Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:49 AM EDT

PDB ID	:	3HM1
Title	:	Crystal structure of human Estrogen Receptor Alpha Ligand-Binding Domain in complex with a Glucocorticoid Receptor Interacting Protein 1 Nr Box II Peptide and estrone ((8R,9S,13S,14S)-3-hydroxy-13-methyl-7,8,9,11,12,14,15,16-octahydro-6H-cyclopenta[a]phenanthren-17-one)
Authors	:	Rajan, S.S.; Kim, Y.; Vanek, K.; Liwanag, M.; Joachimiak, A.; Greene, G.L.
Deposited on	:	2009-05-28
Resolution	:	2.33 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:

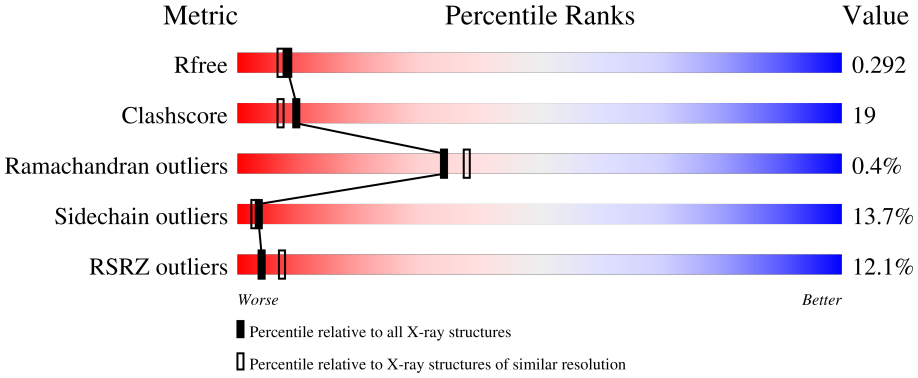
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	253	13% 51% 34% 8% 7%
1	B	253	9% 64% 23% 7% 6%
2	C	13	23% 31% 31% 15% 23%
2	D	13	15% 31% 31% 8% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4062 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	1911	1223	327	339	22	0	3	0
1	B	239	1933	1237	334	340	22	0	2	0

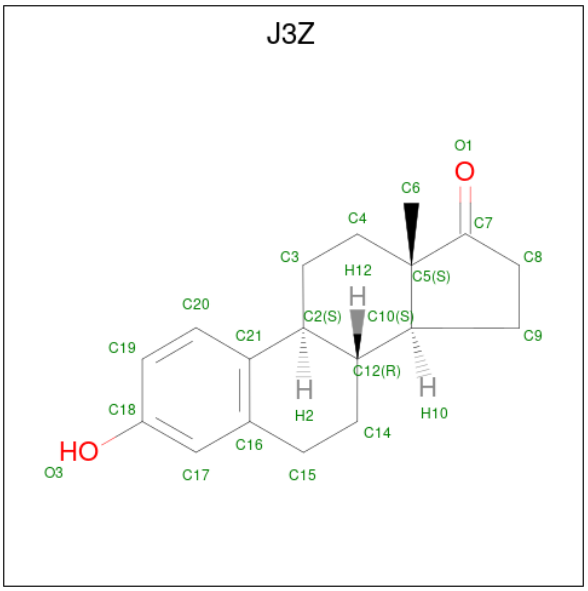
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	SER	TYR	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	89	57	19	13	0	0	0
2	D	9	79	51	16	12	0	0	0

- Molecule 3 is (9beta,13alpha)-3-hydroxyestra-1,3,5(10)-trien-17-one (three-letter code: J3Z) (formula: $C_{18}H_{22}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	B	1	Total C O 20 18 2	0	0

- Molecule 4 is water.

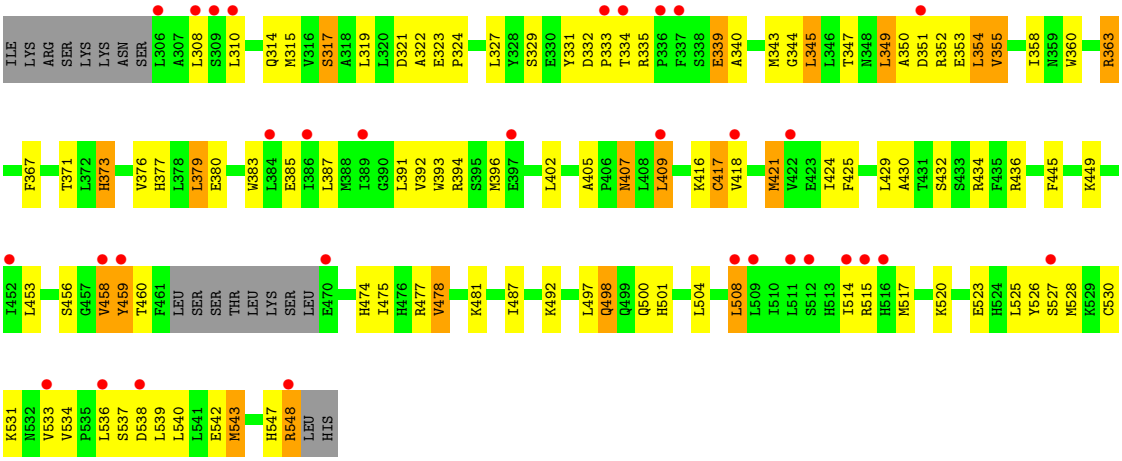
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	2	Total O 2 2	0	0

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.

