1:D:282:MET:CE	2.18	0.74
1:D:237:ASN:OD1	8:D:404:HOH:O	2.09	0.71
1:D:255:ALA:O	8:D:403:HOH:O	2.07	0.71
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.09	0.69
1:D:139:GLN:HG2	1:D:282:MET:HE2	1.75	0.69
1:D:212:ILE:O	1:D:219:THR:OG1	2.10	0.69
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.74	0.69
1:B:173:LYS:NZ	8:B:404:HOH:O	2.24	0.68
1:D:283:ALA:O	1:D:284:PRO:C	2.36	0.68
1:D:168:GLY:O	8:D:405:HOH:O	2.10	0.68
1:A:184:GLU:HG2	8:A:443:HOH:O	1.94	0.67
1:A:140:LEU:HD22	1:B:182:PHE:CE1	2.29	0.67
1:B:229:ARG:NH1	8:B:406:HOH:O	2.27	0.67
1:D:204:ASP:OD2	8:D:407:HOH:O	2.13	0.67
1:D:139:GLN:O	1:D:282:MET:HE1	1.95	0.66
1:B:150:VAL:HG12	3:B:301:2NU:BR1	2.51	0.65
1:D:238:ILE:O	8:D:408:HOH:O	2.14	0.65
1:D:203:LYS:HG3	1:D:263:THR:O	1.97	0.65
1:C:261:SER:HB3	8:C:410:HOH:O	1.96	0.64
1:D:153:ARG:HG2	8:D:443:HOH:O	1.97	0.64
1:D:149:LEU:HG	8:D:441:HOH:O	1.97	0.64
1:B:201:MET:SD	1:B:227:ALA:HA	2.37	0.63
1:C:108:ILE:CD1	1:C:198:THR:HG23	2.29	0.62
1:D:295:ILE:HD11	1:D:298:VAL:HG12	1.82	0.62
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.81	0.62
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.81	0.61
1:D:140:LEU:HD23	1:D:141:VAL:C	2.26	0.61
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.34	0.61
1:C:291:MET:O	1:C:293:HIS:ND1	2.34	0.60
1:D:237:ASN:O	1:D:269:ILE:HA	2.02	0.60
1:D:165:ASN:N	1:D:165:ASN:OD1	2.34	0.60
1:C:249:LEU:HD21	1:C:293:HIS:CD2	2.37	0.60
1:C:142:GLN:O	1:C:145:SER:OG	2.13	0.58
1:D:152:LEU:C	8:D:401:HOH:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLY:HA3	1:C:225:SER:HB2	1.86	0.57
1:D:170:SER:HB3	8:D:415:HOH:O	2.05	0.57
1:C:119:LYS:NZ	1:C:181:ALA:O	2.30	0.56
1:B:200:THR:HG1	1:B:266:THR:HG1	1.51	0.56
1:D:145:SER:HA	8:D:414:HOH:O	2.06	0.56
1:D:195:PHE:CD2	1:D:278:ILE:HD11	2.42	0.55
1:D:286:ILE:HG23	1:D:290:LEU:HD12	1.89	0.55
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.88	0.55
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.06	0.55
1:D:153:ARG:CG	8:D:443:HOH:O	2.53	0.54
1:D:203:LYS:NZ	1:D:259:SER:O	2.39	0.54
