



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:40 PM UTC

PDB ID : 1DKF / pdb_00001dkf
Title : CRYSTAL STRUCTURE OF A HETERODIMERIC COMPLEX OF RAR AND RXR LIGAND-BINDING DOMAINS
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Deposited on : 1999-12-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

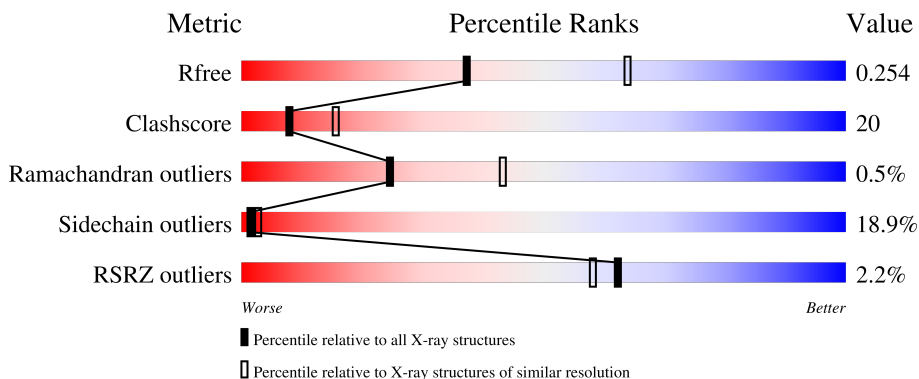
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	233	
2	B	235	

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
4	BMS	B	600	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3743 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 PROTEIN (RETINOID X RECEPTOR-ALPHA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1701	1088	291	312	10	0	0	0

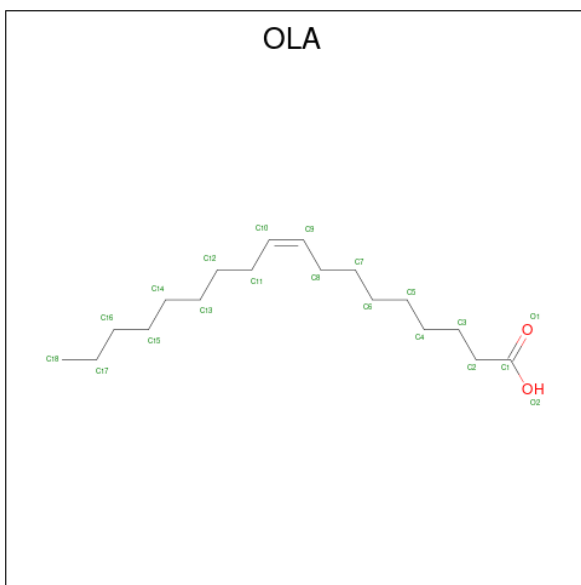
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	PHE	engineered mutation	UNP P28700

- Molecule 2 is a protein called PROTEIN (RETINOIC ACID RECEPTOR-ALPHA).

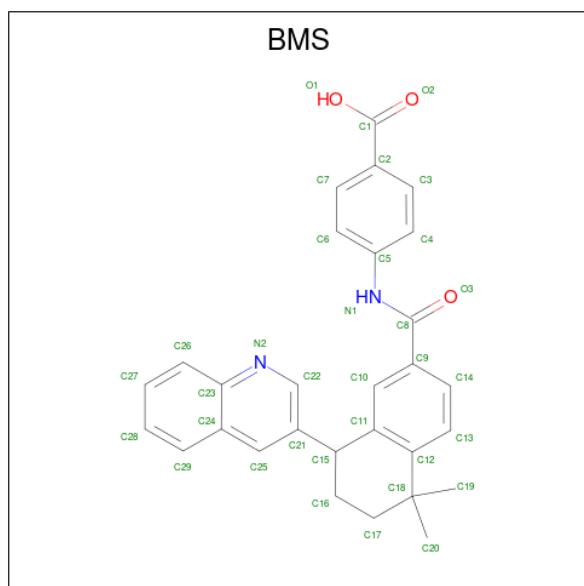
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	232	1831	1164	307	344	16	0	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



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

- Molecule 4 is 4-[(4,4-DIMETHYL-1,2,3,4-TETRAHYDRO-[1,2']BINAPHTHALENYL-7-CARBONYL)-AMINO]-BENZOIC ACID (CCD ID: BMS) (formula: $C_{29}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			34	29	2	3		