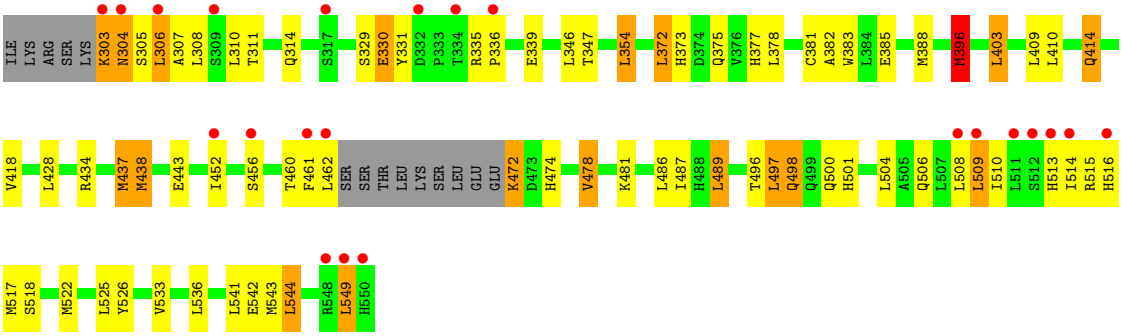
• Molecule 1: Estrogen receptor

Chain A:



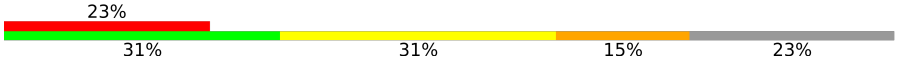
• Molecule 1: Estrogen receptor

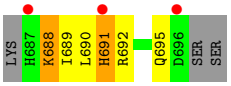
Chain B:



• Molecule 2: Nuclear receptor coactivator 2

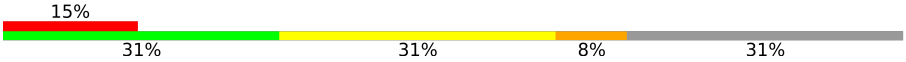
Chain C:

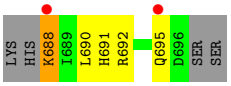




• Molecule 2: Nuclear receptor coactivator 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.27Å 82.67Å 58.99Å 90.00° 109.18° 90.00°	Depositor
Resolution (Å)	33.37 – 2.33 33.37 – 2.33	Depositor EDS
% Data completeness (in resolution range)	86.0 (33.37-2.33) 86.0 (33.37-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.86 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.231 , 0.289 0.240 , 0.292	Depositor DCC
R_{free} test set	966 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4062	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: CME, J3Z

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	0.30	0/1926	0.51	0/2595
1	B	0.31	0/1946	0.49	0/2624
2	C	0.21	0/90	0.35	0/119
2	D	0.24	0/79	0.39	0/104
All	All	0.30	0/4041	0.50	0/5442

