



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:54 PM EDT

PDB ID : 7FT4 / pdb_00007ft4
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z48847594
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.17 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:

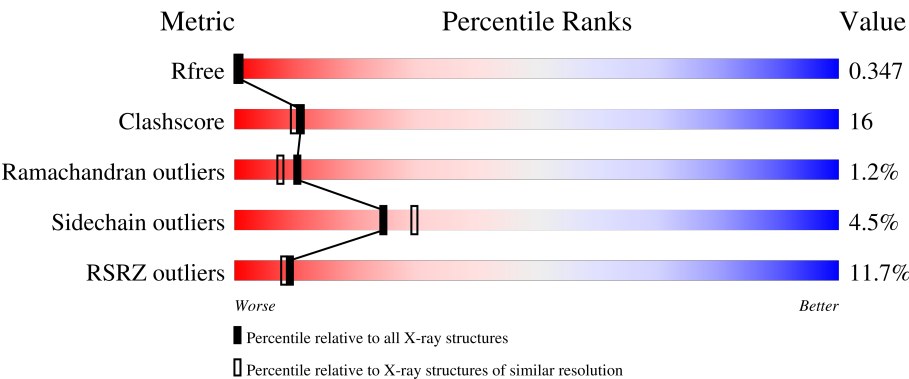
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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.

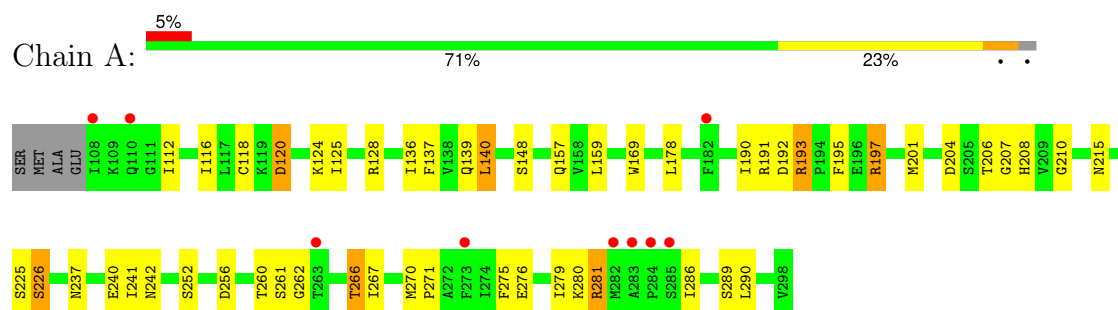
Mol	Chain	Length	Quality of chain
1	A	195	5% 71% 23% ..
1	B	195	6% 70% 25% ..
1	C	195	6% 75% 22% ..
1	D	195	30% 49% 46% ..

ENTRY-COMPOSITION INFOmissingINFO

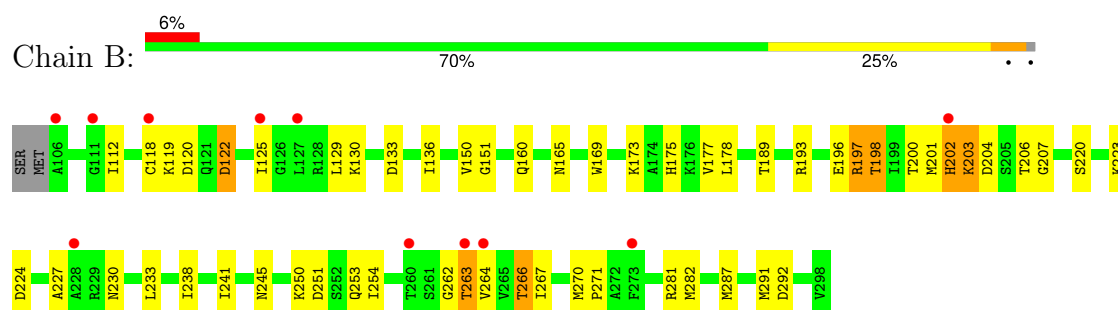
2 Residue-property plots [i](#)

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.