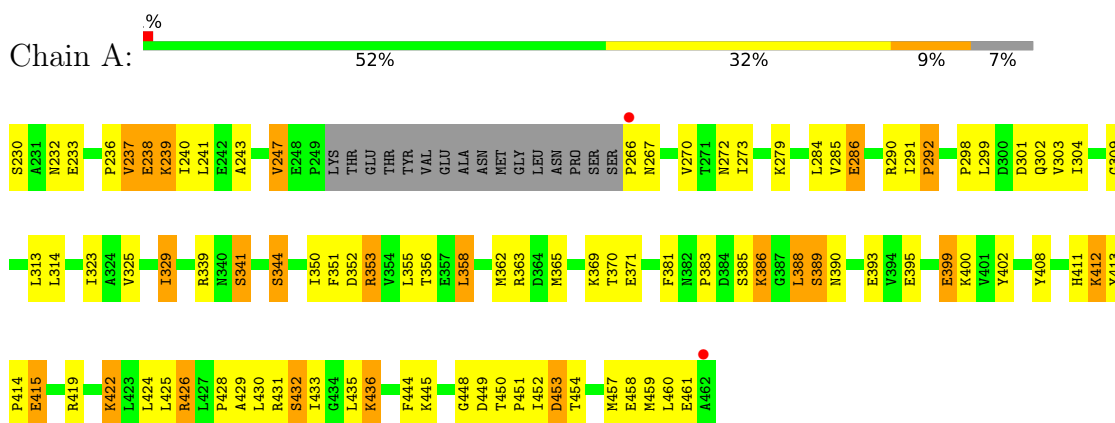
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	78	Total	O	0	0
			78	78		

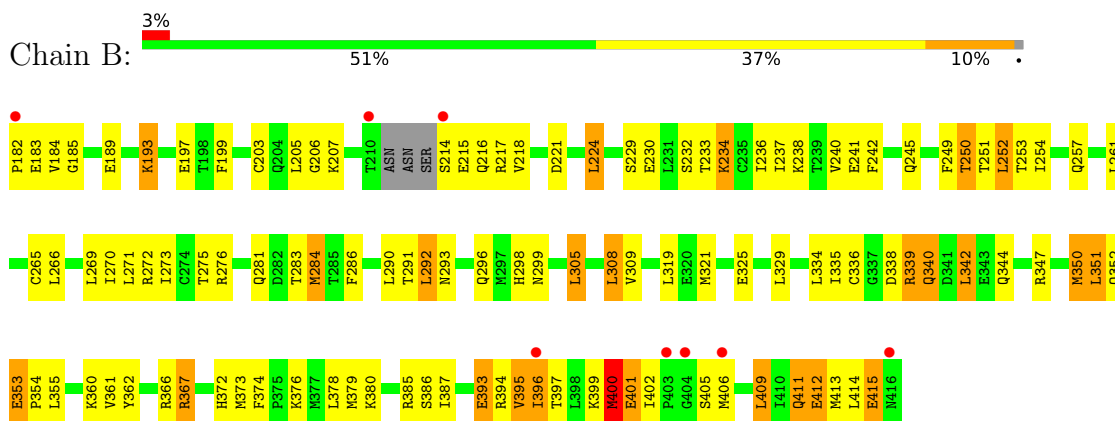
3 Residue-property plots

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: PROTEIN (RETINOID X RECEPTOR-ALPHA)



- Molecule 2: PROTEIN (RETINOIC ACID RECEPTOR-ALPHA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.60Å 116.60Å 207.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 88.0 (20.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.50Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.203 , 0.262 0.203 , 0.254	Depositor DCC
R_{free} test set	1427 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: OLA, BMS

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	0.49	0/1734	0.92	5/2344 (0.2%)
2	B	0.53	1/1860 (0.1%)	0.97	6/2511 (0.2%)
All	All	0.51	1/3594 (0.0%)	0.95	11/4855 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	MET	SD-CE	5.91	1.94	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	GLU	N-CA-C	-6.77	105.02	113.28
2	B	367	ARG	CA-C-N	6.66	126.92	119.32
2	B	367	ARG	C-N-CA	6.66	126.92	119.32
1	A	412	LYS	N-CA-C	6.24	119.06	111.82
2	B	224	LEU	N-CA-C	-5.95	104.14	111.40
2	B	380	LYS	N-CA-C	-5.66	105.10	112.23
1	A	413	TYR	CA-C-N	5.54	125.89	119.47
1	A	413	TYR	C-N-CA	5.54	125.89	119.47
1	A	240	ILE	N-CA-C	-5.37	106.46	111.45
2	B	206	GLY	N-CA-C	-5.19	100.88	113.18
1	A	266	PRO	N-CA-CB	5.17	108.69	103.00

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	1701	0	1734	64	0
2	B	1831	0	1888	81	0
3	A	20	0	33	1	0
4	B	34	0	24	1	0
5	A	79	0	0	2	0
5	B	78	0	0	3	0
All	All	3743	0	3679	143	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 20.