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	1911	0	1951	95	0
1	B	1933	0	1981	66	0
2	C	89	0	95	4	0
2	D	79	0	88	6	0
3	A	20	0	22	1	0
3	B	20	0	22	2	0
4	A	8	0	0	1	0
4	B	2	0	0	0	0
All	All	4062	0	4159	159	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 (159) 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)
2:D:688:LYS:HG2	2:D:691:HIS:HB2	1.46	0.95
1:B:335:ARG:HG3	1:B:336:PRO:HD2	1.59	0.83
1:B:330:GLU:HG2	1:B:330:GLU:O	1.82	0.78
1:A:481:LYS:HZ2	1:A:481:LYS:HB3	1.48	0.78
1:A:393:TRP:O	1:A:396:MET:HB2	1.84	0.77
1:A:331:TYR:HB2	1:A:345:LEU:HD21	1.67	0.76
2:C:688:LYS:HG3	2:C:691:HIS:HB3	1.67	0.76
1:B:410:LEU:HD22	1:B:414:GLN:HG2	1.69	0.74
1:B:335:ARG:HG3	1:B:336:PRO:CD	2.17	0.74
2:D:688:LYS:HG3	2:D:691:HIS:H	1.54	0.73
1:A:526:TYR:CE2	1:A:530:CME:HE3	2.25	0.71
1:B:304:ASN:H	1:B:304:ASN:HD22	1.35	0.71
1:A:377:HIS:NE2	1:A:460:THR:HG23	2.06	0.71
1:A:498:GLN:HA	1:A:501[A]:HIS:NE2	2.07	0.70
1:B:525:LEU:HD11	1:B:536:LEU:HD11	1.72	0.70
1:A:391:LEU:HA	1:A:394:ARG:NH1	2.08	0.68
1:B:474:HIS:O	1:B:478:VAL:HG12	1.93	0.68
1:A:508:LEU:HG	1:B:509:LEU:CD1	2.24	0.67
1:A:526:TYR:HE2	1:A:530:CME:HE3	1.57	0.67
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.76	0.66
1:B:522:MET:HA	1:B:522:MET:CE	2.27	0.65
1:A:322:ALA:HA	1:A:363:ARG:NH2	2.12	0.64
1:A:481:LYS:HB3	1:A:481:LYS:NZ	2.13	0.64
1:A:354:LEU:O	1:A:358:ILE:HG12	1.97	0.64
1:B:383:TRP:NE1	1:B:543:MET:HB3	2.15	0.62
1:A:349:LEU:HD11	1:A:405:ALA:HB2	1.81	0.62
1:B:304:ASN:HD22	1:B:304:ASN:N	1.98	0.62
1:A:459[A]:TYR:CE2	1:B:513[A]:HIS:HB3	2.35	0.62
1:A:525:LEU:HD13	3:A:2:J3Z:H36	1.82	0.61
1:A:308:LEU:HD21	1:A:477:ARG:HB3	1.83	0.61
1:B:438:MET:HG3	1:B:438:MET:O	2.00	0.61
1:B:443:GLU:HB3	1:B:489:LEU:HD21	1.83	0.60
1:A:487:ILE:CD1	1:A:504:LEU:HD22	2.32	0.59
1:B:347:THR:HG21	1:B:536:LEU:HD21	1.85	0.59
1:A:429:LEU:HD12	1:A:430:ALA:N	2.17	0.58
2:D:688:LYS:CG	2:D:691:HIS:H	2.16	0.58
1:B:497:LEU:HD22	1:B:501[A]:HIS:HE2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:THR:O	1:B:500:GLN:HG3	2.04	0.56
1:A:360:TRP:CZ2	1:A:449:LYS:HG2	2.40	0.56
1:A:371:THR:HG22	1:A:373:HIS:H	1.71	0.56
1:B:346:LEU:HB3	3:B:1:J3Z:H23	1.87	0.56
1:B:388:MET:HG2	1:B:428:LEU:HD21	1.87	0.56
1:A:391:LEU:HD11	1:A:402:LEU:HB3	1.88	0.56
1:B:437:MET:O	1:B:437:MET:HG2	2.06	0.55
1:B:549:LEU:HD22	1:B:549:LEU:N	2.22	0.55
1:A:329:SER:H	1:A:407:ASN:HD21	1.52	0.55
1:B:526:TYR:CD2	1:B:549:LEU:HD23	2.42	0.55
1:A:459[A]:TYR:CE1	1:B:513[A]:HIS:CD2	2.95	0.54
1:B:339:GLU:HA	1:B:418:VAL:HG22	1.90	0.53
1:B:311:THR:HG23	1:B:314:GLN:OE1	2.08	0.53
1:A:527:SER:O	1:A:531:LYS:HG2	2.08	0.53
1:B:377:HIS:CD2	1:B:461:PHE:CE2	2.97	0.53
1:B:497:LEU:HD22	1:B:501[A]:HIS:NE2	2.23	0.53
1:A:314:GLN:HA	1:A:317:SER:HB2	1.90	0.53
1:A:456:SER:HA	1:A:515:ARG:NH2	2.25	0.52
1:A:344:GLY:HA2	1:A:534:VAL:HG21	1.90	0.52
1:A:351:ASP:OD2	1:A:540:LEU:HB2	2.09	0.52
1:A:329:SER:H	1:A:407:ASN:ND2	2.07	0.52
1:A:498:GLN:HA	1:A:501[A]:HIS:CD2	2.45	0.52
1:A:329:SER:HB3	1:A:407:ASN:HD21	1.75	0.52
1:B:522:MET:HA	1:B:522:MET:HE2	1.92	0.51
1:A:315:MET:HE3	1:A:481:LYS:NZ	2.26	0.51
1:A:344:GLY:CA	1:A:534:VAL:HG21	2.42	0.50
1:A:514:ILE:HA	1:A:517:MET:HE2	1.93	0.50
1:A:487:ILE:HD13	1:A:504:LEU:HD22	1.92	0.50
1:B:486:LEU:HD23	1:B:504:LEU:HD12	1.92	0.50
1:A:352:ARG:NH2	4:A:5:HOH:O	2.43	0.50
1:A:474:HIS:O	1:A:478:VAL:HG12	2.11	0.50
1:A:459[B]:TYR:HE2	1:B:434:ARG:HG2	1.76	0.49
1:A:498:GLN:HA	1:A:501[A]:HIS:CE1	2.48	0.49
1:B:382:ALA:HB2	1:B:456:SER:OG	2.12	0.49
1:B:506:GLN:O	1:B:510:ILE:HG13	2.13	0.48
1:A:416:LYS:O	1:A:417:CME:C	2.61	0.48
1:A:497:LEU:O	1:A:500:GLN:HB2	2.14	0.48
1:A:421:MET:CE	1:A:421:MET:HA	2.43	0.48
1:B:498:GLN:HA	1:B:501[B]:HIS:ND1	2.28	0.48
1:A:393:TRP:HB2	1:A:445:PHE:CE1	2.48	0.48
1:A:391:LEU:HA	1:A:394:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:O	1:A:380:GLU:HG3	2.14	0.48
