



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:34 PM UTC

PDB ID : 8PTA / pdb_00008pta
Title : JNK1 covalently bound to BD837 cyclohexenone based inhibitor
Authors : Sok, P.; Poti, A.; Remenyi, A.
Deposited on : 2023-07-13
Resolution : 2.41 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

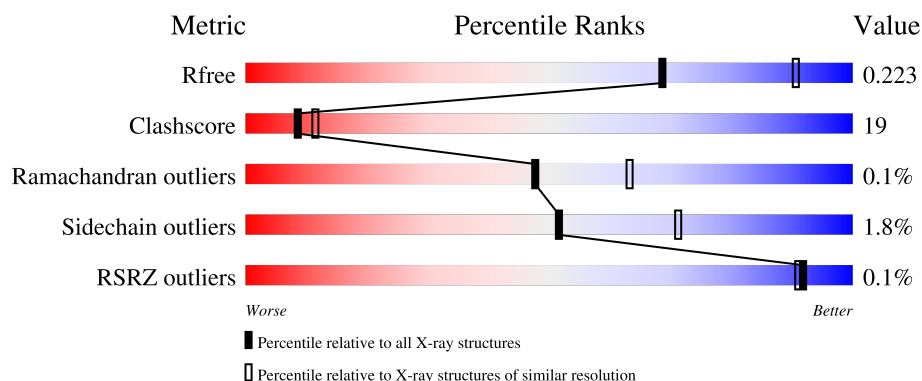
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	366	66% 30% ..
1	B	366	64% 32% ..
1	C	366	50% 44% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8442 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.

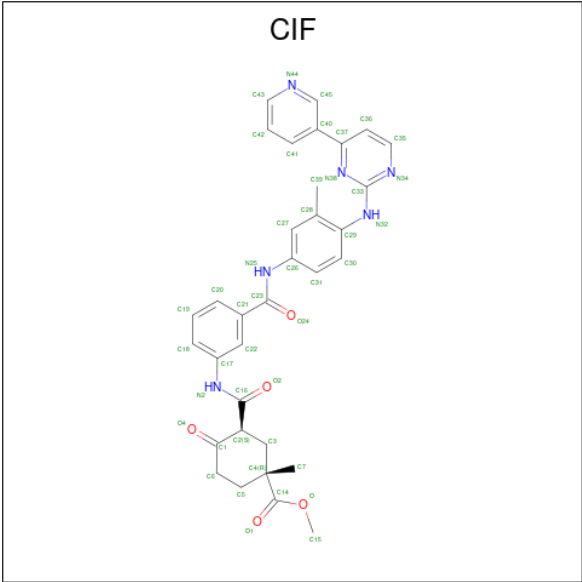
- Molecule 1 is a protein called Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2765	1781	456	507	21			
1	B	352	Total	C	N	O	S	0	0	0
			2777	1790	460	507	20			
1	C	351	Total	C	N	O	S	0	0	0
			2735	1758	456	502	19			

There are 9 discrepancies between the modelled and reference sequences:

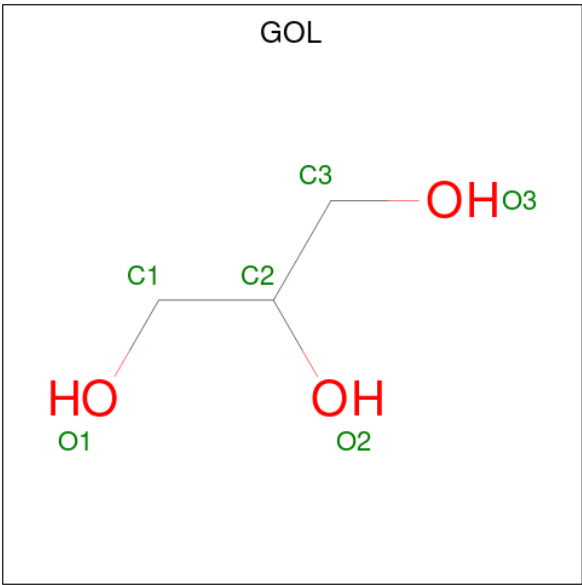
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P45983
A	0	SER	-	expression tag	UNP P45983
A	208	ILE	LEU	variant	UNP P45983
B	-1	GLY	-	expression tag	UNP P45983
B	0	SER	-	expression tag	UNP P45983
B	208	ILE	LEU	variant	UNP P45983
C	-1	GLY	-	expression tag	UNP P45983
C	0	SER	-	expression tag	UNP P45983
C	208	ILE	LEU	variant	UNP P45983

- Molecule 2 is methyl (1R,3S)-1-methyl-3-[[3-[[3-methyl-4-[(4-pyridin-3-yl)pyrimidin-2-yl)amino]phenyl]carbamoyl]phenyl]carbamoyl]-4-oxidanylidene-cyclohexane-1-carboxylate (CCD ID: CIF) (formula: $C_{33}H_{32}N_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	33	6	5		
2	B	1	Total	C	N	O	0	0
			44	33	6	5		
2	C	1	Total	C	N	O	0	0
			44	33	6	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

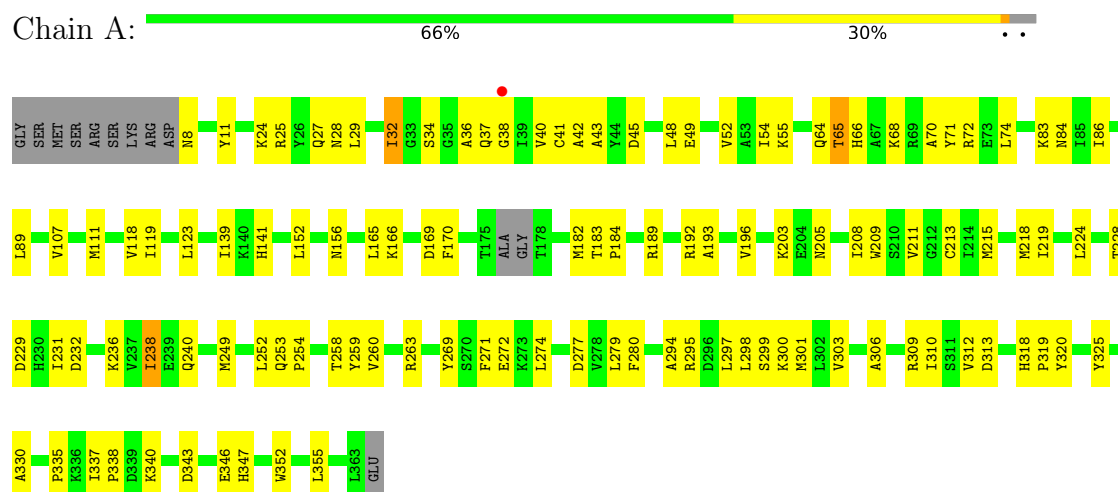
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	12	Total 12	O 12	0	0
4	C	7	Total 7	O 7	0	0

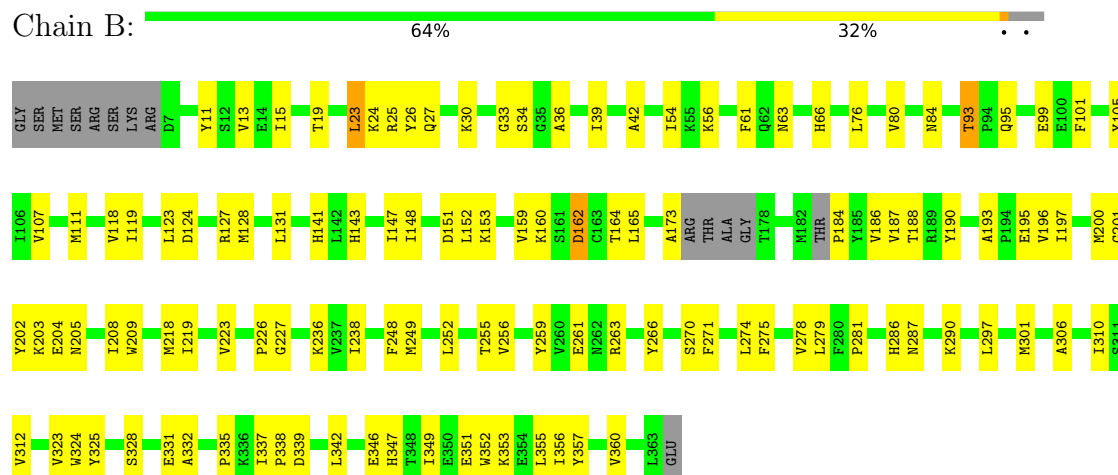
3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase 8



