Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:50 PM EDT

PDB ID	:	3O50
Title	:	Crystal structure of benzamide 9 bound to AuroraA
Authors	:	Huang, X.
Deposited on	:	2010-07-27
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

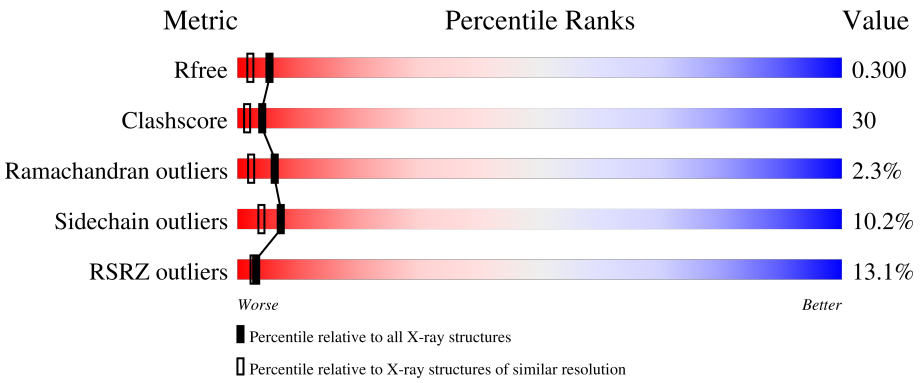
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	267	12% 47% 38% 7% 8%
1	B	267	13% 48% 39% 6% 7%

2 Entry composition (i)

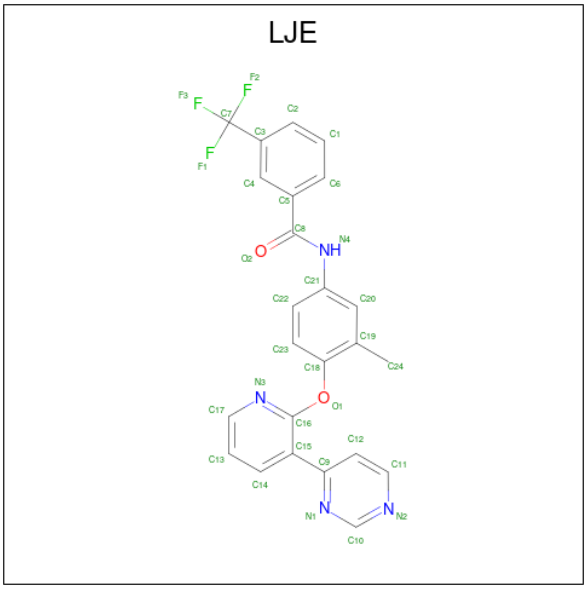
There are 3 unique types of molecules in this entry. The entry contains 4149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cDNA FLJ58295, highly similar to Serine/threonine-protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1982	1280	339	359	4	0	0	0
1	B	249	2009	1294	346	364	5	0	0	0

- Molecule 2 is N-{3-methyl-4-[(3-pyrimidin-4-ylpyridin-2-yl)oxy]phenyl}-3-(trifluoromethyl) benzamide (three-letter code: LJE) (formula: $C_{24}H_{17}F_3N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	33	24	3	4	2	0	0
2	B	1	33	24	3	4	2	0	0

- Molecule 3 is water.

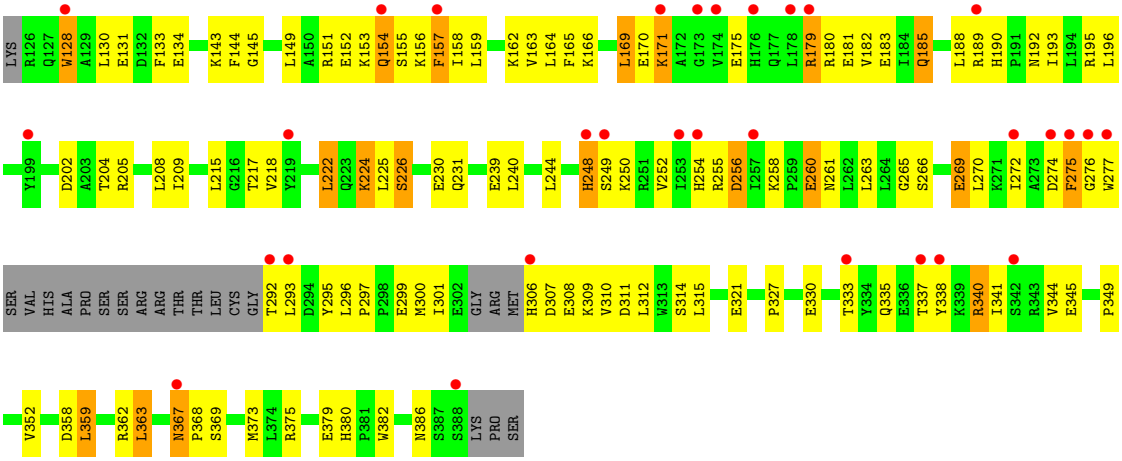
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	45	45	45	0	0
			Total	O		
3	B	47	47	47	1	0

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.

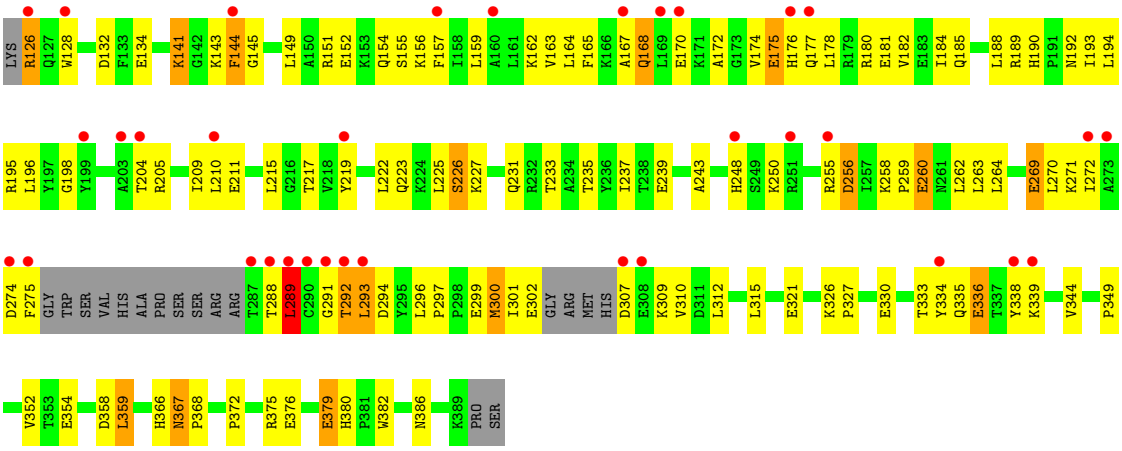
• Molecule 1: cDNA FLJ58295, highly similar to Serine/threonine-protein kinase 6