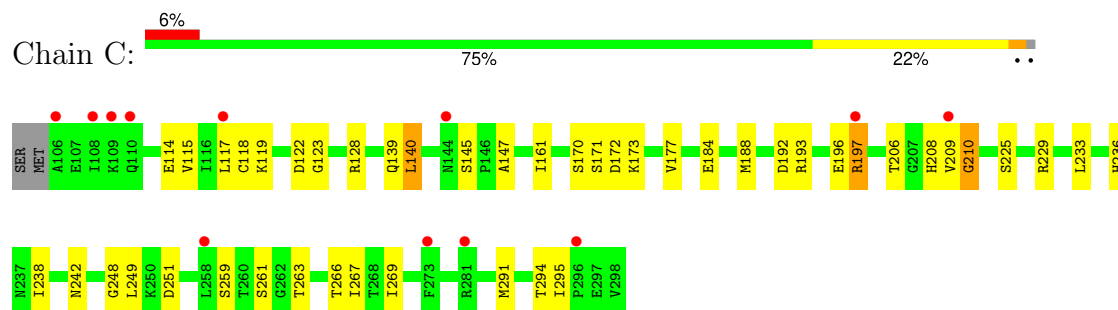
• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1

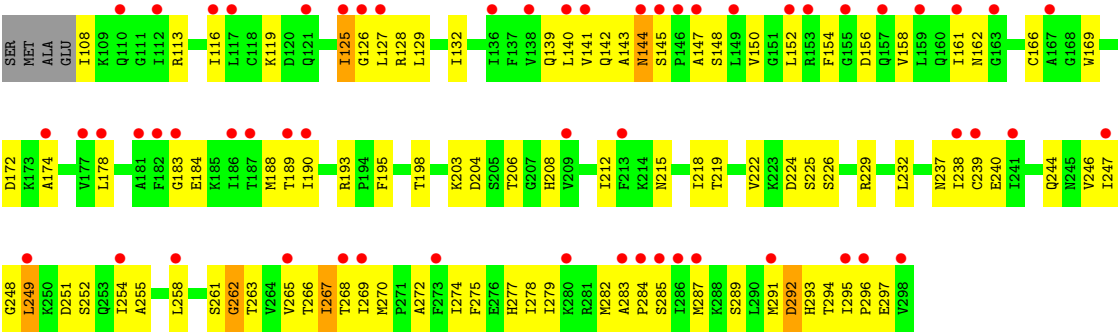


• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1





3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.16Å 49.09Å 115.07Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	45.16 – 2.17 45.16 – 2.17	Depositor EDS
% Data completeness (in resolution range)	80.2 (45.16-2.17) 80.2 (45.16-2.17)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.249 , 0.347 0.254 , 0.347	Depositor DCC
R_{free} test set	2340 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	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	0.94	EDS
Total number of atoms	6337	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 32.45 % 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 9.3739e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: O0J, DGL, EDO, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/1502	1.10	1/2019 (0.0%)
1	B	0.60	0/1516	1.13	1/2038 (0.0%)
1	C	0.59	0/1535	1.12	1/2063 (0.0%)
1	D	0.62	0/1502	1.19	3/2019 (0.1%)
All	All	0.60	0/6055	1.13	6/8139 (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	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	THR	CB-CA-C	7.25	121.65	109.84
1	D	292	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	292	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	172	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	172	ASP	CB-CA-C	-5.50	101.33	110.68
1	A	120	ASP	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	B	197	ARG	Sidechain
1	C	197[A]	ARG	Sidechain
1	D	113	ARG	Sidechain

4.2 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	38	0
1	B	1495	0	1541	41	0
1	C	1514	0	1558	27	0
1	D	1481	0	1530	102	0
2	A	16	0	0	4	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
3	C	12	0	18	0	0
3	D	8	0	12	0	0
4	B	10	0	7	2	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	2	0
7	D	6	0	4	0	0
8	A	42	0	0	7	0
8	B	90	0	0	8	0
8	C	67	0	0	3	0
8	D	73	0	0	19	0
All	All	6337	0	6229	203	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 16.

