



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:17 PM EDT

PDB ID : 3F5X / pdb_00003f5x
Title : CDK-2-Cyclin complex with indazole inhibitor 9 bound at its active site
Authors : Kiefer, J.R.; Day, J.E.; Caspers, N.L.; Mathis, K.J.; Kretzmer, K.K.; Weinberg, R.A.; Reitz, B.A.; Stegeman, R.A.; Trujillo, J.I.; Huang, W.; Thorarensen, A.; Xing, L.; Wrightstone, A.; Christine, L.; Compton, R.; Li, X.
Deposited on : 2008-11-04
Resolution : 2.40 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

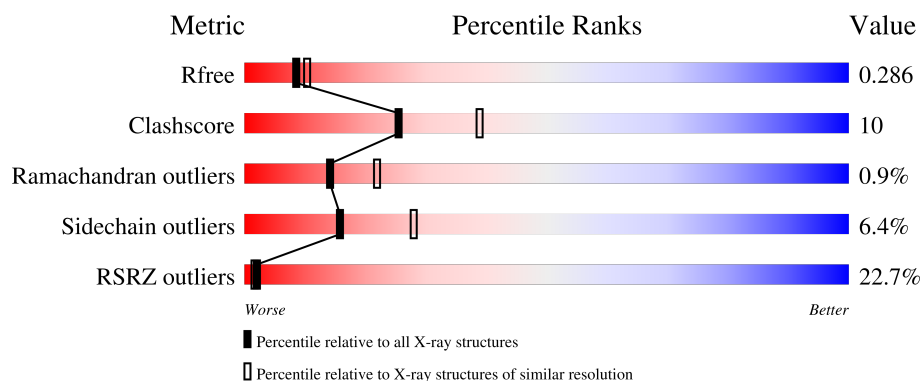
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	298	28% 80% 16% • •
1	C	298	24% 73% 20% 5% •
2	B	256	18% 84% 15% •
2	D	256	20% 83% 15% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9069 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.

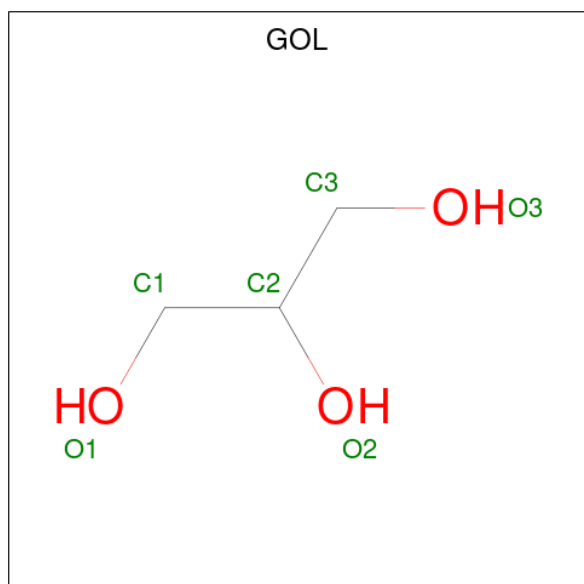
- Molecule 1 is a protein called Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2390	1555	406	421	8			
1	C	298	Total	C	N	O	S	0	0	0
			2398	1559	408	423	8			

- Molecule 2 is a protein called Cyclin-A2.

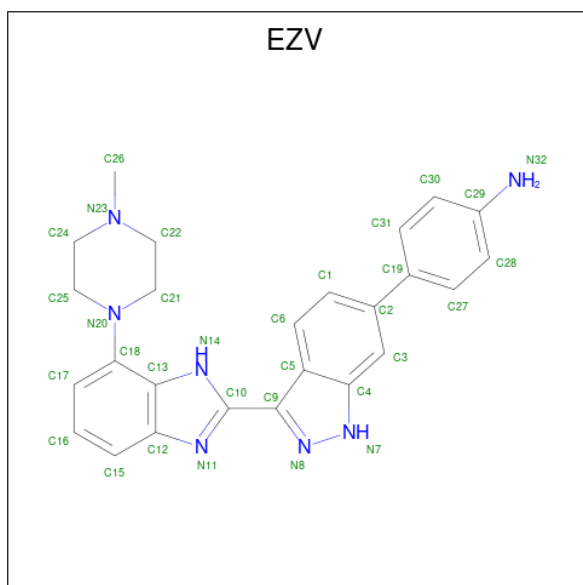
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2070	1340	337	382	11			
2	D	255	Total	C	N	O	S	0	0	0
			2062	1336	336	379	11			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



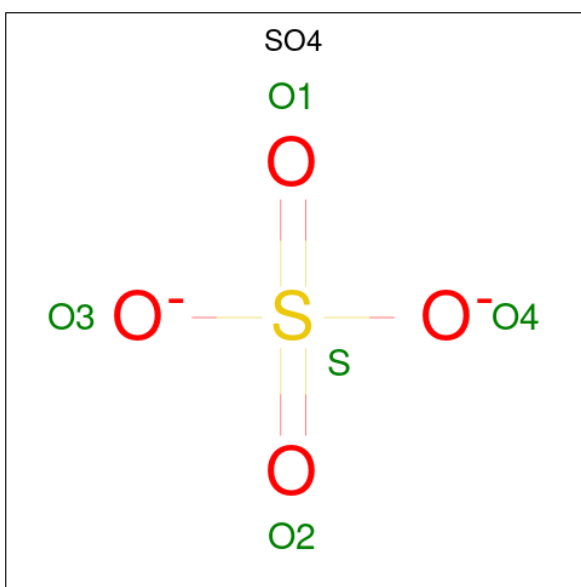
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-{3-[7-(4-methylpiperazin-1-yl)-1H-benzimidazol-2-yl]-1H-indazol-6-yl}aniline (CCD ID: EZV) (formula: C₂₅H₂₅N₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			32	25	7		
4	C	1	Total	C	N	0	0
			32	25	7		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

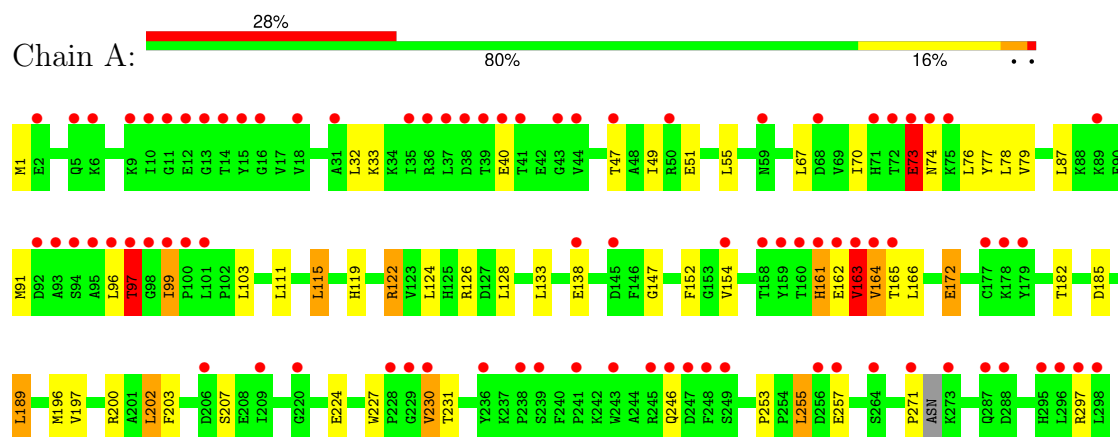
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	10	Total	O	0	0
			10	10		
6	C	3	Total	O	0	0
			3	3		
6	D	14	Total	O	0	0
			14	14		