1:D:114:GLU:O	8:D:409:HOH:O	2.18	0.54
1:C:251:ASP:OD1	8:C:401:HOH:O	2.19	0.53
1:A:128:ARG:HG2	1:B:182:PHE:CZ	2.43	0.53
1:C:119:LYS:HB3	1:C:123:GLY:HA2	1.91	0.53
1:D:130:LYS:NZ	8:D:416:HOH:O	2.42	0.52
1:A:117:LEU:HD13	1:A:188:MET:HE3	1.92	0.52
1:D:252:SER:HB3	8:D:419:HOH:O	2.10	0.52
1:D:261:SER:OG	1:D:265:VAL:HG22	2.10	0.51
1:D:250:LYS:O	1:D:254:ILE:HG13	2.10	0.51
1:C:292:ASP:OD1	1:C:294:THR:HG22	2.11	0.51
1:D:214:LYS:O	1:D:217:LYS:N	2.39	0.51
1:D:283:ALA:O	1:D:285:SER:N	2.43	0.51
1:D:226:SER:OG	6:D:303:SO4:O2	2.15	0.51
1:A:282:MET:HE3	1:A:287:MET:CG	2.42	0.50
1:D:244:GLN:O	1:D:246:VAL:HG13	2.11	0.50
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.94	0.50
1:D:170:SER:HB2	8:D:452:HOH:O	2.12	0.50
1:D:141:VAL:HG21	1:D:152:LEU:O	2.12	0.49
1:B:192:ASP:O	1:B:193:ARG:C	2.55	0.49
1:C:256:ASP:O	1:C:260:THR:HG23	2.13	0.49
1:D:241:ILE:HD11	1:D:254:ILE:HG23	1.94	0.49
1:D:158:VAL:CG1	1:D:188:MET:HE2	2.43	0.49
1:D:270:MET:SD	1:D:275:PHE:CA	2.99	0.49
1:D:261:SER:CB	1:D:265:VAL:HG22	2.43	0.49
1:C:198:THR:HG22	1:C:268:THR:OG1	2.13	0.49
1:B:204:ASP:O	1:B:207:GLY:N	2.45	0.48
1:A:250:LYS:HG3	1:A:253:GLN:OE1	2.13	0.48
1:D:195:PHE:HD2	1:D:278:ILE:HD11	1.79	0.48
1:D:143:ALA:O	1:D:144:ASN:ND2	2.46	0.48
1:B:204:ASP:OD1	1:B:206:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ILE:O	1:D:145:SER:HB2	2.14	0.48
1:D:252:SER:CB	8:D:419:HOH:O	2.62	0.47
1:A:133:ASP:HB3	1:C:234:THR:O	2.13	0.47
1:C:210:GLY:HA3	1:C:225:SER:CB	2.43	0.47
1:C:125:ILE:HD11	1:C:178:LEU:HD13	1.96	0.47
1:A:155:GLY:HA3	1:A:196:GLU:OE2	2.15	0.46
1:D:254:ILE:O	1:D:255:ALA:C	2.58	0.46
1:D:117:LEU:HD21	1:D:147:ALA:HA	1.97	0.46
1:C:160:GLN:HG3	1:C:165:ASN:HA	1.98	0.46
1:D:218:ILE:HD13	1:D:232:LEU:HD11	1.97	0.46
1:C:283:ALA:HB3	1:C:286:ILE:HG12	1.98	0.46
1:D:251:ASP:HA	1:D:254:ILE:HD12	1.97	0.46
1:B:115:VAL:HG21	1:B:152:LEU:HD21	1.98	0.46
1:B:245:ASN:OD1	1:B:245:ASN:C	2.58	0.46
1:C:143:ALA:HB2	1:C:292:ASP:HA	1.97	0.46
1:D:204:ASP:N	1:D:208:HIS:O	2.48	0.46
1:D:239:CYS:HB2	1:D:268:THR:HG22	1.98	0.46
1:D:139:GLN:CG	1:D:282:MET:HE2	2.45	0.45