1:B:525:LEU:HG	1:B:544:LEU:CD2	2.44	0.48
1:A:525:LEU:HD12	1:A:528:MET:CE	2.44	0.48
1:A:528:MET:HG3	1:A:533:VAL:HG23	1.95	0.48
1:B:487:ILE:HG23	1:B:500:GLN:NE2	2.29	0.47
1:A:331:TYR:CB	1:A:345:LEU:HD21	2.43	0.47
1:B:498:GLN:HA	1:B:501[B]:HIS:CE1	2.50	0.47
1:A:349:LEU:O	1:A:353:GLU:HG3	2.15	0.47
1:B:385:GLU:HG3	1:B:518:SER:HB2	1.98	0.46
1:A:343:MET:SD	1:A:418:VAL:HG21	2.55	0.46
1:B:410:LEU:HD23	1:B:414:GLN:HE21	1.80	0.46
1:A:538:ASP:O	1:A:538:ASP:OD2	2.34	0.46
1:B:329:SER:C	1:B:331:TYR:H	2.19	0.46
1:A:379:LEU:O	1:A:383:TRP:HB3	2.16	0.46
1:A:352:ARG:O	1:A:355:VAL:HG13	2.16	0.45
1:A:385:GLU:CG	1:A:514:ILE:HG22	2.44	0.45
1:A:367:PHE:CE1	1:A:453:LEU:HD11	2.51	0.45
1:A:523:GLU:CD	1:A:548[B]:ARG:HH12	2.20	0.45
1:B:514:ILE:HA	1:B:517:MET:HE2	1.99	0.45
1:A:308:LEU:HD21	1:A:477:ARG:HE	1.82	0.45
1:A:343:MET:HE2	1:A:528:MET:SD	2.57	0.45
1:A:351:ASP:OD1	1:A:537:SER:HB3	2.16	0.45
1:A:458:VAL:HG23	1:A:475:ILE:HD12	1.99	0.44
1:B:305:SER:C	1:B:307:ALA:H	2.20	0.44
1:B:307:ALA:HA	1:B:310:LEU:CD1	2.47	0.44
1:B:403:LEU:HD12	1:B:409:LEU:HD11	1.98	0.44
2:D:688:LYS:HD2	2:D:690:LEU:HB3	2.00	0.44
1:A:409:LEU:H	1:A:409:LEU:CD1	2.31	0.44
2:C:691:HIS:O	2:C:695:GLN:HG3	2.18	0.44
1:A:459[B]:TYR:CE2	1:B:434:ARG:HG2	2.51	0.44
1:A:396:MET:O	1:A:436:ARG:HD3	2.18	0.44
1:A:528:MET:HE3	1:A:536:LEU:HD21	2.00	0.44
1:A:458:VAL:HG12	1:A:459[B]:TYR:CD1	2.53	0.44
1:A:347:THR:HG21	1:A:528:MET:HE1	1.99	0.43
1:B:385:GLU:HB3	1:B:452:ILE:HG21	2.00	0.43
1:A:339:GLU:HG3	1:A:340:ALA:N	2.34	0.43
1:A:332:ASP:C	1:A:334:THR:H	2.21	0.43
1:A:421:MET:CE	1:A:424:ILE:HD12	2.48	0.43
1:A:456:SER:HA	1:A:515:ARG:HH22	1.83	0.43
1:A:525:LEU:HD12	1:A:528:MET:HE2	2.00	0.43
2:C:691:HIS:CD2	2:C:692:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HG2	1:A:418:VAL:HG21	2.01	0.43
1:B:510:ILE:O	1:B:514:ILE:HG13	2.18	0.43
1:B:472:LYS:N	1:B:472:LYS:HE2	2.34	0.43
1:A:459[B]:TYR:HE2	1:B:434:ARG:CG	2.32	0.43
1:A:497:LEU:HD13	1:B:497:LEU:HD21	2.00	0.43
1:A:387:LEU:HD12	1:A:387:LEU:HA	1.90	0.43
1:A:421:MET:HA	1:A:421:MET:HE2	2.00	0.43
1:A:520:LYS:HA	1:A:520:LYS:HD3	1.83	0.42
1:A:339:GLU:HG3	1:A:340:ALA:H	1.84	0.42
1:B:306:LEU:O	1:B:306:LEU:HG	2.19	0.42
1:B:541:LEU:HD12	1:B:541:LEU:HA	1.87	0.42
2:D:688:LYS:CG	2:D:691:HIS:HB2	2.33	0.42
1:A:315:MET:O	1:A:319:LEU:HG	2.20	0.42
1:A:380:GLU:O	1:A:547:HIS:HE1	2.03	0.42
1:A:409:LEU:H	1:A:409:LEU:HD12	1.84	0.42
1:B:525:LEU:HD22	3:B:1:J3Z:H36	2.02	0.42
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.82	0.42
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.83	0.42
1:B:522:MET:HE1	1:B:525:LEU:HD23	2.01	0.42
1:B:544:LEU:HD13	1:B:544:LEU:HA	1.78	0.42
1:A:392:VAL:HG13	1:A:432:SER:HA	2.02	0.41
1:A:409:LEU:HD13	1:A:409:LEU:O	2.20	0.41
1:A:350:ALA:O	1:A:354:LEU:HB2	2.20	0.41
1:A:543:MET:CE	2:C:690:LEU:HD22	2.50	0.41
1:B:310:LEU:O	1:B:481:LYS:HE2	2.20	0.41
1:B:396:MET:HE3	1:B:396:MET:HB3	1.94	0.41
1:B:372:LEU:HD21	2:D:695:GLN:CD	2.40	0.41
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.87	0.41
1:A:515:ARG:HD2	1:B:516:HIS:HB2	2.02	0.41
1:A:391:LEU:HD12	1:A:391:LEU:O	2.21	0.41
1:B:303:LYS:HB2	1:B:303:LYS:HE3	1.94	0.41
1:B:456:SER:HA	1:B:515:ARG:NH2	2.36	0.41
1:A:501[B]:HIS:CD2	1:B:501[B]:HIS:HB3	2.56	0.41
1:B:305:SER:C	1:B:307:ALA:N	2.74	0.41
1:A:407:ASN:H	1:A:407:ASN:HD22	1.69	0.41
1:B:403:LEU:CD1	1:B:409:LEU:HD11	2.51	0.40
1:A:323:GLU:HA	1:A:324:PRO:HD3	1.84	0.40
1:A:459[A]:TYR:CE1	1:B:513[A]:HIS:HD2	2.39	0.40
1:B:372:LEU:HD22	1:B:375:GLN:NE2	2.37	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	230/253 (91%)	224 (97%)	5 (2%)	1 (0%)	34	38
1	B	234/253 (92%)	225 (96%)	8 (3%)	1 (0%)	34	38
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	479/532 (90%)	464 (97%)	13 (3%)	2 (0%)	34	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	MET
1	A	333	PRO