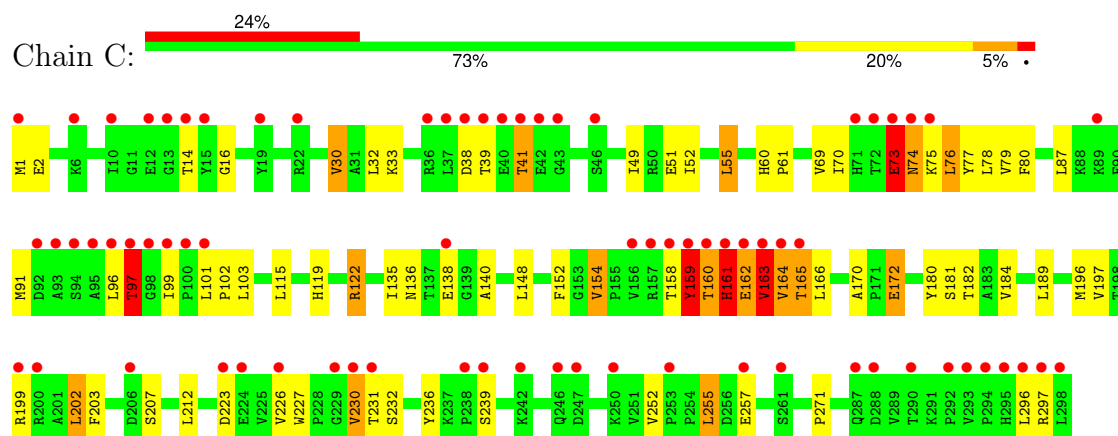
3 Residue-property plots [i](#)

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.

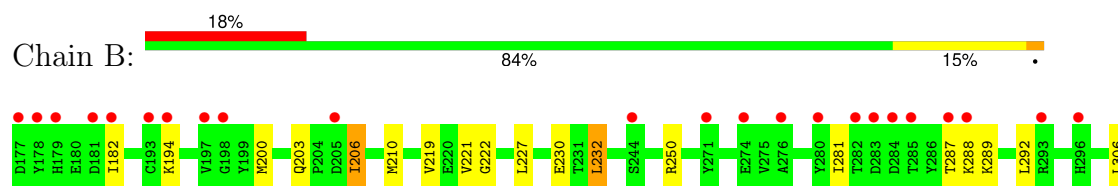
• Molecule 1: Cell division protein kinase 2

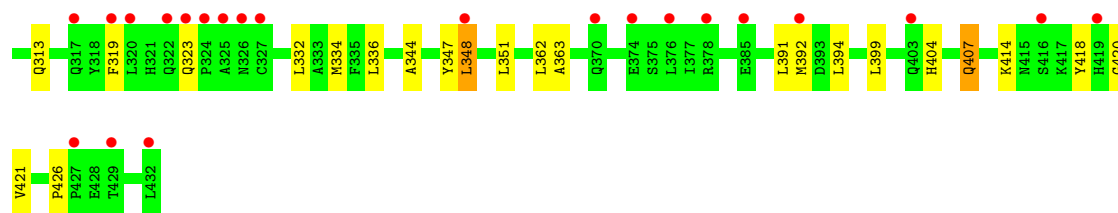


• Molecule 1: Cell division protein kinase 2

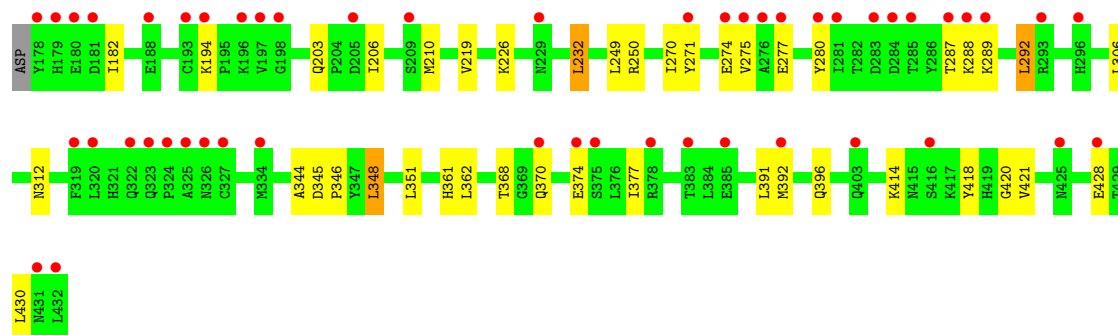
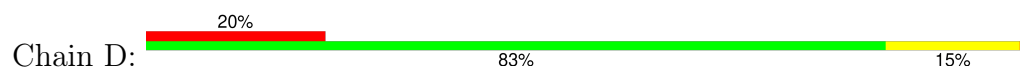


• Molecule 2: Cyclin-A2





● Molecule 2: Cyclin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.05Å 184.05Å 214.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.40) 99.2 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.283 0.268 , 0.286	Depositor DCC
R_{free} test set	4169 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9069	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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: EZV, SO4, GOL

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	0.56	0/2451	0.80	3/3324 (0.1%)
1	C	0.55	0/2460	0.83	6/3338 (0.2%)
2	B	0.50	0/2119	0.76	0/2875
2	D	0.53	0/2111	0.82	3/2864 (0.1%)
All	All	0.54	0/9141	0.80	12/12401 (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	C	2	1
2	D	1	0
All	All	3	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	280	TYR	N-CA-C	10.04	123.47	111.82
1	C	163	VAL	N-CA-C	8.19	126.38	109.34
2	D	392	MET	N-CA-C	6.62	118.49	111.28
1	C	160	THR	CB-CA-C	6.06	121.84	109.55
1	C	97	THR	N-CA-CB	5.92	120.50	110.49
1	A	253	PRO	N-CA-C	5.75	117.71	110.70
2	D	280	TYR	N-CA-CB	5.55	118.88	110.28
1	C	159	TYR	N-CA-C	5.33	117.63	109.95
1	A	163	VAL	N-CA-C	5.27	120.30	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	GLY	N-CA-C	5.26	117.69	110.69
1	C	159	TYR	N-CA-CB	5.16	118.44	110.60
1	A	99	ILE	N-CA-C	-5.03	104.31	108.63

