Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 01:12 AM EDT

PDB ID	:	2G5O
Title	:	Human estrogen receptor alpha ligand-binding domain in complex with 2-(but-1-enyl)-17beta-estradiol and a glucocorticoid receptor interacting protein 1 NR BOX II Peptide
Authors	:	Rajan, S.S.; Hsieh, R.W.; Sharma, S.K.; Greene, G.L.
Deposited on	:	2006-02-23
Resolution	:	2.30 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:

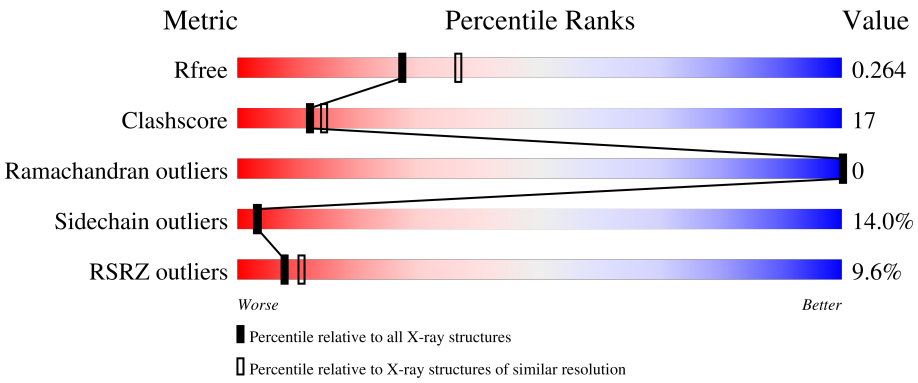
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	257	10% 61% 23% 8% 7%
1	B	257	7% 67% 21% 5% 7%
2	C	13	15% 46% 31% 23%
2	D	13	8% 38% 15% 15% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DRQ	A	201	-	-	X	-
3	DRQ	B	555	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4099 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	238	1918	1225	328	343	22	0	1	0
1	B	239	1933	1235	331	343	24	0	2	0

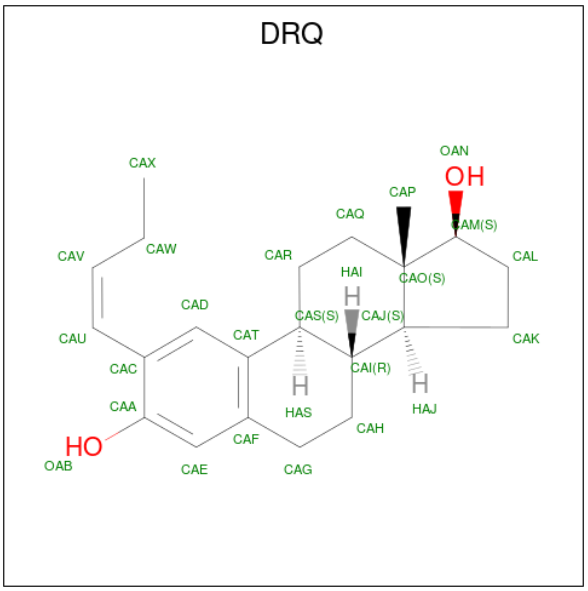
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	CME	CYS	modified residue	UNP P03372
A	417	CME	CYS	modified residue	UNP P03372
A	530	CME	CYS	modified residue	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	381	CME	CYS	modified residue	UNP P03372
B	417	CME	CYS	modified residue	UNP P03372
B	530	CME	CYS	modified residue	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 (9ALPHA,13BETA,17BETA)-2-[(1Z)-BUT-1-EN-1-YL]ESTRA-1,3,5(10)-TRIENE-3,17-DIOL (three-letter code: DRQ) (formula: $C_{22}H_{30}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 24 22 2	0	0
3	B	1	Total C O 24 22 2	0	0

- Molecule 4 is water.

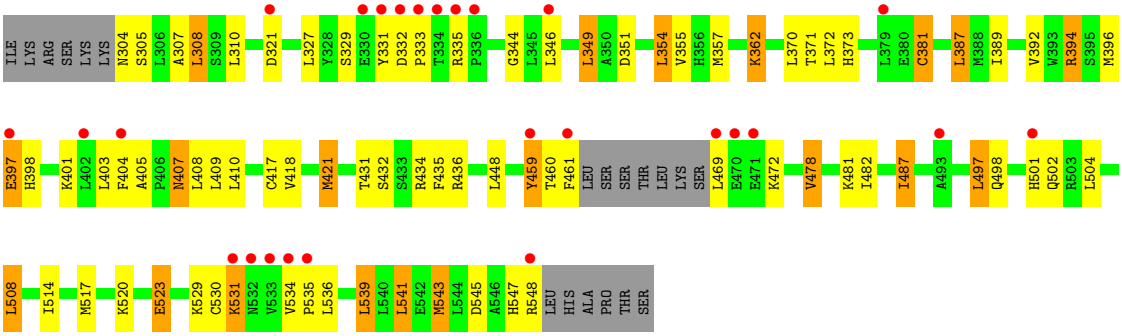
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	13	Total O 13 13	0	0

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.