All (203) 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	1.79	0.98
1:B:150:VAL:O	8:B:401:HOH:O	1.89	0.90
1:D:128:ARG:O	1:D:129:LEU:HD23	1.79	0.82
1:B:133:ASP:OD1	3:B:301:EDO:O2	1.97	0.82
1:B:173:LYS:O	1:B:177:VAL:HG23	1.81	0.80
1:C:128:ARG:HB2	1:C:140:LEU:HB3	1.65	0.79
1:A:280:LYS:HA	8:A:433:HOH:O	1.82	0.79
1:B:133:ASP:OD1	8:B:402:HOH:O	2.01	0.77
1:D:127:LEU:CD1	1:D:188:MET:HE1	2.15	0.76
1:D:139:GLN:O	1:D:282:MET:HE1	1.85	0.76
1:D:287:MET:SD	8:D:473:HOH:O	2.44	0.75
1:D:238:ILE:O	8:D:402:HOH:O	2.05	0.75
1:D:215:ASN:O	8:D:403:HOH:O	2.06	0.73
1:C:229:ARG:NH2	8:C:401:HOH:O	2.21	0.73
1:D:208:HIS:CG	8:D:419:HOH:O	2.41	0.72
1:B:282:MET:HE3	1:B:287:MET:HB2	1.72	0.72
1:D:152:LEU:C	8:D:401:HOH:O	2.27	0.71
1:A:128:ARG:HB3	1:A:140:LEU:HB3	1.72	0.70
1:D:150:VAL:O	8:D:404:HOH:O	2.09	0.70
1:D:139:GLN:HG2	1:D:282:MET:HE2	1.76	0.68
1:D:226:SER:OG	6:D:303:SO4:O2	2.10	0.67
1:D:237:ASN:OD1	8:D:405:HOH:O	2.12	0.67
1:D:272:ALA:HB1	8:D:422:HOH:O	1.95	0.67
1:A:197:ARG:NH2	8:A:402:HOH:O	2.19	0.67
1:B:262:GLY:O	1:B:263:THR:C	2.39	0.66
1:D:139:GLN:HG2	1:D:282:MET:CE	2.27	0.65
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.78	0.65
1:D:204:ASP:OD2	8:D:406:HOH:O	2.13	0.64
1:D:283:ALA:O	1:D:284:PRO:C	2.40	0.64
1:D:141:VAL:HG21	1:D:152:LEU:O	1.97	0.64
1:D:237:ASN:O	1:D:269:ILE:HA	1.98	0.64
1:B:160:GLN:NE2	1:B:165:ASN:OD1	2.29	0.63
1:B:202:HIS:O	1:B:203:LYS:O	2.15	0.63
1:A:128:ARG:HD3	2:A:301:O0J:C6	2.29	0.63
1:D:295:ILE:HG23	1:D:296:PRO:HD2	1.81	0.62
1:D:254:ILE:O	1:D:255:ALA:C	2.41	0.61
1:D:203:LYS:HG3	1:D:263:THR:O	2.02	0.60
1:B:119:LYS:NZ	1:B:178:LEU:O	2.31	0.60
1:B:202:HIS:O	1:B:203:LYS:C	2.44	0.59
1:D:144:ASN:ND2	8:D:411:HOH:O	2.35	0.59
1:B:196:GLU:OE1	8:B:404:HOH:O	2.17	0.59
1:C:118:CYS:SG	1:C:184:GLU:O	2.59	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:O	1:A:207:GLY:N	2.29	0.59
1:D:248:GLY:HA2	1:D:287:MET:HE2	1.85	0.59
1:B:204:ASP:OD2	8:B:403:HOH:O	2.16	0.59
1:A:125:ILE:HD11	1:A:178:LEU:HD13	1.85	0.58
1:A:204:ASP:OD1	1:A:208:HIS:N	2.33	0.58
1:D:108:ILE:HG12	1:D:193:ARG:CZ	2.34	0.58
1:B:200:THR:O	1:B:230:ASN:ND2	2.36	0.58
1:A:128:ARG:HB2	2:A:301:O0J:C7	2.34	0.57
1:D:252:SER:O	1:D:255:ALA:HB3	2.05	0.57
1:D:126:GLY:HA3	1:D:145:SER:HB2	1.85	0.57
1:D:272:ALA:C	8:D:422:HOH:O	2.48	0.57
2:A:301:O0J:O	1:B:118:CYS:SG	2.63	0.57