Chain A:



• Molecule 1: cDNA FLJ58295, highly similar to Serine/threonine-protein kinase 6

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.32Å 125.00Å 76.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 95.8 (29.58-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.351 0.248 , 0.300	Depositor DCC
R_{free} test set	981 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4149	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LJE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.55	0/2029	0.75	0/2747
1	B	0.49	0/2055	0.69	0/2779
All	All	0.52	0/4084	0.72	0/5526

There are no bond length outliers.

There are no bond angle outliers.

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	1982	0	1950	123	0
1	B	2009	0	1987	116	0
2	A	33	0	17	4	0
2	B	33	0	17	1	0
3	A	45	0	0	3	0
3	B	47	0	0	3	0
All	All	4149	0	3971	240	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 30.

All (240) 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:B:293:LEU:HD23	1:B:293:LEU:H	1.19	1.07
1:B:141:LYS:HD2	1:B:141:LYS:H	1.32	0.95
1:B:185:GLN:OE1	1:B:275:PHE:HA	1.69	0.92
1:A:293:LEU:HD12	1:A:296:LEU:HD12	1.50	0.92
1:A:255:ARG:O	1:A:256:ASP:HB2	1.67	0.89
1:B:336:GLU:OE1	1:B:339:LYS:HD3	1.75	0.87
1:B:301:ILE:HG13	1:B:302:GLU:N	1.92	0.82
1:B:333:THR:HG22	1:B:335:GLN:H	1.45	0.82
1:B:301:ILE:HG13	1:B:302:GLU:H	1.45	0.81
1:B:297:PRO:HG3	1:B:310:VAL:HG13	1.62	0.81
1:B:380:HIS:HD2	1:B:382:TRP:H	1.29	0.81
1:A:333:THR:HG22	1:A:335:GLN:H	1.44	0.80
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.47	0.80
1:A:225:LEU:O	1:A:226:SER:HB3	1.83	0.79
1:A:308:GLU:OE2	3:A:393:HOH:O	2.02	0.78
1:B:255:ARG:O	1:B:256:ASP:HB3	1.86	0.76
1:B:293:LEU:H	1:B:293:LEU:CD2	1.97	0.75
1:B:204:THR:HG23	1:B:205:ARG:HG3	1.69	0.74
1:A:274:ASP:O	1:A:276:GLY:N	2.17	0.72
1:A:180:ARG:HH11	1:A:277:TRP:CB	2.03	0.70
1:A:375:ARG:CZ	1:A:379:GLU:OE2	2.39	0.70
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.56	0.70
1:A:185:GLN:HG3	1:A:275:PHE:CD2	2.26	0.70
1:A:164:LEU:HB3	1:A:169:LEU:HD21	1.72	0.69
1:A:308:GLU:O	1:A:311:ASP:OD1	2.09	0.69
1:A:297:PRO:HG3	1:A:310:VAL:HG13	1.74	0.68
1:A:367:ASN:HD22	1:A:367:ASN:C	1.97	0.68
1:B:217:THR:HG22	1:B:263:LEU:CD2	2.24	0.67
1:A:258:LYS:HB2	1:A:260:GLU:OE1	1.95	0.67
1:A:327:PRO:HG2	1:A:330:GLU:HB2	1.77	0.67
1:B:225:LEU:O	1:B:226:SER:HB3	1.94	0.66
1:A:218:VAL:HG21	1:A:270:LEU:HD11	1.77	0.65
1:A:380:HIS:CD2	1:A:382:TRP:H	2.13	0.65
1:A:190:HIS:CD2	1:A:192:ASN:HB2	2.33	0.64
1:A:217:THR:HG22	1:A:263:LEU:CD2	2.27	0.64
1:A:293:LEU:HA	1:A:296:LEU:HD12	1.79	0.64
1:B:333:THR:HG22	1:B:335:GLN:N	2.12	0.64
1:A:367:ASN:C	1:A:367:ASN:ND2	2.51	0.63
1:B:299:GLU:N	1:B:299:GLU:OE1	2.31	0.63
1:B:172:ALA:O	1:B:174:VAL:HG13	1.99	0.63
1:B:344:VAL:HG21	1:B:366:HIS:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASP:OD2	1:B:380:HIS:HE1	1.82	0.63
1:A:240:LEU:HG	1:A:270:LEU:HD23	1.82	0.62
1:B:375:ARG:O	1:B:379:GLU:HG3	1.98	0.62
1:A:192:ASN:O	1:A:272:ILE:HG22	2.00	0.62
1:B:134:GLU:CD	1:B:151:ARG:HH21	2.03	0.62
1:B:297:PRO:HG2	1:B:300:MET:HB2	1.79	0.62
1:A:275:PHE:CD1	2:A:1:LJE:H6	2.33	0.62
1:A:190:HIS:CD2	1:A:192:ASN:H	2.18	0.62
1:A:258:LYS:HG3	1:A:261:ASN:HD22	1.64	0.62
1:B:141:LYS:HD2	1:B:141:LYS:N	2.10	0.62
1:B:312:LEU:N	1:B:312:LEU:HD22	2.14	0.61
1:B:275:PHE:N	1:B:275:PHE:CD1	2.68	0.61
1:A:170:GLU:HG2	1:A:175:GLU:OE1	2.00	0.61
1:A:367:ASN:HD22	1:A:368:PRO:N	1.97	0.61
1:A:190:HIS:HD2	1:A:192:ASN:HB2	1.65	0.60
1:A:269:GLU:N	1:A:269:GLU:OE1	2.34	0.60
1:A:255:ARG:O	1:A:256:ASP:CB	2.43	0.60
1:B:176:HIS:CE1	1:B:177:GLN:HG3	2.35	0.60
1:A:258:LYS:NZ	1:A:292:THR:HG22	2.16	0.60
1:B:380:HIS:CD2	1:B:382:TRP:H	2.17	0.60
1:B:177:GLN:O	1:B:181:GLU:HG3	2.02	0.59
1:A:340:ARG:HD2	1:A:345:GLU:HG3	1.84	0.58
1:A:358:ASP:OD1	1:A:362:ARG:NH1	2.34	0.58
1:B:157:PHE:HD2	1:B:159:LEU:HD23	1.67	0.58
1:B:128:TRP:CD1	1:B:209:ILE:HD13	2.38	0.58
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.19	0.58