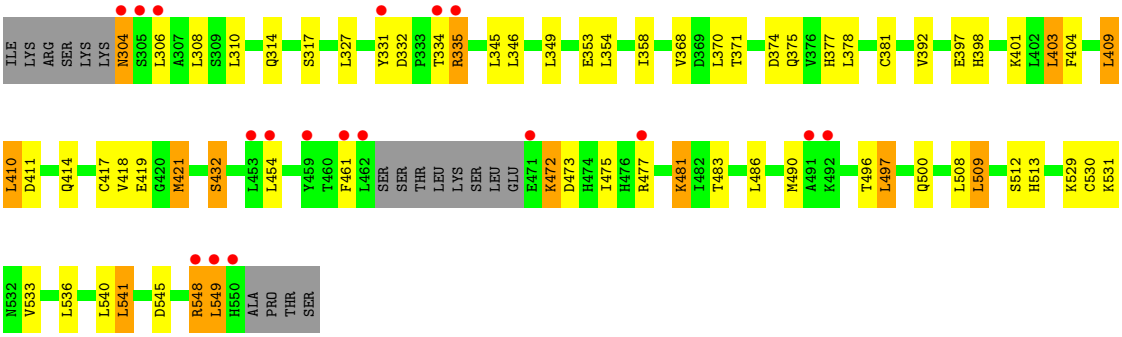
• Molecule 1: Estrogen receptor

Chain A:



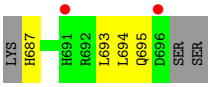
• Molecule 1: Estrogen receptor

Chain B:



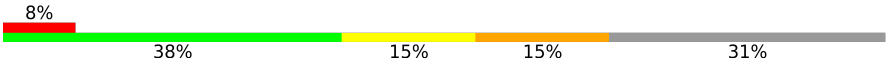
• Molecule 2: Nuclear receptor coactivator 2

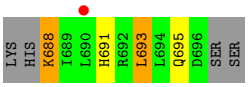
Chain C:



• Molecule 2: Nuclear receptor coactivator 2

Chain D:


8%
38%
15%
15%
31%


LYS
HIS
K688
I689
L690
H691
R692
L693
L694
Q695
D696
SER
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.07Å 83.35Å 58.83Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	19.65 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.65-2.30) 97.4 (19.65-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.264 0.209 , 0.264	Depositor DCC
R_{free} test set	1134 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4099	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: DRQ, CME

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	0.40	0/1925	0.56	0/2596
1	B	0.40	0/1935	0.54	0/2610
2	C	0.30	0/90	0.46	0/119
2	D	0.39	0/79	0.65	0/104
All	All	0.40	0/4029	0.55	0/5429