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	211/226 (93%)	181 (86%)	30 (14%)	3	3
1	B	214/226 (95%)	187 (87%)	27 (13%)	4	3
2	C	10/13 (77%)	7 (70%)	3 (30%)	0	0
2	D	9/13 (69%)	7 (78%)	2 (22%)	1	0
All	All	444/478 (93%)	382 (86%)	62 (14%)	3	3

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	317	SER
1	A	321	ASP
1	A	327	LEU
1	A	335	ARG
1	A	339	GLU
1	A	345	LEU
1	A	349	LEU
1	A	354	LEU
1	A	355	VAL
1	A	363	ARG
1	A	373	HIS
1	A	379	LEU
1	A	407	ASN
1	A	409	LEU
1	A	421	MET
1	A	425	PHE
1	A	434	ARG
1	A	458	VAL
1	A	459[A]	TYR
1	A	459[B]	TYR
1	A	478	VAL
1	A	492	LYS
1	A	498	GLN
1	A	508	LEU
1	A	539	LEU
1	A	542	GLU
1	A	543	MET
1	A	548[A]	ARG
1	A	548[B]	ARG
1	B	303	LYS
1	B	304	ASN
1	B	306	LEU
1	B	308	LEU
1	B	330	GLU
1	B	354	LEU
1	B	372	LEU
1	B	373	HIS
1	B	378	LEU
1	B	396	MET
1	B	403	LEU
1	B	414	GLN
1	B	437	MET

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Mol	Chain	Res	Type
1	B	438	MET
1	B	460	THR
1	B	462	LEU
1	B	472	LYS
1	B	478	VAL
1	B	489	LEU
1	B	497	LEU
1	B	498	GLN
1	B	508	LEU
1	B	509	LEU
1	B	533	VAL
1	B	542	GLU
1	B	544	LEU
1	B	549	LEU
2	C	688	LYS
2	C	689	ILE
2	C	691	HIS
2	D	688	LYS
2	D	692	ARG

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

Mol	Chain	Res	Type
1	A	375	GLN
1	A	407	ASN
1	A	474	HIS
1	A	499	GLN
1	A	502	GLN
1	A	519	ASN
1	A	547	HIS
1	B	304	ASN
1	B	375	GLN
1	B	377	HIS
1	B	414	GLN
1	B	476	HIS
1	B	500	GLN
1	B	502	GLN
1	B	506	GLN
1	B	519	ASN
1	B	532	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	A	417	1	8,9,10	0.60	0	5,9,11	1.75	1 (20%)
1	CME	B	417	1	8,9,10	0.50	0	5,9,11	0.66	0
1	CME	A	530	1	8,9,10	0.51	0	5,9,11	0.39	0
1	CME	B	381	1	8,9,10	0.55	0	5,9,11	2.21	1 (20%)
1	CME	A	381	1	8,9,10	0.52	0	5,9,11	0.51	0
1	CME	B	530	1	8,9,10	0.41	0	5,9,11	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	417	1	-	2/5/8/10	-
1	CME	B	417	1	-	0/5/8/10	-
1	CME	A	530	1	-	2/5/8/10	-
1	CME	B	381	1	-	1/5/8/10	-
1	CME	A	381	1	-	1/5/8/10	-
1	CME	B	530	1	-	0/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	381	CME	CB-SG-SD	-4.77	91.46	103.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	CME	CB-SG-SD	3.39	112.61	103.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	417	CME	CA-CB-SG-SD
1	B	381	CME	N-CA-CB-SG
1	A	530	CME	CA-CB-SG-SD
1	A	381	CME	CZ-CE-SD-SG
1	A	417	CME	CZ-CE-SD-SG
1	A	530	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	417	CME	1	0
1	A	530	CME	2	0

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	$\#\|Z\| > 2$
3	J3Z	A	2	-	23,23,23	0.88	0	36,36,36	1.52	7 (19%)
3	J3Z	B	1	-	23,23,23	0.92	1 (4%)	36,36,36	1.50	9 (25%)

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
3	J3Z	A	2	-	-	-	0/4/4/4
3	J3Z	B	1	-	-	-	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	J3Z	C21-C2	-2.01	1.49	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	J3Z	C8-C7-C5	3.70	112.24	108.59
3	B	1	J3Z	C2-C12-C10	-3.66	103.44	108.73
3	A	2	J3Z	C2-C12-C10	-3.25	104.03	108.73
3	A	2	J3Z	C9-C10-C5	3.14	106.89	104.08
3	B	1	J3Z	C5-C10-C12	-2.88	110.04	113.12
3	B	1	J3Z	C8-C7-C5	2.83	111.38	108.59
3	B	1	J3Z	C15-C14-C12	2.71	115.11	110.59
3	B	1	J3Z	C9-C8-C7	-2.67	103.01	105.70
3	B	1	J3Z	C6-C5-C7	2.63	110.01	105.18
3	A	2	J3Z	C14-C12-C2	2.54	111.76	109.28
3	A	2	J3Z	C5-C10-C12	-2.51	110.44	113.12
3	A	2	J3Z	C9-C8-C7	-2.22	103.47	105.70
3	B	1	J3Z	C14-C12-C2	2.15	111.38	109.28
3	B	1	J3Z	O1-C7-C8	-2.10	123.16	125.76
3	A	2	J3Z	C15-C14-C12	2.08	114.05	110.59
3	B	1	J3Z	C9-C10-C5	2.05	105.92	104.08

There are no chirality outliers.