All (143) 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:353:ARG:HH22	1:A:432:SER:HB3	1.12	1.05
1:A:353:ARG:NH2	1:A:432:SER:HB3	1.81	0.96
2:B:395:VAL:HG22	2:B:406:MET:HE1	1.56	0.86
2:B:411:GLN:O	2:B:415:GLU:HG2	1.83	0.79
2:B:393:GLU:O	2:B:396:ILE:HG13	1.82	0.79
2:B:293:ASN:CG	2:B:296:GLN:HE21	1.91	0.77
2:B:261:LEU:HD12	2:B:414:LEU:HD22	1.68	0.75
2:B:379:MET:HA	2:B:379:MET:HE2	1.70	0.74
2:B:399:LYS:HA	2:B:405:SER:OG	1.88	0.73
1:A:353:ARG:HH22	1:A:432:SER:CB	1.98	0.72
1:A:323:ILE:HG23	1:A:363:ARG:HB2	1.72	0.71
1:A:230:SER:HA	1:A:233:GLU:HG3	1.73	0.70
1:A:350:ILE:H	1:A:350:ILE:HD12	1.56	0.70
1:A:267:ASN:C	1:A:267:ASN:HD22	2.01	0.69
2:B:240:VAL:HG22	2:B:261:LEU:HD13	1.74	0.69
2:B:271:LEU:O	2:B:275:THR:HG23	1.94	0.68
2:B:273:ILE:HG13	2:B:284:MET:HG2	1.76	0.67
2:B:400:MET:HG2	2:B:401:GLU:N	2.09	0.66
2:B:308:LEU:HD23	2:B:387:ILE:HG12	1.77	0.66
2:B:207:LYS:HG2	2:B:291:THR:OG1	1.96	0.65
1:A:431:ARG:HG2	1:A:431:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ILE:O	2:B:241:GLU:HG3	1.96	0.64
2:B:352:GLN:HA	2:B:355:LEU:HD12	1.79	0.64
1:A:303:VAL:HG23	1:A:460:LEU:HD12	1.81	0.63
2:B:276:ARG:HG3	2:B:276:ARG:HH11	1.64	0.62
1:A:358:LEU:HD22	1:A:433:ILE:HD13	1.81	0.62
1:A:232:ASN:ND2	1:A:236:PRO:HA	2.15	0.61
2:B:395:VAL:CG2	2:B:406:MET:HE1	2.31	0.60
2:B:412:GLU:HA	2:B:415:GLU:HG3	1.83	0.60
1:A:431:ARG:HG2	1:A:431:ARG:NH1	2.16	0.59
2:B:281:GLN:HB3	2:B:283:THR:HG23	1.85	0.59
1:A:385:SER:HB2	1:A:388:LEU:HD22	1.85	0.59
2:B:399:LYS:HA	2:B:405:SER:HG	1.66	0.59
2:B:409:LEU:CD1	2:B:413:MET:HE2	2.34	0.58
1:A:371:GLU:OE2	1:A:419:ARG:HD3	2.03	0.58
2:B:250:THR:HA	2:B:257:GLN:NE2	2.19	0.57
2:B:319:LEU:HD11	2:B:376:LYS:HD3	1.86	0.57
2:B:339:ARG:HG2	2:B:339:ARG:HH11	1.68	0.57
1:A:353:ARG:HE	1:A:436:LYS:HE3	1.69	0.57
2:B:266:LEU:O	2:B:270:ILE:HG13	2.05	0.57
1:A:371:GLU:CD	1:A:419:ARG:HH11	2.11	0.57
1:A:329:ILE:HD12	1:A:351:PHE:CZ	2.40	0.56
2:B:276:ARG:HG3	2:B:276:ARG:NH1	2.20	0.55
1:A:267:ASN:ND2	1:A:272:ASN:HD21	2.04	0.55
1:A:298:PRO:HG2	1:A:301:ASP:HB2	1.89	0.55
1:A:390:ASN:ND2	1:A:393:GLU:HB2	2.22	0.55
2:B:218:VAL:H	2:B:299:ASN:HD21	1.55	0.55
2:B:249:PHE:O	2:B:252:LEU:HB2	2.08	0.54
2:B:361:VAL:HG23	2:B:362:TYR:N	2.24	0.53
2:B:261:LEU:HD12	2:B:414:LEU:CD2	2.40	0.52
1:A:415:GLU:CD	1:A:415:GLU:H	2.17	0.51
2:B:308:LEU:CD2	2:B:387:ILE:HG12	2.41	0.51
2:B:393:GLU:HB3	5:B:144:HOH:O	2.09	0.50
1:A:358:LEU:O	1:A:362:MET:HG3	2.11	0.50
2:B:182:PRO:HD2	2:B:184:VAL:HG12	1.92	0.50
1:A:323:ILE:O	1:A:363:ARG:NH1	2.42	0.50
2:B:237:ILE:HA	2:B:413:MET:HE1	1.94	0.50
1:A:304:ILE:HG21	1:A:388:LEU:HD13	1.94	0.49
1:A:429:ALA:O	1:A:433:ILE:HD12	2.12	0.49
2:B:215:GLU:HG3	2:B:216:GLN:N	2.26	0.49
2:B:286:PHE:HD1	2:B:290:LEU:O	1.95	0.49
2:B:319:LEU:HD12	2:B:373:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:C	1:A:428:PRO:HD2	2.38	0.49
2:B:409:LEU:HD11	2:B:413:MET:HE2	1.94	0.49
2:B:325:GLU:CD	2:B:366:ARG:HH11	2.21	0.49
1:A:309:GLY:O	1:A:313:LEU:HG	2.13	0.49
1:A:365:MET:O	1:A:419:ARG:NH2	2.45	0.48
2:B:292:LEU:HG	2:B:296:GLN:HB3	1.95	0.48
2:B:362:TYR:CE1	2:B:366:ARG:HD2	2.49	0.48
1:A:399:GLU:HG2	2:B:372:HIS:HB2	1.96	0.48
1:A:459:MET:HE2	5:A:92:HOH:O	2.14	0.47
1:A:371:GLU:OE1	1:A:419:ARG:NH1	2.47	0.47
1:A:451:PRO:HG2	1:A:454:THR:OG1	2.13	0.47
2:B:336:CYS:SG	2:B:338:ASP:HB2	2.54	0.47
1:A:270:VAL:HA	1:A:444:PHE:CE2	2.50	0.47
