



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:31 PM UTC

PDB ID : 8W03 / pdb_00008w03
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-1154
Authors : Min, C.K.; Nwachukwu, J.C.; Hou, Y.; Russo, R.J.; Papa, A.; Min, J.; Peng, R.; Kim, S.H.; Ziegler, Y.; Rangarajan, E.S.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on : 2024-02-13
Resolution : 1.68 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.48.1

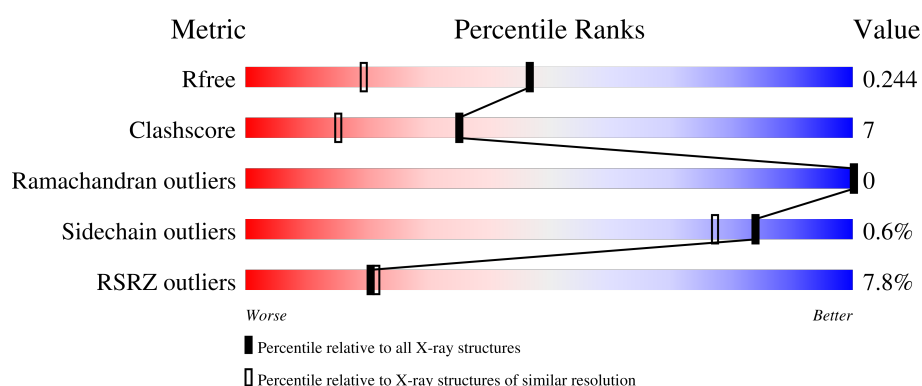
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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	242	7% 82% 17%
1	B	242	8% 87% 9% .
1	C	242	6% 87% 12%
1	D	242	9% 82% 11% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15422 atoms, of which 7505 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.

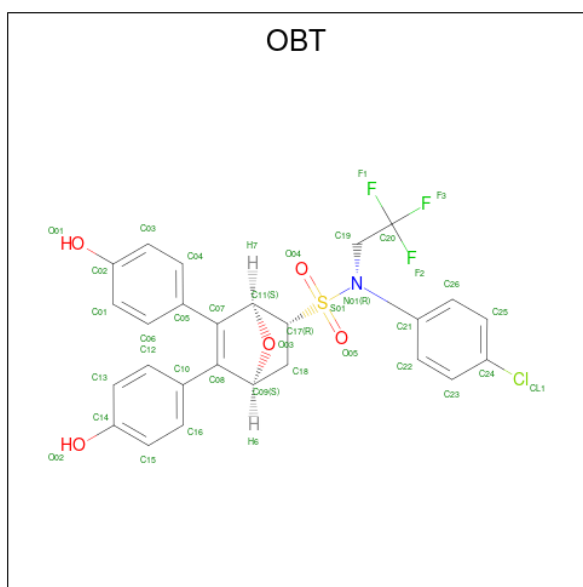
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	H	N	O	S	0	1	0
			3758	1204	1876	322	339	17			
1	B	232	Total	C	H	N	O	S	0	0	0
			3663	1166	1843	309	330	15			
1	C	241	Total	C	H	N	O	S	0	1	0
			3804	1214	1906	322	345	17			
1	D	224	Total	C	H	N	O	S	0	0	0
			3579	1140	1802	303	318	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (1S,2R,4S)-N-(4-chlorophenyl)-5,6-bis(4-hydroxyphenyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (CCD ID: OBT) (formula: C₂₆H₂₁ClF₃NO₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	S	0	0		
			40	18	15	1	5	1				
2	B	1	Total	C	Cl	H	N	O	S	0	0	
			54	25	1	21	1	5	1			
2	C	1	Total	C	Cl	H	N	O	S	0	0	
			54	25	1	21	1	5	1			
2	D	1	Total	C	Cl	F	H	N	O	S	0	0
			58	26	1	3	21	1	5	1		

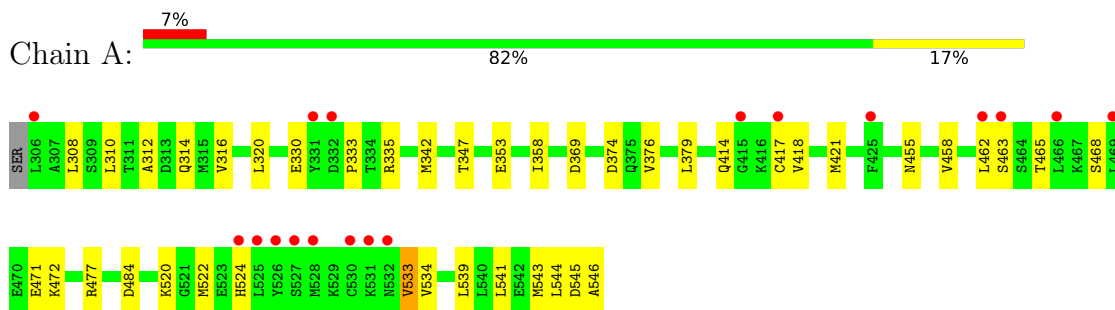
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	B	109	Total	O	0	0
			109	109		
3	C	107	Total	O	0	0
			107	107		
3	D	90	Total	O	0	0
			90	90		

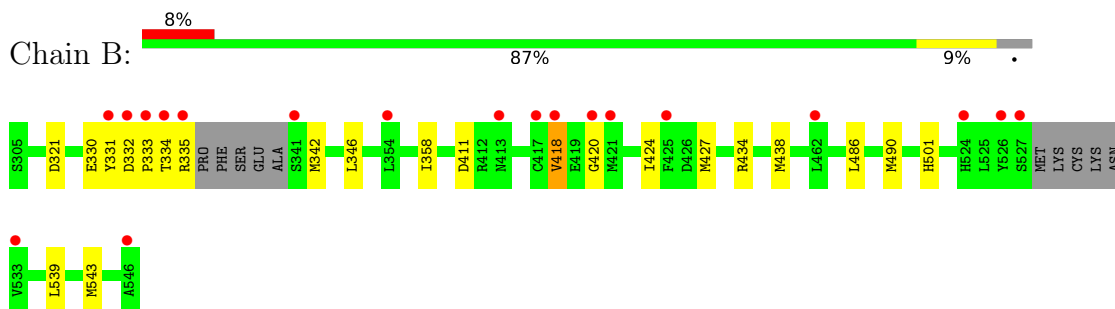
3 Residue-property plots

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.