There are no torsion outliers.

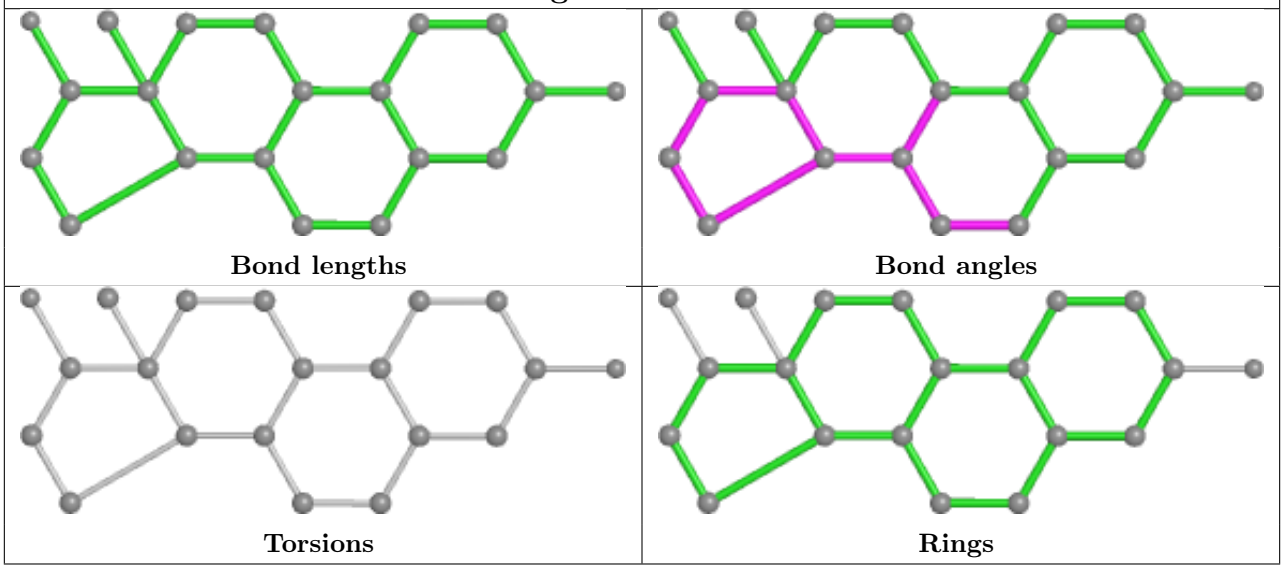
There are no ring outliers.

2 monomers are involved in 3 short contacts:

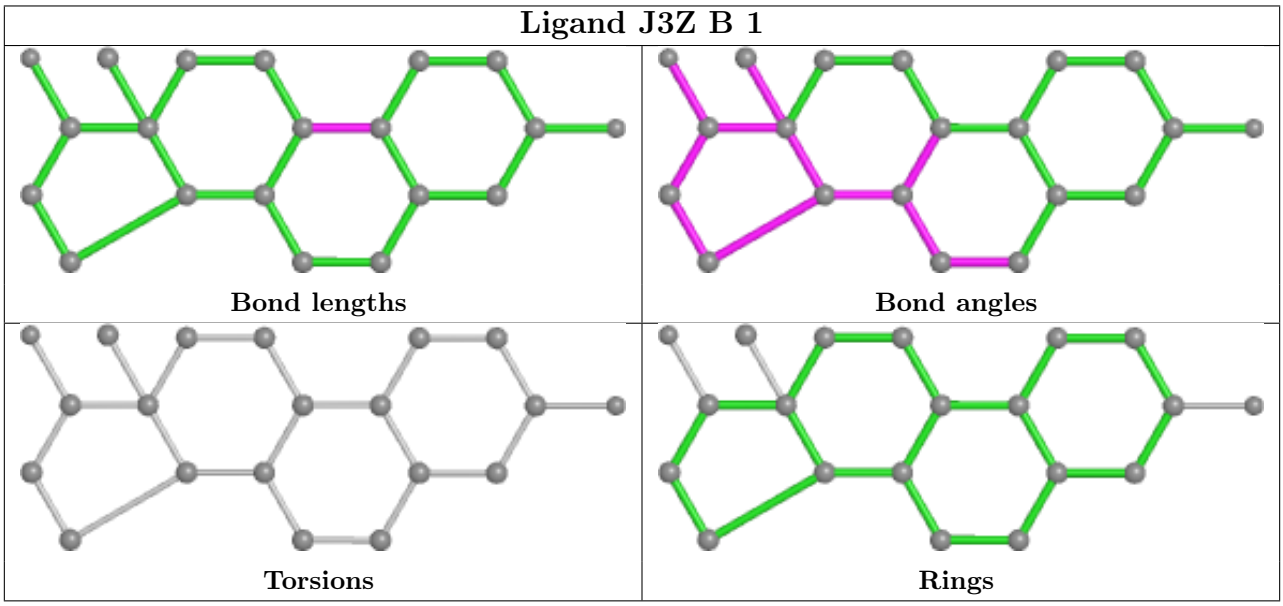
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	J3Z	1	0
3	B	1	J3Z	2	0