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.19	0.58
1:A:190:HIS:HD2	1:A:192:ASN:H	1.50	0.58
1:A:133:PHE:HZ	1:A:209:ILE:HD13	1.68	0.57
1:A:307:ASP:OD1	1:A:308:GLU:OE1	2.23	0.57
1:B:307:ASP:OD2	1:B:309:LYS:HB2	2.03	0.57
1:B:157:PHE:CD2	1:B:159:LEU:HD23	2.40	0.57
1:B:176:HIS:HB2	3:B:96:HOH:O	2.03	0.57
1:A:239:GLU:OE1	1:A:270:LEU:HB2	2.04	0.57
1:B:296:LEU:HD22	1:B:300:MET:CE	2.35	0.56
1:B:145:GLY:HA3	1:B:163:VAL:O	2.06	0.56
1:A:293:LEU:HD12	1:A:296:LEU:CD1	2.31	0.56
1:B:358:ASP:OD2	1:B:380:HIS:CE1	2.58	0.56
1:A:309:LYS:HA	1:A:312:LEU:HD23	1.88	0.56
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.06	0.55
1:A:308:GLU:OE1	1:A:308:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASN:C	1:B:367:ASN:HD22	2.09	0.55
1:B:170:GLU:N	1:B:175:GLU:OE2	2.39	0.55
1:A:269:GLU:CD	1:A:269:GLU:H	2.09	0.54
1:A:375:ARG:NH1	1:A:379:GLU:OE2	2.40	0.54
1:A:258:LYS:HZ3	1:A:292:THR:HG22	1.72	0.54
1:B:262:LEU:CD2	1:B:272:ILE:HG22	2.37	0.54
1:B:296:LEU:HD22	1:B:300:MET:HE2	1.88	0.54
1:B:126:ARG:HD2	1:B:126:ARG:N	2.23	0.54
1:A:225:LEU:O	1:A:226:SER:CB	2.56	0.54
1:B:235:THR:O	1:B:239:GLU:HG3	2.07	0.54
1:B:259:PRO:HD2	1:B:260:GLU:OE2	2.08	0.54
1:A:170:GLU:O	1:A:171:LYS:C	2.47	0.53
1:A:231:GLN:HA	1:A:386:ASN:O	2.07	0.53
1:B:367:ASN:HD22	1:B:368:PRO:N	2.06	0.53
1:B:204:THR:HG23	1:B:205:ARG:CG	2.38	0.53
1:A:367:ASN:ND2	1:A:369:SER:H	2.07	0.53
1:B:195:ARG:HB3	1:B:211:GLU:HB2	1.90	0.53
1:A:193:ILE:HG12	1:A:272:ILE:CG2	2.39	0.53
1:A:128:TRP:HA	1:A:128:TRP:CE3	2.44	0.53
1:A:155:SER:O	1:A:156:LYS:HB2	2.09	0.53
1:B:225:LEU:O	1:B:226:SER:CB	2.56	0.53
1:B:185:GLN:NE2	1:B:188:LEU:HD12	2.23	0.53
1:A:195:ARG:HG2	1:A:196:LEU:N	2.25	0.52
1:B:312:LEU:HG	1:B:372:PRO:O	2.08	0.52
1:A:164:LEU:N	1:A:164:LEU:HD12	2.25	0.52
1:A:244:LEU:HD13	1:A:311:ASP:HB2	1.92	0.52
1:A:297:PRO:O	1:A:301:ILE:HG23	2.10	0.52
1:B:165:PHE:HB2	1:B:168:GLN:HE21	1.73	0.52
1:A:196:LEU:HD12	1:A:209:ILE:O	2.10	0.51
1:B:211:GLU:OE1	1:B:271:LYS:HE3	2.11	0.51
1:A:260:GLU:HG3	3:A:400:HOH:O	2.11	0.51
1:B:293:LEU:HD23	1:B:293:LEU:N	2.04	0.51
1:B:312:LEU:N	1:B:312:LEU:CD2	2.73	0.51
1:A:311:ASP:OD1	1:A:312:LEU:HD22	2.10	0.51
1:B:301:ILE:CG1	1:B:302:GLU:N	2.71	0.51
1:B:128:TRP:CZ3	1:B:132:ASP:HB3	2.46	0.50
1:A:349:PRO:HG2	1:A:352:VAL:HG23	1.92	0.50
1:B:196:LEU:HG	1:B:210:LEU:CD2	2.41	0.50
1:A:189:ARG:HH21	1:A:189:ARG:HG2	1.77	0.50
1:A:181:GLU:HB3	1:A:275:PHE:O	2.12	0.50
1:A:185:GLN:NE2	1:A:188:LEU:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:CG2	1:A:270:LEU:HD11	2.42	0.49
1:B:239:GLU:OE1	1:B:269:GLU:HG3	2.12	0.49
1:B:275:PHE:CD2	2:B:1:LJE:H6	2.47	0.49
1:A:134:GLU:HG3	1:A:153:LYS:HD3	1.94	0.49
1:B:217:THR:HA	1:B:262:LEU:O	2.12	0.49
1:A:258:LYS:HG3	1:A:261:ASN:ND2	2.27	0.49
1:A:260:GLU:H	1:A:260:GLU:CD	2.12	0.49
1:B:231:GLN:HG3	1:B:386:ASN:O	2.13	0.49
1:B:288:THR:O	1:B:289:LEU:O	2.31	0.49
1:B:344:VAL:CG2	1:B:366:HIS:HB2	2.43	0.49
1:A:162:LYS:HD3	1:A:164:LEU:HD11	1.94	0.49
1:B:217:THR:HG22	1:B:263:LEU:HD23	1.94	0.49
1:A:222:LEU:HD11	1:A:321:GLU:HG2	1.93	0.49
1:A:309:LYS:HG2	1:A:368:PRO:O	2.13	0.49
1:B:233:THR:O	1:B:237:ILE:HG12	2.13	0.48
1:B:126:ARG:N	1:B:126:ARG:CD	2.76	0.48
1:B:359:LEU:O	1:B:359:LEU:HD22	2.13	0.48
1:A:128:TRP:HA	1:A:128:TRP:HE3	1.78	0.48
1:A:311:ASP:O	1:A:314:SER:HB2	2.14	0.48
1:A:380:HIS:HD2	1:A:382:TRP:H	1.57	0.48
1:A:133:PHE:CZ	1:A:209:ILE:HD13	2.49	0.48
1:A:162:LYS:HD2	2:A:1:LJE:H22	1.96	0.48
1:B:167:ALA:HA	1:B:170:GLU:CD	2.34	0.47
1:B:128:TRP:HE3	1:B:132:ASP:OD2	1.97	0.47
1:A:131:GLU:O	1:A:153:LYS:NZ	2.42	0.47
1:A:274:ASP:C	1:A:276:GLY:N	2.67	0.47
1:B:326:LYS:HD2	1:B:330:GLU:OE1	2.14	0.47
1:B:192:ASN:HB2	1:B:243:ALA:HB2	1.97	0.47
1:B:312:LEU:CD2	1:B:312:LEU:H	2.27	0.47
1:B:349:PRO:HG2	1:B:352:VAL:HG23	1.95	0.47
1:A:166:LYS:NZ	1:A:202:ASP:O	2.47	0.47
1:A:265:GLY:HA3	1:A:269:GLU:OE1	2.15	0.47
1:A:297:PRO:HG2	1:A:300:MET:HB2	1.97	0.47
1:B:196:LEU:HG	1:B:210:LEU:HD23	1.95	0.47
1:A:295:TYR:HE2	1:A:321:GLU:OE2	1.98	0.47