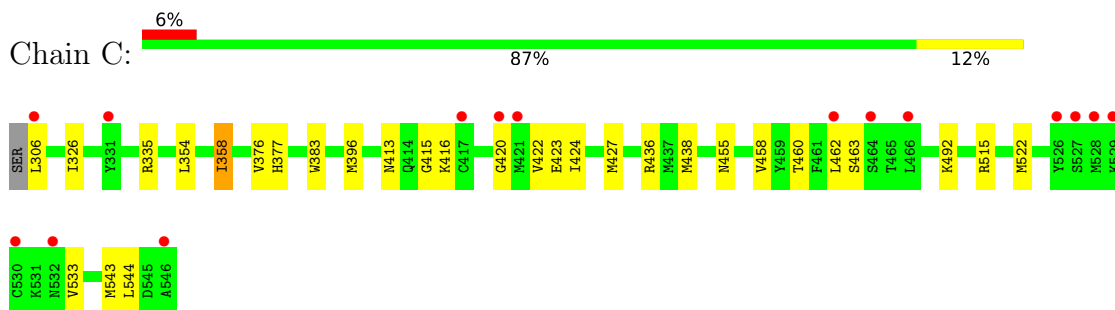
- Molecule 1: Estrogen receptor



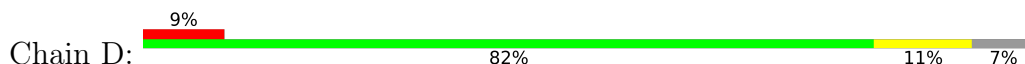
- Molecule 1: Estrogen receptor

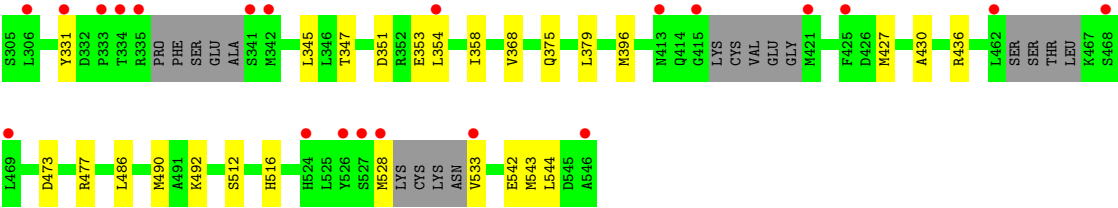


- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.49Å 58.77Å 93.21Å 86.61° 75.17° 62.96°	Depositor
Resolution (Å)	38.36 – 1.68 38.36 – 1.68	Depositor EDS
% Data completeness (in resolution range)	59.8 (38.36-1.68) 59.7 (38.36-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.201 , 0.245 0.202 , 0.244	Depositor DCC
R_{free} test set	3267 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.085 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15422	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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: OBT, YCM

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	0.60	0/1910	0.65	0/2589
1	B	0.62	0/1840	0.67	0/2487
1	C	0.66	0/1926	0.68	0/2608
1	D	0.63	0/1796	0.67	0/2423
All	All	0.62	0/7472	0.67	0/10107

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	LEU	Peptide

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	1882	1876	1875	39	0
1	B	1820	1843	1843	27	1
1	C	1898	1906	1904	23	0
1	D	1777	1802	1801	25	0
2	A	25	15	0	2	0
2	B	33	21	0	2	0
2	C	33	21	0	3	0
2	D	37	21	0	5	0
3	A	106	0	0	12	3
3	B	109	0	0	12	3
3	C	107	0	0	4	1
3	D	90	0	0	4	0
All	All	7917	7505	7423	109	4

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 7.

All (109) 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:C:462:LEU:HD21	1:D:430:ALA:HB2	1.14	1.12
1:B:332:ASP:OD2	3:B:701:HOH:O	1.65	1.10
1:B:332:ASP:OD2	3:B:702:HOH:O	1.71	1.07
1:C:463:SER:OG	3:C:701:HOH:O	1.79	0.98
1:B:427:MET:SD	3:B:760:HOH:O	2.27	0.90
1:A:316:VAL:O	3:A:701:HOH:O	1.90	0.86
1:B:331:TYR:O	3:B:703:HOH:O	1.94	0.85
1:C:306:LEU:N	3:C:702:HOH:O	2.11	0.82
1:B:335:ARG:N	3:B:701:HOH:O	2.11	0.82
1:B:334:THR:N	3:B:701:HOH:O	2.12	0.82
1:A:463:SER:HA	1:A:468:SER:HB2	1.62	0.82
1:C:462:LEU:HD21	1:D:430:ALA:CB	2.04	0.81
1:C:462:LEU:CD2	1:D:430:ALA:HB2	2.04	0.80
1:A:316:VAL:HG12	3:A:701:HOH:O	1.83	0.79
1:A:539:LEU:HD11	1:A:543:MET:HE2	1.67	0.76
1:D:354:LEU:HG	1:D:543:MET:HE1	1.67	0.75
1:B:342:MET:HE2	1:B:418:VAL:HG21	1.68	0.75
1:D:427:MET:HE1	1:D:516:HIS:CD2	2.23	0.74
1:A:320:LEU:HG	3:A:701:HOH:O	1.89	0.72
1:D:473:ASP:OD2	3:D:701:HOH:O	2.09	0.70
1:B:330:GLU:O	3:B:704:HOH:O	2.09	0.69
1:D:353:GLU:OE1	2:D:600:OBT:O02	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:OD1	3:A:702:HOH:O	2.11	0.67
1:D:351:ASP:OD2	3:D:702:HOH:O	2.12	0.67
1:D:542:GLU:OE1	3:D:703:HOH:O	2.12	0.66
1:D:533:VAL:HG11	2:D:600:OBT:O01	1.98	0.64
1:A:545:ASP:OD1	3:A:703:HOH:O	2.15	0.63
1:C:515:ARG:NH1	1:D:512:SER:OG	2.31	0.63
1:B:418:VAL:HG12	1:B:420:GLY:H	1.62	0.62
1:A:463:SER:HA	1:A:468:SER:CB	2.28	0.62
1:D:331:TYR:HB3	1:D:345:LEU:HD21	1.81	0.61
1:B:342:MET:HE2	1:B:418:VAL:CG2	2.30	0.61
1:D:492:LYS:N	1:D:492:LYS:HD2	2.16	0.60
1:A:463:SER:O	1:A:472:LYS:NZ	2.35	0.60
1:B:486:LEU:O	1:B:490:MET:HG3	2.01	0.59
1:A:539:LEU:CD1	1:A:543:MET:HE2	2.33	0.58
1:C:415:GLY:HA2	2:C:600:OBT:CL1	2.41	0.57
1:B:335:ARG:NH2	3:B:708:HOH:O	2.37	0.56
1:D:375:GLN:HB3	1:D:544:LEU:HD21	1.86	0.56
1:A:316:VAL:C	3:A:701:HOH:O	2.40	0.56
1:A:546:ALA:HB2	3:A:710:HOH:O	2.05	0.56
1:C:492:LYS:NZ	3:C:703:HOH:O	2.12	0.56
1:A:358:ILE:HD13	1:A:379:LEU:HD13	1.88	0.55
1:A:308:LEU:HD13	1:A:477:ARG:HE	1.71	0.54
1:A:520:LYS:O	1:A:524:HIS:ND1	2.41	0.54
1:A:310:LEU:HD22	1:A:314:GLN:HB3	1.89	0.53
1:C:413:ASN:HA	1:C:416:LYS:HD2	1.90	0.53
1:A:353:GLU:OE1	2:A:600:OBT:O02	2.27	0.53
1:A:330:GLU:OE1	3:A:704:HOH:O	2.18	0.52
1:A:310:LEU:HD22	1:A:314:GLN:CB	2.39	0.52
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.93	0.50
1:C:455:ASN:O	1:C:458:VAL:HG12	2.11	0.50
1:C:424:ILE:HG21	2:C:600:OBT:O04	2.11	0.49
1:D:486:LEU:O	1:D:490:MET:HG3	2.12	0.49
1:D:477:ARG:HA	1:D:477:ARG:HE	1.78	0.48
1:B:332:ASP:C	3:B:701:HOH:O	2.56	0.48
1:B:332:ASP:OD2	1:B:332:ASP:C	2.56	0.48
1:C:377:HIS:NE2	1:C:460:THR:OG1	2.45	0.48
1:A:533:VAL:HG13	2:A:600:OBT:O01	2.15	0.47
1:A:312:ALA:O	1:A:316:VAL:HG23	2.14	0.47
1:C:422:VAL:HG12	1:C:423:GLU:OE2	2.15	0.47
1:A:541:LEU:HA	1:A:544:LEU:HD12	1.97	0.47
1:B:333:PRO:N	3:B:714:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ARG:NH2	3:C:705:HOH:O	2.30	0.46
1:C:358:ILE:HG12	1:C:543:MET:HE3	1.97	0.46
1:A:333:PRO:HG2	1:A:335:ARG:HD3	1.96	0.46
1:B:342:MET:HE3	1:B:342:MET:HB3	1.91	0.46
1:C:354:LEU:HG	1:C:543:MET:HE1	1.97	0.46
1:A:522:MET:HE1	1:A:534:VAL:HG21	1.97	0.46
1:C:420:GLY:HA2	1:C:423:GLU:OE1	2.16	0.46
1:B:424:ILE:HG21	2:B:600:OBT:O04	2.16	0.46
1:A:376:VAL:HG22	1:A:544:LEU:CD1	2.46	0.45
1:A:522:MET:HE1	1:A:534:VAL:CG2	2.47	0.45
1:C:423:GLU:O	1:C:427:MET:HG3	2.15	0.45
1:D:473:ASP:O	1:D:477:ARG:HG2	2.17	0.44
1:A:316:VAL:CG1	3:A:701:HOH:O	2.55	0.44
1:B:420:GLY:HA3	2:B:600:OBT:C25	2.48	0.44
1:D:368:VAL:HG22	3:D:718:HOH:O	2.18	0.44
1:A:342:MET:HE1	1:A:417:CYS:HB2	1.99	0.44
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.35	0.44
1:B:321:ASP:OD2	3:B:705:HOH:O	2.20	0.44
1:B:334:THR:C	3:B:701:HOH:O	2.54	0.44
1:B:342:MET:HE1	1:B:346:LEU:HD11	2.00	0.44
1:C:438:MET:HE2	1:C:438:MET:HB3	1.95	0.44
1:D:358:ILE:HD13	1:D:379:LEU:HD13	1.99	0.44
1:C:383:TRP:CZ2	1:C:522:MET:HE1	2.53	0.43
1:C:533:VAL:HG13	2:C:600:OBT:O01	2.18	0.43
1:A:320:LEU:CG	3:A:701:HOH:O	2.55	0.43
1:B:434:ARG:O	1:B:438:MET:HG3	2.19	0.43
1:A:455:ASN:O	1:A:458:VAL:HG12	2.19	0.42
1:A:330:GLU:HG3	3:A:744:HOH:O	2.19	0.42
1:A:320:LEU:CD1	3:A:701:HOH:O	2.67	0.42
1:A:484:ASP:OD1	1:B:501:HIS:HE1	2.01	0.42
1:D:347:THR:HA	2:D:600:OBT:O01	2.19	0.42
1:D:358:ILE:CD1	1:D:379:LEU:HD13	2.50	0.42
1:D:533:VAL:CG1	2:D:600:OBT:O01	2.66	0.42
1:B:539:LEU:HD12	1:B:539:LEU:O	2.19	0.42
1:A:342:MET:HE1	1:A:414:GLN:O	2.20	0.42
1:D:396:MET:O	1:D:436:ARG:HD3	2.19	0.42
1:B:358:ILE:HG13	1:B:543:MET:HE2	2.01	0.41
1:A:418:VAL:CG1	1:A:421:MET:HG3	2.51	0.41
1:D:396:MET:HE3	1:D:436:ARG:HA	2.03	0.41
1:A:358:ILE:HG23	1:A:544:LEU:HD23	2.03	0.41
1:C:396:MET:O	1:C:436:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:MET:SD	2:D:600:OBT:F3	2.69	0.40
1:A:347:THR:HG23	1:A:533:VAL:HG22	2.03	0.40
1:B:539:LEU:HD12	1:B:543:MET:HG3	2.03	0.40
1:A:347:THR:CG2	1:A:533:VAL:HG22	2.50	0.40
1:B:411:ASP:OD1	1:B:411:ASP:C	2.64	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:PRO:O	3:C:701:HOH:O[1_466]	1.85	0.35
3:A:800:HOH:O	3:B:717:HOH:O[1_645]	1.95	0.25
3:A:785:HOH:O	3:B:808:HOH:O[1_645]	2.05	0.15
3:A:786:HOH:O	3:B:771:HOH:O[1_645]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	239/242 (99%)	236 (99%)	3 (1%)	0	100	100
1	B	225/242 (93%)	222 (99%)	3 (1%)	0	100	100
1	C	239/242 (99%)	236 (99%)	3 (1%)	0	100	100
1	D	213/242 (88%)	212 (100%)	1 (0%)	0	100	100
All	All	916/968 (95%)	906 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	202/217 (93%)	200 (99%)	2 (1%)	73	62
1	B	199/217 (92%)	198 (100%)	1 (0%)	86	81
1	C	207/217 (95%)	205 (99%)	2 (1%)	73	62
1	D	195/217 (90%)	195 (100%)	0	100	100
All	All	803/868 (92%)	798 (99%)	5 (1%)	84	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	THR
1	A	533	VAL
1	B	418	VAL
1	C	326	ILE
1	C	358	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
1	B	501	HIS
1	B	516	HIS
1	B	519	ASN
1	C	375	GLN
1	C	513	HIS
1	D	474	HIS
1	D	488	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	YCM	A	381	1	7,9,10	0.95	0	5,10,12	0.72	0
1	YCM	C	381	1	7,9,10	1.25	0	5,10,12	0.51	0
1	YCM	D	381	1	7,9,10	1.19	0	5,10,12	0.83	0
1	YCM	B	381	1	7,9,10	1.14	0	5,10,12	1.06	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	YCM	A	381	1	-	1/6/8/10	-
1	YCM	C	381	1	-	2/6/8/10	-
1	YCM	D	381	1	-	2/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	CE-CD-SG-CB
1	C	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-OZ1
1	B	381	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OBT	A	600	-	27,28,41	2.83	11 (40%)	33,43,63	2.68	8 (24%)
2	OBT	C	600	-	35,37,41	3.28	19 (54%)	46,56,63	3.25	16 (34%)
2	OBT	D	600	-	39,41,41	3.29	15 (38%)	53,63,63	3.21	19 (35%)
2	OBT	B	600	-	35,37,41	2.74	18 (51%)	46,56,63	3.12	14 (30%)

