



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:23 AM UTC

PDB ID : 2QA8 / pdb_00002qa8
Title : Crystal Structure of the Estrogen Receptor Alpha Ligand Binding Domain Mutant 537S Complexed with Genistein
Authors : Nettles, K.W.; Bruning, J.B.; Nowak, J.; Sharma, S.K.; Hahm, J.B.; Shi, Y.; Kulp, K.; Hochberg, R.B.; Zhou, H.; Katzenellenbogen, J.A.; Katzenellenbogen, B.S.; Kim, Y.; Joachimiak, A.; Greene, G.L.
Deposited on : 2007-06-14
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

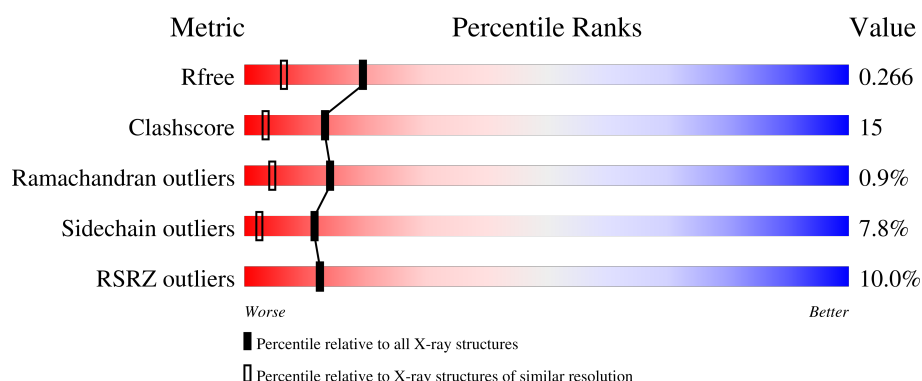
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	6% 68% 18% • 11%
2	B	258	11% 59% 28% • 9%
3	C	13	23% 46% 23% 8% 23%
3	D	13	31% 23% 15% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4015 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
1	A	230	Total	C	N	O	S	0	2	0
			1843	1178	314	330	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	cloning artifact	UNP P03372
A	530	CME	CYS	modified residue	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	4	0
			1894	1215	322	336	21			

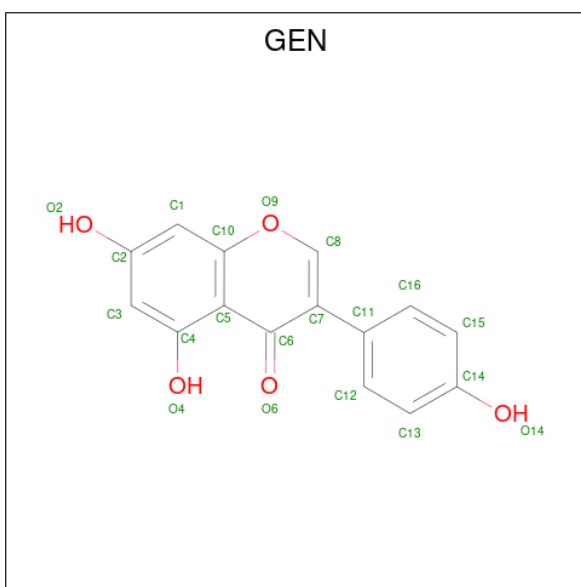
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	SER	-	cloning artifact	UNP P03372
B	381	CME	CYS	modified residue	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 3 is a protein called nuclear receptor coactivator 2.

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

- Molecule 4 is GENISTEIN (CCD ID: GEN) (formula: C₁₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	15	5		
4	B	1	Total	C	O	0	0
			20	15	5		

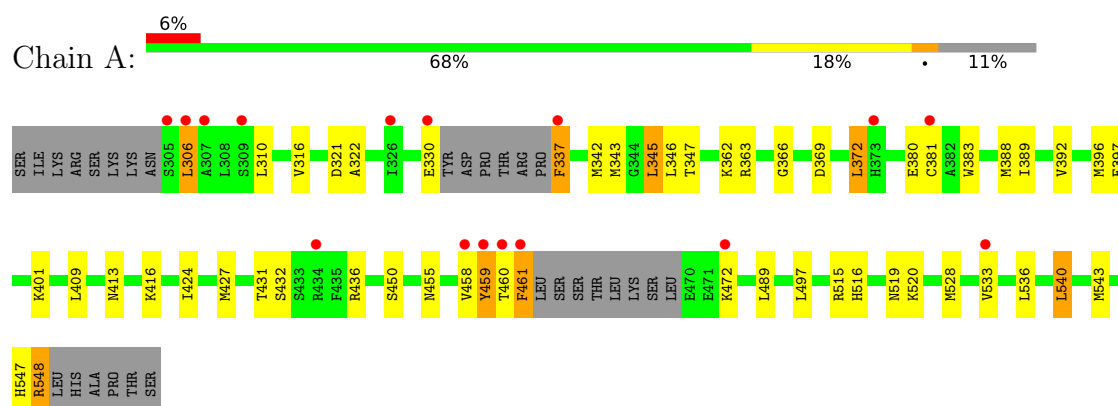
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	32	Total	O	0	0
			32	32		