1:A:145:GLY:HA3	1:A:163:VAL:O	2.15	0.46
1:B:275:PHE:N	1:B:275:PHE:HD1	2.12	0.46
1:A:367:ASN:HD22	1:A:368:PRO:CD	2.28	0.46
1:B:248:HIS:C	1:B:250:LYS:H	2.18	0.46
1:B:215:LEU:N	1:B:215:LEU:HD12	2.30	0.46
1:B:256:ASP:OD2	1:B:258:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:O	1:B:223:GLN:HG2	2.16	0.46
1:A:185:GLN:HE21	1:A:188:LEU:HD12	1.80	0.46
1:A:230:GLU:OE1	1:A:382:TRP:NE1	2.47	0.46
1:A:165:PHE:O	1:A:169:LEU:HD22	2.16	0.45
2:A:1:LJE:H22	2:A:1:LJE:O2	2.15	0.45
1:B:167:ALA:HA	1:B:170:GLU:OE2	2.16	0.45
1:B:144:PHE:O	1:B:164:LEU:HG	2.16	0.45
1:B:260:GLU:OE2	1:B:260:GLU:N	2.49	0.45
1:A:154:GLN:HE21	1:A:154:GLN:HB3	1.60	0.45
1:A:250:LYS:O	1:A:252:VAL:HG23	2.15	0.45
1:B:134:GLU:CD	1:B:151:ARG:NH2	2.69	0.45
1:A:143:LYS:O	1:A:144:PHE:HB2	2.17	0.45
1:B:185:GLN:HE22	1:B:188:LEU:HD12	1.82	0.45
1:A:380:HIS:CD2	1:A:382:TRP:HB3	2.52	0.45
1:A:128:TRP:CD1	1:A:209:ILE:CD1	3.00	0.44
1:A:128:TRP:HD1	1:A:209:ILE:HD12	1.81	0.44
1:A:180:ARG:NH1	1:A:277:TRP:CB	2.75	0.44
1:B:164:LEU:HD12	1:B:164:LEU:N	2.33	0.44
1:B:178:LEU:O	1:B:182:VAL:HG23	2.18	0.44
1:A:380:HIS:HD2	1:A:382:TRP:HB3	1.82	0.44
1:B:297:PRO:HB2	1:B:299:GLU:OE1	2.17	0.44
1:B:176:HIS:H	1:B:176:HIS:HD1	1.64	0.44
1:A:307:ASP:CG	1:A:308:GLU:OE1	2.57	0.44
1:A:224:LYS:HE3	1:A:224:LYS:HB3	1.82	0.43
1:B:258:LYS:HZ1	1:B:292:THR:HG21	1.83	0.43
1:B:258:LYS:NZ	1:B:292:THR:HG21	2.33	0.43
1:A:299:GLU:HG3	1:A:306:HIS:HB3	2.00	0.43
1:A:338:TYR:CD2	1:A:338:TYR:C	2.91	0.43
1:A:344:VAL:HG12	1:A:344:VAL:O	2.17	0.43
1:B:333:THR:HG22	1:B:334:TYR:N	2.32	0.43
1:A:190:HIS:HD2	1:A:192:ASN:N	2.16	0.43
1:B:258:LYS:HB2	1:B:260:GLU:HG2	2.00	0.43
1:A:265:GLY:CA	1:A:269:GLU:OE1	2.67	0.43
1:A:128:TRP:CD1	1:A:209:ILE:HD12	2.54	0.43
1:A:215:LEU:HD22	1:A:265:GLY:O	2.19	0.42
1:B:134:GLU:OE2	1:B:151:ARG:NH2	2.52	0.42
1:B:193:ILE:HG12	1:B:272:ILE:HD11	2.01	0.42
1:B:211:GLU:OE1	1:B:271:LYS:CE	2.67	0.42
1:A:248:HIS:ND1	1:A:249:SER:N	2.67	0.42
1:A:359:LEU:O	1:A:363:LEU:HD22	2.19	0.42
1:B:128:TRP:CH2	1:B:152:GLU:OE2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:HIS:CD2	1:A:272:ILE:HD11	2.55	0.42
1:A:155:SER:C	1:A:157:PHE:H	2.22	0.42
1:A:311:ASP:HA	1:A:314:SER:HB2	2.02	0.41
1:B:155:SER:O	1:B:156:LYS:HB2	2.20	0.41
1:B:227:LYS:HD3	3:B:405:HOH:O	2.20	0.41
1:B:309:LYS:HB3	1:B:368:PRO:HB3	2.02	0.41
1:A:182:VAL:HG12	1:A:183:GLU:N	2.34	0.41
1:A:306:HIS:CE1	3:A:108:HOH:O	2.72	0.41
1:B:222:LEU:HD21	1:B:321:GLU:HG2	2.01	0.41
1:A:162:LYS:HD2	2:A:1:LJE:C22	2.50	0.41
1:B:192:ASN:HA	1:B:270:LEU:O	2.21	0.41
1:A:202:ASP:OD1	1:A:202:ASP:C	2.59	0.41
1:A:195:ARG:HG2	1:A:196:LEU:H	1.83	0.41
1:B:198:GLY:C	1:B:209:ILE:HD12	2.41	0.41
1:A:255:ARG:CB	1:A:300:MET:HE3	2.50	0.41
1:A:292:THR:HG23	1:A:292:THR:O	2.20	0.41
1:A:358:ASP:OD2	1:A:380:HIS:HE1	2.04	0.41
1:B:162:LYS:HG2	1:B:164:LEU:CD1	2.50	0.41
1:B:301:ILE:HD12	1:B:338:TYR:CD1	2.55	0.41
1:B:264:LEU:HA	1:B:269:GLU:O	2.20	0.41
1:B:309:LYS:HA	1:B:309:LYS:HD2	1.79	0.41
1:B:165:PHE:HB2	1:B:168:GLN:NE2	2.35	0.41
1:B:180:ARG:O	1:B:184:ILE:HG12	2.21	0.41
1:B:190:HIS:HD2	1:B:192:ASN:H	1.67	0.41
1:B:194:LEU:HD12	1:B:194:LEU:HA	1.85	0.41
1:B:327:PRO:HB2	3:B:62:HOH:O	2.21	0.41
1:B:376:GLU:HA	1:B:379:GLU:OE1	2.21	0.41
1:B:154:GLN:HG3	1:B:154:GLN:O	2.20	0.41
1:B:327:PRO:HG2	1:B:330:GLU:HB2	2.01	0.41
1:B:126:ARG:HE	1:B:126:ARG:HB3	1.57	0.40
1:A:151:ARG:HD3	1:A:158:ILE:HD11	2.03	0.40
1:A:163:VAL:HG11	1:A:205:ARG:HD3	2.03	0.40
1:A:248:HIS:ND1	1:A:248:HIS:C	2.73	0.40
1:B:168:GLN:HE21	1:B:168:GLN:HB2	1.32	0.40
1:A:337:THR:O	1:A:341:ILE:HG13	2.21	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	240/267 (90%)	221 (92%)	15 (6%)	4 (2%)	9 4
1	B	243/267 (91%)	223 (92%)	13 (5%)	7 (3%)	4 1
All	All	483/534 (90%)	444 (92%)	28 (6%)	11 (2%)	6 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP
1	A	275	PHE
1	B	256	ASP
1	B	289	LEU
1	A	171	LYS
1	B	143	LYS
1	B	226	SER
1	B	294	ASP
1	A	226	SER
1	B	144	PHE
1	B	291	GLY