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	97	THR	CA
1	C	163	VAL	CA
2	D	280	TYR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	HIS	Peptide
1	C	161	HIS	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	2390	0	2443	54	0
1	C	2398	0	2450	72	0
2	B	2070	0	2091	33	0
2	D	2062	0	2087	33	0
3	A	6	0	8	2	0
3	C	6	0	8	0	0
4	A	32	0	25	5	0
4	C	32	0	25	3	0
5	D	5	0	0	0	0
6	A	41	0	0	0	0
6	B	10	0	0	0	0
6	C	3	0	0	0	0
6	D	14	0	0	0	0
All	All	9069	0	9137	174	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 (174) 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:163:VAL:HG23	1:A:164:VAL:HG23	1.46	0.96
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.49	0.95
2:B:210:MET:HE1	2:B:250:ARG:CB	2.01	0.90
1:A:126:ARG:O	1:A:164:VAL:HG22	1.76	0.85
1:C:33:LYS:NZ	4:C:300:EZV:H28	1.94	0.83
1:A:33:LYS:NZ	4:A:300:EZV:H28	1.96	0.80
1:C:148:LEU:HD11	1:C:163:VAL:CG2	2.13	0.79
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.64	0.78
1:C:152:PHE:CE2	2:D:182:ILE:CD1	2.67	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.76
1:C:148:LEU:CD1	1:C:163:VAL:HB	2.15	0.76
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.69	0.75
1:C:1:MET:HE3	1:C:77:TYR:CD1	2.22	0.74
1:A:1:MET:HE1	1:A:70:ILE:HD13	1.68	0.74
1:A:163:VAL:CG2	1:A:164:VAL:HG23	2.18	0.74
1:C:152:PHE:CE2	2:D:182:ILE:HD11	2.23	0.73
1:A:197:VAL:HG11	1:A:255:LEU:HD13	1.72	0.72
1:C:1:MET:CE	1:C:70:ILE:HD13	2.19	0.72
2:D:210:MET:HE1	2:D:250:ARG:CB	2.20	0.72
1:C:33:LYS:HZ1	4:C:300:EZV:H28	1.55	0.71
1:C:1:MET:HE1	1:C:70:ILE:CD1	2.21	0.71
1:A:128:LEU:HD13	1:A:189:LEU:HD13	1.73	0.70
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.27	0.70
1:C:227:TRP:O	1:C:230:VAL:HG22	1.92	0.69
1:C:148:LEU:HD11	1:C:163:VAL:HG21	1.73	0.69
2:B:194:LYS:HE3	2:B:351:LEU:HD21	1.74	0.68
1:A:33:LYS:HZ1	4:A:300:EZV:H28	1.58	0.68
1:C:197:VAL:HG11	1:C:255:LEU:HD13	1.76	0.68
1:C:163:VAL:O	1:C:164:VAL:C	2.36	0.67
1:C:158:THR:HG22	1:C:180:TYR:CD1	2.31	0.65
1:C:158:THR:HA	1:C:180:TYR:CE1	2.31	0.65
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.79	0.65
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.80	0.64
1:A:1:MET:CE	1:A:70:ILE:HD13	2.29	0.62
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.34	0.62
2:B:210:MET:HE1	2:B:250:ARG:HB3	1.82	0.62
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.35	0.61
1:A:96:LEU:O	1:A:97:THR:HG23	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:PHE:CZ	2:D:182:ILE:HD11	2.35	0.61
2:B:221:VAL:HG11	2:B:281:ILE:HD13	1.83	0.60
1:C:51:GLU:O	1:C:55:LEU:HB2	2.02	0.60
1:A:163:VAL:O	1:A:164:VAL:C	2.44	0.59
1:A:51:GLU:OE2	4:A:300:EZV:N32	2.34	0.59
1:A:163:VAL:CG2	1:A:164:VAL:N	2.65	0.59
1:C:227:TRP:CG	1:C:230:VAL:HG13	2.39	0.58
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.86	0.57
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.87	0.57
1:A:152:PHE:CE2	2:B:182:ILE:CD1	2.87	0.57
1:A:73:GLU:CG	1:A:74:ASN:H	2.17	0.57
1:A:91:MET:HE3	1:A:196:MET:HG2	1.87	0.56
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.86	0.56
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.86	0.56
1:A:122:ARG:HB3	2:B:182:ILE:HD13	1.88	0.56
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.88	0.55
2:B:319:PHE:HE2	2:B:334:MET:HE1	1.71	0.55
1:C:30:VAL:HG21	1:C:79:VAL:CG1	2.36	0.55
1:C:73:GLU:CG	1:C:74:ASN:H	2.20	0.55
1:C:148:LEU:HD11	1:C:163:VAL:CB	2.37	0.55
2:B:200:MET:SD	2:B:206:ILE:HD12	2.46	0.55
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.43	0.54
2:D:275:VAL:HG11	2:D:292:LEU:HD13	1.89	0.54
1:C:223:ASP:H	1:C:226:VAL:HG12	1.73	0.54
1:A:47:THR:HG23	1:A:147:GLY:CA	2.37	0.54
1:C:159:TYR:CE1	1:C:162:GLU:HG3	2.42	0.54
1:C:159:TYR:HB3	2:D:270:ILE:HD13	1.90	0.54
1:A:1:MET:HE1	1:A:70:ILE:CD1	2.37	0.54
2:D:194:LYS:HE3	2:D:351:LEU:HD21	1.90	0.54
1:A:152:PHE:CZ	2:B:182:ILE:HD11	2.43	0.53
1:A:73:GLU:HG2	1:A:74:ASN:H	1.73	0.53
1:C:166:LEU:HD21	1:C:207:SER:C	2.33	0.53
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.91	0.53
1:A:1:MET:HE3	1:A:77:TYR:CD1	2.44	0.53
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.91	0.52
1:A:51:GLU:OE2	4:A:300:EZV:H28	2.10	0.52
1:A:91:MET:HE3	1:A:196:MET:CG	2.39	0.52
1:C:162:GLU:OE1	1:C:163:VAL:HG23	2.10	0.52
1:A:51:GLU:O	1:A:55:LEU:HB2	2.09	0.51
1:C:148:LEU:HD11	1:C:163:VAL:HB	1.89	0.51
1:A:33:LYS:HZ3	4:A:300:EZV:H28	1.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD22	1:A:119:HIS:CE1	2.46	0.51
1:C:69:VAL:HG13	1:C:76:LEU:HD21	1.92	0.51
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.93	0.51
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.22	0.51
2:D:287:THR:HG22	2:D:289:LYS:H	1.76	0.50
1:C:162:GLU:CD	1:C:163:VAL:HG23	2.37	0.50