1:A:352:ASP:O	1:A:356:THR:HG23	2.15	0.47
2:B:319:LEU:HA	2:B:373:MET:HE1	1.97	0.47
1:A:247:VAL:O	1:A:247:VAL:HG13	2.15	0.47
2:B:184:VAL:HG13	2:B:185:GLY:N	2.30	0.47
2:B:218:VAL:H	2:B:299:ASN:ND2	2.13	0.47
2:B:240:VAL:HG21	2:B:413:MET:HE3	1.95	0.47
1:A:383:PRO:HB3	1:A:395:GLU:HB2	1.98	0.46
1:A:236:PRO:HB2	1:A:239:LYS:HB2	1.97	0.46
1:A:411:HIS:O	1:A:414:PRO:HD3	2.14	0.46
1:A:431:ARG:O	1:A:435:LEU:HG	2.16	0.46
1:A:232:ASN:ND2	1:A:238:GLU:OE2	2.49	0.46
1:A:386:LYS:HE2	1:A:386:LYS:HB3	1.59	0.46
1:A:452:ILE:HG22	1:A:453:ASP:N	2.31	0.46
2:B:402:ILE:O	2:B:405:SER:HB3	2.16	0.46
2:B:221:ASP:HB3	2:B:224:LEU:HB2	1.98	0.45
2:B:234:LYS:HE2	5:B:119:HOH:O	2.15	0.45
1:A:323:ILE:HG23	1:A:363:ARG:CB	2.45	0.45
3:A:700:OLA:H111	3:A:700:OLA:H81	1.83	0.45
2:B:367:ARG:HH11	2:B:367:ARG:HG3	1.81	0.44
2:B:415:GLU:HG2	2:B:415:GLU:H	1.55	0.44
2:B:238:LYS:HE2	2:B:241:GLU:OE1	2.17	0.44
2:B:414:LEU:HD12	2:B:414:LEU:HA	1.80	0.44
2:B:250:THR:O	2:B:257:GLN:NE2	2.50	0.44
2:B:353:GLU:HB3	2:B:354:PRO:HD3	1.99	0.44
2:B:360:LYS:HA	2:B:374:PHE:CD2	2.53	0.44
1:A:241:LEU:HD12	1:A:241:LEU:O	2.18	0.43
1:A:267:ASN:HD21	1:A:272:ASN:HD21	1.65	0.43
1:A:339:ARG:HH11	1:A:339:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:LEU:O	2:B:309:VAL:HG23	2.18	0.43
1:A:402:TYR:OH	2:B:379:MET:HG3	2.19	0.43
1:A:291:ILE:HA	1:A:292:PRO:HD2	1.86	0.43
2:B:293:ASN:H	2:B:296:GLN:NE2	2.16	0.43
2:B:342:LEU:HD12	2:B:342:LEU:HA	1.91	0.43
1:A:285:VAL:HB	5:A:92:HOH:O	2.17	0.43
2:B:339:ARG:HG2	2:B:339:ARG:NH1	2.34	0.43
2:B:340:GLN:HE21	2:B:340:GLN:HB2	1.63	0.43
1:A:408:TYR:OH	1:A:412:LYS:HD2	2.19	0.42
1:A:298:PRO:O	1:A:302:GLN:HG3	2.19	0.42
1:A:399:GLU:HG2	2:B:372:HIS:CB	2.50	0.42
2:B:199:PHE:CE2	2:B:272:ARG:HB3	2.53	0.42
1:A:424:LEU:C	1:A:426:ARG:H	2.28	0.42
2:B:182:PRO:CD	2:B:184:VAL:HG12	2.49	0.42
2:B:335:ILE:HG22	2:B:335:ILE:O	2.19	0.42
1:A:243:ALA:HB2	1:A:290:ARG:HB2	2.00	0.42
2:B:217:ARG:HD3	2:B:298:HIS:CG	2.55	0.42
1:A:426:ARG:HD3	1:A:426:ARG:HA	1.68	0.42
2:B:242:PHE:O	2:B:245:GLN:HB2	2.20	0.42
1:A:301:ASP:OD1	1:A:389:SER:HB3	2.20	0.41
1:A:381:PHE:O	1:A:383:PRO:HD3	2.20	0.41
2:B:182:PRO:HD2	2:B:184:VAL:CG1	2.49	0.41
2:B:203:CYS:HB3	5:B:27:HOH:O	2.20	0.41
2:B:250:THR:C	2:B:252:LEU:H	2.28	0.41
1:A:303:VAL:CG2	1:A:460:LEU:HD12	2.50	0.41
2:B:350:MET:N	2:B:350:MET:HE2	2.35	0.41
1:A:371:GLU:CD	1:A:419:ARG:NH1	2.77	0.41
2:B:193:LYS:O	2:B:197:GLU:HB2	2.21	0.41
1:A:286:GLU:O	1:A:290:ARG:HG3	2.20	0.41
1:A:422:LYS:NZ	1:A:422:LYS:HB2	2.36	0.41
2:B:229:SER:HA	4:B:600:BMS:H29	2.03	0.41
2:B:361:VAL:CG2	2:B:362:TYR:N	2.83	0.41
1:A:448:GLY:C	1:A:450:THR:H	2.29	0.41
2:B:232:SER:O	2:B:233:THR:C	2.62	0.41
2:B:351:LEU:HD23	2:B:351:LEU:HA	1.91	0.41
2:B:394:ARG:O	2:B:397:THR:HB	2.21	0.40
1:A:237:VAL:HG13	1:A:370:THR:CG2	2.51	0.40
2:B:319:LEU:HB3	2:B:321:MET:HG3	2.03	0.40
2:B:409:LEU:HD12	2:B:413:MET:HE2	2.01	0.40
1:A:341:SER:O	1:A:344:SER:HB3	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	213/233 (91%)	198 (93%)	13 (6%)	2 (1%)	14	27
2	B	228/235 (97%)	218 (96%)	10 (4%)	0	100	100
All	All	441/468 (94%)	416 (94%)	23 (5%)	2 (0%)	24	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	VAL
1	A	292	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	185/199 (93%)	151 (82%)	34 (18%)	1	3
2	B	207/211 (98%)	167 (81%)	40 (19%)	1	2
All	All	392/410 (96%)	318 (81%)	74 (19%)	1	3