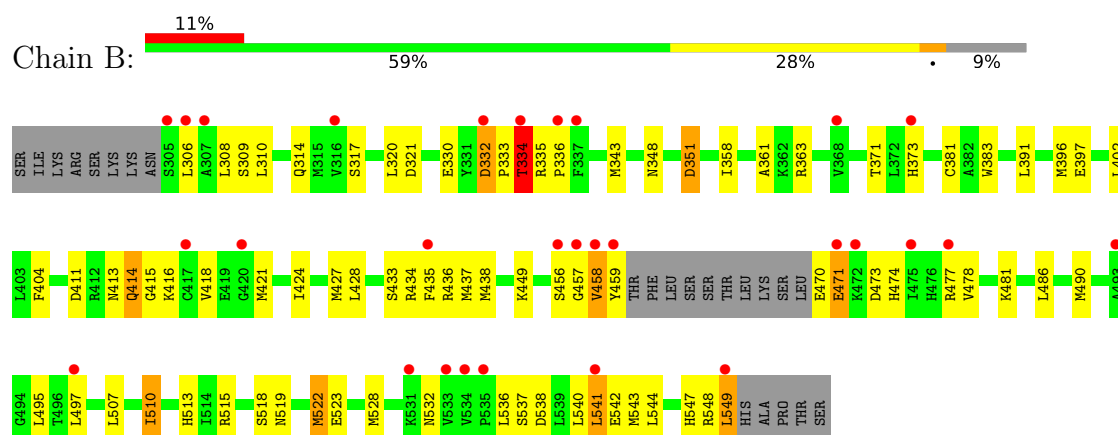
3 Residue-property plots [i](#)

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.

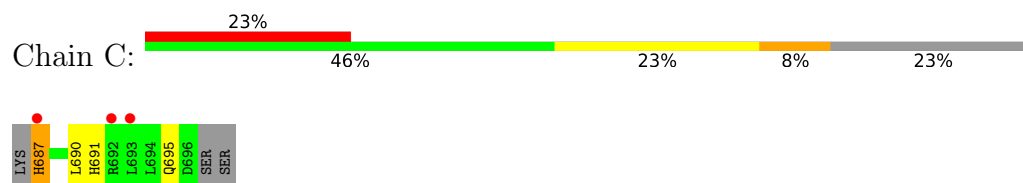
- Molecule 1: Estrogen receptor



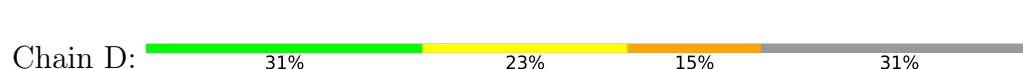
- Molecule 2: Estrogen receptor



- Molecule 3: nuclear receptor coactivator 2



- Molecule 3: nuclear receptor coactivator 2



LYS	HIS	K688	I689	L690	L693	L694	Q695	D696	SER	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.67Å 77.96Å 58.00Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	19.89 – 1.85 19.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.89-1.85) 96.8 (19.89-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.264 0.211 , 0.266	Depositor DCC
R_{free} test set	1935 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GEN, 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	0.67	0/1870	0.91	0/2518
2	B	0.59	0/1933	0.90	2/2609 (0.1%)
3	C	0.58	0/90	0.97	0/119
3	D	0.47	0/79	0.80	0/104
All	All	0.63	0/3972	0.90	2/5350 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	332	ASP	CA-C-N	5.36	126.54	119.84
2	B	332	ASP	C-N-CA	5.36	126.54	119.84

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	1843	0	1887	44	0
2	B	1894	0	1953	78	0
3	C	89	0	95	3	0
3	D	79	0	88	5	0
4	A	20	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	9	0	0
5	A	38	0	0	1	0
5	B	32	0	0	4	0
All	All	4015	0	4040	118	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 15.