1:D:161:ILE:HD13	1:D:178:LEU:HD21	1.86	0.57
1:D:252:SER:CB	8:D:410:HOH:O	2.53	0.56
1:A:128:ARG:NE	1:A:139:GLN:OE1	2.38	0.56
1:D:158:VAL:O	1:D:166:CYS:SG	2.61	0.56
1:A:157:GLN:HG2	1:A:159:LEU:HD23	1.88	0.56
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.86	0.56
1:D:251:ASP:N	6:D:304:SO4:O2	2.39	0.55
1:D:261:SER:OG	1:D:265:VAL:HG22	2.07	0.55
1:D:287:MET:O	1:D:291:MET:HB2	2.06	0.55
1:B:151:GLY:HA3	8:B:401:HOH:O	2.06	0.55
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.07	0.55
1:A:128:ARG:HD3	2:A:301:O0J:C5	2.38	0.54
1:B:193:ARG:HB3	1:B:196:GLU:HB2	1.89	0.54
1:D:274:ILE:O	1:D:275:PHE:C	2.51	0.54
1:D:169:TRP:HE3	1:D:174:ALA:HB2	1.73	0.54
1:D:116:ILE:O	1:D:150:VAL:HG11	2.07	0.54
1:D:206:THR:OG1	1:D:208:HIS:ND1	2.40	0.53
1:D:287:MET:HG3	1:D:291:MET:CE	2.38	0.53
1:D:293:HIS:NE2	8:D:408:HOH:O	2.31	0.53
1:A:112:ILE:HD11	1:A:191:ARG:NH2	2.24	0.53
1:A:215:ASN:O	8:A:401:HOH:O	2.18	0.53
1:B:287:MET:HG3	1:B:291:MET:HE2	1.91	0.53
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.41	0.53
1:D:140:LEU:HD23	1:D:141:VAL:C	2.34	0.53
1:D:270:MET:SD	1:D:275:PHE:HA	2.49	0.53
1:A:286:ILE:HG23	1:A:290:LEU:CD1	2.39	0.52
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.08	0.52
1:D:261:SER:CB	1:D:265:VAL:HG22	2.38	0.52
1:D:239:CYS:HB2	1:D:268:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:THR:HA	1:D:267:ILE:O	2.10	0.52
1:C:193:ARG:HG2	1:C:196:GLU:OE1	2.10	0.52
1:B:202:HIS:C	1:B:203:LYS:O	2.53	0.51
1:B:129:LEU:H	1:B:175:HIS:CE1	2.29	0.51
1:D:127:LEU:HD11	1:D:188:MET:HE1	1.90	0.51
1:B:136:ILE:HD11	1:B:169:TRP:O	2.11	0.51
1:D:161:ILE:HG22	1:D:162:ASN:HD22	1.74	0.51
1:A:226:SER:OG	8:A:403:HOH:O	2.19	0.51
1:A:276:GLU:OE2	8:A:404:HOH:O	2.19	0.51
1:B:250:LYS:O	1:B:251:ASP:C	2.54	0.51
1:D:195:PHE:HD2	1:D:278:ILE:HD11	1.76	0.51
1:D:203:LYS:HE3	1:D:265:VAL:CG2	2.41	0.51
1:A:270:MET:O	1:A:271:PRO:C	2.54	0.50
1:D:119:LYS:HG3	1:D:183:GLY:HA3	1.93	0.50
1:D:212:ILE:O	1:D:219:THR:OG1	2.21	0.50
1:A:136:ILE:HD11	1:A:169:TRP:O	2.12	0.50
1:A:169:TRP:O	8:A:405:HOH:O	2.20	0.50
1:D:215:ASN:CB	8:D:403:HOH:O	2.60	0.50
1:A:197:ARG:HG2	1:C:197[B]:ARG:HH12	1.77	0.49
1:D:145:SER:OG	1:D:147:ALA:HB3	2.11	0.49
1:B:130:LYS:NZ	4:B:303:DGL:OXT	2.38	0.49
1:D:255:ALA:O	8:D:407:HOH:O	2.20	0.49
1:A:241:ILE:O	1:A:242:ASN:C	2.55	0.49
1:D:127:LEU:HD12	1:D:188:MET:HE1	1.91	0.49