1:A:115:LEU:HD12	1:A:189:LEU:HD22	1.94	0.50
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.94	0.50
2:B:203:GLN:HG2	2:B:206:ILE:HG13	1.94	0.50
2:B:221:VAL:CG1	2:B:281:ILE:HD13	2.42	0.49
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.95	0.49
2:B:319:PHE:CE2	2:B:334:MET:HE1	2.47	0.49
1:C:158:THR:HG22	1:C:180:TYR:CE1	2.46	0.49
2:B:418:TYR:O	2:B:421:VAL:HG13	2.12	0.49
1:C:159:TYR:CZ	1:C:162:GLU:HG3	2.47	0.49
1:A:163:VAL:HG22	1:A:164:VAL:N	2.28	0.48
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.94	0.48
2:B:399:LEU:HD23	2:B:426:PRO:HG2	1.95	0.48
2:B:210:MET:CE	2:B:250:ARG:HB2	2.31	0.48
2:D:210:MET:CE	2:D:250:ARG:HB2	2.43	0.48
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.95	0.48
2:B:287:THR:HG22	2:B:289:LYS:H	1.79	0.48
1:C:161:HIS:HB2	2:D:271:TYR:OH	2.14	0.48
1:A:96:LEU:O	1:A:96:LEU:HG	2.14	0.48
1:A:111:LEU:CD2	1:A:133:LEU:HD22	2.44	0.48
1:C:197:VAL:CG1	1:C:255:LEU:HD13	2.42	0.48
1:A:73:GLU:CG	1:A:74:ASN:N	2.78	0.47
1:C:73:GLU:HG2	1:C:74:ASN:H	1.79	0.47
1:A:166:LEU:HD21	1:A:207:SER:C	2.40	0.47
1:C:164:VAL:O	1:C:165:THR:C	2.55	0.47
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.49	0.47
2:D:287:THR:HG22	2:D:288:LYS:N	2.30	0.47
1:C:148:LEU:CD1	1:C:163:VAL:CG2	2.91	0.46
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.50	0.46
1:C:33:LYS:HZ3	4:C:300:EZV:H28	1.78	0.46
1:C:135:ILE:HD12	1:C:296:LEU:HD21	1.97	0.46
1:A:152:PHE:CE2	2:B:182:ILE:HD11	2.50	0.46
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.99	0.46
1:A:164:VAL:O	1:A:165:THR:C	2.59	0.46
1:A:40:GLU:O	2:B:288:LYS:HD3	2.16	0.45
1:C:158:THR:HG22	1:C:180:TYR:CG	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:SER:O	1:C:184:VAL:HG22	2.16	0.45
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.47	0.45
1:C:119:HIS:CE1	1:C:182:THR:HB	2.51	0.45
2:B:222:GLY:HA2	2:B:227:LEU:HD12	1.99	0.45
1:C:159:TYR:CG	2:D:270:ILE:CG2	3.00	0.45
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.99	0.45
1:A:47:THR:HG23	1:A:147:GLY:HA3	1.99	0.45
2:B:194:LYS:CE	2:B:351:LEU:HD21	2.45	0.45
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.47	0.44
2:B:287:THR:HG22	2:B:288:LYS:N	2.31	0.44
2:D:418:TYR:O	2:D:421:VAL:HG13	2.16	0.44
2:B:404:HIS:O	2:B:407:GLN:NE2	2.45	0.44
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.48	0.44
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.47	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.99	0.44
1:C:101:LEU:N	1:C:102:PRO:CD	2.81	0.44
2:D:203:GLN:HG2	2:D:206:ILE:CG1	2.48	0.44
1:A:122:ARG:HB3	2:B:182:ILE:CD1	2.49	0.43
1:C:172:GLU:HG2	1:C:271:PRO:HG3	2.00	0.43
2:D:275:VAL:HG11	2:D:292:LEU:CD1	2.47	0.43
1:C:30:VAL:HG22	1:C:80:PHE:O	2.19	0.43
1:A:197:VAL:CG1	1:A:255:LEU:HD13	2.46	0.43
1:C:122:ARG:HD2	1:C:122:ARG:O	2.19	0.43
1:C:91:MET:HE3	1:C:196:MET:HG2	2.01	0.43
1:C:1:MET:HE2	1:C:70:ILE:HG21	2.01	0.43
1:C:159:TYR:CG	2:D:270:ILE:HG21	2.53	0.43
2:D:362:LEU:HD13	2:D:430:LEU:HD21	2.01	0.43
1:C:202:LEU:HD13	1:C:203:PHE:CZ	2.54	0.42
1:C:231:THR:HA	1:C:236:TYR:CD1	2.53	0.42
1:C:122:ARG:HB3	2:D:182:ILE:HD13	2.01	0.42
1:C:159:TYR:CD1	2:D:270:ILE:CG2	3.02	0.42
1:A:67:LEU:HB3	3:A:299:GOL:C1	2.50	0.42
1:C:38:ASP:OD2	1:C:41:THR:OG1	2.32	0.42
2:B:414:LYS:HA	2:B:420:GLY:HA2	2.02	0.42
2:D:368:THR:HB	2:D:370:GLN:HE21	1.85	0.42
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.35	0.42
1:C:163:VAL:O	1:C:164:VAL:O	2.38	0.42
1:C:148:LEU:CD1	1:C:163:VAL:CB	2.89	0.41
2:B:319:PHE:HE2	2:B:334:MET:CE	2.30	0.41
1:C:39:THR:HG22	1:C:39:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:TYR:OH	2:B:394:LEU:HA	2.20	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.55	0.41
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.19	0.41
1:C:96:LEU:O	1:C:96:LEU:HG	2.19	0.41
1:A:124:LEU:HD21	1:A:182:THR:HA	2.03	0.41
1:A:67:LEU:HB3	3:A:299:GOL:H12	2.03	0.41
1:C:154:VAL:HG21	2:D:312:ASN:ND2	2.36	0.41
2:D:194:LYS:CE	2:D:351:LEU:HD21	2.50	0.41
1:A:138:GLU:N	1:A:138:GLU:CD	2.79	0.40
1:C:97:THR:HG23	1:C:199:ARG:NH1	2.36	0.40
2:D:274:GLU:HG3	2:D:277:GLU:HG2	2.03	0.40
2:D:345:ASP:HA	2:D:346:PRO:HA	1.93	0.40
2:D:362:LEU:CD1	2:D:430:LEU:HD21	2.51	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	293/298 (98%)	279 (95%)	10 (3%)	4 (1%)	9	13
1	C	296/298 (99%)	282 (95%)	8 (3%)	6 (2%)	6	7
2	B	254/256 (99%)	251 (99%)	3 (1%)	0	100	100
2	D	253/256 (99%)	251 (99%)	2 (1%)	0	100	100
All	All	1096/1108 (99%)	1063 (97%)	23 (2%)	10 (1%)	14	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	97	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	VAL
1	C	164	VAL
1	A	97	THR
1	C	73	GLU
1	A	73	GLU
1	A	161	HIS
1	C	161	HIS
1	C	165	THR