All (118) 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:B:391[B]:LEU:CD1	2:B:402[B]:LEU:HD22	1.57	1.35
1:A:547:HIS:O	1:A:548:ARG:HG3	1.60	1.00
1:A:519:ASN:ND2	2:B:519:ASN:HD22	1.60	1.00
1:A:519:ASN:HD22	2:B:519:ASN:ND2	1.61	0.99
2:B:391[B]:LEU:CD1	2:B:402[B]:LEU:CD2	2.42	0.97
2:B:391[B]:LEU:HD11	2:B:402[B]:LEU:CD2	1.94	0.97
2:B:391[B]:LEU:HD11	2:B:402[B]:LEU:HD22	0.97	0.95
1:A:396:MET:O	1:A:436:ARG:HD3	1.68	0.94
1:A:519:ASN:HD22	2:B:519:ASN:HD22	0.95	0.90
2:B:457:GLY:O	2:B:459:TYR:N	2.08	0.87
2:B:343:MET:HE1	2:B:421:MET:CE	2.08	0.83
2:B:343:MET:HE1	2:B:421:MET:HE1	1.61	0.83
2:B:434:ARG:HH11	2:B:437:MET:HE3	1.42	0.82
2:B:332:ASP:OD2	2:B:334:THR:HG23	1.82	0.80
2:B:351:ASP:OD2	2:B:537:SER:HB2	1.82	0.80
2:B:391[B]:LEU:HD13	2:B:402[B]:LEU:HD22	1.61	0.79
3:C:687:HIS:CE1	3:C:691:HIS:HB3	2.18	0.79
1:A:497:LEU:HD11	2:B:497:LEU:HD11	1.67	0.77
2:B:391[B]:LEU:HD13	2:B:402[B]:LEU:CD2	2.14	0.75
2:B:473:ASP:O	2:B:477:ARG:HG3	1.86	0.74
1:A:372:LEU:HD21	3:C:691:HIS:NE2	2.02	0.74
2:B:413:ASN:HA	2:B:416:LYS:HE3	1.68	0.74
2:B:538:ASP:O	2:B:542:GLU:HG3	1.88	0.73
2:B:411:ASP:H	2:B:414:GLN:HE21	1.34	0.72
1:A:397:GLU:HG2	5:A:605:HOH:O	1.91	0.70
2:B:486:LEU:O	2:B:490:MET:HG3	1.91	0.70
2:B:334:THR:O	2:B:334:THR:OG1	2.09	0.70
1:A:413:ASN:HD22	1:A:416:LYS:NZ	1.90	0.70
2:B:456:SER:HA	2:B:515:ARG:NH2	2.08	0.69
1:A:388:MET:O	1:A:392:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TRP:CD1	1:A:543:MET:HE3	2.31	0.66
2:B:548:ARG:O	2:B:549:LEU:HB2	1.97	0.65
2:B:309:SER:HB2	5:B:659:HOH:O	1.97	0.64
2:B:396:MET:O	2:B:436:ARG:HD3	1.99	0.63
2:B:333:PRO:O	2:B:335:ARG:N	2.31	0.62
2:B:397:GLU:HG2	5:B:648:HOH:O	1.99	0.62
1:A:459:TYR:CZ	2:B:513:HIS:HB2	2.36	0.60
2:B:343:MET:HE1	2:B:421:MET:HE2	1.83	0.60
2:B:456:SER:HB2	5:B:635:HOH:O	2.03	0.57
2:B:433:SER:O	2:B:437:MET:HG3	2.03	0.57
2:B:470:GLU:N	2:B:473:ASP:HB3	2.19	0.57
1:A:383:TRP:CG	1:A:543:MET:HE3	2.39	0.57
1:A:392:VAL:HG23	1:A:432:SER:CA	2.36	0.56
1:A:396:MET:HE3	1:A:436:ARG:HA	1.88	0.56
1:A:459:TYR:CE2	2:B:513:HIS:HB2	2.41	0.55
2:B:343:MET:HE2	2:B:343:MET:HA	1.88	0.55
1:A:413:ASN:HD22	1:A:416:LYS:HZ2	1.52	0.55
1:A:337:PHE:HE1	1:A:345:LEU:CD2	2.20	0.55
2:B:310:LEU:HD22	2:B:314:GLN:HB3	1.90	0.54
2:B:536:LEU:HB2	2:B:541:LEU:HD13	1.90	0.54
2:B:358:ILE:HD11	3:D:690:LEU:HD12	1.89	0.53
2:B:522[B]:MET:HE3	2:B:544:LEU:HA	1.91	0.53
1:A:389:ILE:HA	1:A:392:VAL:CG1	2.39	0.53
2:B:373:HIS:C	2:B:373:HIS:HD1	2.17	0.53
2:B:383:TRP:NE1	2:B:543:MET:HB3	2.24	0.52
2:B:358:ILE:HG23	3:D:694:LEU:HD13	1.92	0.52
2:B:308:LEU:HA	2:B:481:LYS:HD2	1.92	0.52
1:A:401:LYS:HD3	1:A:409:LEU:HG	1.90	0.51
1:A:343:MET:HE2	1:A:528:MET:HG3	1.92	0.51
1:A:347:THR:HG21	1:A:536:LEU:CD2	2.41	0.51
2:B:456:SER:HA	2:B:515:ARG:HH22	1.75	0.51
1:A:389:ILE:HA	1:A:392:VAL:HG12	1.91	0.51
1:A:413:ASN:ND2	1:A:416:LYS:NZ	2.59	0.51
2:B:343:MET:HE2	2:B:343:MET:CA	2.40	0.51
2:B:373:HIS:C	2:B:373:HIS:ND1	2.68	0.51