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E344	E350	E351	W352	K353	E354	L355	I356	Y357	K358	E359	V360	N361	ASP	LEU	GLU
V256	R257	T258	Y259	R263	Y266	F271	E272	K273	L274	F275	P276	D277	V278	L279	F280
T178	S179	F180	M181	M182	THR	PRO	TYR	V186	V187	T188	R189	Y190	Y191	R192	A193
L98	E99	F100	F101	Q102	D103	V104	Y105	V106	V107	M111	M114	V118	L123	D124	H125
GLY	SER	MET	SER	ARG	SER	LYS	ARG	ASP	N8	F10	G16	D17	L23	K24	R25
V281	P281	F280	L279	D277	V278	N361	V360	ASP	LEU	GLU	E285	K288	L289	K290	A291
M301	K300	S211	S210	W209	I208	D207	V206	E204	K203	Y202	G201	M200	S129	M128	R127
M301	K300	S211	S210	W209	I208	D207	V206	E204	K203	Y202	G201	M200	S129	M128	R127
I304	D305	A306	R309	I310	A315	H318	P319	Y320	I321	W324	E329	P335	K336	I337	L342
F61	P60	L57	K56	I54	K55	Y71	R72	R73	L74	V75	L76	M77	H82	K83	N84
G177	A176	T175	R174	A173	L172	G171	F170	D169	I167	K166	L165	K160	V159	V158	R150
S97	K96	Q95	P94	T93	F92	V91	L89	G87	I86	I85	N84	K83	H82	K83	R82

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	106.26Å 106.26Å 99.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.89 – 2.41 46.89 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.89-2.41) 99.7 (46.89-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.210 , 0.226 0.211 , 0.223	Depositor DCC
R_{free} test set	1979 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l 0.130 for h,-h-k,-l 0.129 for -k,-h,-l	Xtriage
Reported twinning fraction	0.459 for -h,-k,l	Depositor
Outliers	0 of 48500 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8442	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CIF

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	0.34	1/2829 (0.0%)	0.58	1/3844 (0.0%)
1	B	0.41	1/2840 (0.0%)	0.65	1/3851 (0.0%)
1	C	0.48	2/2797 (0.1%)	0.73	1/3799 (0.0%)
All	All	0.41	4/8466 (0.0%)	0.66	3/11494 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLY	CA-C	9.01	1.59	1.52
1	C	226	PRO	C-N	-8.06	1.29	1.33
1	C	201	GLY	C-O	5.44	1.27	1.23
1	A	34	SER	CA-CB	-5.30	1.49	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	VAL	N-CA-C	-6.18	104.91	112.76
1	B	201	GLY	CA-C-O	-6.09	117.92	122.37
1	A	37	GLN	N-CA-C	-5.36	106.43	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2765	0	2697	79	0
1	B	2777	0	2737	86	0
1	C	2735	0	2668	143	0
2	A	44	0	0	2	0
2	B	44	0	0	6	0
2	C	44	0	0	3	0
3	A	6	0	8	0	0
4	A	8	0	0	0	0
4	B	12	0	0	0	0
4	C	7	0	0	0	0
All	All	8442	0	8110	313	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 19.