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	262/263 (100%)	243 (93%)	19 (7%)	13	22
1	C	263/263 (100%)	234 (89%)	29 (11%)	6	9
2	B	230/230 (100%)	222 (96%)	8 (4%)	32	53
2	D	229/230 (100%)	222 (97%)	7 (3%)	35	57
All	All	984/986 (100%)	921 (94%)	63 (6%)	16	28

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	76	LEU
1	A	78	LEU
1	A	87	LEU
1	A	97	THR
1	A	115	LEU
1	A	122	ARG
1	A	154	VAL
1	A	162	GLU
1	A	163	VAL
1	A	172	GLU
1	A	189	LEU
1	A	200	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	202	LEU
1	A	230	VAL
1	A	246	GLN
1	A	255	LEU
1	A	257	GLU
1	A	297	ARG
2	B	206	ILE
2	B	232	LEU
2	B	292	LEU
2	B	323	GLN
2	B	348	LEU
2	B	391	LEU
2	B	392	MET
2	B	407	GLN
1	C	2	GLU
1	C	14	THR
1	C	30	VAL
1	C	41	THR
1	C	55	LEU
1	C	73	GLU
1	C	74	ASN
1	C	75	LYS
1	C	76	LEU
1	C	87	LEU
1	C	97	THR
1	C	122	ARG
1	C	138	GLU
1	C	154	VAL
1	C	159	TYR
1	C	160	THR
1	C	161	HIS
1	C	162	GLU
1	C	163	VAL
1	C	172	GLU
1	C	202	LEU
1	C	212	LEU
1	C	230	VAL
1	C	232	SER
1	C	239	SER
1	C	252	VAL
1	C	255	LEU
1	C	257	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	297	ARG
2	D	226	LYS
2	D	232	LEU
2	D	249	LEU
2	D	292	LEU
2	D	348	LEU
2	D	396	GLN
2	D	428	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	85	GLN
2	B	208	ASN
2	B	312	ASN
2	B	317	GLN
2	B	323	GLN
2	B	370	GLN
2	B	403	GLN
2	B	404	HIS
2	B	406	GLN
1	C	287	GLN
2	D	208	ASN
2	D	233	HIS
2	D	370	GLN
2	D	406	GLN
2	D	415	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	EZV	C	300	-	37,37,37	1.18	4 (10%)	51,54,54	2.31	19 (37%)
3	GOL	C	299	-	5,5,5	0.35	0	5,5,5	0.14	0
3	GOL	A	299	-	5,5,5	0.38	0	5,5,5	0.38	0
5	SO4	D	1	-	4,4,4	0.24	0	6,6,6	0.11	0
4	EZV	A	300	-	37,37,37	1.16	4 (10%)	51,54,54	2.32	19 (37%)

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	EZV	A	300	-	-	0/11/22/22	0/6/6/6
3	GOL	C	299	-	-	0/4/4/4	-
4	EZV	C	300	-	-	0/11/22/22	0/6/6/6
3	GOL	A	299	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	300	EZV	C10-N14	-3.04	1.31	1.36
4	A	300	EZV	C10-N14	-3.04	1.31	1.36
4	C	300	EZV	C10-N11	2.71	1.36	1.32
4	A	300	EZV	C10-N11	2.65	1.36	1.32
4	C	300	EZV	C13-C12	-2.60	1.38	1.40
4	A	300	EZV	C5-C4	-2.50	1.38	1.41
4	C	300	EZV	C5-C4	-2.43	1.38	1.41
4	A	300	EZV	C13-C12	-2.27	1.38	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	EZV	C13-C12-N11	-7.91	104.50	109.91
4	A	300	EZV	C13-C12-N11	-7.44	104.83	109.91
4	C	300	EZV	C12-C13-N14	5.88	110.30	105.40
4	A	300	EZV	C12-C13-N14	5.83	110.26	105.40
4	A	300	EZV	C9-N8-N7	-4.37	102.87	106.07
4	C	300	EZV	C15-C12-C13	4.34	124.21	120.24
4	A	300	EZV	C15-C12-C13	4.32	124.20	120.24
4	A	300	EZV	C4-N7-N8	4.07	114.92	111.90
4	C	300	EZV	C12-N11-C10	3.94	108.68	104.68
4	A	300	EZV	C24-N23-C22	3.81	115.61	109.54
4	C	300	EZV	C9-N8-N7	-3.56	103.47	106.07
4	C	300	EZV	C4-N7-N8	3.49	114.49	111.90
4	A	300	EZV	C12-N11-C10	3.38	108.11	104.68
4	C	300	EZV	C1-C6-C5	-3.03	115.87	120.86
4	A	300	EZV	C1-C6-C5	-3.01	115.90	120.86
4	C	300	EZV	C21-C22-N23	-2.82	106.33	110.86
4	C	300	EZV	N14-C10-N11	-2.81	110.21	113.22
4	C	300	EZV	C24-N23-C22	2.69	113.82	109.54
4	C	300	EZV	C21-N20-C18	-2.63	109.95	116.19
4	A	300	EZV	C16-C15-C12	-2.60	114.19	118.97
4	A	300	EZV	C17-C18-C13	-2.57	114.84	119.01
4	A	300	EZV	C21-N20-C18	-2.56	110.11	116.19
4	C	300	EZV	C3-C4-C5	2.55	124.55	122.52
4	C	300	EZV	C17-C18-C13	-2.54	114.89	119.01
4	C	300	EZV	C16-C15-C12	-2.49	114.39	118.97
4	A	300	EZV	C2-C3-C4	-2.48	115.20	119.59
4	C	300	EZV	C16-C17-C18	2.46	123.25	118.28
4	C	300	EZV	C2-C3-C4	-2.44	115.28	119.59
4	A	300	EZV	C16-C17-C18	2.40	123.12	118.28
4	C	300	EZV	C25-C24-N23	-2.28	107.19	110.86
4	C	300	EZV	C5-C4-N7	-2.26	104.96	106.59
4	C	300	EZV	C6-C1-C2	2.26	124.02	121.12
4	A	300	EZV	C21-C22-N23	-2.26	107.23	110.86
4	A	300	EZV	C3-C4-C5	2.24	124.31	122.52
4	A	300	EZV	N14-C10-N11	-2.08	111.00	113.22
4	A	300	EZV	C5-C4-N7	-2.07	105.10	106.59
4	A	300	EZV	C1-C2-C3	2.05	121.06	118.23
4	A	300	EZV	C18-C13-N14	-2.01	128.64	130.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