2:B:518:SER:O	2:B:522[A]:MET:HG2	2.11	0.50
1:A:392:VAL:HG23	1:A:432:SER:HA	1.94	0.50
2:B:519:ASN:O	2:B:523:GLU:HG2	2.12	0.50
2:B:424:ILE:HA	2:B:427:MET:CE	2.42	0.49
2:B:358:ILE:HD11	3:D:690:LEU:CD1	2.43	0.49
2:B:330:GLU:HG2	2:B:348:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASP:OD2	2:B:332:ASP:C	2.56	0.49
2:B:474:HIS:O	2:B:478:VAL:HG23	2.13	0.48
2:B:348:ASN:ND2	5:B:613:HOH:O	2.28	0.48
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.96	0.48
1:A:459:TYR:C	1:A:461:PHE:H	2.22	0.47
1:A:413:ASN:ND2	1:A:416:LYS:HZ1	2.13	0.47
2:B:424:ILE:HA	2:B:427:MET:HE2	1.97	0.47
1:A:322:ALA:HB1	1:A:363:ARG:HB2	1.97	0.46
2:B:402[B]:LEU:HD21	2:B:428:LEU:HB3	1.98	0.46
2:B:457:GLY:C	2:B:459:TYR:N	2.73	0.46
2:B:435:PHE:HE1	2:B:510:ILE:HG21	1.81	0.45
2:B:343:MET:SD	2:B:528:MET:HG3	2.55	0.45
2:B:371:THR:HG23	2:B:471:GLU:OE1	2.16	0.45
1:A:520:LYS:N	1:A:520:LYS:HD2	2.31	0.45
2:B:537:SER:HB3	2:B:540:LEU:HB2	1.98	0.45
2:B:481:LYS:HB3	2:B:481:LYS:HE3	1.78	0.44
1:A:392:VAL:HG21	1:A:431:THR:HG22	1.99	0.44
1:A:396:MET:HE2	1:A:396:MET:HB3	1.86	0.44
1:A:337:PHE:HE1	1:A:345:LEU:HD22	1.83	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.76	0.43
2:B:434:ARG:HH11	2:B:437:MET:CE	2.23	0.43
3:D:695:GLN:O	3:D:696:ASP:C	2.61	0.43
2:B:358:ILE:CD1	3:D:690:LEU:HD12	2.48	0.43
2:B:391[A]:LEU:HD13	2:B:404:PHE:HA	2.00	0.43
1:A:306:LEU:H	1:A:306:LEU:HD22	1.83	0.43
1:A:547:HIS:C	1:A:548:ARG:HG3	2.39	0.43
2:B:361:ALA:C	2:B:363:ARG:N	2.73	0.43
2:B:458:VAL:HG22	2:B:458:VAL:O	2.19	0.42
1:A:515:ARG:O	1:A:516:HIS:C	2.63	0.42
2:B:415:GLY:O	2:B:421:MET:HB3	2.19	0.42
1:A:366:GLY:O	1:A:369:ASP:HB2	2.19	0.42
2:B:414:GLN:H	2:B:414:GLN:HG2	1.61	0.42
2:B:438:MET:HE1	2:B:507:LEU:HD23	2.01	0.42
2:B:490:MET:HB3	2:B:495[A]:LEU:HD12	2.02	0.41
1:A:455:ASN:O	1:A:458:VAL:HG12	2.20	0.41
2:B:343:MET:HE3	2:B:418:VAL:HG11	2.02	0.41
1:A:380:GLU:HG3	3:C:690:LEU:HD23	2.02	0.41
1:A:458:VAL:HG13	1:A:459:TYR:N	2.36	0.41
2:B:373:HIS:ND1	2:B:373:HIS:O	2.54	0.41
2:B:522[B]:MET:HE2	2:B:547:HIS:CD2	2.56	0.41
1:A:392:VAL:CG2	1:A:432:SER:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:PHE:HB2	1:A:472:LYS:HE3	2.02	0.40
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.90	0.40
2:B:306:LEU:HD13	2:B:306:LEU:HA	1.82	0.40
1:A:424:ILE:HA	1:A:427:MET:HE3	2.04	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	224/258 (87%)	222 (99%)	1 (0%)	1 (0%)	30	17
2	B	234/258 (91%)	223 (95%)	8 (3%)	3 (1%)	9	2
3	C	8/13 (62%)	8 (100%)	0	0	100	100
3	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	473/542 (87%)	460 (97%)	9 (2%)	4 (1%)	14	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	334	THR
2	B	458	VAL
1	A	460	THR
2	B	336	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	207/232 (89%)	189 (91%)	18 (9%)	9	2
2	B	214/232 (92%)	201 (94%)	13 (6%)	17	5
3	C	10/13 (77%)	8 (80%)	2 (20%)	1	0
3	D	9/13 (69%)	6 (67%)	3 (33%)	0	0
All	All	440/490 (90%)	404 (92%)	36 (8%)	11	2