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	208/236 (88%)	184 (88%)	24 (12%)	5 3
1	B	212/236 (90%)	193 (91%)	19 (9%)	9 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	420/472 (89%)	377 (90%)	43 (10%)	7 4

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	TRP
1	A	130	LEU
1	A	149	LEU
1	A	152	GLU
1	A	154	GLN
1	A	157	PHE
1	A	159	LEU
1	A	169	LEU
1	A	179	ARG
1	A	185	GLN
1	A	204	THR
1	A	208	LEU
1	A	222	LEU
1	A	224	LYS
1	A	248	HIS
1	A	260	GLU
1	A	266	SER
1	A	269	GLU
1	A	315	LEU
1	A	340	ARG
1	A	359	LEU
1	A	363	LEU
1	A	367	ASN
1	A	373	MET
1	B	126	ARG
1	B	141	LYS
1	B	149	LEU
1	B	168	GLN
1	B	175	GLU
1	B	189	ARG
1	B	260	GLU
1	B	269	GLU
1	B	274	ASP
1	B	289	LEU
1	B	292	THR
1	B	293	LEU
1	B	300	MET

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Mol	Chain	Res	Type
1	B	315	LEU
1	B	336	GLU
1	B	354	GLU
1	B	359	LEU
1	B	367	ASN
1	B	379	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	185	GLN
1	A	190	HIS
1	A	192	ASN
1	A	201	HIS
1	A	223	GLN
1	A	261	ASN
1	A	367	ASN
1	A	370	GLN
1	A	380	HIS
1	B	168	GLN
1	B	177	GLN
1	B	190	HIS
1	B	192	ASN
1	B	223	GLN
1	B	231	GLN
1	B	332	ASN
1	B	367	ASN
1	B	370	GLN
1	B	380	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	LJE	B	1	-	35,36,36	2.61	19 (54%)	43,51,51	2.49	20 (46%)
2	LJE	A	1	-	35,36,36	3.37	24 (68%)	43,51,51	2.35	14 (32%)