1:D:189:THR:O	1:D:190:ILE:HD13	2.17	0.45
1:D:270:MET:HE1	1:D:278:ILE:HD12	1.98	0.45
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.99	0.45
1:D:127:LEU:HD21	1:D:152:LEU:HD13	1.98	0.45
1:D:119:LYS:NZ	1:D:179:LYS:O	2.49	0.45
1:D:166:CYS:HA	1:D:169:TRP:CE2	2.51	0.45
1:C:108:ILE:HD13	1:C:197[B]:ARG:HA	1.98	0.45
1:C:252:SER:HB3	8:D:454:HOH:O	2.17	0.45
1:C:206:THR:OG1	1:C:208:HIS:CE1	2.70	0.44
1:D:140:LEU:HD23	1:D:140:LEU:C	2.42	0.44
1:B:154:PHE:CD1	1:B:247:ILE:CD1	3.00	0.44
1:C:249:LEU:HD21	1:C:293:HIS:NE2	2.32	0.44
1:B:259:SER:OG	1:B:260:THR:N	2.51	0.44
1:A:169:TRP:CZ3	1:A:177:VAL:HG21	2.53	0.44
1:B:203:LYS:NZ	1:B:259:SER:O	2.51	0.44
1:A:128:ARG:HG2	1:B:182:PHE:CE1	2.52	0.44
1:A:282:MET:HE3	1:A:287:MET:HG2	1.99	0.44
1:D:198:THR:HA	1:D:267:ILE:O	2.18	0.43
1:D:197:ARG:HB3	8:D:457:HOH:O	2.18	0.43
1:D:148:SER:O	1:D:151:GLY:N	2.46	0.43
1:A:173:LYS:O	1:A:177:VAL:HG23	2.19	0.43
1:D:244:GLN:HB2	1:D:295:ILE:HG22	2.00	0.43
1:D:142:GLN:HG3	1:D:290:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:O	1:D:268:THR:HA	2.19	0.43
1:A:259:SER:C	1:A:261:SER:H	2.27	0.43
1:D:270:MET:CE	1:D:278:ILE:HD12	2.48	0.42
1:B:203:LYS:C	8:B:403:HOH:O	2.62	0.42
1:D:158:VAL:HG13	1:D:188:MET:HE2	2.01	0.42
1:A:210:GLY:HA3	1:A:225:SER:CB	2.49	0.42
1:B:263:THR:HB	8:B:465:HOH:O	2.19	0.42
1:D:113:ARG:HH11	1:D:113:ARG:HB3	1.84	0.42
1:D:120:ASP:OD1	1:D:120:ASP:C	2.63	0.42
1:D:125:ILE:HD11	1:D:178:LEU:HD13	2.02	0.42
1:B:173:LYS:O	1:B:177:VAL:HG23	2.19	0.42
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.92	0.42
1:A:121:GLN:HG3	8:A:442:HOH:O	2.19	0.42
1:D:192:ASP:O	1:D:193:ARG:C	2.63	0.42
1:C:243:GLY:O	2:C:301:EDO:O1	2.28	0.42
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.20	0.41
1:D:224:ASP:O	1:D:229:ARG:NH1	2.52	0.41
1:D:284:PRO:CD	8:D:476:HOH:O	2.68	0.41
1:B:150:VAL:CG1	3:B:301:2NU:BR1	3.21	0.41
1:C:145:SER:O	1:C:149:LEU:HG	2.21	0.41
1:D:108:ILE:HG12	1:D:198:THR:HG23	2.03	0.41
1:D:113:ARG:HH11	1:D:113:ARG:CB	2.34	0.41
1:A:201:MET:HE3	1:A:201:MET:HB2	1.94	0.41