All (313) 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:C:72:ARG:HH22	1:C:172:LEU:HA	1.39	0.88
1:C:129:SER:HB2	1:C:324:TRP:HE1	1.41	0.85
1:B:111:MET:H	2:B:401:CIF:C35	1.95	0.78
1:C:178:THR:HG23	1:C:180:PHE:H	1.49	0.77
1:C:189:ARG:HA	1:C:192:ARG:HG3	1.65	0.76
1:B:147:ILE:HD12	1:B:173:ALA:HB1	1.68	0.75
1:B:23:LEU:HD23	1:B:24:LYS:H	1.52	0.75
1:C:186:VAL:HB	1:C:188:THR:HG23	1.70	0.74
1:B:119:ILE:HG12	1:B:218:MET:HG2	1.71	0.73
1:C:75:VAL:HG23	1:C:76:LEU:HD12	1.71	0.72
1:B:118:VAL:HG21	1:B:159:VAL:HG21	1.71	0.70
1:B:337:ILE:HD12	1:B:338:PRO:HD2	1.73	0.70
1:C:351:GLU:O	1:C:354:GLU:HG2	1.92	0.69
1:C:195:GLU:HA	1:C:200:MET:HE3	1.74	0.69
1:C:280:PHE:HB3	1:C:281:PRO:HD2	1.76	0.67
1:C:241:LEU:HD21	1:C:271:PHE:CZ	2.30	0.67
1:B:111:MET:HE3	1:B:160:LYS:HG3	1.76	0.66
1:A:89:LEU:HB2	1:A:107:VAL:HG23	1.76	0.66
1:C:220:LYS:HA	1:C:279:LEU:HD13	1.77	0.65
1:B:39:ILE:HB	1:B:56:LYS:HB3	1.79	0.64
1:C:83:LYS:HE3	1:C:329:GLU:HG2	1.79	0.64
1:C:57:LEU:HB3	1:C:104:VAL:HG23	1.79	0.64
1:A:189:ARG:HA	1:A:192:ARG:HG2	1.79	0.64
1:B:76:LEU:O	1:B:80:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TYR:CE1	1:B:24:LYS:HA	2.32	0.63
1:B:19:THR:O	1:B:56:LYS:NZ	2.30	0.63
1:A:340:LYS:HA	1:A:343:ASP:HB2	1.81	0.62
1:C:219:ILE:HG22	1:C:279:LEU:HB3	1.81	0.62
1:A:303:VAL:O	1:A:309:ARG:NH1	2.32	0.62
1:C:301:MET:HG2	1:C:310:ILE:HD11	1.81	0.62
1:A:29:LEU:HD12	1:A:41:CYS:SG	2.40	0.61
1:A:40:VAL:HG12	1:A:55:LYS:HG3	1.83	0.61
1:C:342:LEU:HG	1:C:344:GLU:H	1.66	0.61
1:C:126:GLU:HG3	1:C:324:TRP:CH2	2.35	0.60
1:B:162:ASP:OD1	1:B:162:ASP:N	2.34	0.60
1:B:123:LEU:HB2	1:B:128:MET:HE3	1.84	0.60
1:B:208:ILE:HD11	1:B:312:VAL:HG12	1.83	0.60
1:C:276:PRO:HD2	1:C:279:LEU:HD12	1.84	0.59
1:B:226:PRO:O	1:B:236:LYS:NZ	2.33	0.59
1:B:200:MET:HE1	1:B:248:PHE:HE1	1.66	0.59
1:A:119:ILE:HG12	1:A:218:MET:HG2	1.85	0.59
1:A:252:LEU:HD12	1:A:253:GLN:H	1.67	0.58
1:C:189:ARG:HA	1:C:192:ARG:CG	2.34	0.58
1:C:193:ALA:HA	1:C:209:TRP:CD1	2.39	0.58
1:B:30:LYS:O	1:B:42:ALA:N	2.32	0.58
1:C:169:ASP:OD1	1:C:170:PHE:N	2.37	0.58
1:C:194:PRO:HD3	1:C:209:TRP:CD2	2.38	0.58
1:B:148:ILE:HD11	1:B:204:GLU:HG2	1.86	0.58
1:A:213:CYS:HA	1:A:224:LEU:HD12	1.87	0.57
1:C:111:MET:O	2:C:401:CIF:N32	2.38	0.57
1:C:180:PHE:HE2	1:C:196:VAL:HB	1.69	0.57
1:A:156:ASN:ND2	1:A:169:ASP:OD2	2.38	0.57
1:B:259:TYR:CZ	1:B:263:ARG:HD2	2.40	0.57
1:C:126:GLU:HG3	1:C:324:TRP:HH2	1.69	0.57
1:C:178:THR:OG1	1:C:179:SER:N	2.39	0.56
1:A:192:ARG:NH2	1:A:196:VAL:HG21	2.21	0.56
1:C:219:ILE:HG22	1:C:279:LEU:CB	2.35	0.56
1:A:25:ARG:O	1:A:45:ASP:HA	2.06	0.56
1:C:310:ILE:HD13	1:C:315:ALA:HB2	1.88	0.56
1:C:252:LEU:HB3	1:C:257:ARG:HB2	1.88	0.56
1:A:111:MET:HE3	1:A:166:LYS:HD2	1.87	0.56
1:C:128:MET:O	1:C:132:LEU:HG	2.06	0.56
1:B:23:LEU:HD22	1:B:25:ARG:HG2	1.88	0.55
1:C:296:ASP:O	1:C:300:LYS:HG3	2.05	0.55
1:C:73:GLU:HG3	1:C:74:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:CE1	1:A:355:LEU:HG	2.41	0.55
2:B:401:CIF:N38	2:B:401:CIF:C39	2.70	0.55
1:C:125:HIS:CD2	1:C:281:PRO:HG3	2.41	0.55
1:B:339:ASP:HA	1:B:342:LEU:HB3	1.88	0.55
1:C:147:ILE:HG23	1:C:173:ALA:HA	1.89	0.55
1:C:241:LEU:HD21	1:C:271:PHE:HZ	1.72	0.55
1:C:158:VAL:HG13	1:C:168:LEU:HD11	1.87	0.55
1:C:189:ARG:O	1:C:233:GLN:NE2	2.40	0.55
1:B:23:LEU:HD23	1:B:24:LYS:N	2.20	0.54
1:C:77:MET:HE3	1:C:86:ILE:HG23	1.90	0.54
1:C:98:LEU:HA	1:C:101:PHE:HB2	1.89	0.54
1:C:209:TRP:HB2	1:C:309:ARG:NH1	2.22	0.54
1:C:99:GLU:HG2	1:C:100:GLU:HG3	1.89	0.54
1:C:271:PHE:HA	1:C:274:LEU:HB2	1.90	0.54
2:A:401:CIF:C33	2:A:401:CIF:C39	2.85	0.54
2:A:401:CIF:C39	2:A:401:CIF:N38	2.71	0.54
1:C:72:ARG:HG2	1:C:76:LEU:HD13	1.90	0.54
1:B:202:TYR:O	1:B:203:LYS:HD2	2.08	0.53
2:C:401:CIF:C39	2:C:401:CIF:C33	2.85	0.53
1:C:190:TYR:CD1	1:C:226:PRO:HA	2.43	0.53
1:C:244:PRO:HG3	1:C:304:ILE:HG21	1.89	0.53
1:B:39:ILE:HG13	1:B:56:LYS:HD2	1.91	0.53
1:C:72:ARG:O	1:C:75:VAL:HG22	2.08	0.53
1:C:91:VAL:HG23	1:C:106:ILE:HG22	1.91	0.53
1:C:215:MET:O	1:C:219:ILE:HD12	2.09	0.53
1:B:271:PHE:HA	1:B:274:LEU:HB2	1.91	0.53
1:A:232:ASP:OD1	1:A:236:LYS:NZ	2.42	0.53
1:C:150:ARG:NH2	1:C:173:ALA:O	2.41	0.53
1:C:205:ASN:HB2	1:C:309:ARG:HD2	1.90	0.53
1:A:252:LEU:HD12	1:A:253:GLN:N	2.24	0.52
1:B:271:PHE:O	1:B:275:PHE:N	2.35	0.52
1:C:195:GLU:CD	1:C:195:GLU:H	2.17	0.52
1:C:297:LEU:HD13	1:C:318:HIS:CG	2.45	0.52
1:C:359:GLU:C	1:C:361:MET:N	2.66	0.52
1:A:141:HIS:CE1	1:A:335:PRO:HG3	2.44	0.52
1:B:124:ASP:OD2	1:B:127:ARG:NE	2.42	0.52
1:A:64:GLN:NE2	1:A:347:HIS:O	2.38	0.52
1:A:68:LYS:HD3	1:A:346:GLU:HG2	1.92	0.52
1:C:29:LEU:HA	1:C:42:ALA:O	2.10	0.52
1:C:220:LYS:HD2	1:C:279:LEU:CD1	2.40	0.52
1:C:350:GLU:O	1:C:353:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:HIS:CE1	1:B:335:PRO:HD3	2.44	0.52
1:C:238:ILE:HD12	1:C:266:TYR:CD2	2.45	0.52
1:A:215:MET:HE2	1:A:298:LEU:HG	1.91	0.52
1:A:249:MET:HG2	1:A:260:VAL:HG11	1.91	0.52
1:C:210:SER:O	1:C:214:ILE:HG13	2.10	0.52
1:A:25:ARG:HB2	1:A:45:ASP:OD1	2.10	0.51
1:A:118:VAL:HG12	1:A:123:LEU:HD11	1.92	0.51
1:A:84:ASN:HA	1:A:165:LEU:O	2.10	0.51
1:B:61:PHE:CE2	1:B:353:LYS:HD3	2.44	0.51
1:C:203:LYS:O	1:C:206:VAL:HG12	2.11	0.51
1:B:160:LYS:HE3	1:B:164:THR:OG1	2.10	0.51
1:A:29:LEU:HA	1:A:42:ALA:O	2.10	0.51
1:C:202:TYR:O	1:C:203:LYS:NZ	2.34	0.51
1:B:111:MET:N	2:B:401:CIF:C35	2.70	0.50
1:C:77:MET:SD	1:C:88:LEU:HB2	2.52	0.50
1:C:57:LEU:HB3	1:C:104:VAL:CG2	2.41	0.50
1:B:238:ILE:HG13	1:B:266:TYR:CD2	2.47	0.49
1:B:33:GLY:O	1:B:36:ALA:N	2.41	0.49
1:B:99:GLU:CD	1:B:99:GLU:H	2.20	0.49
1:B:143:HIS:CD2	1:B:148:ILE:HD13	2.47	0.49
1:C:54:ILE:HG22	1:C:107:VAL:HB	1.95	0.49
1:C:97:SER:O	1:C:101:PHE:N	2.45	0.49
1:A:228:THR:HG22	1:A:232:ASP:OD2	2.12	0.49
1:C:272:GLU:O	1:C:276:PRO:HA	2.13	0.49
1:A:36:ALA:C	1:A:38:GLY:H	2.19	0.49
1:B:200:MET:HE1	1:B:248:PHE:CE1	2.47	0.49
1:C:194:PRO:O	1:C:197:ILE:HG22	2.11	0.49
1:C:55:LYS:HB3	1:C:106:ILE:HG12	1.95	0.49
1:C:9:ASN:O	1:C:23:LEU:HA	2.13	0.48
1:C:129:SER:CB	1:C:324:TRP:HE1	2.21	0.48
1:B:119:ILE:HG12	1:B:218:MET:CG	2.43	0.48
1:C:271:PHE:CE2	1:C:299:SER:HA	2.49	0.48
1:A:318:HIS:CD2	1:A:319:PRO:HD2	2.49	0.48
1:C:72:ARG:NH2	1:C:171:GLY:O	2.46	0.48
1:A:66:HIS:HE1	1:A:183:THR:HG23	1.78	0.48
1:A:300:LYS:HB3	1:A:310:ILE:CG2	2.43	0.48
1:C:10:PHE:CE2	1:C:94:PRO:HA	2.48	0.48
1:C:272:GLU:OE1	1:C:272:GLU:N	2.47	0.48
1:A:27:GLN:HG2	1:A:28:ASN:H	1.78	0.48
1:A:25:ARG:HH21	1:A:48:LEU:HD13	1.78	0.48
1:A:325:TYR:HE1	1:A:330:ALA:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PHE:HZ	1:C:101:PHE:CE2	2.31	0.47
1:C:77:MET:HE2	1:C:87:GLY:C	2.40	0.47
1:C:40:VAL:HG11	2:C:401:CIF:C42	2.45	0.47
1:A:279:LEU:C	1:A:279:LEU:HD13	2.40	0.47
1:B:54:ILE:HG12	1:B:107:VAL:HG12	1.96	0.47
1:B:111:MET:CE	1:B:160:LYS:HG3	2.42	0.47
1:C:72:ARG:HG2	1:C:76:LEU:CD1	2.44	0.47
1:C:300:LYS:O	1:C:310:ILE:HG13	2.16	0.47
1:B:13:VAL:HG12	1:B:15:ILE:HG23	1.97	0.46
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.82	0.46
1:B:328:SER:O	1:B:332:ALA:HB2	2.15	0.46
1:C:141:HIS:CD2	1:C:335:PRO:HD3	2.50	0.46
1:C:346:GLU:HG2	1:C:347:HIS:N	2.31	0.46
1:A:346:GLU:HA	1:A:352:TRP:HZ2	1.80	0.46
1:B:187:VAL:O	1:B:187:VAL:HG22	2.15	0.46
1:A:36:ALA:C	1:A:38:GLY:N	2.71	0.46
1:C:61:PHE:CE1	1:C:353:LYS:HA	2.50	0.46
1:A:295:ARG:HA	1:A:298:LEU:HD12	1.98	0.46
1:B:11:TYR:OH	1:B:27:GLN:HA	2.15	0.46
1:A:32:ILE:HD12	1:A:32:ILE:HA	1.82	0.46
1:A:52:VAL:HG11	1:A:107:VAL:HB	1.98	0.46
1:C:277:ASP:OD1	1:C:277:ASP:N	2.48	0.46
1:C:172:LEU:HD21	1:C:176:ALA:HB3	1.97	0.45
1:B:351:GLU:O	1:B:355:LEU:N	2.40	0.45
1:B:281:PRO:O	1:B:287:ASN:HB3	2.16	0.45
1:C:280:PHE:CB	1:C:281:PRO:HD2	2.46	0.45
1:C:135:MET:O	1:C:139:ILE:HG23	2.17	0.45
1:C:197:ILE:HD11	1:C:230:HIS:CE1	2.51	0.45
1:C:259:TYR:O	1:C:263:ARG:HG2	2.17	0.45
1:B:153:LYS:HD2	1:B:188:THR:HG21	1.97	0.45
1:C:208:ILE:O	1:C:211:VAL:HG22	2.17	0.45
1:C:359:GLU:C	1:C:361:MET:H	2.24	0.45
1:C:95:GLN:NE2	1:C:102:GLN:HB3	2.32	0.45
1:C:193:ALA:HB3	1:C:196:VAL:HG22	1.98	0.45
1:C:229:ASP:OD1	1:C:231:ILE:HD12	2.17	0.45
1:A:240:GLN:HA	1:A:269:TYR:HD1	1.82	0.45
1:A:312:VAL:HG23	1:A:313:ASP:OD1	2.17	0.45
1:C:357:TYR:O	1:C:360:VAL:HG12	2.17	0.45
1:A:340:LYS:CA	1:A:343:ASP:HB2	2.45	0.44
1:C:256:VAL:O	1:C:259:TYR:N	2.50	0.44
1:B:346:GLU:OE1	1:B:346:GLU:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:O	1:B:360:VAL:HG22	2.18	0.44
1:C:72:ARG:O	1:C:73:GLU:C	2.60	0.44
1:C:275:PHE:O	1:C:295:ARG:HD3	2.16	0.44
1:A:259:TYR:OH	1:A:263:ARG:NH2	2.51	0.44