1:A:256:ASP:O	1:A:260:THR:HG23	2.11	0.49
1:A:281:ARG:CD	1:B:122:ASP:HA	2.42	0.49
1:B:241:ILE:HD11	1:B:254:ILE:HG23	1.95	0.49
1:D:147:ALA:O	1:D:148:SER:C	2.56	0.49
1:B:281:ARG:HD2	4:B:303:DGL:HA	1.94	0.49
1:D:198:THR:HG22	1:D:268:THR:OG1	2.13	0.48
1:C:210:GLY:HA3	1:C:225:SER:CB	2.44	0.48
1:D:252:SER:HB3	8:D:410:HOH:O	2.14	0.48
1:A:193:ARG:NH1	1:A:240:GLU:OE1	2.46	0.48
1:A:120:ASP:OD1	1:A:124:LYS:HB2	2.14	0.48
1:C:192:ASP:O	1:C:193:ARG:C	2.56	0.48
1:D:295:ILE:HG22	1:D:297:GLU:H	1.78	0.47
1:A:266:THR:HG22	8:A:423:HOH:O	2.13	0.47
1:B:262:GLY:HA2	8:B:412:HOH:O	2.13	0.47
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.44	0.47
1:C:173:LYS:O	1:C:177:VAL:HG23	2.15	0.47
1:D:132:ILE:HD12	1:D:277:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HB3	1:A:140:LEU:CB	2.43	0.47
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.96	0.47
1:B:197:ARG:NH2	1:B:233:LEU:HD12	2.30	0.47
1:D:270:MET:SD	1:D:278:ILE:HD12	2.54	0.47
1:B:200:THR:OG1	1:B:266:THR:OG1	2.26	0.46
1:B:223:LYS:O	1:B:224:ASP:C	2.58	0.46
1:B:203:LYS:HB3	1:B:207:GLY:HA2	1.98	0.46
1:D:274:ILE:O	1:D:277:HIS:N	2.48	0.46
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.50	0.46
1:B:238:ILE:HG23	1:B:267:ILE:HG23	1.98	0.46
1:D:265:VAL:HG12	1:D:267:ILE:CG2	2.46	0.46
1:B:201:MET:SD	1:B:227:ALA:HA	2.55	0.46
1:C:248:GLY:O	1:C:249:LEU:C	2.60	0.45
1:D:239:CYS:HA	1:D:247:ILE:CG1	2.45	0.45
1:D:270:MET:HE1	1:D:278:ILE:HD12	1.97	0.45
1:D:291:MET:O	1:D:293:HIS:CD2	2.70	0.45
1:A:261:SER:OG	1:A:262:GLY:N	2.50	0.45
1:C:139:GLN:O	1:C:291:MET:HE1	2.16	0.45
1:A:157:GLN:O	1:A:190:ILE:HA	2.17	0.45
1:B:224:ASP:HB3	8:B:423:HOH:O	2.16	0.45
1:D:272:ALA:CB	8:D:422:HOH:O	2.59	0.44
1:A:281:ARG:HD2	1:B:122:ASP:HA	1.98	0.44
1:D:218:ILE:HD13	1:D:232:LEU:HD21	1.98	0.44
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.99	0.44
1:D:261:SER:C	1:D:262:GLY:O	2.59	0.44
1:D:203:LYS:HD2	1:D:262:GLY:O	2.18	0.43
1:A:206:THR:HG22	1:A:206:THR:O	2.17	0.43
1:A:137:PHE:HZ	1:C:233:LEU:HD11	1.82	0.43
1:C:197[A]:ARG:NH1	8:C:405:HOH:O	2.32	0.43
1:A:286:ILE:HG23	1:A:290:LEU:HD12	2.01	0.43
1:D:193:ARG:HD2	1:D:240:GLU:OE2	2.19	0.43
1:C:236:HIS:CD2	1:C:269:ILE:HD12	2.54	0.43
1:C:242:ASN:ND2	1:C:261:SER:OG	2.51	0.43
1:D:140:LEU:HD12	1:D:282:MET:SD	2.59	0.43
1:C:170:SER:O	1:C:171:SER:C	2.61	0.43
1:A:137:PHE:CE2	1:A:195:PHE:CE2	3.07	0.43