1:D:125:ILE:HD11	1:D:178:LEU:HD22	2.02	0.41
1:D:175:HIS:O	1:D:176:LYS:C	2.64	0.41
1:D:203:LYS:HD2	1:D:263:THR:HA	2.02	0.41
1:D:283:ALA:C	1:D:285:SER:N	2.78	0.41
1:D:150:VAL:O	8:D:410:HOH:O	2.22	0.40
1:D:154:PHE:CD1	1:D:154:PHE:C	2.99	0.40
1:C:214:LYS:HA	1:C:251:ASP:OD2	2.22	0.40
1:D:127:LEU:HD21	1:D:152:LEU:CD1	2.50	0.40
1:C:201:MET:SD	1:C:209:VAL:CG1	3.10	0.40
1:D:267:ILE:HG13	1:D:268:THR:N	2.37	0.40
1:C:261:SER:CB	8:C:410:HOH:O	2.63	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%)	180 (95%)	8 (4%)	2 (1%)	11	7
1	B	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	24	22
1	C	194/195 (100%)	181 (93%)	13 (7%)	0	100	100
1	D	190/195 (97%)	165 (87%)	23 (12%)	2 (1%)	11	7
All	All	766/780 (98%)	709 (93%)	52 (7%)	5 (1%)	18	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	SER
1	A	181	ALA
1	D	249	LEU
1	A	262	GLY
1	D	284	PRO

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%)	162 (98%)	4 (2%)	43	48
1	B	167/168 (99%)	159 (95%)	8 (5%)	23	22
1	C	169/168 (101%)	163 (96%)	6 (4%)	31	33
1	D	166/168 (99%)	157 (95%)	9 (5%)	20	18
All	All	668/672 (99%)	641 (96%)	27 (4%)	27	28

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	130	LYS
1	A	266	THR
1	A	271	PRO
1	B	125	ILE
1	B	140	LEU
1	B	205	SER
1	B	220	SER
1	B	263	THR
1	B	264	VAL
1	B	266	THR
1	B	267	ILE
1	C	117	LEU
1	C	140	LEU
1	C	141	VAL
1	C	214	LYS
1	C	224	ASP
1	C	297	GLU
1	D	122	ASP
1	D	125	ILE
1	D	165	ASN
1	D	171	SER
1	D	206	THR
1	D	252	SER
1	D	267	ILE
1	D	268	THR
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	B	110	GLN
1	B	139	GLN
1	B	160	GLN
1	B	165	ASN
1	C	110	GLN
1	C	139	GLN
1	C	157	GLN
1	C	253	GLN
1	D	144	ASN

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Mol	Chain	Res	Type
1	D	157	GLN
1	D	202	HIS
1	D	215	ASN
1	D	237	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
4	DGL	D	306	-	8,9,9	0.98	0	8,11,11	0.88	0
4	DGL	B	304	-	8,9,9	1.11	0	8,11,11	1.01	0
2	EDO	B	302	-	3,3,3	0.36	0	2,2,2	0.23	0
2	EDO	A	301	-	3,3,3	0.17	0	2,2,2	0.19	0
2	EDO	C	302	-	3,3,3	0.28	0	2,2,2	0.21	0
3	2NU	B	301	-	15,15,15	2.44	3 (20%)	18,21,21	2.41	9 (50%)