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	1918	0	1960	83	0
1	B	1933	0	1981	59	0
2	C	89	0	95	2	0
2	D	79	0	88	8	0
3	A	24	0	30	16	0
3	B	24	0	29	13	0
4	A	19	0	0	2	0
4	B	13	0	0	0	0
All	All	4099	0	4183	142	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 17.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:HG2	1:A:394:ARG:HH21	1.03	1.08
1:B:349:LEU:HG	3:B:555:DRQ:HAV	1.42	1.01
1:A:349:LEU:HB3	3:A:201:DRQ:HAV	1.46	0.96
1:B:418:VAL:HB	1:B:421:MET:HG3	1.50	0.91
1:A:394:ARG:HG2	1:A:394:ARG:NH2	1.86	0.89
1:B:349:LEU:HD23	3:B:555:DRQ:HAW2	1.53	0.89
2:D:688:LYS:NZ	2:D:688:LYS:HB2	1.85	0.89
1:A:394:ARG:HH21	1:A:394:ARG:CG	1.85	0.87
1:A:349:LEU:HD12	3:A:201:DRQ:HAX3	1.58	0.86
1:A:397:GLU:H	1:A:397:GLU:CD	1.79	0.85
1:A:403:LEU:HD12	1:A:409:LEU:HD13	1.59	0.84
1:A:329:SER:H	1:A:407:ASN:HD21	1.28	0.81
1:A:481:LYS:HZ2	1:A:481:LYS:HB3	1.47	0.80
1:A:349:LEU:HB3	3:A:201:DRQ:CAV	2.13	0.78
1:A:394:ARG:CD	4:A:28:HOH:O	2.30	0.78
2:D:688:LYS:HB2	2:D:688:LYS:HZ3	1.48	0.77
1:B:421:MET:CE	3:B:555:DRQ:HAM	2.14	0.76
1:A:394:ARG:HD3	4:A:28:HOH:O	1.87	0.75
1:B:349:LEU:HD23	3:B:555:DRQ:CAW	2.18	0.74
1:B:332:ASP:OD1	1:B:334:THR:HG22	1.89	0.71
1:B:371:THR:O	1:B:375:GLN:HG3	1.91	0.71
1:A:349:LEU:HD13	3:A:201:DRQ:HAV	1.73	0.69
1:B:349:LEU:CD2	3:B:555:DRQ:HAW2	2.23	0.69
1:A:307:ALA:HA	1:A:310:LEU:CD1	2.23	0.69
1:B:371:THR:HG23	1:B:374:ASP:H	1.57	0.68
1:B:421:MET:HE2	3:B:555:DRQ:HAM	1.74	0.68
1:A:346:LEU:HA	3:A:201:DRQ:HAX2	1.75	0.68
1:A:401:LYS:HE3	1:A:409:LEU:HD21	1.77	0.66
1:A:459:TYR:CE1	1:B:513:HIS:ND1	2.62	0.66
1:B:349:LEU:CG	3:B:555:DRQ:HAV	2.23	0.66
1:A:396:MET:O	1:A:436:ARG:HD3	1.95	0.65
1:A:487:ILE:HD12	1:A:504:LEU:HD22	1.79	0.65
1:A:407:ASN:H	1:A:407:ASN:HD22	1.44	0.64
1:A:404:PHE:HD2	3:A:201:DRQ:HAW1	1.63	0.64
1:A:404:PHE:HB3	3:A:201:DRQ:HAW2	1.81	0.62
1:A:514:ILE:HD13	1:A:517:MET:CE	2.31	0.61
1:A:459:TYR:CD1	1:B:513:HIS:CE1	2.89	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:CD1	1:A:409:LEU:HD13	2.31	0.61
1:B:358:ILE:HD13	2:D:693:LEU:HD23	1.83	0.61
1:A:349:LEU:HD11	1:A:405:ALA:HB2	1.83	0.60
1:A:371:THR:HG22	1:A:373:HIS:N	2.17	0.60
1:A:401:LYS:CE	1:A:409:LEU:HD21	2.31	0.60
1:B:536:LEU:HB2	1:B:541:LEU:HD13	1.84	0.59
1:A:371:THR:HG22	1:A:373:HIS:H	1.68	0.59
1:B:404:PHE:HD2	3:B:555:DRQ:HAW1	1.67	0.59
1:A:497:LEU:HD21	1:B:497:LEU:HD11	1.84	0.59
1:B:304:ASN:C	1:B:304:ASN:HD22	2.05	0.59
1:A:459:TYR:CD1	1:B:513:HIS:ND1	2.71	0.59
1:A:307:ALA:HA	1:A:310:LEU:HD12	1.86	0.58
1:A:349:LEU:CB	3:A:201:DRQ:HAV	2.30	0.58
1:A:349:LEU:CD1	3:A:201:DRQ:HAX3	2.31	0.57
1:B:411:ASP:H	1:B:414:GLN:HE21	1.51	0.57
1:A:523:GLU:HA	1:A:523:GLU:OE1	2.05	0.57
1:A:404:PHE:CD2	3:A:201:DRQ:HAW1	2.39	0.57
1:A:397:GLU:CD	1:A:397:GLU:N	2.50	0.56
1:B:327:LEU:HD12	1:B:353:GLU:HG2	1.87	0.56
1:B:392:VAL:HG13	1:B:432:SER:HA	1.88	0.56
1:B:358:ILE:CD1	2:D:693:LEU:HD23	2.35	0.56
1:B:418:VAL:CB	1:B:421:MET:HG3	2.31	0.55
1:A:357:MET:CE	1:A:387:LEU:HD13	2.37	0.55
1:B:308:LEU:HD21	1:B:477:ARG:HB3	1.88	0.55
1:A:531:LYS:N	1:A:531:LYS:HD2	2.21	0.54
1:A:498:GLN:HA	1:A:501:HIS:CE1	2.42	0.54
1:A:401:LYS:HE3	1:A:409:LEU:CD2	2.39	0.53
1:A:349:LEU:HD13	3:A:201:DRQ:CAV	2.39	0.53
1:A:397:GLU:OE1	1:A:398:HIS:CD2	2.62	0.52
1:B:403:LEU:HD12	1:B:409:LEU:HG	1.91	0.52
1:A:404:PHE:HD2	3:A:201:DRQ:CAW	2.22	0.52
1:A:392:VAL:HG11	1:A:431:THR:HG22	1.91	0.52
1:B:496:THR:O	1:B:500:GLN:HG3	2.10	0.52
1:A:536:LEU:HB2	1:A:541:LEU:HD13	1.92	0.51
1:B:472:LYS:HG3	1:B:475:ILE:HG12	1.93	0.51
1:B:421:MET:HE1	3:B:555:DRQ:HAM	1.94	0.50
1:B:419:GLU:OE2	1:B:531:LYS:NZ	2.44	0.50