1:C:145:SER:C	1:C:147:ALA:N	2.77	0.43
1:D:224:ASP:O	1:D:229:ARG:NH1	2.50	0.43
1:D:249:LEU:HD21	1:D:293:HIS:CD2	2.54	0.42
1:D:258:LEU:O	1:D:261:SER:HB3	2.19	0.42
1:C:114:GLU:HG2	1:C:115:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ASP:OD1	1:D:193:ARG:HG3	2.19	0.42
1:C:161:ILE:HG12	1:C:188:MET:HG2	2.01	0.42
1:D:218:ILE:CD1	1:D:232:LEU:HD11	2.50	0.42
1:C:119:LYS:HD3	1:C:123:GLY:O	2.19	0.42
1:D:295:ILE:CG2	1:D:296:PRO:HD2	2.46	0.42
1:C:294:THR:HG22	1:C:295:ILE:N	2.35	0.42
1:D:270:MET:CE	1:D:278:ILE:HD12	2.50	0.42
1:D:272:ALA:O	1:D:274:ILE:N	2.53	0.42
1:D:249:LEU:HD21	1:D:293:HIS:NE2	2.35	0.42
1:D:283:ALA:O	1:D:285:SER:N	2.52	0.42
1:C:238:ILE:HG23	1:C:267:ILE:HG23	2.02	0.42
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.01	0.41
1:D:142:GLN:HG2	1:D:143:ALA:O	2.20	0.41
1:D:203:LYS:HD2	1:D:263:THR:HA	2.02	0.41
1:D:204:ASP:OD1	1:D:204:ASP:C	2.63	0.41
1:D:204:ASP:N	1:D:208:HIS:O	2.52	0.41
1:A:192:ASP:O	1:A:193:ARG:C	2.62	0.41
1:D:244:GLN:NE2	1:D:295:ILE:HD11	2.35	0.41
1:C:251:ASP:HB3	1:D:206:THR:HG21	2.02	0.41
1:D:244:GLN:O	1:D:246:VAL:HG13	2.19	0.41
1:A:237:ASN:CG	1:A:275:PHE:CD2	2.98	0.41
1:B:198:THR:HG23	1:B:266:THR:HG23	2.02	0.41
1:D:195:PHE:CD2	1:D:278:ILE:HD11	2.55	0.41
1:C:197[A]:ARG:NH2	8:C:406:HOH:O	2.47	0.41
1:D:248:GLY:O	1:D:249:LEU:O	2.39	0.41
1:D:261:SER:HB3	1:D:265:VAL:HG22	2.01	0.41
1:B:245:ASN:OD1	1:B:245:ASN:C	2.63	0.41
1:B:253:GLN:NE2	8:B:406:HOH:O	2.51	0.41
1:C:294:THR:CG2	1:C:295:ILE:N	2.84	0.41
1:D:247:ILE:HG22	1:D:287:MET:HE3	2.01	0.41
1:D:275:PHE:CZ	1:D:279:ILE:HG21	2.56	0.41
1:B:270:MET:O	1:B:271:PRO:C	2.64	0.41
1:D:145:SER:O	1:D:148:SER:OG	2.30	0.40
1:D:143:ALA:O	1:D:144:ASN:CB	2.68	0.40
1:D:215:ASN:HB2	8:D:403:HOH:O	2.21	0.40
1:D:222:VAL:O	1:D:225:SER:HB3	2.22	0.40
1:B:201:MET:HE3	1:B:201:MET:HB2	1.92	0.40
1:B:202:HIS:HA	1:B:263:THR:O	2.22	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/195 (97%)	179 (94%)	9 (5%)	2 (1%)	11	9
1	B	192/195 (98%)	179 (93%)	10 (5%)	3 (2%)	7	5
1	C	194/195 (100%)	180 (93%)	13 (7%)	1 (0%)	24	25
1	D	190/195 (97%)	158 (83%)	29 (15%)	3 (2%)	7	5
All	All	766/780 (98%)	696 (91%)	61 (8%)	9 (1%)	10	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	LYS
1	D	249	LEU
1	B	120	ASP
1	D	262	GLY
1	D	144	ASN
1	B	263	THR
1	A	193	ARG
1	A	279	ILE
1	C	210	GLY