2	EDO	D	302	-	3,3,3	0.09	0	2,2,2	0.09	0
2	EDO	D	301	-	3,3,3	0.18	0	2,2,2	0.02	0
7	ALA	D	305	-	5,5,5	0.92	0	6,6,6	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	303	-	3,3,3	0.09	0	2,2,2	0.37	0
5	GLY	D	307	-	4,4,4	1.28	1 (25%)	3,4,4	0.96	0
6	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.09	0
6	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.13	0
2	EDO	C	303	-	3,3,3	0.24	0	2,2,2	0.47	0
2	EDO	C	301	-	3,3,3	0.28	0	2,2,2	0.16	0
5	GLY	C	304	-	4,4,4	1.05	0	3,4,4	0.97	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
4	DGL	D	306	-	-	0/9/9/9	-
4	DGL	B	304	-	-	3/9/9/9	-
2	EDO	B	302	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
3	2NU	B	301	-	-	4/12/14/14	0/2/2/2
2	EDO	D	302	-	-	0/1/1/1	-
2	EDO	D	301	-	-	1/1/1/1	-
7	ALA	D	305	-	-	0/4/4/4	-
2	EDO	B	303	-	-	1/1/1/1	-
5	GLY	D	307	-	-	2/2/2/2	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	C	301	-	-	1/1/1/1	-
5	GLY	C	304	-	-	2/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	2NU	C2-N1	7.83	1.47	1.35
3	B	301	2NU	BR1-C5	2.78	1.94	1.89
3	B	301	2NU	C8-C7	2.60	1.54	1.48
5	D	307	GLY	OXT-C	-2.23	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	2NU	C3-N2-C4	-4.77	122.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	2NU	C5-C6-N3	-3.66	107.94	110.65
3	B	301	2NU	C3-N2-N3	3.55	126.02	120.94
3	B	301	2NU	C1-N1-C2	-3.24	114.92	122.16
3	B	301	2NU	C3-C2-N1	3.15	124.65	118.35
3	B	301	2NU	C7-N1-C2	3.15	126.85	119.59
3	B	301	2NU	O1-C2-N1	-2.48	117.76	121.92
3	B	301	2NU	C5-C4-N2	2.28	107.52	106.13
3	B	301	2NU	O1-C2-C3	-2.01	117.58	120.56

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	2NU	C8-C7-N1-C1
3	B	301	2NU	C8-C7-N1-C2
5	C	304	GLY	O-C-CA-N
5	D	307	GLY	O-C-CA-N
5	D	307	GLY	OXT-C-CA-N
5	C	304	GLY	OXT-C-CA-N
2	C	301	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
3	B	301	2NU	C3-C2-N1-C7
3	B	301	2NU	C3-C2-N1-C1
4	B	304	DGL	CA-CB-CG-CD
2	B	302	EDO	O1-C1-C2-O2
4	B	304	DGL	OXT-C-CA-CB
2	C	302	EDO	O1-C1-C2-O2
2	D	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	B	303	EDO	O1-C1-C2-O2