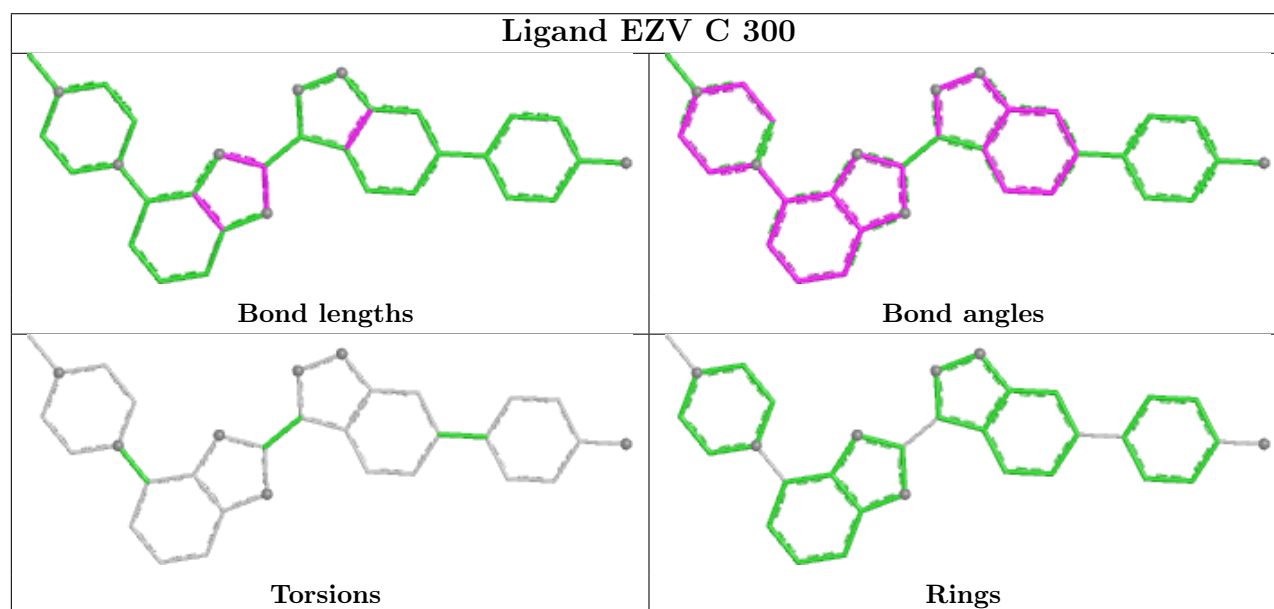
Mol	Chain	Res	Type	Atoms
3	A	299	GOL	O1-C1-C2-O2
3	A	299	GOL	O1-C1-C2-C3
3	A	299	GOL	C1-C2-C3-O3
3	A	299	GOL	O2-C2-C3-O3