4.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/168 (99%)	157 (95%)	9 (5%)	20	22
1	B	167/168 (99%)	159 (95%)	8 (5%)	23	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	169/168 (101%)	162 (96%)	7 (4%)	27	33
1	D	166/168 (99%)	160 (96%)	6 (4%)	31	39
All	All	668/672 (99%)	638 (96%)	30 (4%)	24	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	A	118	CYS
1	A	140	LEU
1	A	148	SER
1	A	226	SER
1	A	252	SER
1	A	266	THR
1	A	281	ARG
1	A	289	SER
1	B	122	ASP
1	B	125	ILE
1	B	198	THR
1	B	202	HIS
1	B	206	THR
1	B	220	SER
1	B	264	VAL
1	B	266	THR
1	C	117	LEU
1	C	122	ASP
1	C	140	LEU
1	C	209	VAL
1	C	259	SER
1	C	263	THR
1	C	266	THR
1	D	125	ILE
1	D	184	GLU
1	D	190	ILE
1	D	266	THR
1	D	267	ILE
1	D	289	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	162	ASN
1	A	180	GLN
1	B	134	ASN
1	B	139	GLN
1	B	162	ASN
1	B	215	ASN
1	B	230	ASN
1	C	110	GLN
1	C	134	ASN
1	C	139	GLN
1	C	202	HIS
1	C	253	GLN
1	D	142	GLN
1	D	162	ASN
1	D	180	GLN
1	D	237	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 13 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLY	C	304	-	4,4,4	0.97	0	3,4,4	1.07	0
5	GLY	D	307	-	4,4,4	1.01	0	3,4,4	1.01	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
5	GLY	C	304	-	-	2/2/2/2	-
5	GLY	D	307	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