1:C:200:MET:HE2	1:C:248:PHE:CZ	2.51	0.44
1:C:205:ASN:ND2	1:C:306:ALA:O	2.50	0.44
1:A:300:LYS:HB3	1:A:310:ILE:HG23	2.00	0.44
1:B:11:TYR:CD1	1:B:24:LYS:HA	2.51	0.44
1:B:84:ASN:HA	1:B:165:LEU:O	2.18	0.44
1:C:82:HIS:O	1:C:85:ILE:HG13	2.16	0.44
1:C:86:ILE:HA	1:C:166:LYS:HD3	1.98	0.44
1:A:277:ASP:OD1	1:A:295:ARG:NH2	2.51	0.44
1:C:143:HIS:CE1	1:C:148:ILE:HA	2.53	0.44
1:A:29:LEU:HD11	1:A:54:ILE:HD12	1.99	0.43
1:A:182:MET:HB3	1:A:184:PRO:HD2	2.00	0.43
1:C:61:PHE:HE1	1:C:353:LYS:HA	1.83	0.43
1:B:93:THR:HG22	1:B:95:GLN:O	2.17	0.43
1:C:114:ASN:O	1:C:118:VAL:HG12	2.18	0.43
1:C:145:ALA:HB2	1:C:335:PRO:HG2	2.01	0.43
1:A:65:THR:HB	1:A:184:PRO:HG2	2.00	0.43
1:A:297:LEU:O	1:A:301:MET:HG2	2.18	0.43
1:C:41:CYS:SG	1:C:54:ILE:HD11	2.58	0.43
1:C:310:ILE:HD12	1:C:310:ILE:O	2.17	0.43
1:C:132:LEU:O	1:C:135:MET:HG2	2.18	0.43
1:C:140:LYS:HB3	1:C:140:LYS:HE3	1.45	0.43
1:A:72:ARG:NH2	1:A:170:PHE:O	2.52	0.43
1:B:111:MET:HE3	1:B:111:MET:HB3	1.90	0.43
1:B:325:TYR:OH	1:B:331:GLU:OE2	2.36	0.43
1:C:23:LEU:HB2	1:C:25:ARG:HG2	2.00	0.43
1:C:76:LEU:HB3	1:C:170:PHE:CD2	2.54	0.43
1:A:208:ILE:O	1:A:211:VAL:HG22	2.19	0.43
1:B:252:LEU:HD22	1:B:256:VAL:CG2	2.49	0.43
2:B:401:CIF:C39	2:B:401:CIF:C33	2.97	0.43
1:C:220:LYS:HD2	1:C:279:LEU:HD13	2.01	0.43
1:A:208:ILE:HG23	1:A:301:MET:HE2	2.01	0.42
1:A:271:PHE:HA	1:A:274:LEU:HB2	2.01	0.42
1:B:205:ASN:ND2	1:B:306:ALA:HB1	2.34	0.42
1:A:32:ILE:O	1:A:32:ILE:HG23	2.18	0.42
1:A:86:ILE:HA	1:A:166:LYS:HD3	2.00	0.42
1:B:323:VAL:HG23	1:B:324:TRP:CD1	2.54	0.42
1:B:111:MET:N	2:B:401:CIF:N34	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:TYR:HA	1:C:44:TYR:O	2.20	0.42
1:C:71:TYR:CE1	1:C:355:LEU:HG	2.54	0.42
1:A:205:ASN:OD1	1:A:306:ALA:HB1	2.19	0.42
1:C:170:PHE:N	1:C:170:PHE:CD1	2.86	0.42
1:C:237:VAL:O	1:C:241:LEU:HB2	2.18	0.42
1:A:271:PHE:CE2	1:A:299:SER:HA	2.55	0.42
1:B:297:LEU:O	1:B:301:MET:HG3	2.19	0.42
1:A:219:ILE:HG21	1:A:280:PHE:CZ	2.54	0.42
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.81	0.42
1:A:346:GLU:HA	1:A:352:TRP:CZ2	2.54	0.42
1:B:301:MET:HG2	1:B:310:ILE:CG2	2.49	0.42
1:C:76:LEU:HB3	1:C:170:PHE:CE2	2.54	0.42
1:C:190:TYR:HD1	1:C:226:PRO:HA	1.82	0.42
1:A:8:ASN:N	1:A:8:ASN:HD22	2.17	0.42
1:A:43:ALA:N	1:A:52:VAL:O	2.51	0.42
1:A:203:LYS:HA	1:A:203:LYS:HD3	1.73	0.42
1:A:238:ILE:H	1:A:238:ILE:HG13	1.63	0.42
1:B:66:HIS:HD2	1:B:184:PRO:HG3	1.84	0.42
1:B:148:ILE:HD12	1:B:204:GLU:HA	2.02	0.42
1:B:249:MET:SD	1:B:261:GLU:HG2	2.60	0.42
1:C:84:ASN:HA	1:C:165:LEU:O	2.19	0.42
1:C:170:PHE:N	1:C:170:PHE:HD1	2.17	0.42
1:C:57:LEU:CB	1:C:104:VAL:HG23	2.47	0.42
1:C:150:ARG:NH2	1:C:172:LEU:HB3	2.35	0.42
1:C:301:MET:CG	1:C:310:ILE:HD11	2.49	0.42
1:C:57:LEU:HD12	1:C:60:PRO:HG3	2.02	0.42
1:B:347:HIS:HB2	1:B:352:TRP:CE2	2.55	0.41
1:C:125:HIS:HD1	1:C:320:TYR:HE1	1.67	0.41
1:C:276:PRO:CD	1:C:279:LEU:HD12	2.50	0.41
1:A:229:ASP:OD1	1:A:231:ILE:HD12	2.20	0.41
1:B:63:ASN:OD1	1:B:63:ASN:C	2.63	0.41
1:B:111:MET:HE1	1:B:160:LYS:HE2	2.02	0.41
1:C:285:GLU:O	1:C:289:LEU:N	2.43	0.41
1:B:131:LEU:HD22	1:B:165:LEU:HD12	2.03	0.41
1:C:203:LYS:HD3	1:C:203:LYS:HA	1.72	0.41
1:A:11:TYR:CD1	1:A:24:LYS:HA	2.54	0.41
1:B:93:THR:HG21	1:B:101:PHE:HD2	1.84	0.41
1:A:249:MET:HE3	1:A:249:MET:HB2	2.00	0.41
1:A:272:GLU:H	1:A:272:GLU:HG3	1.71	0.41
1:A:337:ILE:HB	1:A:340:LYS:CB	2.51	0.41
1:B:151:ASP:OD1	1:B:186:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:HIS:O	1:B:290:LYS:HG2	2.21	0.41
1:B:25:ARG:HG3	1:B:26:TYR:CD2	2.55	0.41
1:B:195:GLU:HA	1:B:200:MET:HE2	2.02	0.41
1:A:193:ALA:HA	1:A:209:TRP:CD1	2.56	0.41
1:B:61:PHE:HB2	1:B:349:ILE:HG13	2.03	0.41
1:B:162:ASP:HB2	1:B:164:THR:HG23	2.03	0.41
1:A:11:TYR:OH	1:A:27:GLN:HA	2.21	0.41
1:A:49:GLU:N	1:A:49:GLU:OE1	2.54	0.41
1:B:56:LYS:HB2	1:B:105:TYR:CE2	2.56	0.41
1:B:193:ALA:HA	1:B:209:TRP:CD1	2.56	0.41
1:B:195:GLU:HB3	1:B:200:MET:HE2	2.03	0.41
1:C:93:THR:HG21	1:C:101:PHE:CE1	2.56	0.41
1:C:172:LEU:HA	1:C:172:LEU:HD12	1.92	0.41
1:C:215:MET:HG2	1:C:298:LEU:HD11	2.02	0.41
1:C:219:ILE:HG21	1:C:280:PHE:CE1	2.55	0.41
1:C:238:ILE:HD12	1:C:266:TYR:HD2	1.86	0.41
1:A:27:GLN:HG2	1:A:28:ASN:N	2.35	0.41
1:B:147:ILE:HG23	1:B:173:ALA:HA	2.02	0.41
1:C:174:ARG:HG3	1:C:175:THR:CG2	2.51	0.41
1:C:288:LYS:O	1:C:291:ALA:HB3	2.21	0.41
1:A:254:PRO:O	1:A:258:THR:HG23	2.21	0.40
1:B:33:GLY:O	1:B:34:SER:C	2.62	0.40
1:B:193:ALA:O	1:B:196:VAL:HG22	2.22	0.40
1:B:219:ILE:HG22	1:B:279:LEU:HB3	2.03	0.40
1:C:133:TYR:HB2	1:C:321:ILE:HG23	2.02	0.40
1:C:160:LYS:HB2	1:C:160:LYS:HE3	1.83	0.40
1:A:139:ILE:HD11	1:A:152:LEU:CD2	2.52	0.40
1:A:279:LEU:HD13	1:A:279:LEU:O	2.22	0.40
1:B:190:TYR:CD2	1:B:223:VAL:HG11	2.56	0.40
1:B:193:ALA:O	1:B:197:ILE:HG12	2.21	0.40
1:B:356:ILE:O	1:B:357:TYR:C	2.62	0.40
1:C:16:GLY:O	1:C:17:ASP:HB2	2.22	0.40
1:C:352:TRP:O	1:C:356:ILE:HG13	2.21	0.40
1:C:123:LEU:HB3	1:C:124:ASP:H	1.78	0.40
1:A:70:ALA:O	1:A:74:LEU:HG	2.21	0.40
1:A:294:ALA:HB2	1:A:320:TYR:CE2	2.57	0.40
1:A:338:PRO:O	1:B:270:SER:HB2	2.22	0.40
1:B:301:MET:HG2	1:B:310:ILE:HG21	2.04	0.40
2:B:401:CIF:O2	2:B:401:CIF:C18	2.67	0.40
1:C:101:PHE:CE2	1:C:357:TYR:HB2	2.56	0.40
1:C:275:PHE:CE2	1:C:298:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HG23	1:C:180:PHE:N	2.27	0.40
1:C:188:THR:OG1	1:C:192:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	350/366 (96%)	340 (97%)	10 (3%)	0	100	100
1	B	346/366 (94%)	336 (97%)	10 (3%)	0	100	100
1	C	347/366 (95%)	336 (97%)	10 (3%)	1 (0%)	36	49
All	All	1043/1098 (95%)	1012 (97%)	30 (3%)	1 (0%)	48	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	178	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/327 (90%)	291 (99%)	4 (1%)	59	77
1	B	299/327 (91%)	294 (98%)	5 (2%)	53	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	290/327 (89%)	283 (98%)	7 (2%)	43 63
All	All	884/981 (90%)	868 (98%)	16 (2%)	51 71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	65	THR
1	A	83	LYS
1	A	238	ILE
1	B	23	LEU
1	B	93	THR
1	B	162	ASP
1	B	255	THR
1	B	278	VAL
1	C	99	GLU
1	C	118	VAL
1	C	240	GLN
1	C	271	PHE
1	C	277	ASP
1	C	337	ILE
1	C	347	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	233	GLN
1	A	318	HIS
1	C	120	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIF	C	401	1	47,48,48	2.12	17 (36%)	64,68,68	2.18	18 (28%)
3	GOL	A	402	-	5,5,5	0.94	0	5,5,5	1.15	1 (20%)
2	CIF	A	401	1	47,48,48	1.98	12 (25%)	64,68,68	2.27	19 (29%)
2	CIF	B	401	1	47,48,48	2.07	16 (34%)	64,68,68	2.34	22 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIF	C	401	1	-	14/32/47/47	0/5/5/5
3	GOL	A	402	-	-	2/4/4/4	-
2	CIF	A	401	1	-	11/32/47/47	0/5/5/5
2	CIF	B	401	1	-	11/32/47/47	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CIF	O-C14	6.36	1.45	1.33
2	B	401	CIF	C26-N25	-4.91	1.31	1.41
2	B	401	CIF	O-C14	4.46	1.41	1.33
2	C	401	CIF	O-C14	4.37	1.41	1.33
2	A	401	CIF	C17-N2	-4.31	1.32	1.41
2	C	401	CIF	C17-N2	-4.23	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	CIF	C26-N25	-4.11	1.33	1.41
2	A	401	CIF	C26-N25	-4.04	1.33	1.41
2	B	401	CIF	C17-N2	-3.52	1.34	1.41
2	C	401	CIF	C3-C4	-3.51	1.50	1.54
2	C	401	CIF	C29-C28	-3.18	1.34	1.40
2	B	401	CIF	C3-C4	-3.08	1.50	1.54
2	C	401	CIF	C20-C21	-2.88	1.35	1.39
2	C	401	CIF	C22-C21	-2.78	1.35	1.39
2	B	401	CIF	C27-C28	-2.72	1.35	1.39
2	B	401	CIF	C27-C26	-2.71	1.35	1.39
2	A	401	CIF	C27-C28	-2.70	1.35	1.39
2	C	401	CIF	C33-N34	-2.56	1.31	1.34
2	C	401	CIF	C27-C28	-2.51	1.36	1.39
2	B	401	CIF	C20-C21	-2.50	1.35	1.39
2	B	401	CIF	C23-N25	-2.50	1.28	1.35
2	A	401	CIF	C27-C26	-2.49	1.35	1.39
2	B	401	CIF	C29-N32	-2.47	1.33	1.39
2	B	401	CIF	C4-C14	-2.43	1.46	1.53
2	A	401	CIF	C29-C28	-2.40	1.35	1.40
2	A	401	CIF	C33-N34	-2.40	1.31	1.34
2	C	401	CIF	C5-C4	-2.37	1.49	1.54
2	A	401	CIF	C20-C21	-2.31	1.35	1.39
2	C	401	CIF	C29-N32	-2.31	1.33	1.39
2	A	401	CIF	C18-C17	-2.30	1.35	1.39
2	C	401	CIF	C27-C26	-2.28	1.35	1.39
2	A	401	CIF	C22-C17	-2.24	1.35	1.39
2	B	401	CIF	O-C15	-2.22	1.40	1.45
2	C	401	CIF	C22-C17	-2.18	1.35	1.39
2	B	401	CIF	C5-C4	-2.17	1.50	1.54
2	B	401	CIF	C29-C28	-2.14	1.36	1.40
2	A	401	CIF	C29-N32	-2.11	1.34	1.39
2	C	401	CIF	C33-N32	-2.11	1.32	1.36
2	C	401	CIF	C41-C40	-2.09	1.35	1.39
2	C	401	CIF	C16-N2	-2.09	1.30	1.35
2	B	401	CIF	C3-C2	-2.07	1.49	1.54
2	B	401	CIF	C31-C26	-2.05	1.35	1.39
2	C	401	CIF	C40-C37	-2.02	1.45	1.49
2	B	401	CIF	C7-C4	-2.01	1.50	1.53
2	A	401	CIF	C16-N2	-2.01	1.31	1.35