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	LJE	B	1	-	-	0/18/22/22	0/4/4/4
2	LJE	A	1	-	-	4/18/22/22	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	LJE	C12-C11	8.57	1.48	1.36
2	A	1	LJE	C10-N1	6.71	1.42	1.32
2	A	1	LJE	C16-N3	6.12	1.41	1.31
2	A	1	LJE	C2-C3	5.35	1.48	1.39
2	A	1	LJE	C4-C3	5.18	1.47	1.39
2	B	1	LJE	C4-C3	4.96	1.46	1.39
2	B	1	LJE	C16-N3	4.56	1.39	1.31
2	B	1	LJE	C4-C5	4.55	1.46	1.39
2	A	1	LJE	C9-N1	4.36	1.44	1.37
2	A	1	LJE	C13-C14	4.19	1.45	1.36
2	B	1	LJE	C2-C3	4.09	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	LJE	C22-C21	4.08	1.46	1.39
2	A	1	LJE	C12-C9	4.06	1.48	1.41
2	A	1	LJE	C4-C5	4.00	1.45	1.39
2	B	1	LJE	C1-C2	3.99	1.45	1.38
2	B	1	LJE	C18-C19	3.55	1.47	1.39
2	B	1	LJE	C6-C5	3.49	1.44	1.39
2	A	1	LJE	C21-N4	-3.30	1.35	1.41
2	A	1	LJE	C1-C2	3.19	1.44	1.38
2	A	1	LJE	C10-N2	3.16	1.39	1.33
2	B	1	LJE	C9-N1	3.12	1.42	1.37
2	B	1	LJE	C13-C14	3.10	1.43	1.36
2	B	1	LJE	C12-C11	3.01	1.40	1.36
2	A	1	LJE	C7-C3	3.00	1.56	1.49
2	B	1	LJE	C24-C19	-2.92	1.45	1.51
2	B	1	LJE	C5-C8	-2.78	1.44	1.50
2	A	1	LJE	C5-C8	-2.77	1.44	1.50
2	A	1	LJE	C11-N2	2.68	1.41	1.33
2	A	1	LJE	C1-C6	2.57	1.43	1.38
2	B	1	LJE	C21-N4	-2.53	1.36	1.41
2	B	1	LJE	C7-C3	2.52	1.55	1.49
2	A	1	LJE	C22-C21	2.51	1.43	1.39
2	B	1	LJE	C10-N1	2.49	1.35	1.32
2	A	1	LJE	C13-C17	2.49	1.44	1.37
2	A	1	LJE	C23-C22	2.46	1.42	1.38
2	B	1	LJE	C20-C21	2.37	1.43	1.39
2	A	1	LJE	C17-N3	2.24	1.39	1.34
2	A	1	LJE	C20-C21	2.24	1.43	1.39
2	B	1	LJE	C1-C6	2.17	1.42	1.38
2	A	1	LJE	C23-C18	2.11	1.43	1.39
2	A	1	LJE	C14-C15	2.08	1.46	1.42
2	A	1	LJE	C6-C5	2.05	1.42	1.39
2	B	1	LJE	C13-C17	2.02	1.43	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	LJE	C10-N1-C9	9.24	125.94	115.43
2	B	1	LJE	C10-N1-C9	6.18	122.45	115.43
2	B	1	LJE	C13-C17-N3	-5.24	115.13	123.42
2	A	1	LJE	C13-C17-N3	-5.18	115.22	123.42
2	B	1	LJE	C11-N2-C10	4.82	125.00	115.35
2	A	1	LJE	C13-C14-C15	4.00	126.31	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	LJE	C15-C16-N3	-3.90	120.12	124.34
2	B	1	LJE	C18-O1-C16	3.66	122.63	117.79
2	B	1	LJE	C17-N3-C16	3.57	127.06	116.28
2	B	1	LJE	C21-C20-C19	-3.31	115.88	121.19
2	B	1	LJE	O1-C16-C15	3.29	120.52	115.43
2	B	1	LJE	C22-C21-C20	3.26	123.60	119.66
2	A	1	LJE	O1-C16-N3	3.23	123.90	119.62
2	B	1	LJE	O1-C18-C23	-3.23	112.29	120.74
2	B	1	LJE	C1-C2-C3	3.18	123.99	120.75
2	A	1	LJE	C17-N3-C16	3.09	125.61	116.28
2	A	1	LJE	C21-C20-C19	-2.92	116.50	121.19
2	A	1	LJE	C20-C19-C18	2.86	121.03	117.80
2	B	1	LJE	C6-C1-C2	-2.73	116.74	120.24
2	B	1	LJE	C5-C4-C3	-2.70	117.53	121.04
2	B	1	LJE	C6-C5-C4	2.65	122.32	119.25
2	A	1	LJE	C18-O1-C16	2.61	121.25	117.79
2	A	1	LJE	F2-C7-C3	-2.60	107.33	112.90
2	B	1	LJE	C22-C23-C18	-2.46	115.41	120.06
2	B	1	LJE	F3-C7-C3	-2.44	107.68	112.90
2	B	1	LJE	F2-C7-C3	-2.43	107.68	112.90
2	A	1	LJE	C22-C21-C20	2.43	122.60	119.66
2	A	1	LJE	C22-C23-C18	-2.35	115.61	120.06
2	B	1	LJE	C5-C8-N4	-2.26	110.41	115.90
2	A	1	LJE	C6-C1-C2	-2.23	117.38	120.24
2	A	1	LJE	C5-C4-C3	-2.08	118.34	121.04
2	B	1	LJE	C24-C19-C18	2.06	123.86	120.94
2	A	1	LJE	C1-C6-C5	2.01	122.34	120.36
2	B	1	LJE	O1-C18-C19	2.01	123.53	118.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	LJE	C4-C5-C8-O2
2	A	1	LJE	C6-C5-C8-O2
2	A	1	LJE	C4-C5-C8-N4
2	A	1	LJE	C6-C5-C8-N4