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	310	LEU
1	A	321	ASP
1	A	330[A]	GLU
1	A	330[B]	GLU
1	A	337	PHE
1	A	342	MET
1	A	345	LEU
1	A	346	LEU
1	A	362	LYS
1	A	372	LEU
1	A	381	CYS
1	A	450	SER
1	A	459	TYR
1	A	461	PHE
1	A	533	VAL
1	A	540	LEU
1	A	548	ARG
2	B	317	SER
2	B	321	ASP
2	B	334	THR
2	B	351	ASP
2	B	414	GLN
2	B	449	LYS
2	B	471	GLU
2	B	510	ILE
2	B	522[A]	MET
2	B	522[B]	MET
2	B	532	ASN
2	B	541	LEU

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Mol	Chain	Res	Type
2	B	549	LEU
3	C	687	HIS
3	C	695	GLN
3	D	693	LEU
3	D	694	LEU
3	D	696	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	413	ASN
1	A	498	GLN
1	A	513	HIS
2	B	348	ASN
2	B	375	GLN
2	B	398	HIS
2	B	414	GLN
2	B	498	GLN
2	B	501	HIS
2	B	513	HIS
2	B	516	HIS
2	B	519	ASN
2	B	532	ASN
3	C	687	HIS
3	C	695	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	CME	B	381	2	8,9,10	0.84	0	6,9,11	1.51	2 (33%)
1	CME	A	530	1	8,9,10	0.66	0	6,9,11	1.19	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
2	CME	B	381	2	-	2/5/8/10	-
1	CME	A	530	1	-	1/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	381	CME	CE-SD-SG	2.23	113.24	103.46
2	B	381	CME	CZ-CE-SD	-2.14	106.22	113.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	381	CME	SD-CE-CZ-OH
1	A	530	CME	SD-CE-CZ-OH
2	B	381	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
4	GEN	A	600	-	22,22,22	1.52	2 (9%)	32,32,32	1.59	7 (21%)
4	GEN	B	600	-	22,22,22	1.60	2 (9%)	32,32,32	1.60	7 (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
4	GEN	A	600	-	-	0/4/4/4	0/3/3/3
4	GEN	B	600	-	-	1/4/4/4	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	GEN	O9-C8	5.07	1.43	1.35
4	A	600	GEN	C8-C7	4.44	1.40	1.34
4	A	600	GEN	O9-C8	4.28	1.42	1.35
4	B	600	GEN	C8-C7	4.25	1.39	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	GEN	O9-C8-C7	-3.88	121.80	125.80
4	A	600	GEN	C10-O9-C8	3.81	122.23	118.27
4	A	600	GEN	C11-C7-C6	3.53	125.81	121.56
4	A	600	GEN	O9-C8-C7	-3.46	122.23	125.80
4	B	600	GEN	C10-O9-C8	3.13	121.52	118.27
4	A	600	GEN	O9-C10-C1	3.11	119.30	115.81
4	B	600	GEN	C4-C5-C10	3.03	120.30	117.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	GEN	O9-C10-C1	3.02	119.20	115.81
4	B	600	GEN	C16-C11-C7	-2.73	117.06	120.98
4	A	600	GEN	C11-C7-C8	-2.65	116.78	119.77
4	A	600	GEN	C5-C6-C7	2.59	118.25	115.79
4	B	600	GEN	C11-C7-C8	-2.42	117.04	119.77
4	B	600	GEN	C11-C7-C6	2.38	124.42	121.56
4	A	600	GEN	O6-C6-C7	-2.12	120.11	122.60

There are no chirality outliers.