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	CIF	C37-N38-C33	7.16	122.32	116.81
2	C	401	CIF	C35-N34-C33	7.03	121.29	115.42
2	A	401	CIF	C37-N38-C33	7.01	122.20	116.81
2	C	401	CIF	N34-C33-N38	-6.58	120.06	126.42
2	A	401	CIF	N34-C33-N38	-6.43	120.20	126.42
2	B	401	CIF	N34-C33-N38	-6.35	120.28	126.42
2	A	401	CIF	C35-N34-C33	5.86	120.31	115.42
2	A	401	CIF	C5-C6-C1	-5.70	99.06	112.52
2	B	401	CIF	C35-N34-C33	5.38	119.92	115.42
2	B	401	CIF	O4-C1-C2	-5.18	115.70	122.12
2	C	401	CIF	C5-C6-C1	-5.11	100.46	112.52
2	C	401	CIF	C37-N38-C33	4.90	120.58	116.81
2	C	401	CIF	C17-N2-C16	-4.54	117.01	127.37
2	C	401	CIF	O-C14-O1	-4.32	116.52	123.95
2	B	401	CIF	C5-C6-C1	-4.01	103.05	112.52
2	B	401	CIF	C5-C4-C3	3.87	116.65	109.08
2	B	401	CIF	C28-C29-N32	3.81	125.28	118.68
2	B	401	CIF	C19-C18-C17	3.60	123.88	119.73
2	B	401	CIF	C6-C5-C4	-3.42	108.75	112.77
2	B	401	CIF	C39-C28-C29	3.39	125.06	121.23
2	A	401	CIF	C17-N2-C16	-3.34	119.73	127.37
2	A	401	CIF	C30-C29-C28	-3.34	116.89	120.70
2	C	401	CIF	C40-C37-N38	3.32	120.83	116.04
2	A	401	CIF	C28-C29-N32	3.31	124.42	118.68
2	A	401	CIF	C6-C5-C4	-3.19	109.02	112.77
2	A	401	CIF	C5-C4-C3	3.09	115.13	109.08
2	C	401	CIF	C27-C28-C29	3.03	121.67	118.24
2	C	401	CIF	C6-C5-C4	-3.02	109.23	112.77
2	C	401	CIF	C39-C28-C29	-2.96	117.88	121.23
2	C	401	CIF	C36-C35-N34	-2.88	120.44	123.97
2	A	401	CIF	C36-C37-N38	-2.85	118.21	121.97
2	A	401	CIF	C2-C16-N2	2.83	118.75	114.82
2	B	401	CIF	C36-C35-N34	-2.79	120.56	123.97
2	B	401	CIF	C6-C1-C2	2.77	121.97	115.83
2	B	401	CIF	C5-C4-C14	-2.74	105.17	110.84
2	A	401	CIF	C39-C28-C27	-2.74	114.75	119.57
2	B	401	CIF	C36-C37-N38	-2.71	118.39	121.97
2	C	401	CIF	C43-N44-C45	2.71	121.60	116.85
2	A	401	CIF	O-C14-O1	-2.69	119.32	123.95
2	B	401	CIF	C30-C29-N32	-2.69	115.95	121.32
2	B	401	CIF	C39-C28-C27	-2.68	114.85	119.57
2	C	401	CIF	O-C14-C4	2.61	120.76	112.76
2	A	401	CIF	C39-C28-C29	2.61	124.18	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	CIF	C20-C21-C22	2.60	122.25	119.25
2	B	401	CIF	O-C14-O1	-2.55	119.56	123.95
2	A	401	CIF	C27-C28-C29	2.49	121.06	118.24
2	C	401	CIF	C30-C29-C28	-2.48	117.86	120.70
2	B	401	CIF	O-C14-C4	2.41	120.14	112.76
2	C	401	CIF	C42-C41-C40	-2.40	117.80	120.54
2	A	401	CIF	C36-C35-N34	-2.40	121.03	123.97
2	C	401	CIF	C5-C4-C3	2.35	113.68	109.08
2	B	401	CIF	C3-C2-C1	2.35	113.00	108.35
2	A	401	CIF	O-C14-C4	2.28	119.72	112.76
2	A	401	CIF	C15-O-C14	2.23	119.58	115.91
2	B	401	CIF	C18-C17-C22	-2.16	117.05	119.66
2	C	401	CIF	C28-C29-N32	2.13	122.37	118.68
2	B	401	CIF	C42-C41-C40	-2.09	118.16	120.54
2	A	401	CIF	C21-C22-C17	2.07	123.11	120.44
3	A	402	GOL	C3-C2-C1	-2.07	104.21	111.80
2	C	401	CIF	C15-O-C14	2.01	119.20	115.91