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 J3Z A 2



Ligand J3Z B 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	232/253 (91%)	0.68	32 (13%)	2	4	40, 65, 115, 139	0
1	B	236/253 (93%)	0.54	22 (9%)	8	14	40, 64, 103, 137	0
2	C	10/13 (76%)	1.65	3 (30%)	0	0	92, 112, 126, 128	0
2	D	9/13 (69%)	1.29	2 (22%)	0	1	77, 94, 106, 108	0
All	All	487/532 (91%)	0.64	59 (12%)	4	7	40, 65, 112, 139	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	PRO	9.4
1	B	462	LEU	7.3
1	B	550	HIS	5.9
1	A	337	PHE	5.1
1	A	459[A]	TYR	4.8
1	B	306	LEU	4.4
1	B	334	THR	4.1
1	A	418	VAL	4.1
1	B	304	ASN	4.1
1	B	303	LYS	4.1
2	C	696	ASP	4.0
2	C	687	HIS	3.9
1	A	470	GLU	3.8
1	A	309	SER	3.7
1	A	334	THR	3.6
1	A	333	PRO	3.4
1	A	409	LEU	3.3
2	C	691	HIS	3.2
1	A	452	ILE	3.1
1	A	533	VAL	3.0
1	B	512	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	515	ARG	2.9
1	A	306	LEU	2.8
1	B	461	PHE	2.7
1	A	548[A]	ARG	2.7
1	B	508	LEU	2.6
1	B	511	LEU	2.6
1	B	456	SER	2.6
1	A	512	SER	2.6
1	A	386	ILE	2.5
1	A	514	ILE	2.5
1	A	527	SER	2.5
1	A	509	LEU	2.5
1	B	332	ASP	2.5
1	A	511	LEU	2.4
1	A	389	ILE	2.4
1	B	514	ILE	2.4
1	A	536	LEU	2.4
1	B	516	HIS	2.4
1	A	310	LEU	2.3
2	D	688	LYS	2.3
1	B	549	LEU	2.3
1	A	422	VAL	2.3
1	B	317	SER	2.3
1	B	513[A]	HIS	2.2
1	B	509	LEU	2.2
1	B	336	PRO	2.2
1	A	308	LEU	2.2
1	A	458	VAL	2.1
1	A	508	LEU	2.1
1	B	548	ARG	2.1
1	A	384	LEU	2.1
1	A	397	GLU	2.1
1	B	452	ILE	2.1
1	A	351	ASP	2.0
1	B	309	SER	2.0
1	A	516	HIS	2.0
2	D	695	GLN	2.0
1	A	538	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	A	417	10/11	0.86	0.26	87,115,118,119	4
1	CME	A	530	10/11	0.90	0.27	88,90,126,196	3
1	CME	B	381	10/11	0.90	0.26	42,75,107,192	3
1	CME	B	530	10/11	0.91	0.14	61,67,109,109	0
1	CME	B	417	10/11	0.94	0.18	69,78,132,155	4
1	CME	A	381	10/11	0.95	0.20	42,53,77,129	4

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

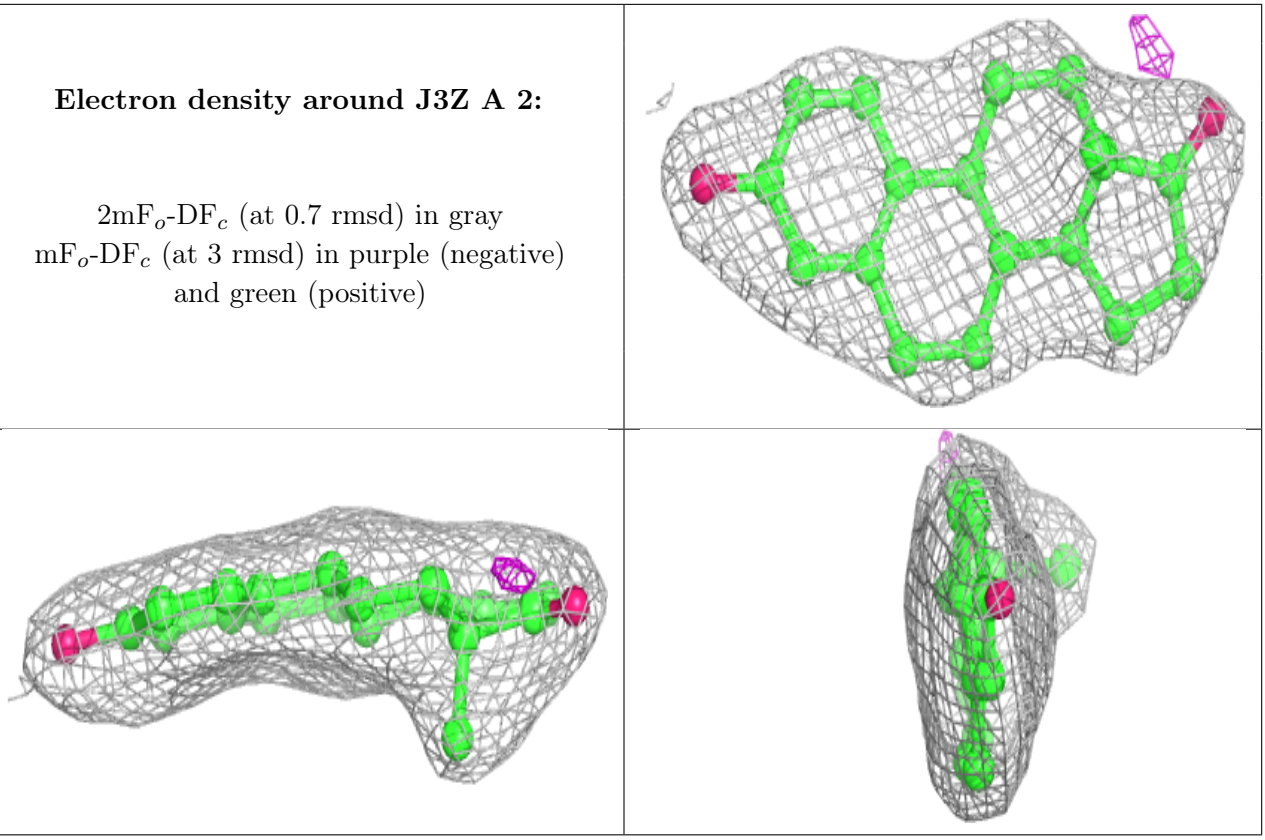
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	J3Z	A	2	20/20	0.93	0.14	38,51,64,65	0
3	J3Z	B	1	20/20	0.94	0.15	41,51,61,63	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.