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	OBT	A	600	-	-	3/12/38/53	0/5/4/5
2	OBT	C	600	-	-	7/22/48/53	0/6/5/5
2	OBT	D	600	-	-	9/27/53/53	0/6/5/5
2	OBT	B	600	-	-	8/22/48/53	0/6/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	OBT	C21-N01	-11.03	1.29	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	OBT	C19-N01	-9.56	1.29	1.47
2	D	600	OBT	C05-C07	-7.82	1.33	1.48
2	D	600	OBT	C10-C08	-7.44	1.34	1.48
2	A	600	OBT	C05-C07	-7.37	1.34	1.48
2	B	600	OBT	C05-C07	-7.28	1.34	1.48
2	C	600	OBT	C05-C07	-7.25	1.35	1.48
2	C	600	OBT	C10-C08	-6.99	1.35	1.48
2	B	600	OBT	C10-C08	-6.79	1.35	1.48
2	A	600	OBT	C10-C08	-6.78	1.35	1.48
2	C	600	OBT	O05-S01	5.73	1.48	1.43
2	D	600	OBT	O05-S01	5.54	1.48	1.43
2	A	600	OBT	S01-N01	5.51	1.69	1.61
2	D	600	OBT	O04-S01	5.37	1.48	1.43
2	D	600	OBT	C17-S01	4.97	1.88	1.77
2	B	600	OBT	C19-N01	-4.35	1.39	1.47
2	C	600	OBT	C17-S01	4.10	1.86	1.77
2	A	600	OBT	C17-S01	4.07	1.86	1.77
2	B	600	OBT	O05-S01	3.92	1.46	1.43
2	C	600	OBT	C06-C05	-3.72	1.33	1.39
2	A	600	OBT	C06-C05	-3.57	1.34	1.39
2	B	600	OBT	C22-C21	-3.39	1.32	1.39
2	B	600	OBT	C17-S01	3.37	1.84	1.77
2	C	600	OBT	C26-C21	-3.26	1.33	1.39
2	C	600	OBT	C23-C22	-3.18	1.33	1.38
2	C	600	OBT	C16-C10	-3.17	1.34	1.39
2	B	600	OBT	C26-C25	-3.15	1.33	1.38
2	D	600	OBT	C06-C05	-3.14	1.34	1.39
2	C	600	OBT	C04-C03	-3.10	1.33	1.38
2	B	600	OBT	C06-C05	-3.06	1.34	1.39
2	C	600	OBT	C06-C01	-3.01	1.34	1.38
2	D	600	OBT	C26-C25	-2.91	1.34	1.38
2	B	600	OBT	C23-C22	-2.89	1.34	1.38
2	A	600	OBT	O05-S01	2.82	1.47	1.43
2	D	600	OBT	C04-C05	-2.81	1.35	1.39
2	D	600	OBT	C23-C22	-2.80	1.34	1.38
2	C	600	OBT	C26-C25	-2.78	1.34	1.38
2	D	600	OBT	S01-N01	2.74	1.73	1.67
2	C	600	OBT	C22-C21	-2.72	1.34	1.39
2	C	600	OBT	C13-C12	-2.69	1.34	1.38
2	B	600	OBT	C04-C05	-2.62	1.35	1.39
2	B	600	OBT	C13-C12	-2.60	1.34	1.38
2	B	600	OBT	C04-C03	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	OBT	C04-C03	-2.54	1.34	1.38
2	D	600	OBT	C06-C01	-2.54	1.34	1.38
2	A	600	OBT	O04-S01	2.54	1.47	1.43
2	B	600	OBT	C06-C01	-2.50	1.34	1.38
2	A	600	OBT	C06-C01	-2.49	1.34	1.38
2	C	600	OBT	C12-C10	-2.46	1.35	1.39
2	B	600	OBT	O03-C11	-2.38	1.40	1.43
2	D	600	OBT	C22-C21	-2.35	1.34	1.39
2	C	600	OBT	C11-C07	2.33	1.53	1.50
2	D	600	OBT	C01-C02	-2.28	1.34	1.39
2	B	600	OBT	C25-C24	-2.27	1.34	1.38
2	C	600	OBT	C15-C14	-2.14	1.35	1.39
2	B	600	OBT	O03-C09	-2.14	1.40	1.44
2	A	600	OBT	C15-C14	-2.13	1.35	1.39
2	B	600	OBT	C12-C10	-2.11	1.36	1.39
2	C	600	OBT	C03-C02	-2.10	1.35	1.39
2	B	600	OBT	C26-C21	-2.10	1.35	1.39
2	A	600	OBT	C03-C02	-2.09	1.35	1.39
2	C	600	OBT	C23-C24	-2.06	1.34	1.38
2	D	600	OBT	C04-C03	-2.03	1.35	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	OBT	O04-S01-C17	-12.88	92.10	107.79
2	C	600	OBT	O05-S01-C17	-11.89	93.31	107.79
2	D	600	OBT	O05-S01-C17	-11.17	94.19	107.79
2	B	600	OBT	O05-S01-N01	11.02	119.75	107.14
2	B	600	OBT	O04-S01-C17	-10.21	95.35	107.79
2	A	600	OBT	O05-S01-C17	-9.96	92.92	107.69
2	B	600	OBT	O05-S01-C17	-9.95	95.66	107.79
2	C	600	OBT	O05-S01-N01	9.45	117.95	107.14
2	C	600	OBT	O04-S01-C17	-9.37	96.38	107.79
2	A	600	OBT	O04-S01-C17	-8.51	95.06	107.69
2	D	600	OBT	O04-S01-N01	8.07	117.03	107.39
2	C	600	OBT	C19-N01-S01	-6.56	108.81	118.23
2	D	600	OBT	C22-C21-N01	4.52	126.73	120.15
2	B	600	OBT	O04-S01-N01	4.44	112.22	107.14
2	D	600	OBT	C19-N01-C21	-4.39	111.86	117.63
2	C	600	OBT	C22-C21-N01	4.25	126.24	120.05
2	D	600	OBT	C20-C19-N01	-4.02	108.23	112.14
2	D	600	OBT	O05-S01-N01	3.76	111.89	107.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	OBT	C19-N01-S01	-3.75	112.84	118.23
2	D	600	OBT	O03-C09-C18	-3.42	98.05	104.73
2	C	600	OBT	O04-S01-N01	3.16	110.76	107.14
2	D	600	OBT	C25-C26-C21	3.09	124.21	120.30
2	D	600	OBT	C12-C10-C08	3.04	124.84	120.91
2	A	600	OBT	O03-C09-C18	-2.97	98.92	104.73
2	D	600	OBT	C15-C16-C10	2.94	123.94	120.80
2	C	600	OBT	O03-C09-C18	-2.83	99.20	104.73
2	B	600	OBT	C26-C21-N01	2.81	124.14	120.05
2	B	600	OBT	O03-C09-C18	-2.79	99.29	104.73
2	C	600	OBT	C26-C21-N01	-2.66	116.17	120.05
2	C	600	OBT	C15-C14-C13	-2.65	115.54	119.77
2	D	600	OBT	C25-C24-C23	-2.57	118.06	121.24
2	C	600	OBT	C12-C10-C08	2.48	124.12	120.91
2	A	600	OBT	C10-C08-C07	2.46	135.17	128.81
2	A	600	OBT	C06-C01-C02	2.45	122.47	119.88
2	C	600	OBT	C09-C08-C07	-2.40	101.92	106.97
2	B	600	OBT	C10-C08-C07	2.40	135.01	128.81
2	A	600	OBT	C05-C07-C08	2.38	134.98	128.81
2	C	600	OBT	C05-C07-C08	2.36	134.92	128.81
2	D	600	OBT	F1-C20-C19	2.34	116.44	112.04
2	C	600	OBT	C12-C13-C14	2.30	122.31	119.88
2	A	600	OBT	C12-C10-C08	2.27	123.84	120.91
2	D	600	OBT	C12-C13-C14	2.26	122.27	119.88
2	D	600	OBT	C26-C21-C22	-2.26	114.87	119.18
2	B	600	OBT	C16-C10-C12	-2.24	115.72	118.57
2	D	600	OBT	C16-C10-C12	-2.23	115.73	118.57
2	D	600	OBT	O05-S01-O04	-2.23	117.49	119.17
2	C	600	OBT	C16-C10-C12	-2.21	115.75	118.57
2	A	600	OBT	C03-C04-C05	2.20	123.14	120.80
2	B	600	OBT	C03-C02-C01	-2.18	116.30	119.77
2	C	600	OBT	C10-C08-C07	2.18	134.44	128.81
2	B	600	OBT	C25-C26-C21	2.17	123.04	120.30
2	B	600	OBT	C23-C22-C21	2.16	123.03	120.30
2	B	600	OBT	C05-C07-C08	2.14	134.34	128.81
2	C	600	OBT	C09-C18-C17	2.10	102.47	100.61
2	B	600	OBT	C25-C24-C23	-2.08	118.67	121.24
2	D	600	OBT	F2-C20-C19	-2.05	108.17	112.04
2	D	600	OBT	C06-C05-C04	-2.03	115.99	118.57