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIF	O1-C14-C4-C3
2	A	401	CIF	C28-C29-N32-C33
2	A	401	CIF	C30-C29-N32-C33
2	B	401	CIF	N2-C16-C2-C1
2	B	401	CIF	O2-C16-C2-C1
2	B	401	CIF	C28-C29-N32-C33
2	B	401	CIF	C30-C29-N32-C33
2	C	401	CIF	N2-C16-C2-C1
2	C	401	CIF	O2-C16-C2-C1
2	C	401	CIF	O-C14-C4-C7
2	C	401	CIF	C28-C29-N32-C33
2	C	401	CIF	C30-C29-N32-C33
2	A	401	CIF	C2-C16-N2-C17
2	C	401	CIF	C2-C16-N2-C17
2	A	401	CIF	O2-C16-N2-C17
2	C	401	CIF	O2-C16-N2-C17
2	A	401	CIF	O-C14-C4-C3
3	A	402	GOL	O1-C1-C2-C3
2	A	401	CIF	N38-C33-N32-C29
2	A	401	CIF	O1-C14-C4-C7

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Mol	Chain	Res	Type	Atoms
2	C	401	CIF	O1-C14-C4-C7
2	C	401	CIF	O1-C14-C4-C3
2	A	401	CIF	O-C14-C4-C7
2	C	401	CIF	O-C14-C4-C3
2	A	401	CIF	N34-C33-N32-C29
2	B	401	CIF	C31-C26-N25-C23
2	B	401	CIF	O1-C14-C4-C3
2	B	401	CIF	C27-C26-N25-C23
2	B	401	CIF	O-C14-C4-C3
2	B	401	CIF	O1-C14-C4-C7
2	B	401	CIF	O-C14-C4-C7
3	A	402	GOL	O1-C1-C2-O2
2	C	401	CIF	N38-C33-N32-C29
2	C	401	CIF	N34-C33-N32-C29
2	C	401	CIF	C20-C21-C23-N25
2	B	401	CIF	O2-C16-C2-C3
2	C	401	CIF	C20-C21-C23-O24
2	A	401	CIF	N2-C16-C2-C1