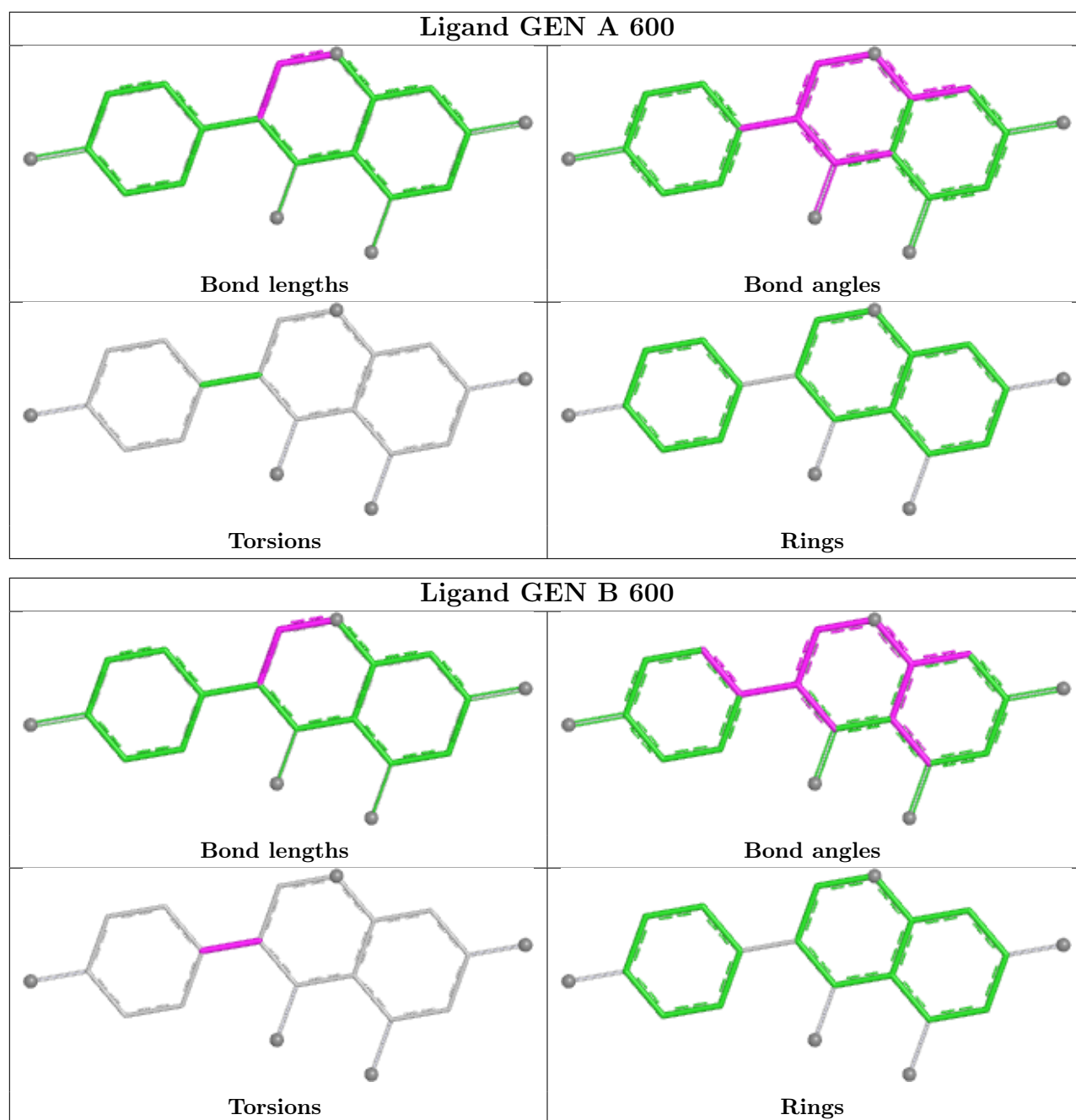
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	GEN	C12-C11-C7-C6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/258 (88%)	0.89	16 (6%) 22 24	37, 44, 71, 96	2 (0%)
2	B	234/258 (90%)	1.07	29 (12%) 8 7	25, 45, 77, 97	4 (1%)
3	C	10/13 (76%)	1.78	3 (30%) 1 1	40, 48, 59, 68	0
3	D	9/13 (69%)	0.98	0 100 100	29, 37, 49, 50	0
All	All	482/542 (88%)	1.00	48 (9%) 12 12	25, 45, 74, 97	6 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	549	LEU	5.9
1	A	337	PHE	5.5
2	B	458	VAL	5.2
2	B	459	TYR	4.4
2	B	337	PHE	4.3
2	B	306	LEU	4.0
1	A	459	TYR	3.9
1	A	373	HIS	3.7
2	B	533	VAL	3.5
2	B	336	PRO	3.4
2	B	471	GLU	3.3
2	B	307	ALA	3.3
2	B	457	GLY	3.3
1	A	306	LEU	3.3
1	A	309	SER	3.1
1	A	460	THR	3.0
2	B	334	THR	3.0
2	B	472	LYS	2.9
2	B	368	VAL	2.9
2	B	305	SER	2.9
3	C	693	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	373	HIS	2.6
2	B	534	VAL	2.6
2	B	541	LEU	2.5
1	A	472	LYS	2.5
2	B	420	GLY	2.5
2	B	497	LEU	2.5
2	B	417	CYS	2.4
1	A	533	VAL	2.4
1	A	381	CYS	2.4
3	C	687	HIS	2.4
2	B	435	PHE	2.4
1	A	305	SER	2.4
1	A	330[A]	GLU	2.3
2	B	475	ILE	2.3
1	A	307	ALA	2.3
2	B	535	PRO	2.2
2	B	493	ALA	2.2
1	A	461	PHE	2.1
1	A	458	VAL	2.1
1	A	326	ILE	2.1
3	C	692	ARG	2.1
2	B	456	SER	2.0
2	B	332	ASP	2.0
2	B	531	LYS	2.0
1	A	434	ARG	2.0
2	B	316	VAL	2.0
2	B	477	ARG	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	530	10/11	0.89	0.14	33,46,76,78	2
2	CME	B	381	10/11	0.90	0.13	39,44,74,76	1