1:A:404:PHE:CD2	3:A:201:DRQ:CAW	2.95	0.49
1:B:473:ASP:O	1:B:477:ARG:HG2	2.12	0.49
1:B:331:TYR:HA	1:B:345:LEU:HD21	1.94	0.49
1:B:401:LYS:HG2	1:B:409:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:HIS:HD2	1:B:461:PHE:HE2	1.59	0.49
1:B:411:ASP:H	1:B:414:GLN:NE2	2.11	0.48
1:A:397:GLU:N	1:A:397:GLU:OE2	2.40	0.48
2:D:688:LYS:HB2	2:D:688:LYS:HZ2	1.72	0.48
1:A:349:LEU:CD1	3:A:201:DRQ:HAV	2.42	0.48
1:A:508:LEU:HG	1:B:509:LEU:HD13	1.95	0.48
1:B:349:LEU:HB3	3:B:555:DRQ:HAX3	1.94	0.48
1:B:472:LYS:HA	1:B:472:LYS:CE	2.44	0.47
1:B:548:ARG:C	1:B:549:LEU:HG	2.32	0.47
1:A:394:ARG:NH2	1:A:403:LEU:O	2.46	0.47
1:B:334:THR:HG23	1:B:335:ARG:NE	2.29	0.47
1:B:349:LEU:HD23	3:B:555:DRQ:CAX	2.44	0.47
2:D:688:LYS:NZ	2:D:688:LYS:CB	2.68	0.47
1:A:539:LEU:O	1:A:543:MET:HB2	2.15	0.47
1:A:398:HIS:HB3	1:A:401:LYS:HE2	1.96	0.47
1:B:481:LYS:NZ	1:B:481:LYS:HB3	2.30	0.47
1:A:418:VAL:HB	1:A:421:MET:HB2	1.96	0.47
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.97	0.47
3:B:555:DRQ:HAX2	3:B:555:DRQ:CAD	2.45	0.46
1:A:362:LYS:HD2	2:C:694:LEU:HD23	1.97	0.46
1:A:502:GLN:HA	1:B:483:THR:HG21	1.97	0.46
1:B:306:LEU:O	1:B:310:LEU:HG	2.15	0.46
1:A:304:ASN:CG	1:A:305:SER:H	2.18	0.46
1:B:377:HIS:HD2	1:B:461:PHE:CE2	2.34	0.46
1:B:477:ARG:HA	1:B:477:ARG:HD3	1.74	0.46
1:B:370:LEU:HD11	1:B:475:ILE:HD11	1.98	0.45
1:A:478:VAL:O	1:A:482:ILE:HG13	2.17	0.45
1:A:407:ASN:HD22	1:A:407:ASN:N	2.07	0.45
1:B:540:LEU:HD23	1:B:540:LEU:HA	1.85	0.45
1:A:381:CME:HE3	1:A:547:HIS:CE1	2.52	0.44
1:A:407:ASN:H	1:A:407:ASN:ND2	2.13	0.44
1:B:398:HIS:CE1	1:B:403:LEU:HD13	2.53	0.44
1:A:394:ARG:NH2	1:A:394:ARG:CG	2.56	0.43
2:D:691:HIS:O	2:D:695:GLN:HG2	2.18	0.43
1:A:344:GLY:HA2	1:A:534:VAL:HG21	2.00	0.43
1:A:372:LEU:HD21	2:C:695:GLN:HG2	1.99	0.43
1:A:389:ILE:HD11	1:A:435:PHE:HZ	1.84	0.43
1:A:331:TYR:CZ	1:A:333:PRO:HA	2.54	0.43
1:A:421:MET:HE1	3:A:201:DRQ:HAL2	2.00	0.43
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.85	0.43
1:A:459:TYR:CE2	1:B:513:HIS:HB3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD22	1:A:469:LEU:N	2.34	0.43
1:B:529:LYS:HG3	1:B:536:LEU:HD12	2.01	0.43
1:A:514:ILE:HD13	1:A:517:MET:HE2	2.00	0.42
1:B:392:VAL:HG13	1:B:432:SER:CA	2.49	0.42
1:B:529:LYS:HE3	1:B:529:LYS:HB3	1.77	0.42
1:A:346:LEU:HD12	3:A:201:DRQ:HAX1	2.01	0.42
1:A:418:VAL:HB	1:A:421:MET:CB	2.49	0.42
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.49	0.42
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.83	0.42
1:B:486:LEU:O	1:B:490:MET:HG3	2.19	0.42
1:A:431:THR:HG21	1:A:514:ILE:HD11	2.00	0.42
1:B:349:LEU:HG	3:B:555:DRQ:CAV	2.32	0.42
2:D:688:LYS:HG2	2:D:691:HIS:HB2	2.01	0.42
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.86	0.41
1:A:331:TYR:CD2	1:A:332:ASP:N	2.88	0.41
1:B:308:LEU:CD2	1:B:477:ARG:HB3	2.51	0.41
1:B:310:LEU:HD22	1:B:314:GLN:HB3	2.02	0.41
1:A:389:ILE:HD11	1:A:435:PHE:CZ	2.55	0.41
1:A:461:PHE:HB2	1:A:472:LYS:NZ	2.35	0.41
1:B:410:LEU:HA	1:B:414:GLN:NE2	2.36	0.41
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.95	0.41
1:B:401:LYS:HB3	1:B:409:LEU:HD22	2.03	0.40
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.82	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	232/257 (90%)	228 (98%)	4 (2%)	0	100	100
1	B	233/257 (91%)	229 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	480/540 (89%)	472 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	212/229 (93%)	179 (84%)	33 (16%)	2	2
1	B	213/229 (93%)	188 (88%)	25 (12%)	5	6
2	C	10/13 (77%)	8 (80%)	2 (20%)	1	1
2	D	9/13 (69%)	7 (78%)	2 (22%)	1	1
All	All	444/484 (92%)	382 (86%)	62 (14%)	3	3