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	VAL
1	A	238	GLU
1	A	239	LYS
1	A	247	VAL

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Mol	Chain	Res	Type
1	A	273	ILE
1	A	279	LYS
1	A	284	LEU
1	A	286	GLU
1	A	299	LEU
1	A	314	LEU
1	A	329	ILE
1	A	341	SER
1	A	344	SER
1	A	353	ARG
1	A	355	LEU
1	A	358	LEU
1	A	369	LYS
1	A	386	LYS
1	A	388	LEU
1	A	389	SER
1	A	399	GLU
1	A	400	LYS
1	A	415	GLU
1	A	422	LYS
1	A	426	ARG
1	A	430	LEU
1	A	432	SER
1	A	436	LYS
1	A	445	LYS
1	A	449	ASP
1	A	453	ASP
1	A	457	MET
1	A	458	GLU
1	A	461	GLU
2	B	189	GLU
2	B	193	LYS
2	B	205	LEU
2	B	214	SER
2	B	230	GLU
2	B	234	LYS
2	B	236	ILE
2	B	250	THR
2	B	251	THR
2	B	252	LEU
2	B	253	THR
2	B	254	ILE

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Mol	Chain	Res	Type
2	B	265	CYS
2	B	269	LEU
2	B	284	MET
2	B	292	LEU
2	B	305	LEU
2	B	308	LEU
2	B	329	LEU
2	B	334	LEU
2	B	339	ARG
2	B	340	GLN
2	B	342	LEU
2	B	344	GLN
2	B	347	ARG
2	B	350	MET
2	B	351	LEU
2	B	353	GLU
2	B	378	LEU
2	B	385	ARG
2	B	386	SER
2	B	393	GLU
2	B	395	VAL
2	B	396	ILE
2	B	400	MET
2	B	401	GLU
2	B	409	LEU
2	B	411	GLN
2	B	412	GLU
2	B	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	272	ASN
1	A	302	GLN
1	A	340	ASN
1	A	390	ASN
2	B	204	GLN
2	B	296	GLN
2	B	299	ASN
2	B	340	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	BMS	B	600	-	38,38,38	5.66	29 (76%)	52,56,56	2.00	10 (19%)
3	OLA	A	700	-	19,19,19	1.67	3 (15%)	19,19,19	1.49	2 (10%)