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	OBT	C11-C17-S01-O04
2	B	600	OBT	C11-C17-S01-O05
2	B	600	OBT	C18-C17-S01-O04
2	B	600	OBT	C18-C17-S01-O05
2	B	600	OBT	C19-N01-S01-C17
2	B	600	OBT	C19-N01-S01-O04
2	B	600	OBT	C22-C21-N01-S01
2	B	600	OBT	C26-C21-N01-S01
2	C	600	OBT	C11-C17-S01-O04
2	C	600	OBT	C11-C17-S01-O05
2	C	600	OBT	C18-C17-S01-O05
2	D	600	OBT	C19-N01-S01-C17
2	D	600	OBT	C21-N01-S01-C17
2	D	600	OBT	C19-N01-S01-O04
2	D	600	OBT	C20-C19-N01-S01
2	D	600	OBT	N01-C19-C20-F1
2	D	600	OBT	N01-C19-C20-F2
2	D	600	OBT	N01-C19-C20-F3
2	C	600	OBT	C18-C17-S01-O04
2	C	600	OBT	C19-N01-S01-C17
2	A	600	OBT	C11-C17-S01-O05
2	A	600	OBT	C18-C17-S01-O05
2	C	600	OBT	C19-N01-S01-O04
2	C	600	OBT	C19-N01-S01-O05
2	A	600	OBT	C18-C17-S01-O04
2	D	600	OBT	C19-N01-S01-O05
2	D	600	OBT	C21-N01-S01-O04