4	B	304	DGL	O-C-CA-CB

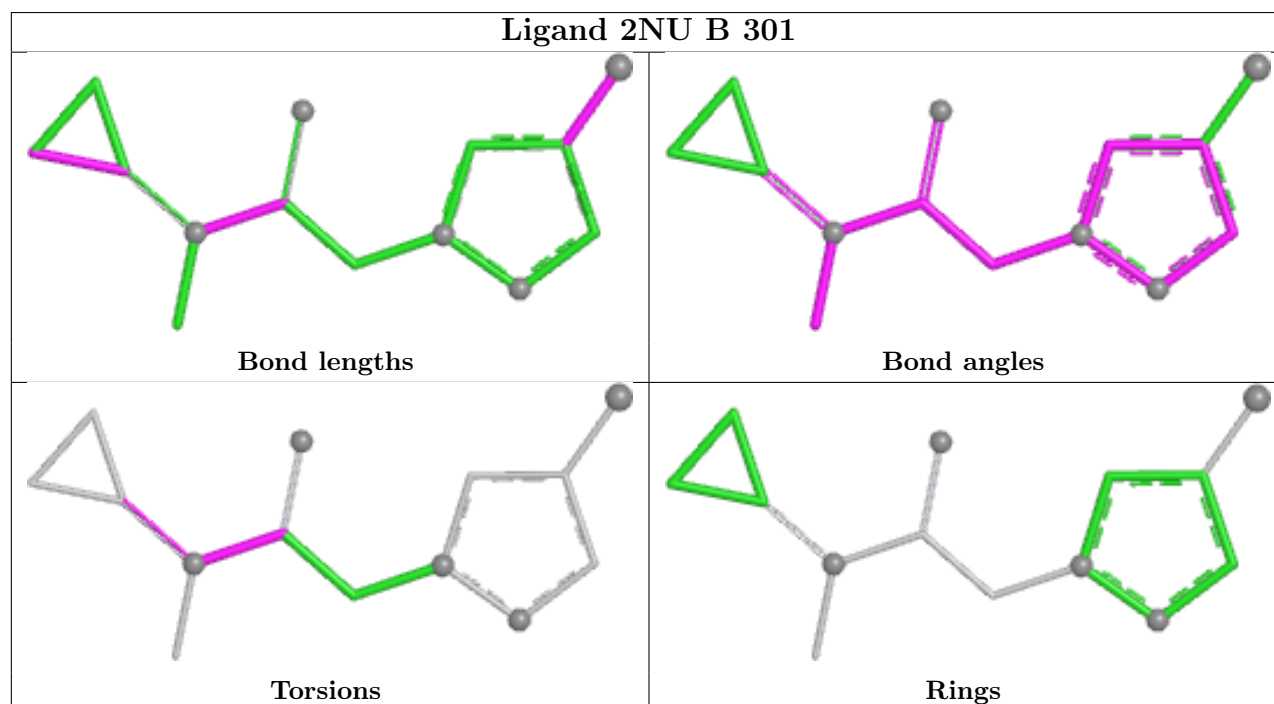
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	2NU	2	0
6	D	303	SO4	1	0
2	C	301	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%)	0.77	18 (9%)	14 15	15, 45, 72, 100	1 (0%)
1	B	193/195 (98%)	0.54	10 (5%)	33 35	13, 43, 63, 96	1 (0%)
1	C	193/195 (98%)	1.12	30 (15%)	5 5	16, 50, 75, 101	3 (1%)
1	D	191/195 (97%)	1.95	88 (46%)	0 0	18, 54, 77, 109	1 (0%)
All	All	768/780 (98%)	1.09	146 (19%)	3 3	13, 48, 74, 109	6 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	LEU	6.2
1	D	190	ILE	6.0
1	D	254	ILE	6.0
1	C	110	GLN	5.8
1	D	125	ILE	5.2
1	D	182	PHE	5.2
1	D	177	VAL	5.1
1	D	178	LEU	5.0
1	C	106	ALA	4.6
1	D	186	ILE	4.5
1	A	108	ILE	4.4
1	A	182	PHE	4.4
1	D	238	ILE	4.4
1	C	108	ILE	4.4
1	C	249	LEU	4.2
1	B	106	ALA	4.2
1	D	241	ILE	4.1
1	D	150	VAL	4.0
1	C	109	LYS	4.0
1	D	260	THR	4.0
1	C	209	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	264	VAL	3.9
1	C	182	PHE	3.9
1	A	109	LYS	3.9
1	C	112	ILE	3.9
1	D	284	PRO	3.8
1	D	273[A]	PHE	3.8
1	D	149	LEU	3.8
1	D	265	VAL	3.7
1	D	108	ILE	3.7
1	D	286	ILE	3.6
1	D	249	LEU	3.6
1	D	267	ILE	3.5
1	D	283	ALA	3.5
1	D	247	ILE	3.5
1	D	213	PHE	3.5
1	D	183	GLY	3.5
1	D	298	VAL	3.5
1	D	126	GLY	3.4
1	D	141	VAL	3.4
1	D	248	GLY	3.4
1	C	254	ILE	3.4
1	D	127	LEU	3.3
1	B	125	ILE	3.3
1	D	116	ILE	3.3
1	D	189	THR	3.2
1	B	111	GLY	3.2
1	D	269	ILE	3.1
1	C	296	PRO	3.1
1	D	268	THR	3.0
1	D	158	VAL	3.0
1	D	287	MET	3.0
1	D	257	ILE	3.0
1	D	207	GLY	3.0
1	D	112	ILE	2.9
1	D	295	ILE	2.9
1	A	110	GLN	2.9
1	A	282	MET	2.9
1	C	294	THR	2.9
1	D	288	LYS	2.9
1	D	161	ILE	2.8
1	D	153	ARG	2.8
1	D	111	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	140	LEU	2.8
1	D	282	MET	2.7
1	D	152	LEU	2.7
1	D	297	GLU	2.7
1	A	112	ILE	2.7
1	D	285	SER	2.7
1	D	239	CYS	2.7
1	D	258	LEU	2.6
1	A	264	VAL	2.6
1	D	155	GLY	2.6
1	A	263	THR	2.6
1	D	159	LEU	2.6
1	D	179	LYS	2.6
1	C	183	GLY	2.6
1	C	259	SER	2.5
1	D	184	GLU	2.5
1	B	108	ILE	2.5
1	C	118	CYS	2.5
1	D	187	THR	2.5
1	C	228	ALA	2.5
1	A	149	LEU	2.5
1	D	291	MET	2.5