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	BMS	B	600	-	1/1/4/5	4/16/32/32	0/5/5/5
3	OLA	A	700	-	-	7/17/17/17	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	BMS	C24-C23	13.18	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	BMS	C11-C12	12.59	1.55	1.40
4	B	600	BMS	C22-C21	9.48	1.52	1.39
4	B	600	BMS	C28-C27	8.29	1.56	1.38
4	B	600	BMS	C13-C12	8.10	1.50	1.39
4	B	600	BMS	C14-C9	7.97	1.51	1.39
4	B	600	BMS	C3-C2	7.86	1.51	1.39
4	B	600	BMS	C10-C11	7.43	1.51	1.39
4	B	600	BMS	C4-C3	6.79	1.49	1.38
4	B	600	BMS	C16-C15	-6.72	1.42	1.54
4	B	600	BMS	C28-C29	6.54	1.50	1.36
4	B	600	BMS	C27-C26	6.44	1.50	1.36
4	B	600	BMS	C7-C2	6.10	1.48	1.39
4	B	600	BMS	C25-C21	5.52	1.48	1.37
3	A	700	OLA	C10-C9	5.27	1.61	1.31
4	B	600	BMS	C6-C5	5.19	1.48	1.39
4	B	600	BMS	C21-C15	-5.11	1.40	1.53
4	B	600	BMS	C22-N2	4.99	1.40	1.31
4	B	600	BMS	C10-C9	4.93	1.46	1.39
4	B	600	BMS	C7-C6	4.56	1.46	1.38
4	B	600	BMS	C4-C5	4.35	1.46	1.39
4	B	600	BMS	C9-C8	-3.86	1.41	1.50
4	B	600	BMS	O2-C1	3.60	1.33	1.22
4	B	600	BMS	C14-C13	3.46	1.44	1.38
4	B	600	BMS	C18-C12	3.32	1.58	1.53
3	A	700	OLA	C2-C1	3.17	1.57	1.50
4	B	600	BMS	C17-C18	2.93	1.61	1.53
4	B	600	BMS	C11-C15	2.80	1.56	1.52
3	A	700	OLA	O1-C1	2.42	1.30	1.22
4	B	600	BMS	C23-N2	2.40	1.41	1.37
4	B	600	BMS	C26-C23	2.29	1.45	1.41
4	B	600	BMS	O3-C8	2.18	1.28	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	BMS	C21-C15-C11	7.73	123.65	113.34
4	B	600	BMS	C16-C15-C11	4.93	121.31	109.06
4	B	600	BMS	C17-C16-C15	4.70	121.97	110.36
4	B	600	BMS	C18-C12-C11	-4.17	118.11	122.75
3	A	700	OLA	O2-C1-C2	3.97	126.55	114.00
3	A	700	OLA	O1-C1-C2	-3.65	111.52	123.09
4	B	600	BMS	C22-N2-C23	3.37	120.86	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	BMS	C24-C23-N2	-2.71	118.31	122.03
4	B	600	BMS	C29-C24-C25	-2.41	117.85	122.00
4	B	600	BMS	C29-C24-C23	2.37	121.63	118.43
4	B	600	BMS	C21-C25-C24	-2.24	118.07	121.47
4	B	600	BMS	C27-C26-C23	-2.09	117.23	120.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	600	BMS	C15

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	BMS	C9-C8-N1-C5
3	A	700	OLA	C11-C12-C13-C14
3	A	700	OLA	C5-C6-C7-C8
3	A	700	OLA	C12-C13-C14-C15
4	B	600	BMS	O3-C8-N1-C5
4	B	600	BMS	C4-C5-N1-C8
4	B	600	BMS	C6-C5-N1-C8
3	A	700	OLA	C3-C4-C5-C6
3	A	700	OLA	O1-C1-C2-C3
3	A	700	OLA	O2-C1-C2-C3
3	A	700	OLA	C4-C5-C6-C7