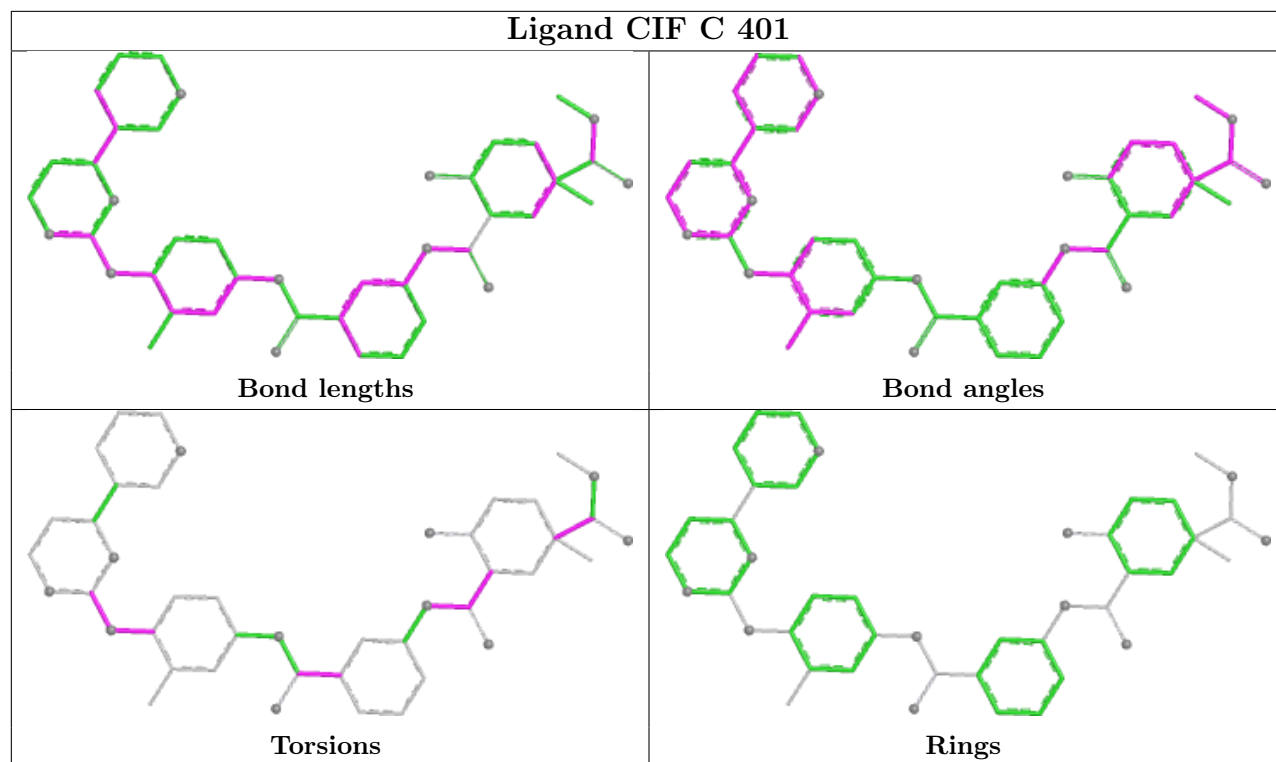
There are no ring outliers.

3 monomers are involved in 11 short contacts:

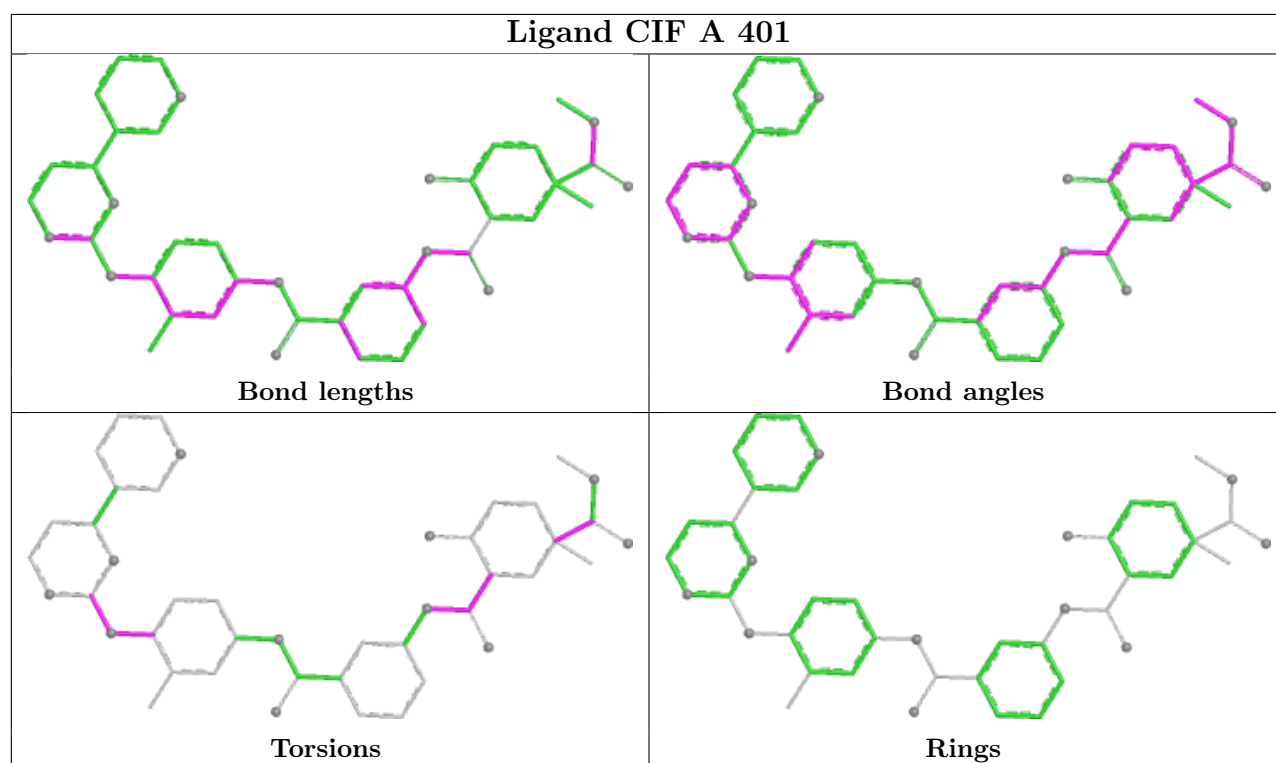
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	CIF	3	0
2	A	401	CIF	2	0
2	B	401	CIF	6	0