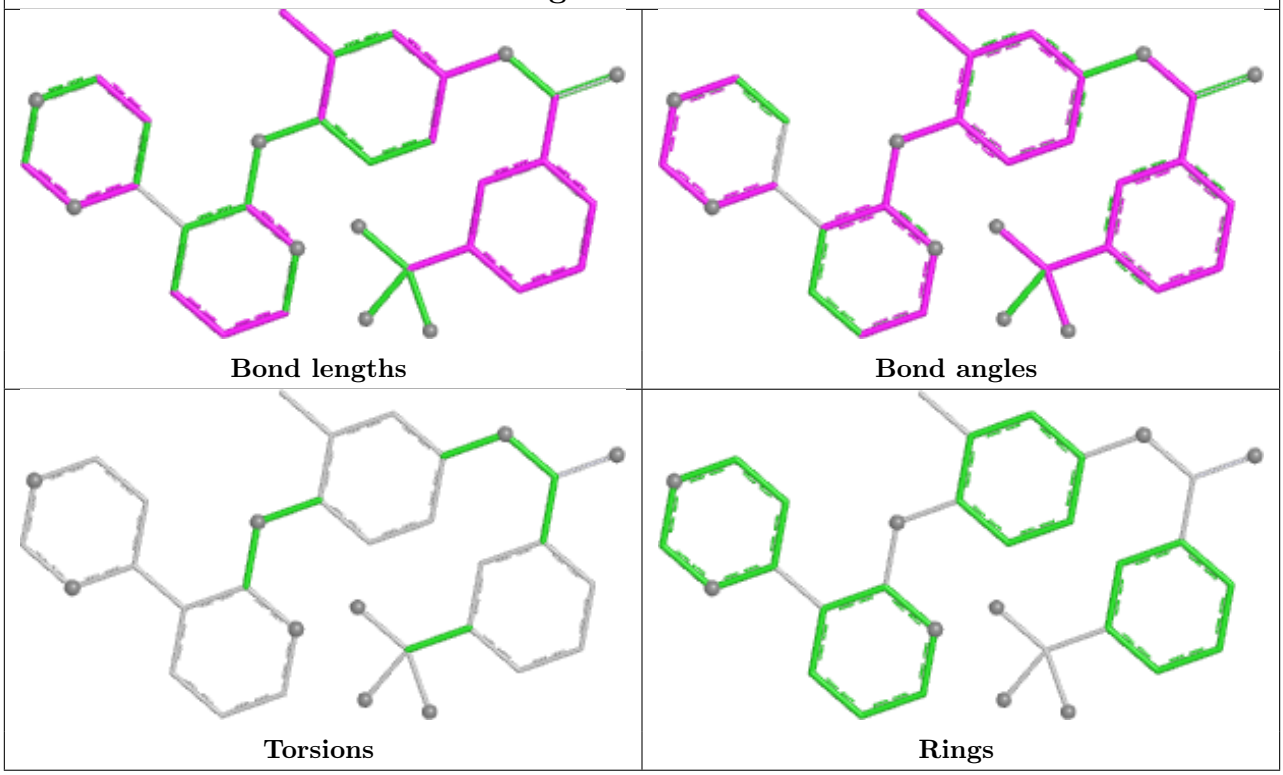
There are no ring outliers.

2 monomers are involved in 5 short contacts:

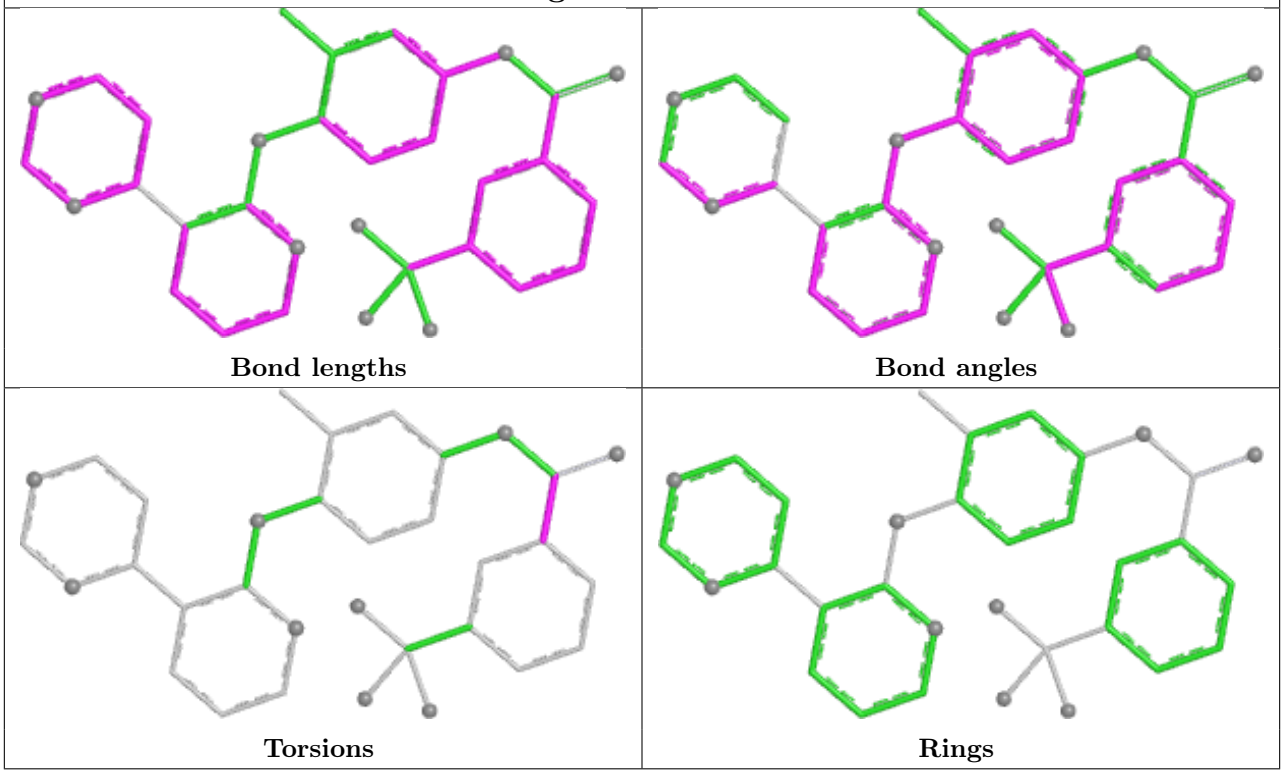
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	LJE	1	0
2	A	1	LJE	4	0

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 then 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 LJE B 1