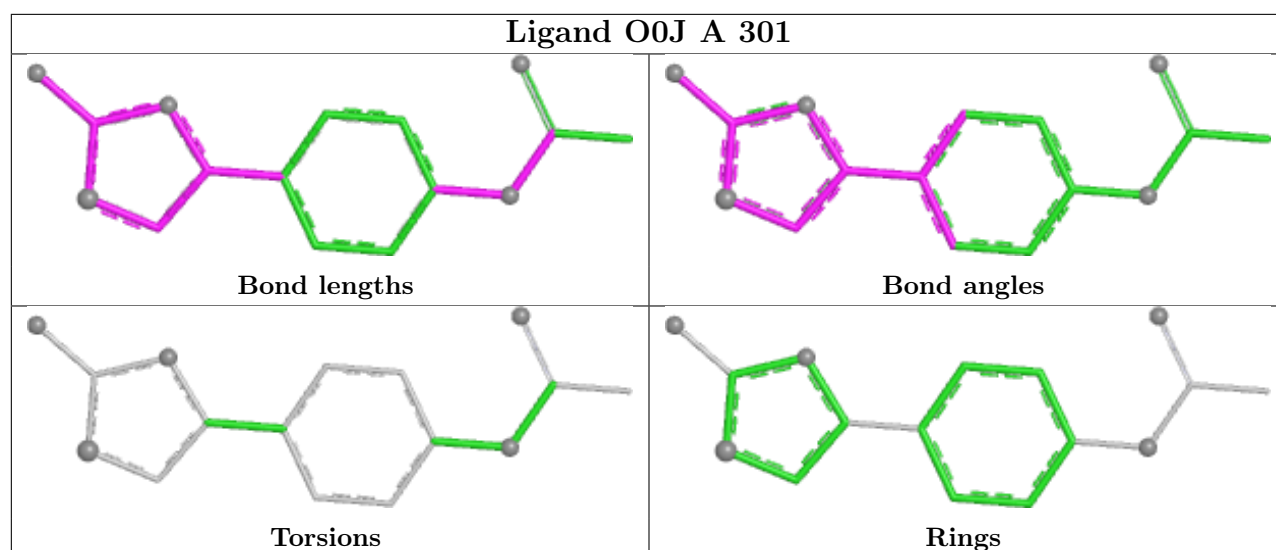
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	304	GLY	O-C-CA-N
5	C	304	GLY	OXT-C-CA-N
5	D	307	GLY	O-C-CA-N
5	D	307	GLY	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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%)	0.52	9 (4%)	36 35	4, 49, 82, 153	1 (0%)
1	B	193/195 (98%)	0.53	11 (5%)	29 28	3, 50, 77, 104	1 (0%)
1	C	193/195 (98%)	0.72	12 (6%)	26 25	4, 51, 82, 110	3 (1%)
1	D	191/195 (97%)	1.65	58 (30%)	1 1	5, 63, 89, 113	1 (0%)
All	All	768/780 (98%)	0.85	90 (11%)	9 8	3, 54, 84, 153	6 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	273[A]	PHE	11.0
1	C	197[A]	ARG	9.7
1	A	273[A]	PHE	9.6
1	C	273[A]	PHE	7.2
1	B	273[A]	PHE	6.7
1	D	149	LEU	6.5
1	C	144[A]	ASN	5.6
1	B	106	ALA	5.6
1	D	141	VAL	5.5
1	D	125	ILE	5.3
1	D	298	VAL	5.0
1	D	189	THR	4.5
1	D	283	ALA	4.4
1	D	178	LEU	4.3
1	D	258	LEU	4.2
1	C	106	ALA	4.2
1	D	116	ILE	4.1
1	D	295	ILE	4.1
1	D	213	PHE	3.9
1	A	283	ALA	3.9
1	D	209	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	3.8
1	B	125	ILE	3.8
1	C	110	GLN	3.8
1	D	286	ILE	3.7
1	D	182	PHE	3.7
1	A	284	PRO	3.6
1	C	108	ILE	3.6
1	D	296	PRO	3.5
1	D	140	LEU	3.5
1	D	269	ILE	3.5
1	B	264	VAL	3.5
1	D	144	ASN	3.5
1	A	282	MET	3.4
1	D	152	LEU	3.3
1	D	190	ILE	3.2
1	D	265	VAL	3.2
1	D	112	ILE	3.2
1	C	209	VAL	3.1
1	D	238	ILE	3.1
1	D	161	ILE	3.1
1	D	285	SER	3.1
1	D	138	VAL	3.1
1	D	186	ILE	3.1
1	D	254	ILE	3.1
1	A	182	PHE	3.0
1	D	117	LEU	3.0
1	D	153	ARG	2.9
1	B	111	GLY	2.9
1	D	174	ALA	2.9
1	D	280	LYS	2.8
1	D	239	CYS	2.8
1	D	167	ALA	2.8
1	D	187	THR	2.7
1	B	263	THR	2.7
1	D	177	VAL	2.7
1	C	109	LYS	2.7
1	C	258	LEU	2.6
1	D	287	MET	2.6
1	D	126	GLY	2.5
1	C	281	ARG	2.5
1	A	285	SER	2.5
1	D	291	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	2.5
1	D	284	PRO	2.4
1	D	145	SER	2.3
1	B	202	HIS	2.3
1	B	118	CYS	2.3
1	D	147	ALA	2.3
1	C	117	LEU	2.3
1	D	127	LEU	2.3
1	D	183	GLY	2.2
1	D	249	LEU	2.2
1	D	268	THR	2.2
1	D	159	LEU	2.2
1	C	296	PRO	2.2
1	D	241	ILE	2.2
1	D	110	GLN	2.1
1	B	260	THR	2.1
1	A	110	GLN	2.1
1	D	136	ILE	2.1
1	D	121	GLN	2.1
1	D	146	PRO	2.1
1	D	157	GLN	2.1
1	D	163	GLY	2.1
1	D	181	ALA	2.1
1	A	263	THR	2.1
1	D	155	GLY	2.1
1	D	247	ILE	2.1
1	B	228	ALA	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

5.4 Other polymers [i](#)

There are no such residues in this entry.