6.3 Carbohydrates [i](#)

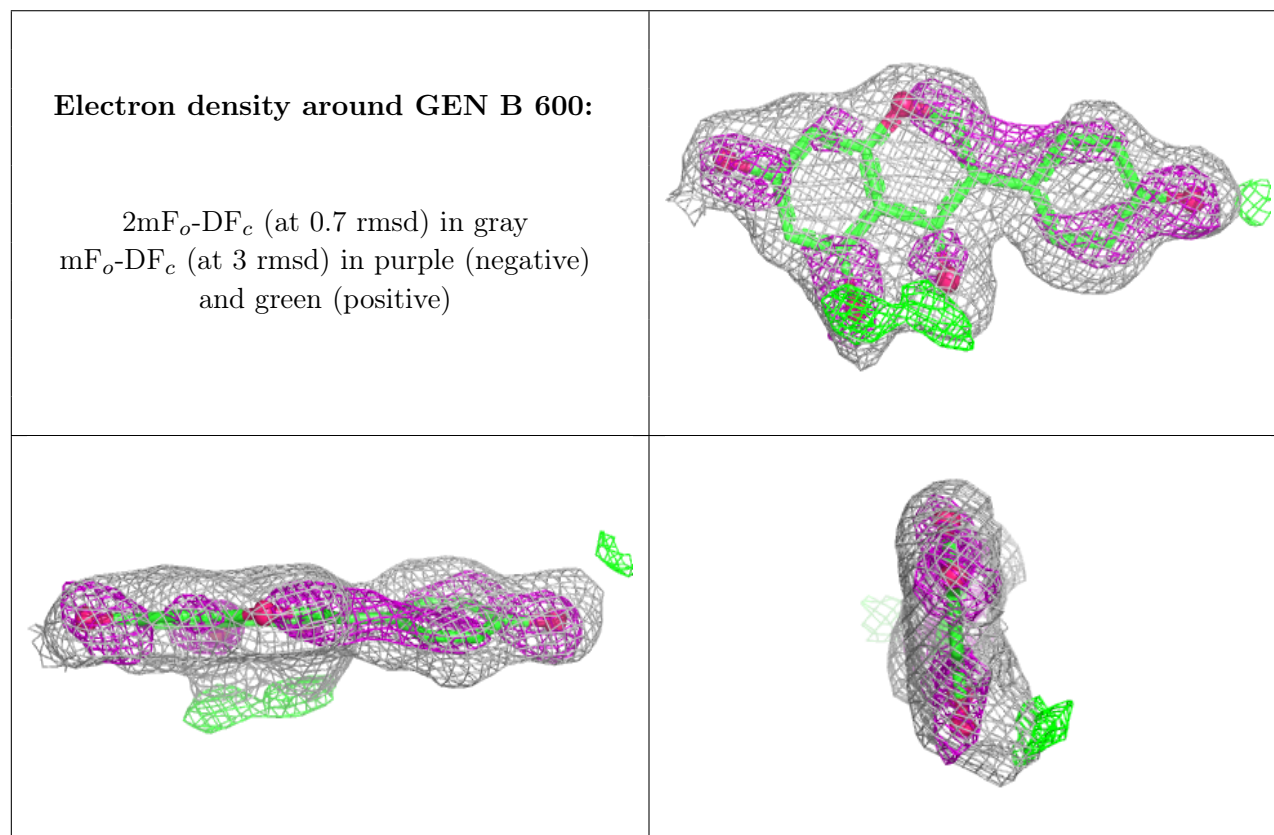
There are no oligosaccharides in this entry.