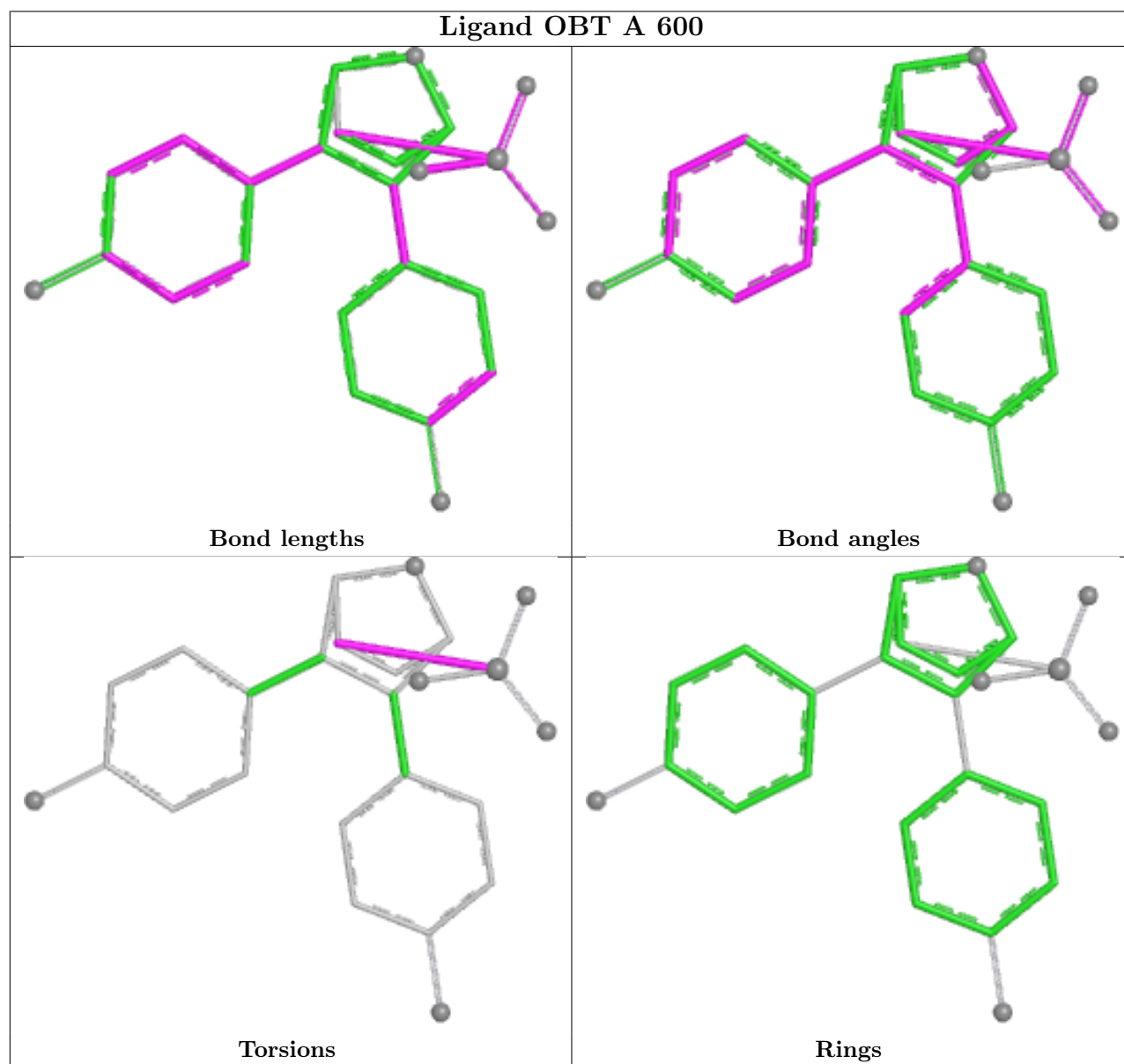
There are no ring outliers.

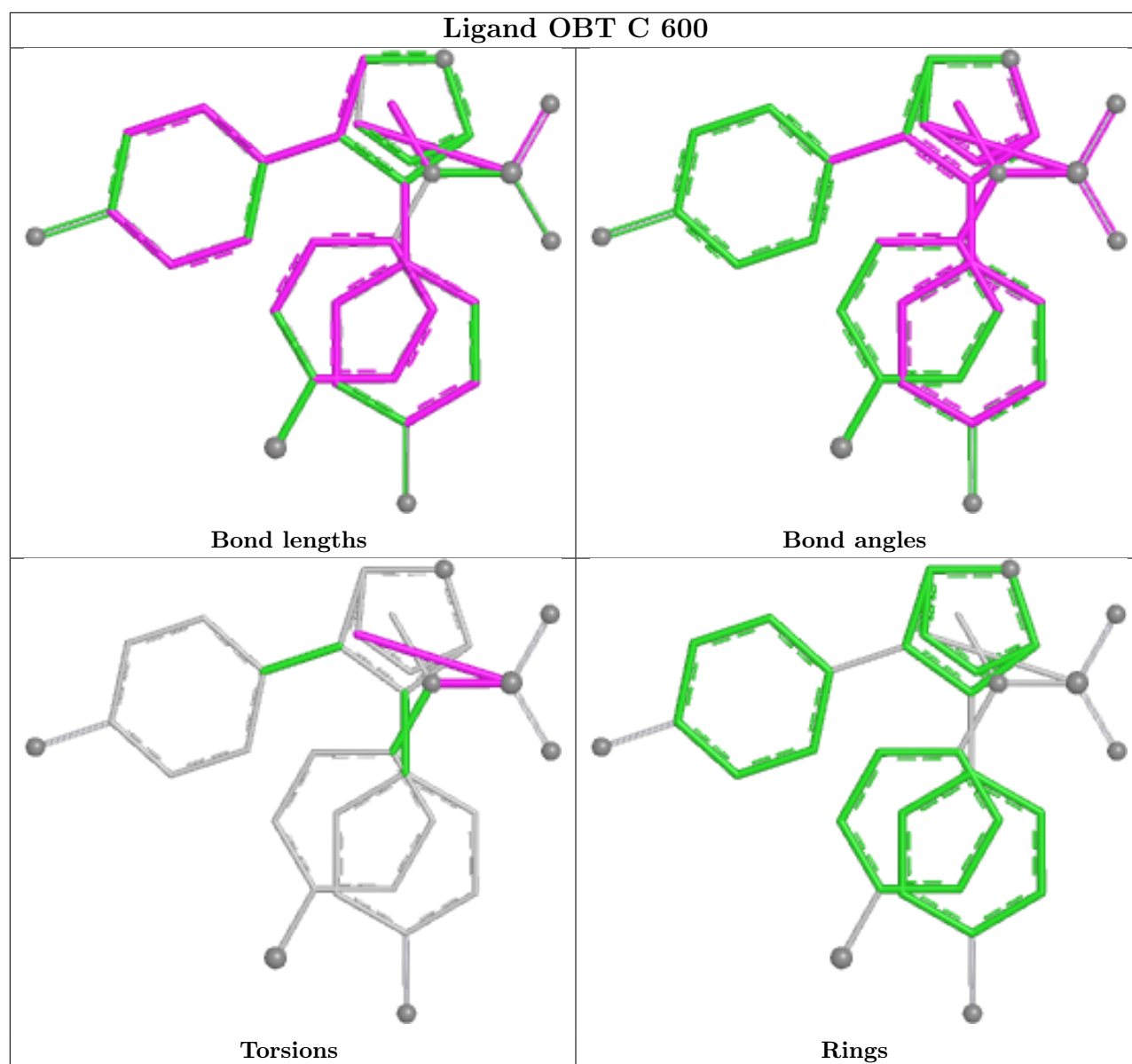
4 monomers are involved in 12 short contacts:

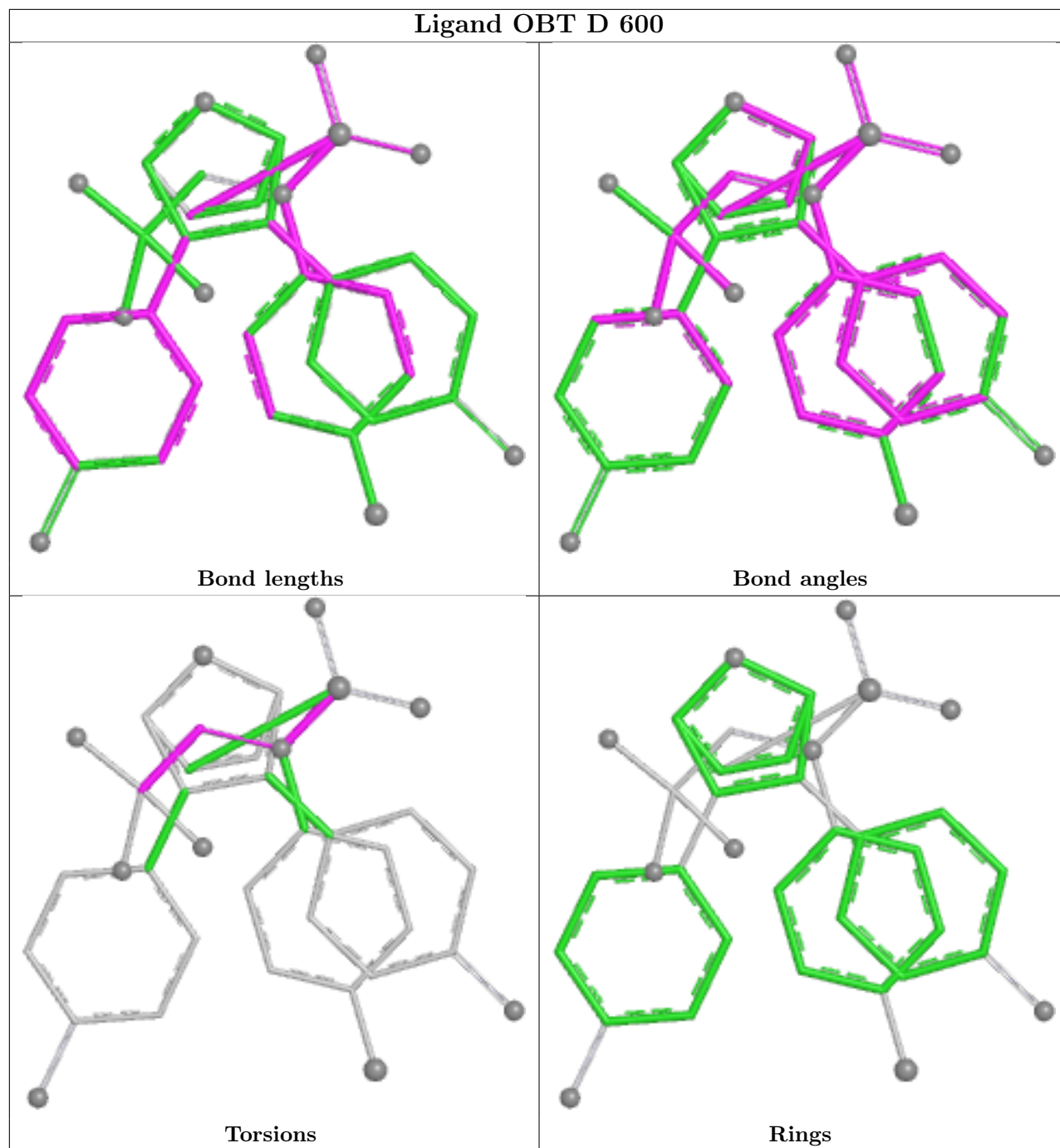
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	OBT	2	0
2	C	600	OBT	3	0
2	D	600	OBT	5	0
2	B	600	OBT	2	0

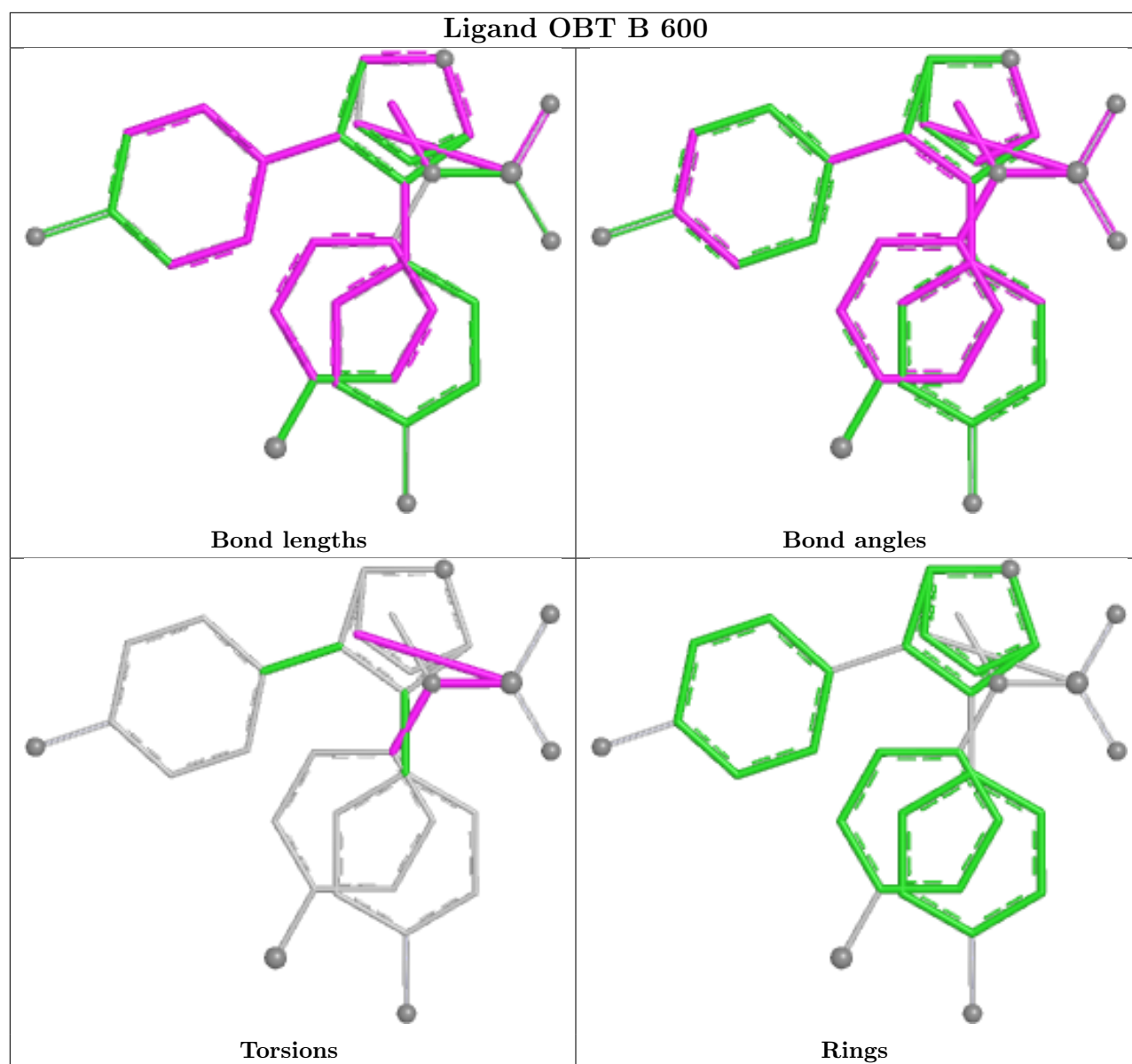
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	240/242 (99%)	0.40	18 (7%) 22 23	14, 36, 62, 106	1 (0%)
1	B	231/242 (95%)	0.27	19 (8%) 19 20	18, 33, 79, 114	0
1	C	240/242 (99%)	0.17	15 (6%) 27 29	14, 32, 62, 82	1 (0%)
1	D	223/242 (92%)	0.37	21 (9%) 15 16	16, 35, 75, 112	0
All	All	934/968 (96%)	0.30	73 (7%) 20 21	14, 34, 66, 114	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	LEU	7.6
1	B	526	TYR	6.0
1	D	331	TYR	5.0
1	B	417	CYS	4.7
1	D	334	THR	4.7
1	A	530	CYS	4.5
1	C	462	LEU	4.5
1	A	462	LEU	4.3
1	B	421	MET	4.2
1	A	526	TYR	3.9
1	B	334	THR	3.8
1	D	335	ARG	3.8
1	C	526	TYR	3.7
1	B	341	SER	3.7
1	D	415	GLY	3.6
1	D	546	ALA	3.4
1	C	527	SER	3.4
1	B	413	ASN	3.3
1	C	532	ASN	3.1
1	B	420	GLY	3.1
1	B	462	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	331	TYR	3.1
1	B	425	PHE	3.1
1	B	527	SER	3.1
1	A	527	SER	3.0
1	A	528	MET	2.9
1	C	331	TYR	2.9
1	A	417	CYS	2.9
1	D	425	PHE	2.9
1	D	421	MET	2.9
1	D	526	TYR	2.8
1	D	333	PRO	2.8
1	A	306	LEU	2.8
1	C	420	GLY	2.8
1	B	335	ARG	2.8
1	B	333	PRO	2.7
1	B	546	ALA	2.7
1	A	532	ASN	2.7
1	B	418	VAL	2.7
1	A	463	SER	2.6
1	A	466	LEU	2.6
1	D	527	SER	2.6
1	C	529	LYS	2.6
1	A	524	HIS	2.5
1	D	528	MET	2.5
1	A	469	LEU	2.5
1	D	533	VAL	2.5
1	D	413	ASN	2.5
1	C	421	MET	2.4
1	D	342	MET	2.4
1	D	468	SER	2.4
1	C	306	LEU	2.4
1	C	530	CYS	2.4
1	C	464	SER	2.3
1	C	466	LEU	2.3
1	D	524	HIS	2.3
1	A	331	TYR	2.3
1	B	524	HIS	2.2
1	D	469	LEU	2.2
1	C	417	CYS	2.2
1	A	425	PHE	2.2
1	B	533	VAL	2.2
1	A	332	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	354	LEU	2.2
1	D	306	LEU	2.2
1	A	415	GLY	2.2
1	D	354	LEU	2.1
1	C	528	MET	2.1
1	D	341	SER	2.1
1	B	332	ASP	2.1
1	A	525	LEU	2.1
1	A	531	LYS	2.0
1	C	546	ALA	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	YCM	C	381	10/11	0.91	0.13	19,26,54,54	0
1	YCM	D	381	10/11	0.94	0.12	24,36,60,60	0
1	YCM	A	381	10/11	0.95	0.10	14,25,45,45	0
1	YCM	B	381	10/11	0.95	0.07	18,29,43,43	0