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

Mol	Chain	Res	Type
1	A	308	LEU
1	A	321	ASP
1	A	327	LEU
1	A	335	ARG
1	A	349	LEU
1	A	351	ASP
1	A	354	LEU
1	A	355	VAL
1	A	362	LYS
1	A	370	LEU
1	A	387	LEU
1	A	394	ARG
1	A	397	GLU
1	A	407	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	LEU
1	A	421	MET
1	A	432	SER
1	A	434	ARG
1	A	459	TYR
1	A	460	THR
1	A	478	VAL
1	A	487	ILE
1	A	497	LEU
1	A	508	LEU
1	A	520	LYS
1	A	523	GLU
1	A	529	LYS
1	A	531	LYS
1	A	539	LEU
1	A	541	LEU
1	A	543	MET
1	A	545	ASP
1	A	548	ARG
1	B	304	ASN
1	B	317	SER
1	B	335	ARG
1	B	346	LEU
1	B	354	LEU
1	B	368	VAL
1	B	378	LEU
1	B	397	GLU
1	B	403	LEU
1	B	409	LEU
1	B	410	LEU
1	B	421	MET
1	B	432	SER
1	B	454	LEU
1	B	472	LYS
1	B	481	LYS
1	B	497	LEU
1	B	508	LEU
1	B	509	LEU
1	B	512	SER
1	B	533	VAL
1	B	541	LEU
1	B	545	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	548	ARG
1	B	549	LEU
2	C	687	HIS
2	C	693	LEU
2	D	688	LYS
2	D	693	LEU

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	314	GLN
1	A	373	HIS
1	A	375	GLN
1	A	398	HIS
1	A	407	ASN
1	A	488	HIS
1	A	499	GLN
1	A	501	HIS
1	A	502	GLN
1	A	513	HIS
1	A	519	ASN
1	B	304	ASN
1	B	375	GLN
1	B	398	HIS
1	B	414	GLN
1	B	500	GLN
1	B	502	GLN
1	B	506	GLN
1	B	519	ASN
1	B	547	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)

7 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	B	381[A]	-	8,9,10	0.76	0	5,9,11	3.97	2 (40%)
1	CME	B	530	1	8,9,10	0.82	0	5,9,11	3.36	2 (40%)
1	CME	A	381	1	8,9,10	0.82	0	5,9,11	4.30	2 (40%)
1	CME	A	530	1	8,9,10	0.82	0	5,9,11	4.00	2 (40%)
1	CME	A	417	1	8,9,10	0.75	0	5,9,11	4.75	2 (40%)
1	CME	B	381[B]	-	8,9,10	0.76	0	5,9,11	3.50	2 (40%)
1	CME	B	417	1	8,9,10	0.92	1 (12%)	5,9,11	3.66	2 (40%)

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	B	381[A]	-	-	3/5/8/10	-
1	CME	B	530	1	-	2/5/8/10	-
1	CME	A	381	1	-	3/5/8/10	-
1	CME	A	530	1	-	2/5/8/10	-
1	CME	A	417	1	-	2/5/8/10	-
1	CME	B	381[B]	-	-	2/5/8/10	-
1	CME	B	417	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	CME	CB-SG	-2.05	1.75	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	CME	CB-SG-SD	9.06	127.28	103.82
1	A	530	CME	CB-SG-SD	7.39	122.96	103.82
1	A	381	CME	CB-SG-SD	7.22	122.53	103.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	381[A]	CME	CB-SG-SD	7.08	122.18	103.82
1	B	381[B]	CME	CB-SG-SD	6.37	120.33	103.82
1	B	417	CME	CB-SG-SD	6.23	119.96	103.82
1	A	381	CME	CE-SD-SG	5.98	130.98	103.45
1	B	530	CME	CB-SG-SD	5.96	119.26	103.82
1	A	417	CME	CE-SD-SG	5.37	128.17	103.45
1	B	381[A]	CME	CE-SD-SG	5.15	127.16	103.45
1	B	417	CME	CE-SD-SG	4.78	125.49	103.45
1	A	530	CME	CE-SD-SG	4.74	125.27	103.45
1	B	381[B]	CME	CE-SD-SG	4.32	123.35	103.45
1	B	530	CME	CE-SD-SG	4.31	123.29	103.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381	CME	1	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	DRQ	B	555	-	27,27,27	1.32	3 (11%)	41,41,41	1.56	7 (17%)
3	DRQ	A	201	-	27,27,27	1.37	4 (14%)	41,41,41	1.74	9 (21%)