1	B	109	LYS	2.5
1	B	202	HIS	2.5
1	D	208	HIS	2.5
1	D	296	PRO	2.4
1	D	154	PHE	2.4
1	D	245	ASN	2.4
1	C	184	GLU	2.4
1	D	174	ALA	2.4
1	D	181	ALA	2.4
1	C	143	ALA	2.4
1	C	147	ALA	2.4
1	D	264	VAL	2.4
1	D	109	LYS	2.4
1	D	185	LYS	2.4
1	D	164	GLU	2.3
1	A	258	LEU	2.3
1	D	119	LYS	2.3
1	D	160	GLN	2.3
1	A	283	ALA	2.3
1	A	183	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	146	PRO	2.3
1	D	123	GLY	2.3
1	D	263	THR	2.3
1	B	118	CYS	2.3
1	A	290	LEU	2.3
1	D	188	MET	2.3
1	D	175	HIS	2.2
1	C	273[A]	PHE	2.2
1	D	214	LYS	2.2
1	D	250	LYS	2.2
1	A	228	ALA	2.2
1	A	118	CYS	2.2
1	A	273[A]	PHE	2.2
1	C	263	THR	2.2
1	C	286	ILE	2.2
1	D	212	ILE	2.2
1	D	142	GLN	2.2
1	B	199	ILE	2.1
1	C	210	GLY	2.1
1	C	128	ARG	2.1
1	D	118	CYS	2.1
1	B	230	ASN	2.1
1	A	184	GLU	2.1
1	D	110	GLN	2.1
1	D	278	ILE	2.1
1	D	143	ALA	2.1
1	D	167	ALA	2.1
1	D	289	SER	2.1
1	C	256	ASP	2.1
1	C	241	ILE	2.1
1	D	115	VAL	2.1
1	C	127	LEU	2.0
1	C	144[A]	ASN	2.0
1	D	165	ASN	2.0
1	D	191	ARG	2.0
1	C	185	LYS	2.0
1	A	180	GLN	2.0
1	C	121	GLN	2.0
1	C	251	ASP	2.0
1	D	294	THR	2.0
1	D	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](#)

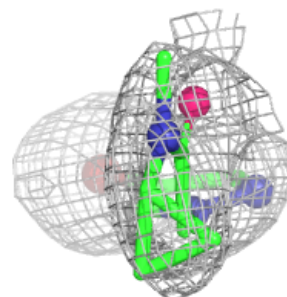
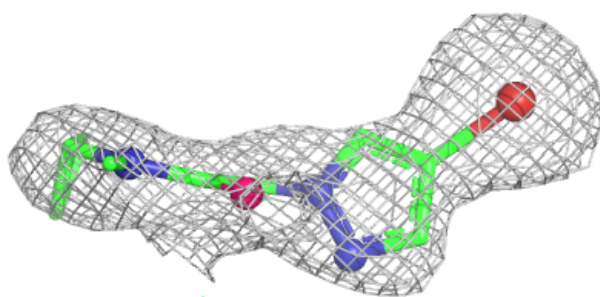
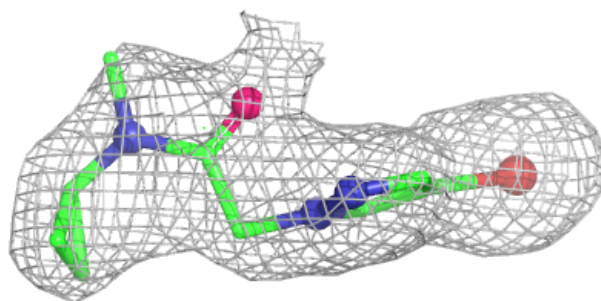
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	304	5/5	0.55	0.15	91,96,105,108	0
6	SO4	D	303	5/5	0.73	0.13	76,78,86,93	0
4	DGL	D	306	10/10	0.75	0.16	53,80,88,89	0
7	ALA	D	305	6/6	0.80	0.16	79,81,81,84	0
5	GLY	C	304	5/5	0.81	0.14	51,53,69,72	0
4	DGL	B	304	10/10	0.82	0.14	44,65,69,70	0
2	EDO	C	301	4/4	0.82	0.15	44,47,47,50	0
5	GLY	D	307	5/5	0.85	0.14	47,51,55,57	0
2	EDO	D	301	4/4	0.88	0.14	39,46,49,56	0
2	EDO	A	301	4/4	0.88	0.13	45,47,47,49	0
2	EDO	B	302	4/4	0.92	0.11	29,36,38,43	0
2	EDO	C	302	4/4	0.92	0.12	34,38,41,43	0
2	EDO	D	302	4/4	0.93	0.10	45,51,52,54	0
2	EDO	C	303	4/4	0.94	0.13	49,53,57,58	0
3	2NU	B	301	14/14	0.94	0.14	54,58,60,61	14
2	EDO	B	303	4/4	0.94	0.08	37,39,40,40	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 2NU 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.