Ligand LJE A 1



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	246/267 (92%)	0.89	31 (12%)	3	3	12, 25, 47, 57	0
1	B	249/267 (93%)	1.09	34 (13%)	3	2	11, 25, 48, 64	0
All	All	495/534 (92%)	0.99	65 (13%)	3	3	11, 25, 48, 64	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	CYS	10.7
1	B	289	LEU	8.7
1	B	308	GLU	6.9
1	B	288	THR	6.3
1	B	287	THR	6.1
1	B	334	TYR	5.2
1	B	126	ARG	5.1
1	B	251	ARG	5.0
1	A	275	PHE	5.0
1	A	277	TRP	4.8
1	B	291	GLY	4.8
1	B	275	PHE	4.7
1	B	292	THR	4.3
1	B	157	PHE	4.3
1	B	128	TRP	4.0
1	B	176	HIS	3.9
1	A	293	LEU	3.8
1	A	306	HIS	3.6
1	A	257	ILE	3.6
1	A	292	THR	3.5
1	A	199	TYR	3.5
1	A	157	PHE	3.4
1	A	248	HIS	3.3
1	B	307	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	253	ILE	3.3
1	A	338	TYR	3.3
1	A	176	HIS	3.2
1	B	169	LEU	3.1
1	A	128	TRP	3.1
1	A	249	SER	3.1
1	B	199	TYR	3.0
1	B	338	TYR	3.0
1	B	203	ALA	3.0
1	B	248	HIS	2.9
1	A	274	ASP	2.9
1	B	272	ILE	2.9
1	A	388	SER	2.9
1	A	179	ARG	2.8
1	A	178	LEU	2.5
1	A	154	GLN	2.5
1	A	337	THR	2.4
1	B	293	LEU	2.4
1	A	171	LYS	2.3
1	A	173	GLY	2.3
1	B	170	GLU	2.3
1	A	219	TYR	2.3
1	A	254	HIS	2.3
1	B	144	PHE	2.2
1	A	272	ILE	2.2
1	B	160	ALA	2.2
1	B	204	THR	2.2
1	A	276	GLY	2.2
1	A	174	VAL	2.2
1	A	367	ASN	2.1
1	B	274	ASP	2.1
1	B	339	LYS	2.1
1	B	255	ARG	2.1
1	B	219	TYR	2.1
1	A	342	SER	2.1
1	B	210	LEU	2.0
1	A	333	THR	2.0
1	B	167	ALA	2.0
1	B	273	ALA	2.0
1	A	189	ARG	2.0
1	B	177	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

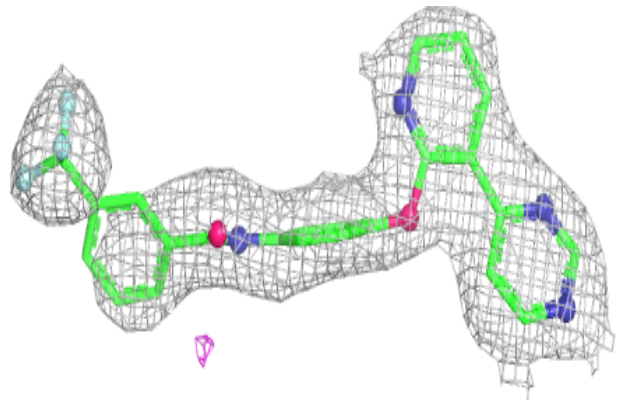
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

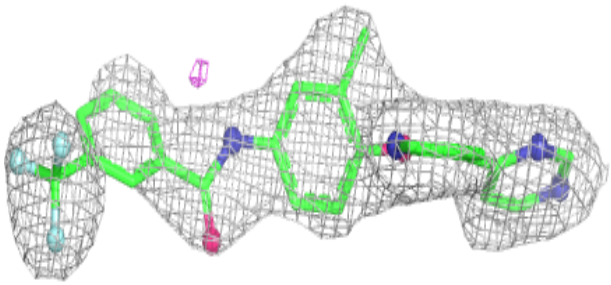
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LJE	A	1	33/33	0.91	0.19	10,23,37,40	0
2	LJE	B	1	33/33	0.92	0.17	8,17,31,32	0

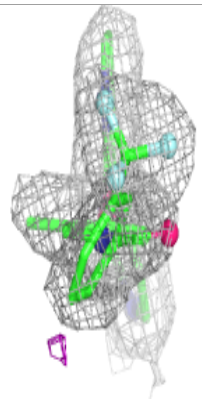
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LJE A 1:

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

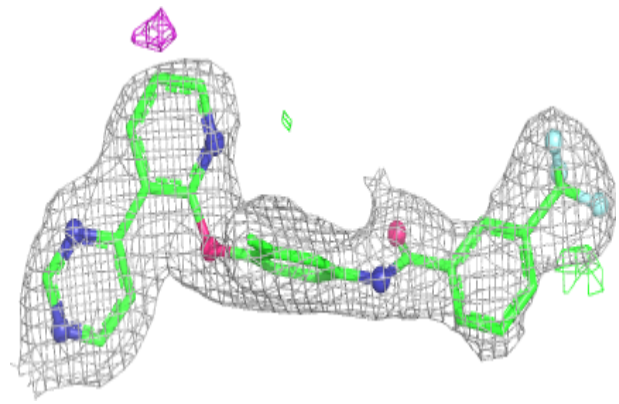


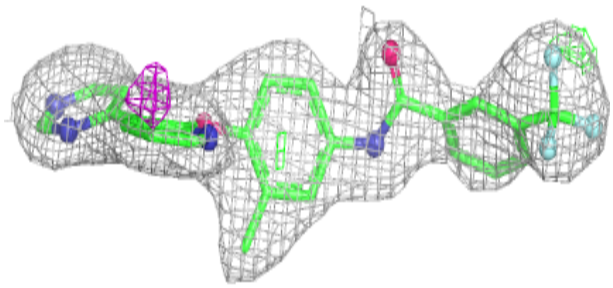


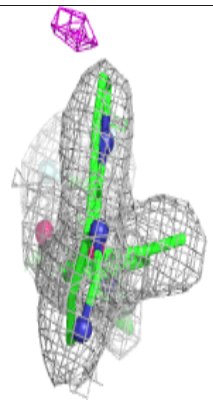


Electron density around LJE B 1:

$2mF_o$-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.