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	DRQ	B	555	-	-	3/4/44/44	0/4/4/4
3	DRQ	A	201	-	-	2/4/44/44	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	555	DRQ	CAC-CAU	-4.87	1.39	1.47
3	A	201	DRQ	CAC-CAU	-4.74	1.39	1.47
3	A	201	DRQ	CAW-CAV	-2.54	1.39	1.51
3	B	555	DRQ	CAW-CAV	-2.48	1.39	1.51
3	A	201	DRQ	CAU-CAV	2.34	1.39	1.31
3	A	201	DRQ	CAT-CAS	2.25	1.55	1.52
3	B	555	DRQ	CAU-CAV	2.07	1.38	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	DRQ	CAW-CAV-CAU	-5.23	120.15	125.86
3	A	201	DRQ	CAL-CAM-CAO	-5.10	100.48	104.53
3	B	555	DRQ	CAW-CAV-CAU	-4.91	120.50	125.86
3	B	555	DRQ	CAL-CAM-CAO	-4.28	101.13	104.53
3	A	201	DRQ	CAH-CAI-CAS	3.36	112.56	109.28
3	A	201	DRQ	CAJ-CAO-CAM	-2.70	96.42	99.27
3	B	555	DRQ	CAH-CAI-CAS	2.60	111.81	109.28
3	A	201	DRQ	CAG-CAF-CAE	-2.55	114.81	119.91
3	A	201	DRQ	CAG-CAF-CAT	2.49	124.86	121.13
3	A	201	DRQ	CAO-CAJ-CAI	-2.47	110.72	114.38
3	B	555	DRQ	CAG-CAF-CAT	2.26	124.51	121.13
3	B	555	DRQ	CAG-CAF-CAE	-2.23	115.44	119.91
3	B	555	DRQ	CAG-CAH-CAI	2.21	114.27	110.59
3	A	201	DRQ	CAD-CAC-CAA	2.16	120.62	118.86
3	B	555	DRQ	CAC-CAU-CAV	-2.14	120.90	125.52
3	A	201	DRQ	CAK-CAJ-CAI	-2.04	115.72	119.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	DRQ	CAA-CAC-CAU-CAV
3	B	555	DRQ	CAA-CAC-CAU-CAV
3	B	555	DRQ	CAD-CAC-CAU-CAV
3	A	201	DRQ	CAD-CAC-CAU-CAV
3	B	555	DRQ	CAU-CAV-CAW-CAX

There are no ring outliers.

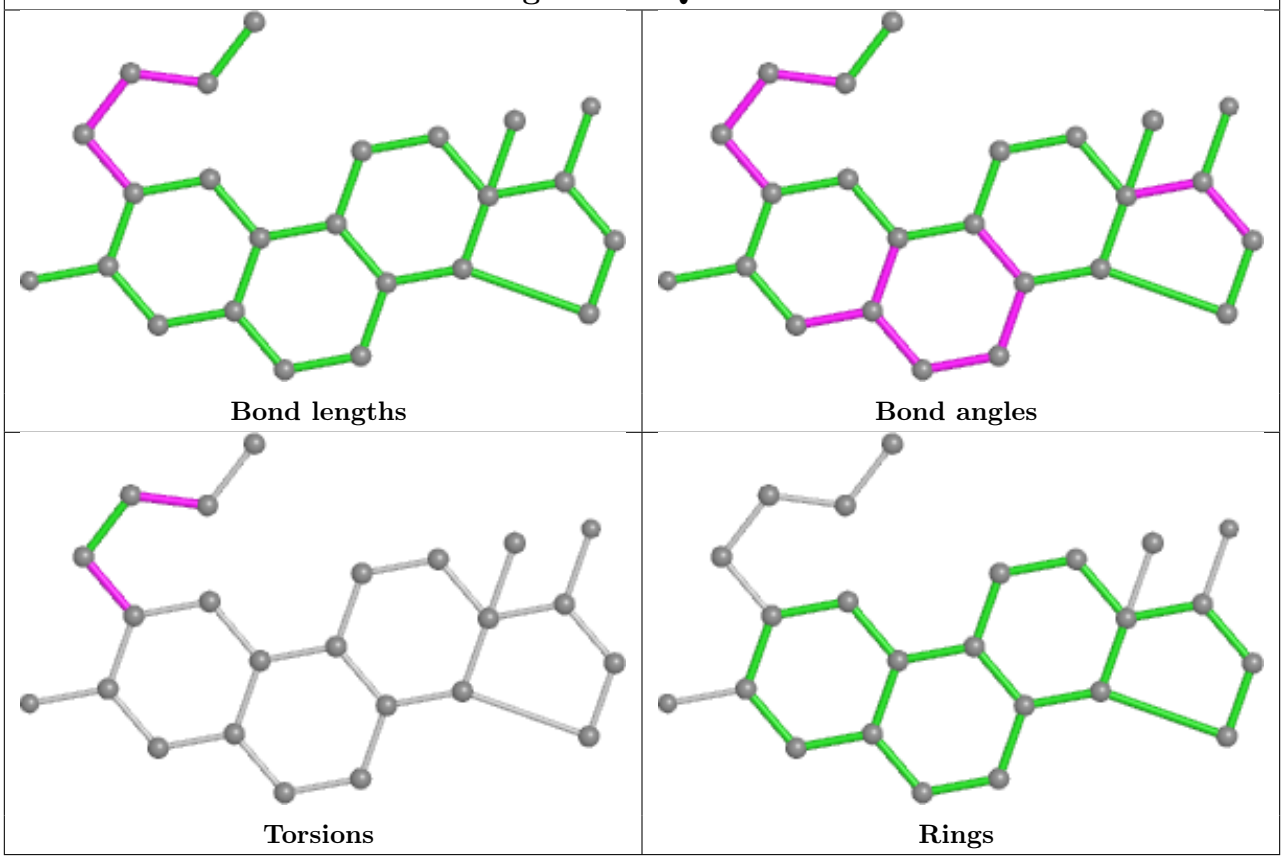
2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	555	DRQ	13	0
3	A	201	DRQ	16	0