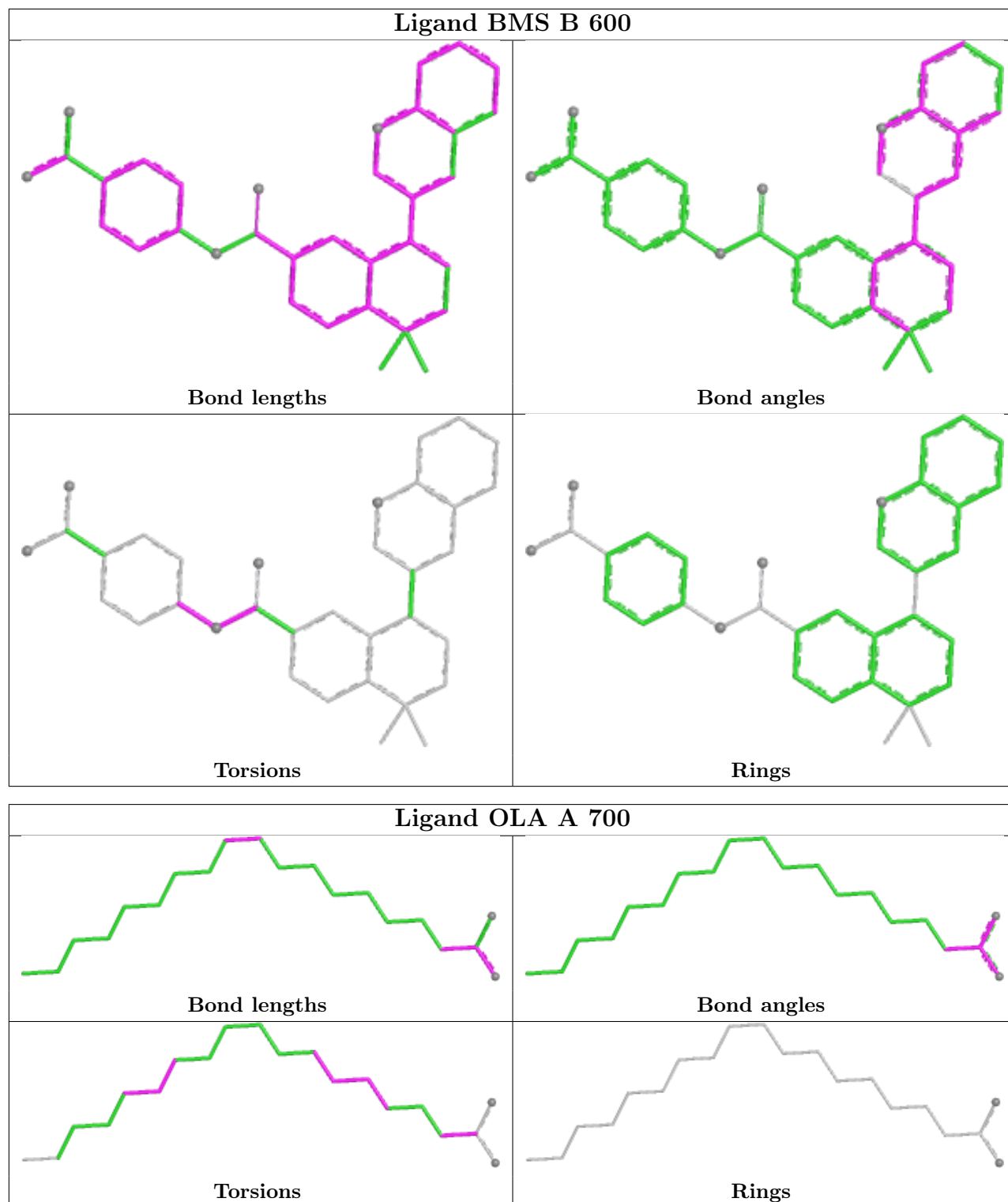
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	BMS	1	0
3	A	700	OLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	217/233 (93%)	-0.09	2 (0%) 81 78	27, 46, 67, 82	0
2	B	232/235 (98%)	-0.19	8 (3%) 48 43	26, 41, 71, 79	0
All	All	449/468 (95%)	-0.14	10 (2%) 62 58	26, 43, 69, 82	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	SER	3.5
2	B	416	ASN	3.1
2	B	210	THR	3.1
2	B	182	PRO	3.0
1	A	266	PRO	2.5
1	A	462	ALA	2.4
2	B	396	ILE	2.4
2	B	406	MET	2.3
2	B	403	PRO	2.2
2	B	404	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

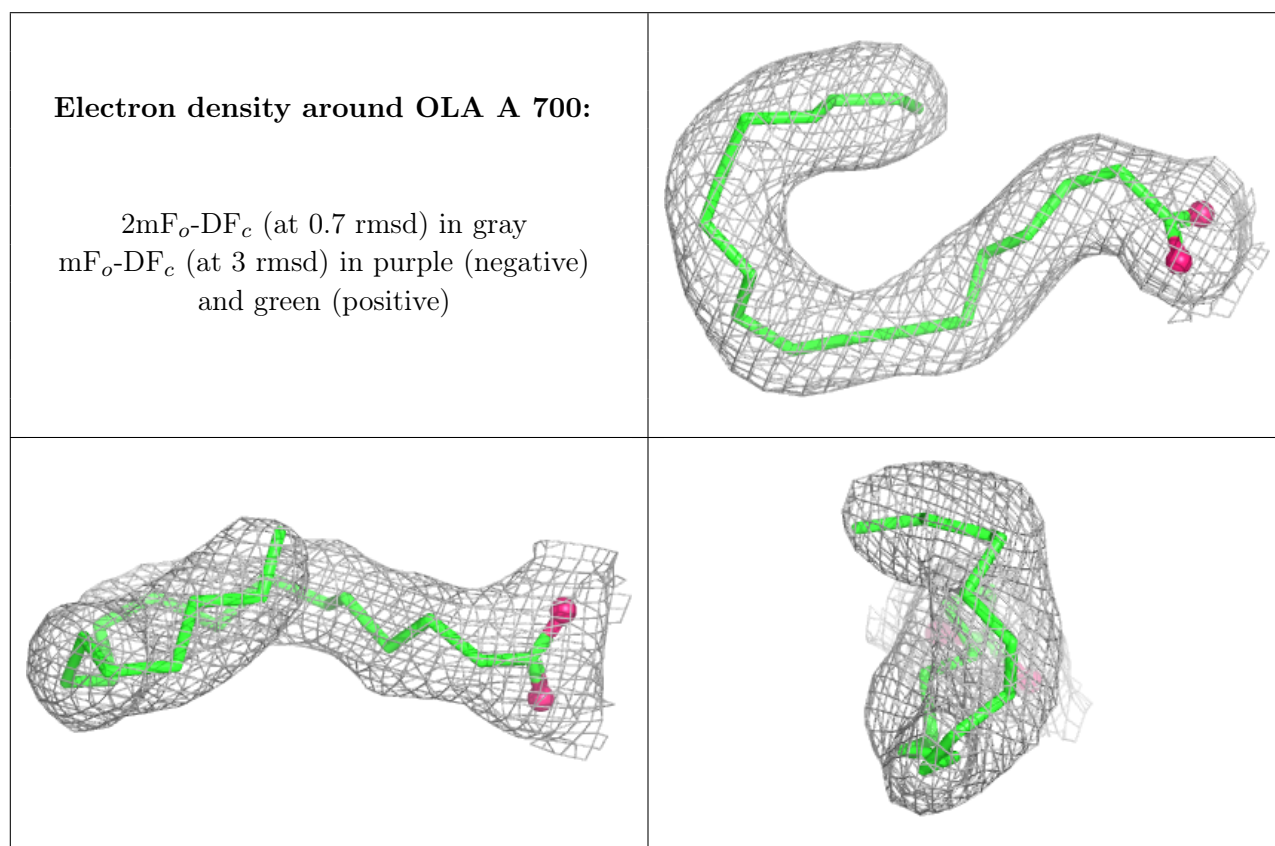
There are no oligosaccharides in this entry.