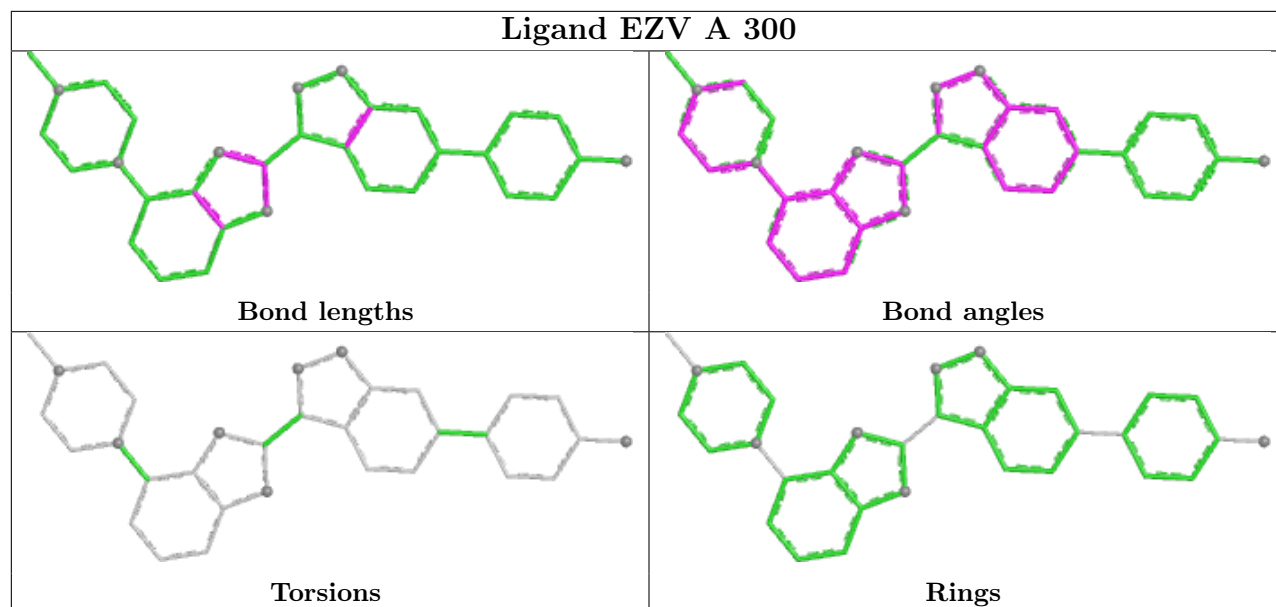
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	300	EZV	3	0
3	A	299	GOL	2	0
4	A	300	EZV	5	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	297/298 (99%)	1.54	83 (27%) 1 1	42, 52, 71, 77	0
1	C	298/298 (100%)	1.57	73 (24%) 2 1	42, 53, 74, 92	0
2	B	256/256 (100%)	1.09	45 (17%) 4 3	41, 51, 68, 78	0
2	D	255/256 (99%)	1.30	50 (19%) 3 2	40, 50, 66, 75	0
All	All	1106/1108 (99%)	1.39	251 (22%) 2 2	40, 52, 70, 92	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	10.1
1	C	162	GLU	8.8
2	B	323	GLN	8.7
2	D	323	GLN	8.5
2	D	324	PRO	8.5
1	A	15	TYR	8.0
1	C	71	HIS	7.8
1	A	39	THR	7.7
2	D	178	TYR	7.5
1	C	96	LEU	7.4
1	A	160	THR	7.3
1	A	161	HIS	7.3
1	C	163	VAL	7.3
2	D	283	ASP	7.2
1	A	159	TYR	7.2
2	D	193	CYS	7.2
1	A	41	THR	6.9
1	C	161	HIS	6.8
1	A	92	ASP	6.3
1	A	162	GLU	6.3
1	C	15	TYR	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	160	THR	6.2
1	C	41	THR	6.1
1	A	13	GLY	5.9
1	C	159	TYR	5.9
1	C	164	VAL	5.9
2	D	179	HIS	5.8
1	C	38	ASP	5.7
1	C	298	LEU	5.7
2	D	374	GLU	5.6
1	C	40	GLU	5.5
1	C	72	THR	5.5
2	B	178	TYR	5.4
1	A	287	GLN	5.3
1	C	97	THR	5.2
2	B	177	ASP	5.2
2	D	392	MET	5.1
1	A	256	ASP	5.1
1	A	71	HIS	5.1
1	C	14	THR	5.0
1	A	38	ASP	4.9
2	D	280	TYR	4.9
1	A	298	LEU	4.9
1	A	163	VAL	4.8
2	B	324	PRO	4.7
2	D	322	GLN	4.6
1	C	257	GLU	4.6
1	A	2	GLU	4.6
1	A	164	VAL	4.5
2	D	281	ILE	4.5
1	C	295	HIS	4.4
2	D	378	ARG	4.4
2	D	287	THR	4.3
2	D	284	ASP	4.3
2	D	274	GLU	4.3
2	D	327	CYS	4.2
2	D	271	TYR	4.2
1	A	247	ASP	4.1
1	A	248	PHE	4.1
2	B	432	LEU	4.1
1	A	257	GLU	4.0
1	C	206	ASP	4.0
1	C	297	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	320	LEU	3.9
1	A	36	ARG	3.9
1	A	273	LYS	3.9
1	A	97	THR	3.9
2	D	385	GLU	3.9
2	D	229	ASN	3.8
1	A	96	LEU	3.8
2	B	271	TYR	3.8
2	D	194	LYS	3.7
1	C	230	VAL	3.7
1	A	89	LYS	3.7
2	B	179	HIS	3.6
1	A	209	ILE	3.6
2	B	287	THR	3.6
2	B	284	ASP	3.6
1	C	287	GLN	3.6
2	D	285	THR	3.5
1	A	295	HIS	3.5
1	C	74	ASN	3.5
1	C	13	GLY	3.5
2	B	283	ASP	3.5
1	A	73	GLU	3.5
2	D	277	GLU	3.5
1	C	101	LEU	3.5
1	A	12	GLU	3.4
1	A	74	ASN	3.4
1	C	157	ARG	3.4
1	A	230	VAL	3.4
1	C	98	GLY	3.4
1	A	5	GLN	3.4
1	A	229	GLY	3.4
2	B	280	TYR	3.3
1	C	92	ASP	3.3
1	C	239	SER	3.3
2	B	193	CYS	3.3
1	A	246	GLN	3.3
1	C	39	THR	3.3
1	C	95	ALA	3.3
2	B	182	ILE	3.3
2	B	378	ARG	3.3
2	D	428	GLU	3.3
2	D	288	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	296	HIS	3.2
1	A	158	THR	3.2
2	D	403	GLN	3.2
1	C	42	GLU	3.2
2	D	431	ASN	3.2
1	C	93	ALA	3.1
1	A	9	LYS	3.1
2	D	334	MET	3.1
1	A	72	THR	3.1
1	C	36	ARG	3.1
1	A	14	THR	3.0
2	D	180	GLU	3.0
1	C	293	VAL	3.0
2	B	385	GLU	3.0
2	D	432	LEU	3.0
1	C	288	ASP	3.0
1	C	158	THR	2.9
1	A	10	ILE	2.9
1	C	238	PRO	2.9
1	C	250	LYS	2.9
1	A	145	ASP	2.9
2	D	209	SER	2.8
1	C	165	THR	2.8
1	C	200	ARG	2.8
2	B	194	LYS	2.8
2	B	205	ASP	2.8
1	C	43	GLY	2.7
1	C	292	PRO	2.7
1	A	154	VAL	2.7
2	D	325	ALA	2.7
2	D	289	LYS	2.7
2	B	403	GLN	2.7
1	A	220	GLY	2.7
1	C	73	GLU	2.7
2	B	370	GLN	2.7
1	A	43	GLY	2.7
1	A	75	LYS	2.7
1	C	1	MET	2.7
1	A	249	SER	2.7
2	D	275	VAL	2.7
1	A	206	ASP	2.6
1	C	296	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	197	VAL	2.6
1	A	236	TYR	2.6
2	D	188	GLU	2.6
1	C	231	THR	2.6
2	B	322	GLN	2.6
2	D	181	ASP	2.6
1	C	224	GLU	2.6
1	A	297	ARG	2.6
2	B	293	ARG	2.6
1	A	101	LEU	2.6
1	A	228	PRO	2.5
2	B	198	GLY	2.5
2	B	427	PRO	2.5
1	A	35	ILE	2.5
2	B	274	GLU	2.5
1	C	6	LYS	2.5
2	B	282	THR	2.5
1	C	199	ARG	2.5
1	A	241	PRO	2.5
1	C	294	PRO	2.5
2	B	416	SER	2.5
1	C	12	GLU	2.5
1	C	75	LYS	2.5
2	B	320	LEU	2.5
2	B	429	THR	2.5
1	A	100	PRO	2.4
1	A	238	PRO	2.4
2	D	276	ALA	2.4
1	A	98	GLY	2.4
1	C	89	LYS	2.4
2	B	317	GLN	2.4
2	D	326	ASN	2.4
1	A	31	ALA	2.4
1	A	16	GLY	2.4
1	C	226	VAL	2.4
1	A	47	THR	2.4
2	B	285	THR	2.4
1	C	10	ILE	2.4
2	D	293	ARG	2.4
1	A	138	GLU	2.4
1	C	99	ILE	2.3
2	D	205	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	327	CYS	2.3
1	C	242	LYS	2.3
1	A	239	SER	2.3
1	C	37	LEU	2.3
2	B	348	LEU	2.3
1	C	19	TYR	2.3
2	B	276	ALA	2.3
1	C	246	GLN	2.3
2	B	244	SER	2.3
2	D	375	SER	2.3
1	C	247	ASP	2.3
1	A	93	ALA	2.3
1	A	165	THR	2.3
1	A	94	SER	2.3
2	D	416	SER	2.3
1	A	6	LYS	2.3
2	D	196	LYS	2.3
2	D	370	GLN	2.2
1	A	264	SER	2.2
1	A	18	VAL	2.2
1	A	245	ARG	2.2
2	D	425	ASN	2.2
1	A	179	TYR	2.2
2	B	419	HIS	2.2
1	C	94	SER	2.2
2	B	181	ASP	2.2
2	B	296	HIS	2.2
1	A	177	CYS	2.2
2	B	376	LEU	2.2
2	B	319	PHE	2.2
1	A	44	VAL	2.2
2	D	383	THR	2.2
1	C	22	ARG	2.2
2	D	319	PHE	2.2
1	A	37	LEU	2.1
1	A	296	LEU	2.1
1	C	290	THR	2.1
1	A	99	ILE	2.1
1	A	50	ARG	2.1
1	A	271	PRO	2.1
1	C	253	PRO	2.1
1	C	156	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	326	ASN	2.1
1	A	11	GLY	2.1
1	C	229	GLY	2.1
1	C	46	SER	2.1
1	A	178	LYS	2.1
1	C	100	PRO	2.1
2	B	197	VAL	2.1
1	A	243	TRP	2.1
2	B	325	ALA	2.1
2	D	198	GLY	2.1
2	B	288	LYS	2.1
2	B	392	MET	2.1
1	C	138	GLU	2.1
2	B	374	GLU	2.1
1	A	95	ALA	2.0
1	A	59	ASN	2.0
1	C	261	SER	2.0
1	A	68	ASP	2.0
1	A	288	ASP	2.0
1	C	223	ASP	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.