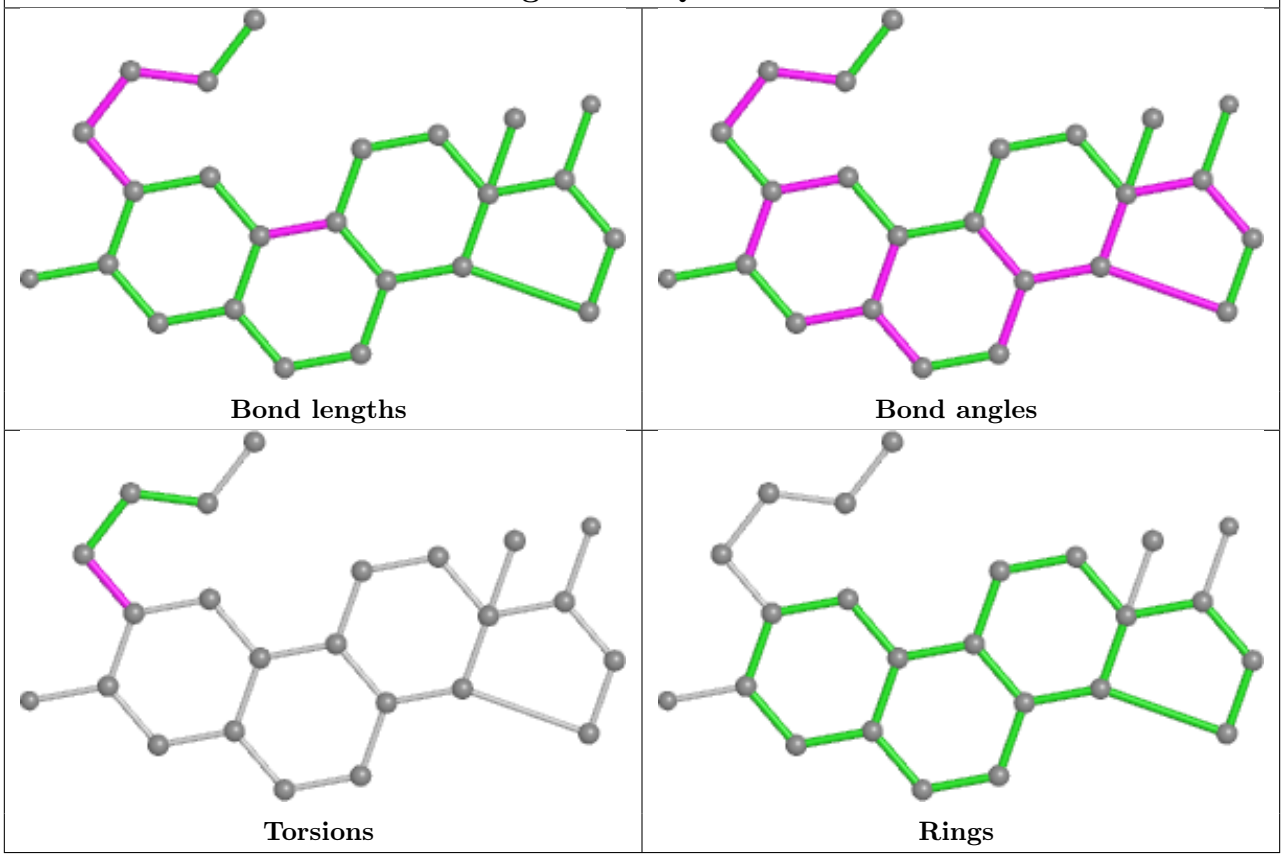
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DRQ B 555



Ligand DRQ A 201



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	235/257 (91%)	0.67	26 (11%)	5	7	36, 47, 70, 78	0
1	B	236/257 (91%)	0.61	18 (7%)	13	18	36, 47, 70, 74	0
2	C	10/13 (76%)	1.46	2 (20%)	1	1	53, 62, 71, 74	0
2	D	9/13 (69%)	1.08	1 (11%)	5	7	56, 62, 71, 75	0
All	All	490/540 (90%)	0.67	47 (9%)	8	10	36, 47, 71, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	HIS	9.5
1	B	471	GLU	6.0
1	A	469	LEU	6.0
1	A	533	VAL	5.7
1	B	306	LEU	5.5
1	B	548	ARG	5.1
1	B	304	ASN	4.8
1	A	334	THR	4.6
1	B	462	LEU	4.3
1	A	470	GLU	4.2
1	A	459	TYR	4.1
1	A	331	TYR	3.8
1	A	335	ARG	3.8
1	A	346	LEU	3.7
1	A	333	PRO	3.6
1	B	335	ARG	3.5
2	C	696	ASP	3.5
1	A	330	GLU	3.1
1	A	531	LYS	2.9
1	A	501	HIS	2.9
1	B	477	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	454	LEU	2.8
1	A	548	ARG	2.7
1	A	532	ASN	2.6
1	A	471	GLU	2.6
1	A	397	GLU	2.5
1	A	535	PRO	2.5
1	A	332	ASP	2.5
1	B	491	ALA	2.5
1	A	461	PHE	2.4
1	A	534	VAL	2.4
1	A	336	PRO	2.3
1	B	334	THR	2.3
1	B	459	TYR	2.3
1	A	493	ALA	2.3
1	B	305	SER	2.3
1	B	549	LEU	2.2
1	B	461	PHE	2.2
1	B	453	LEU	2.2
1	B	492	LYS	2.2
2	C	691	HIS	2.1
1	B	331	TYR	2.1
1	A	379	LEU	2.1
2	D	690	LEU	2.1
1	A	321	ASP	2.1
1	A	404	PHE	2.1
1	A	402	LEU	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	B	381[A]	10/11	0.77	0.28	39,41,44,44	6
1	CME	B	381[B]	10/11	0.77	0.28	39,44,50,50	6
1	CME	A	381	10/11	0.84	0.22	40,48,62,62	0
1	CME	A	417	10/11	0.86	0.26	55,58,60,60	0
1	CME	A	530	10/11	0.87	0.31	52,53,54,54	5
1	CME	B	417	10/11	0.88	0.18	54,57,60,60	5
1	CME	B	530	10/11	0.91	0.19	50,51,52,52	5