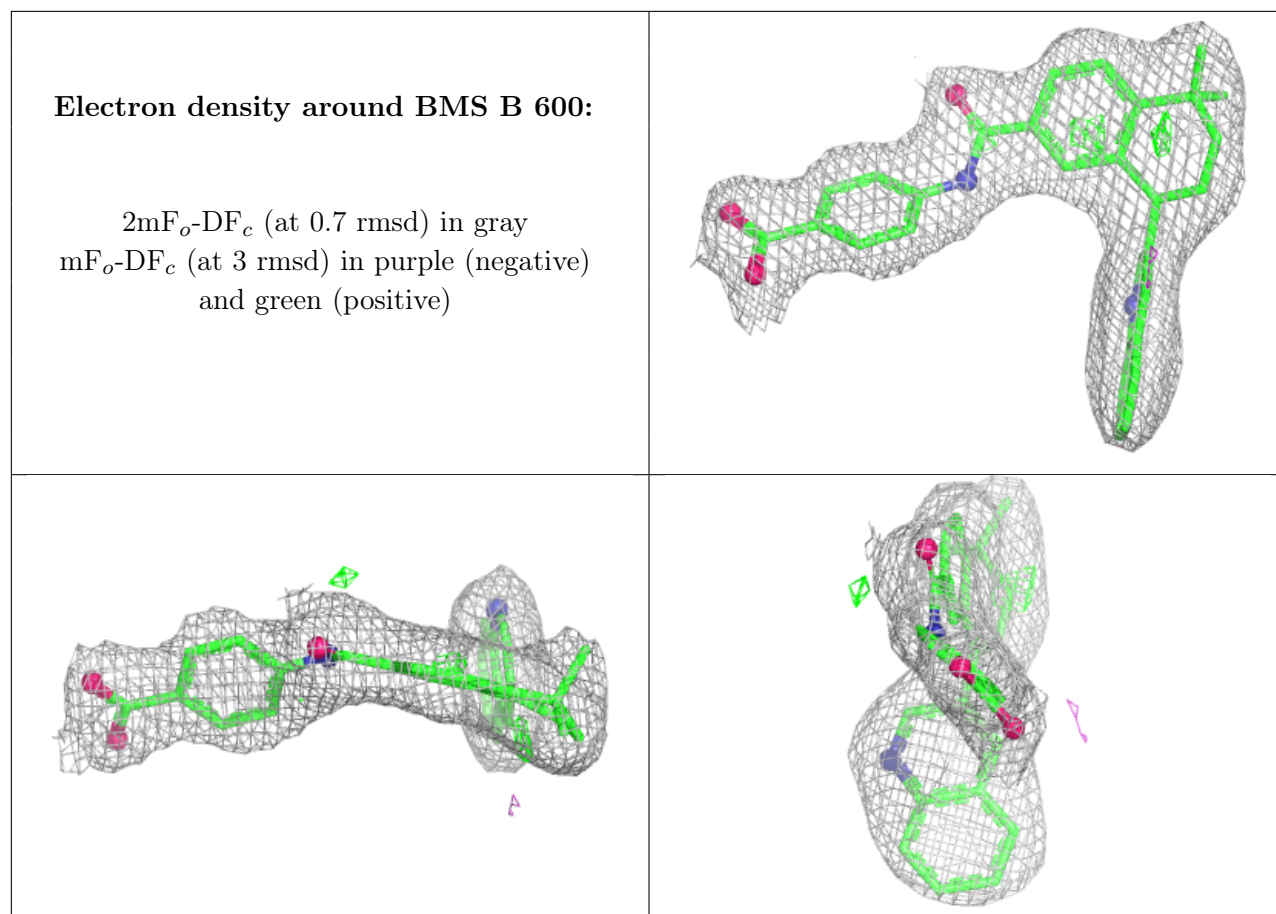
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLA	A	700	20/20	0.95	0.07	30,35,39,39	0
4	BMS	B	600	34/34	0.95	0.08	28,32,39,42	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.