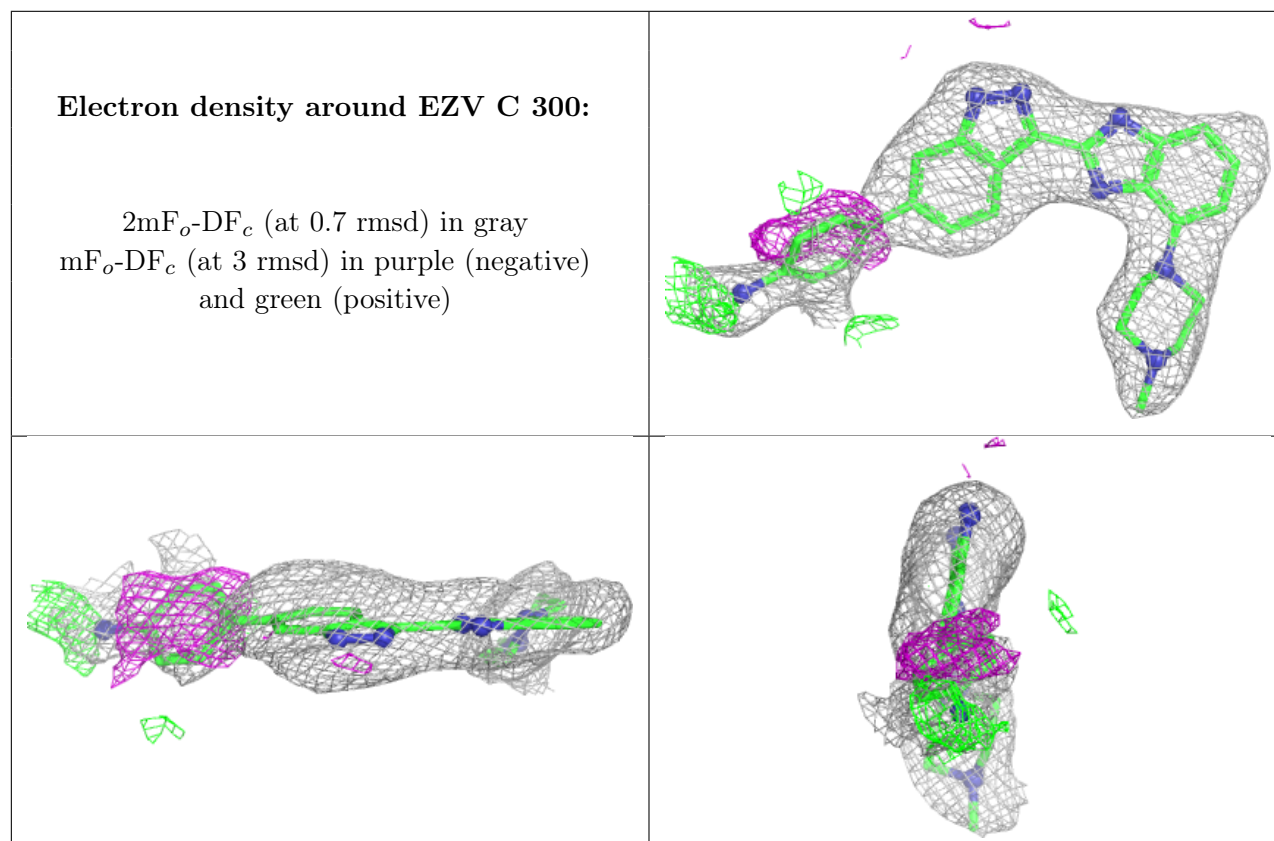
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EZV	C	300	32/32	0.80	0.22	72,73,75,75	0
5	SO4	D	1	5/5	0.83	0.17	106,106,107,107	0
3	GOL	A	299	6/6	0.88	0.16	52,53,54,55	0

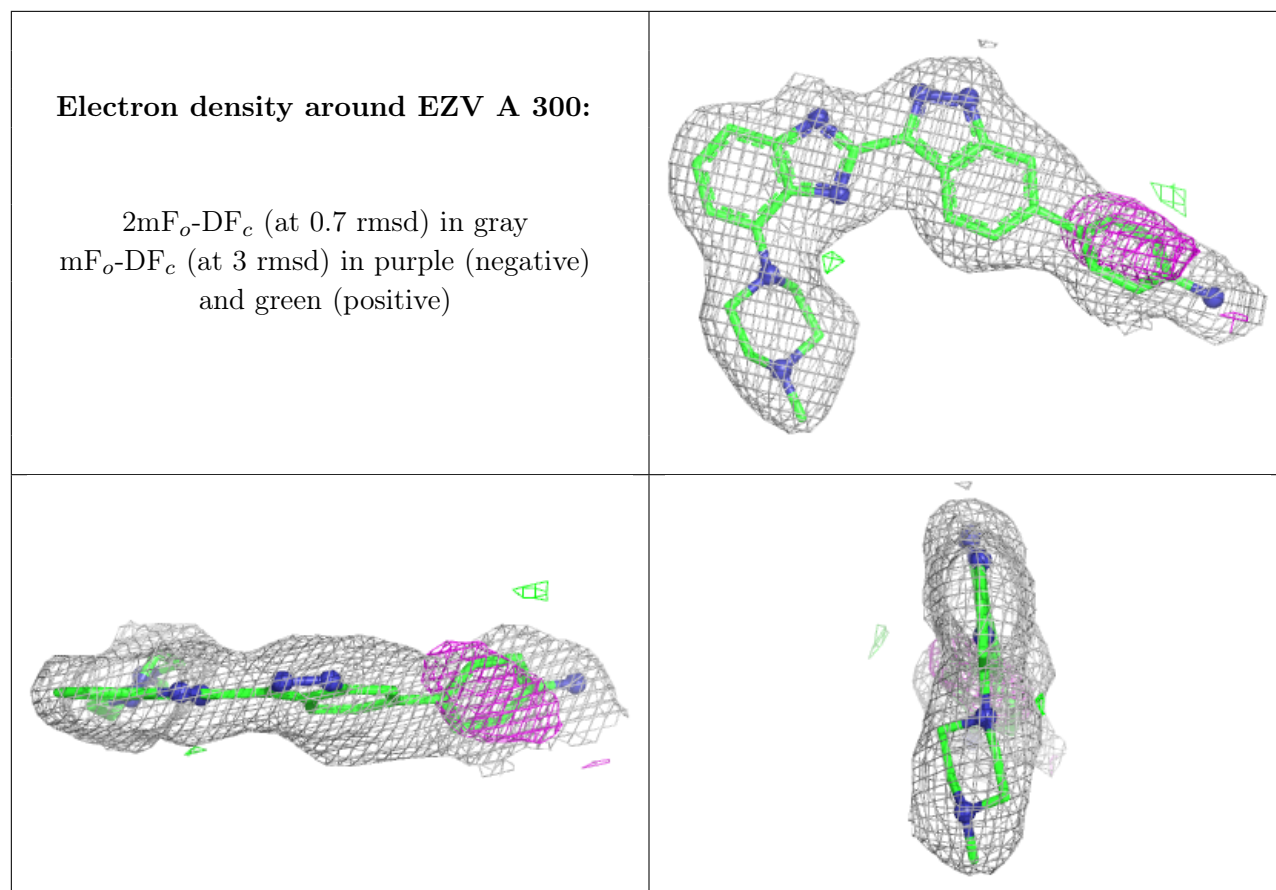
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	299	6/6	0.88	0.11	65,66,66,66	0
4	EZV	A	300	32/32	0.91	0.11	46,49,50,51	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.