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

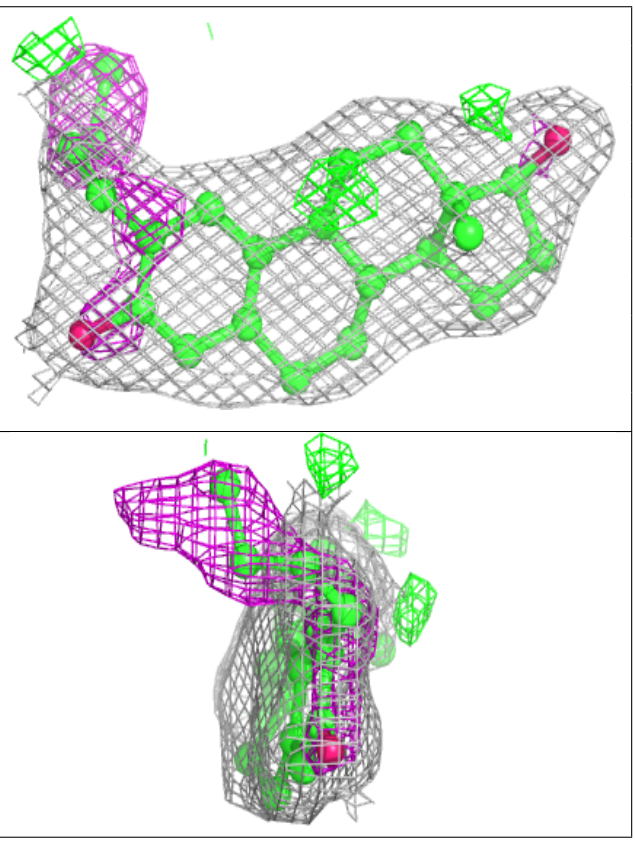
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DRQ	A	201	24/24	0.86	0.18	46,46,51,53	0
3	DRQ	B	555	24/24	0.89	0.16	44,46,51,53	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.

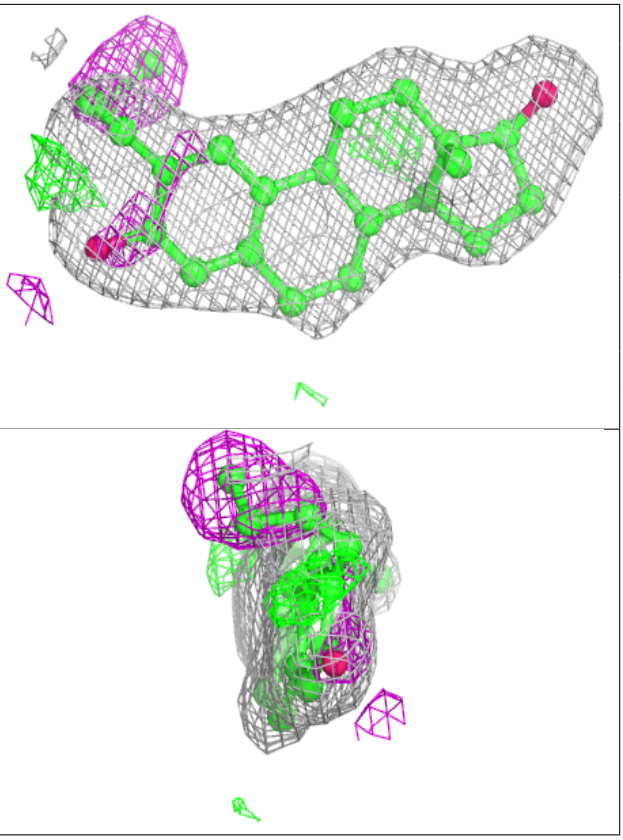
Electron density around DRQ A 201:

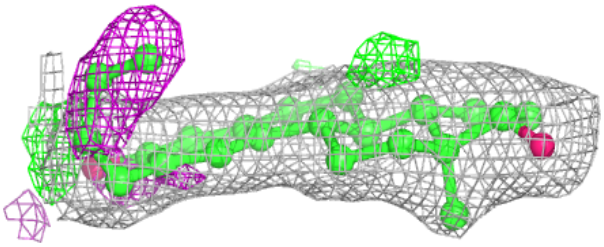
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DRQ B 555:

$2mF_o$-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.