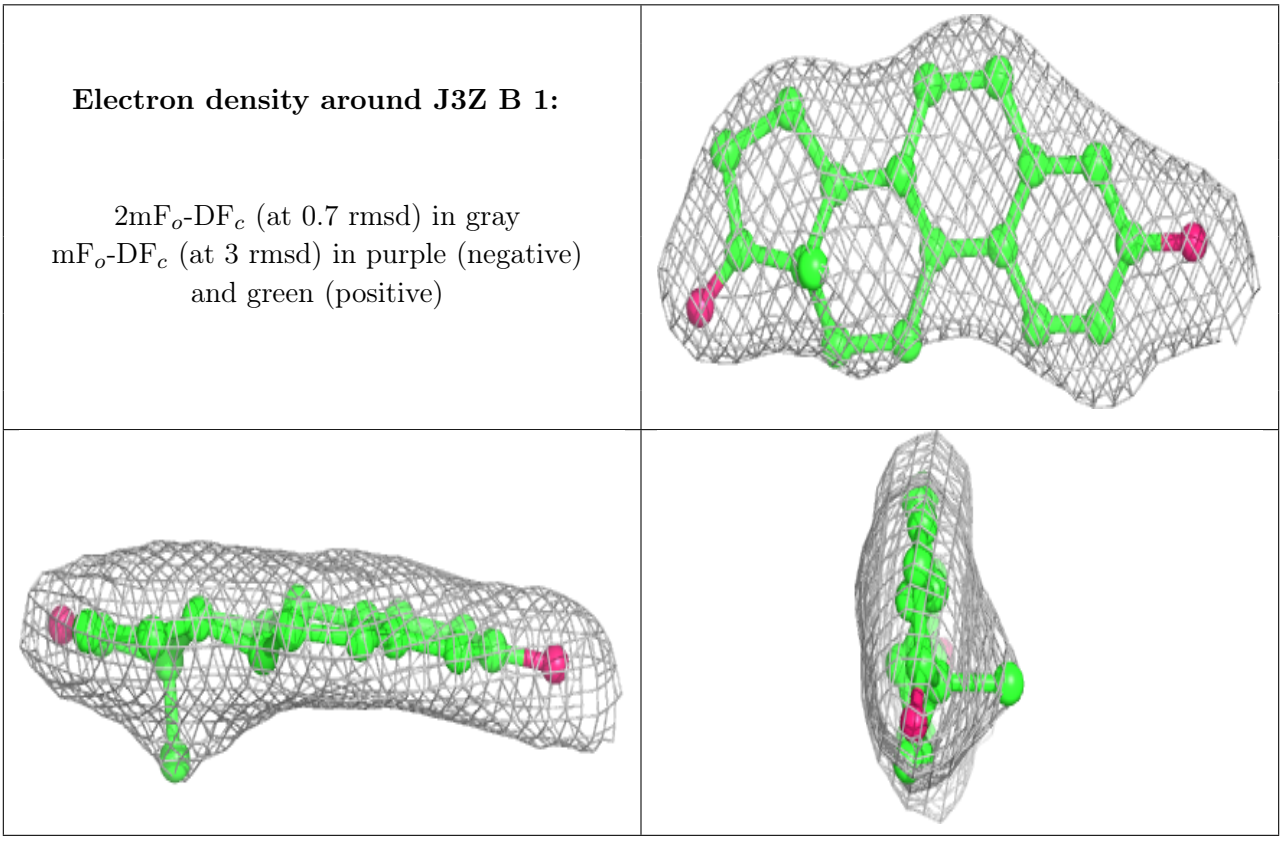
Electron density around J3Z A 2:

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



Electron density around J3Z 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.