6.3 Carbohydrates [i](#)

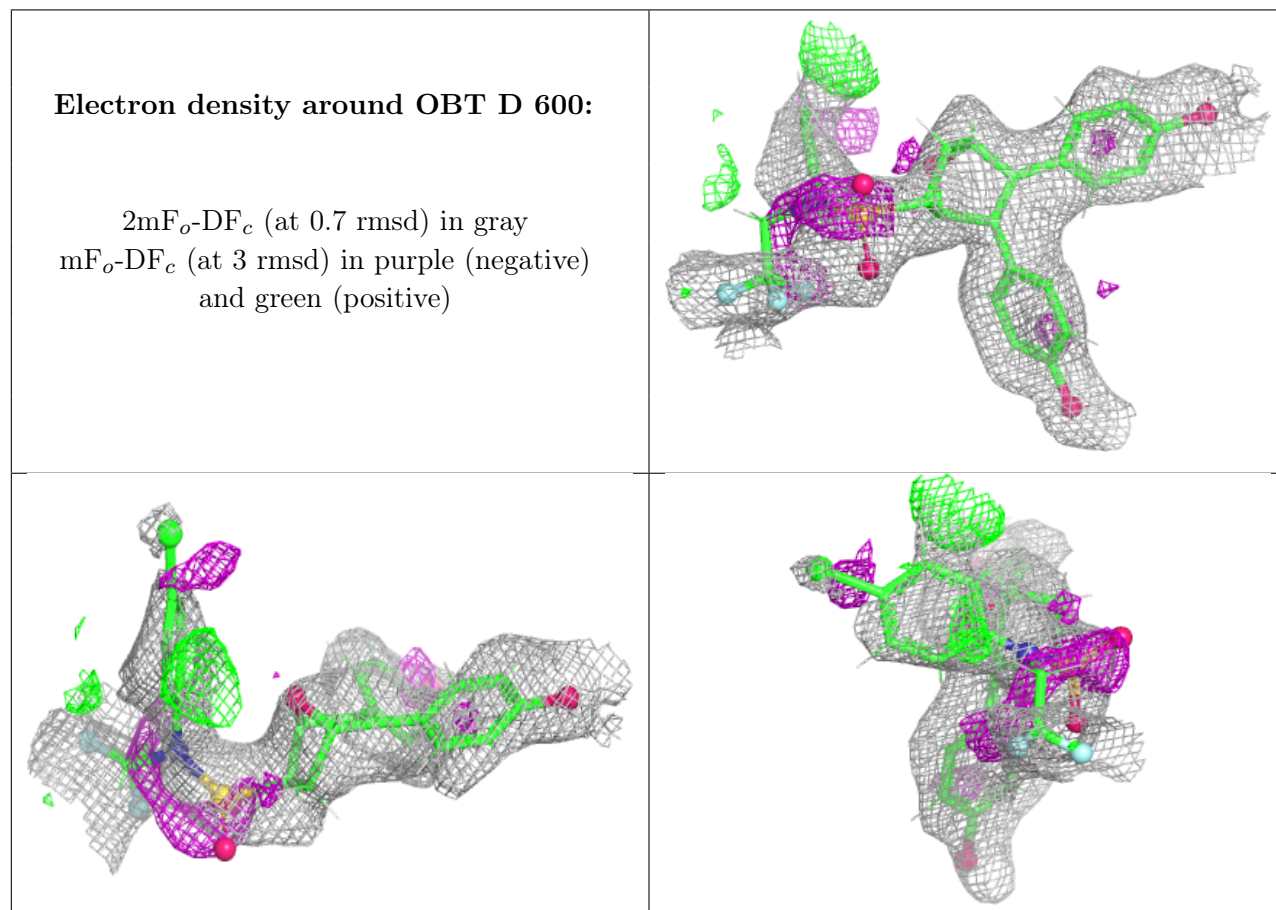
There are no oligosaccharides in this entry.

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.