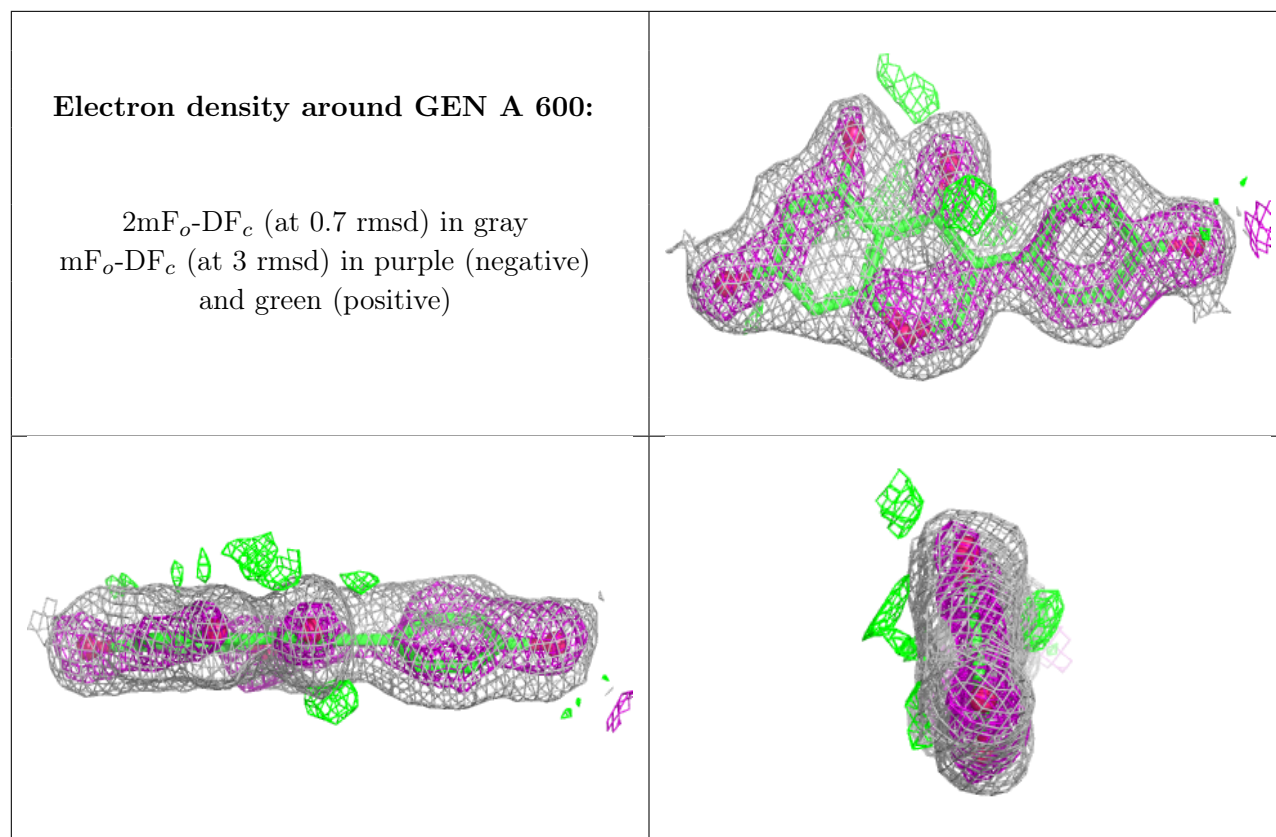
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GEN	B	600	20/20	0.91	0.10	11,30,39,46	0
4	GEN	A	600	20/20	0.92	0.10	16,23,35,37	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.