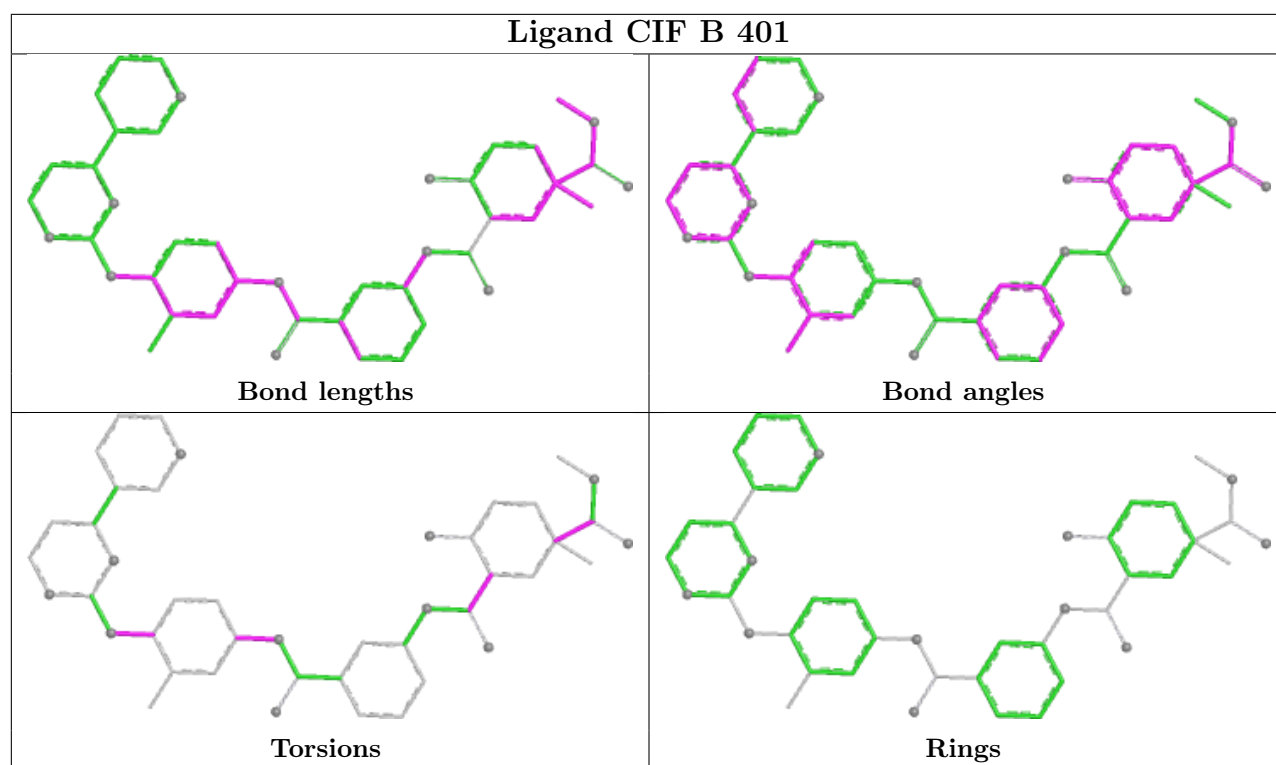
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand CIF C 401



Ligand CIF A 401





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	354/366 (96%)	-0.46	1 (0%) 90 88	55, 76, 104, 159	0
1	B	352/366 (96%)	-0.50	0 100 100	51, 74, 107, 129	0
1	C	351/366 (95%)	-0.28	0 100 100	71, 96, 129, 183	0
All	All	1057/1098 (96%)	-0.41	1 (0%) 92 91	51, 83, 117, 183	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	2.2

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
2	CIF	C	401	44/44	0.97	0.08	72,81,86,87	0
3	GOL	A	402	6/6	0.97	0.06	61,62,66,69	0

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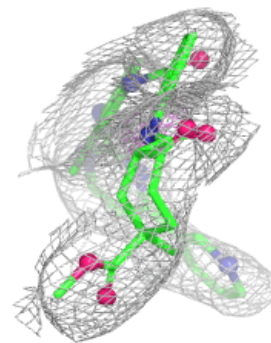
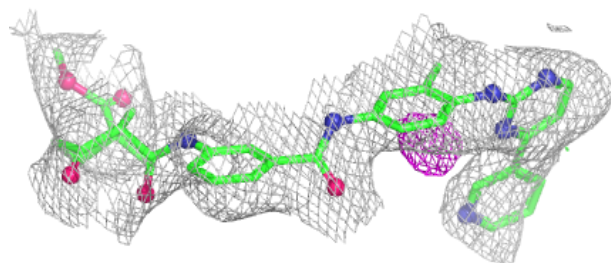
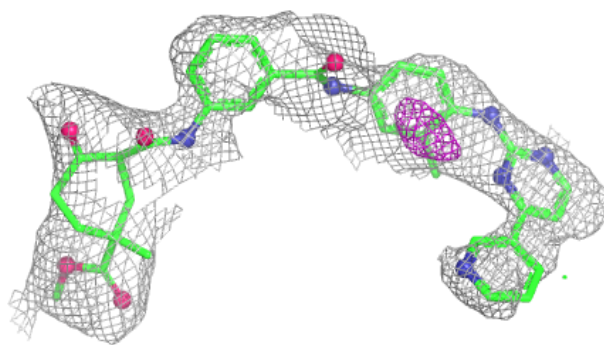
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIF	A	401	44/44	0.98	0.07	63,77,92,110	0
2	CIF	B	401	44/44	0.98	0.07	71,78,92,110	0

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.

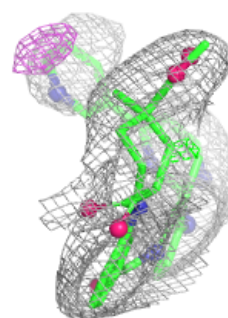
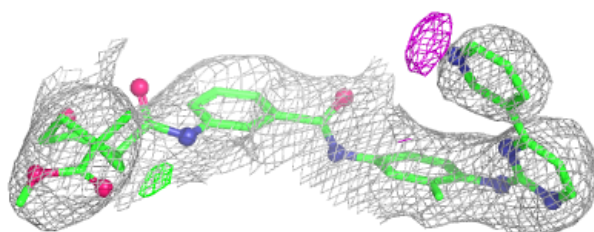
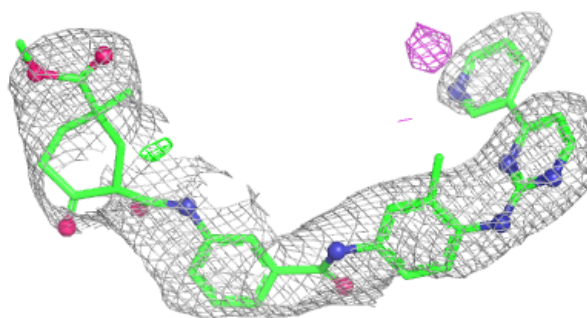
Electron density around CIF C 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

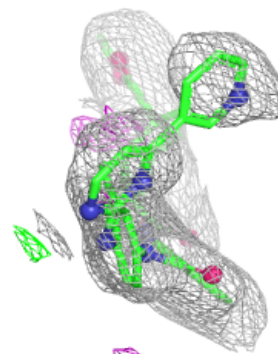
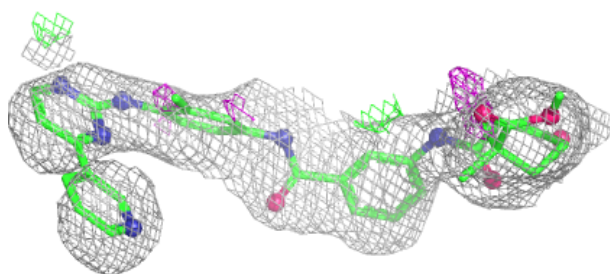
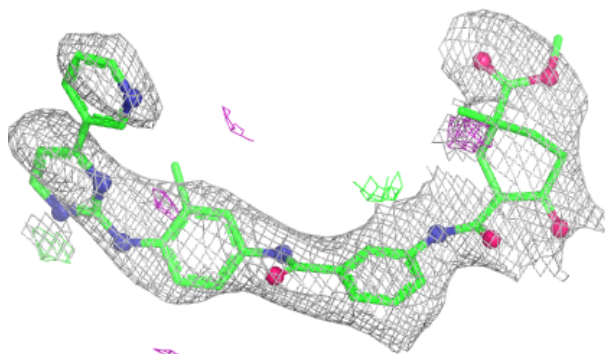


Electron density around CIF A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CIF B 401:**

$2mF_o-DF_c$ (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.