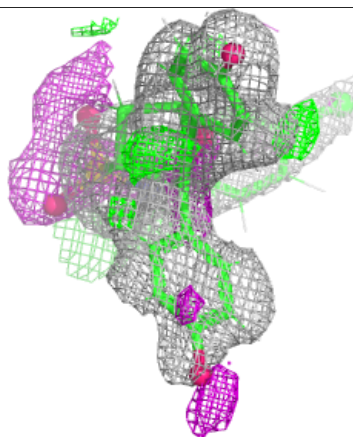
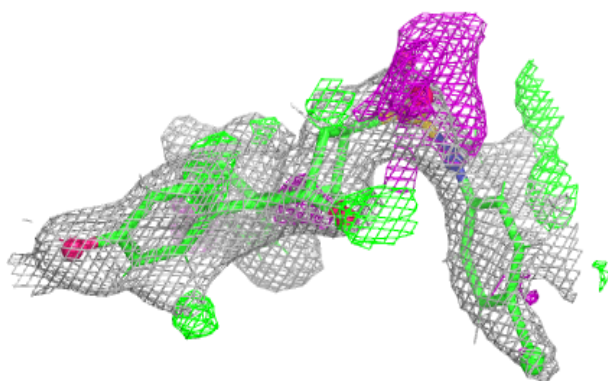
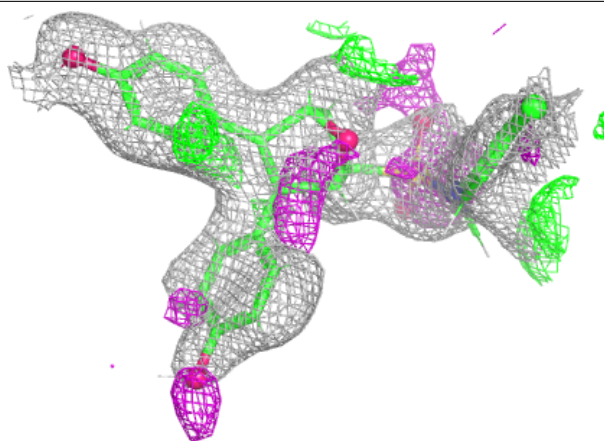
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OBT	D	600	37/37	0.78	0.16	31,55,87,95	0
2	OBT	C	600	33/37	0.80	0.15	27,47,73,78	0
2	OBT	B	600	33/37	0.81	0.17	30,59,117,141	0
2	OBT	A	600	25/37	0.83	0.13	27,40,56,66	0

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.



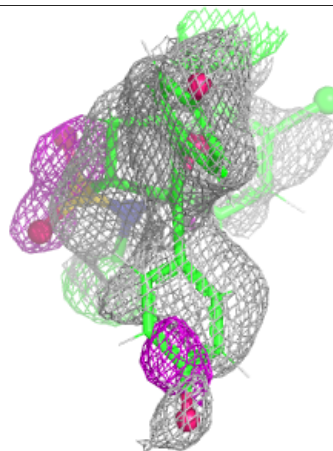
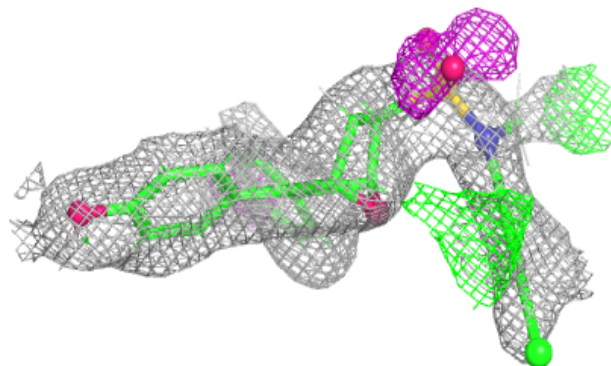
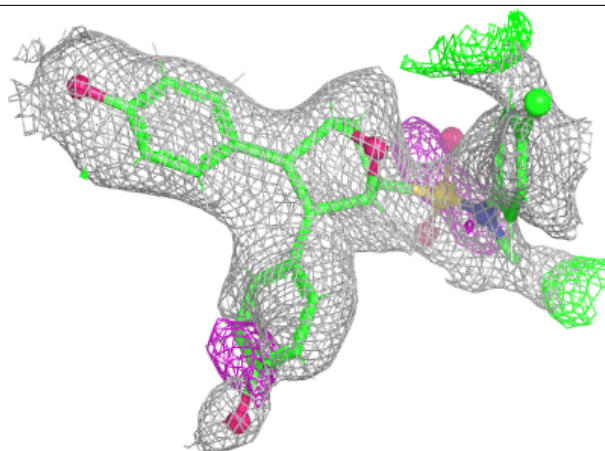
Electron density around OBT C 600:

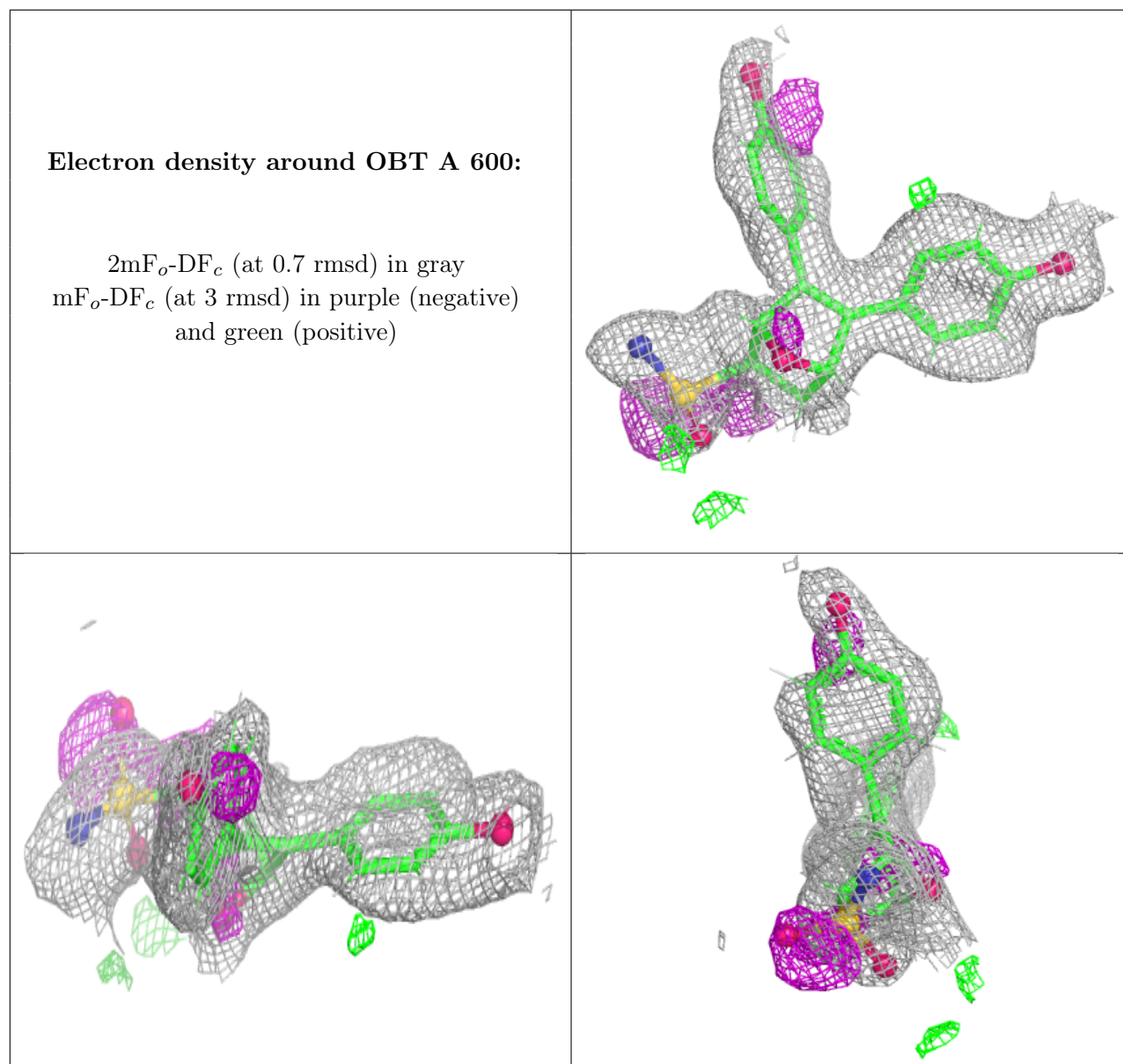
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OBT B 600:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.