



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:12 PM UTC

PDB ID : 1PQ6 / pdb_00001pq6
Title : HUMAN LXR BETA HORMONE RECEPTOR / GW3965 COMPLEX
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.; Gustafsson, J.-A.; Carlquist, M.
Deposited on : 2003-06-18
Resolution : 2.40 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)
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

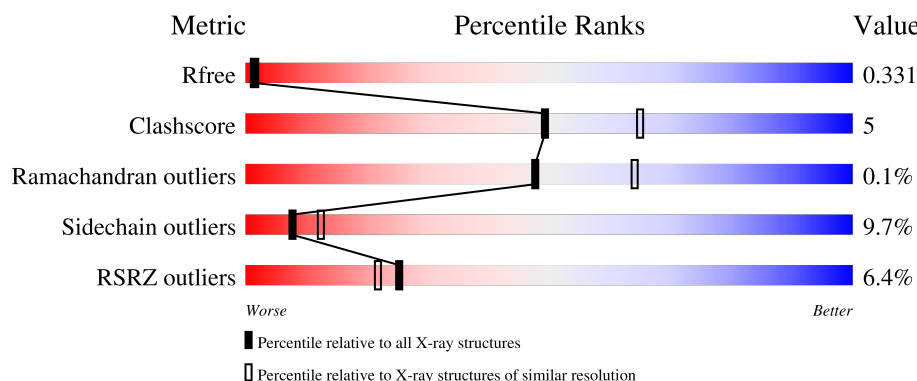
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	253	 3% 71% 19% • 8%
1	B	253	 5% 81% 13% • 5%
1	C	253	 5% 66% 15% • 18%
1	D	253	 10% 67% 18% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7673 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.

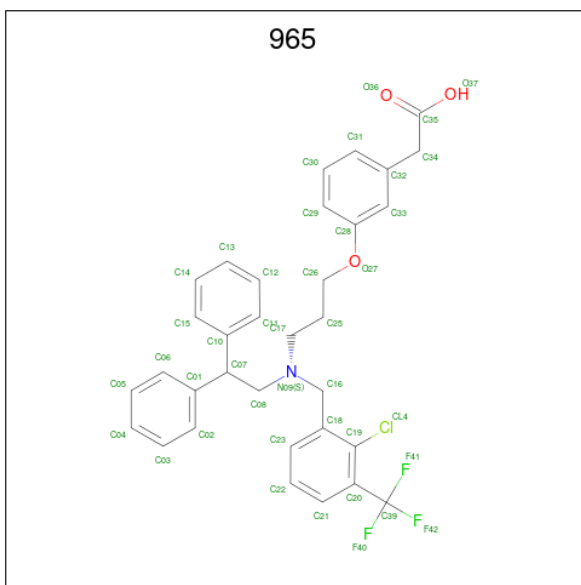
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1879	1203	330	339	7			
1	B	241	Total	C	N	O	S	0	0	0
			1950	1246	341	356	7			
1	C	208	Total	C	N	O	S	0	0	0
			1698	1082	300	309	7			
1	D	227	Total	C	N	O	S	0	0	0
			1848	1188	323	330	7			

There are 16 discrepancies between the modelled and reference sequences:

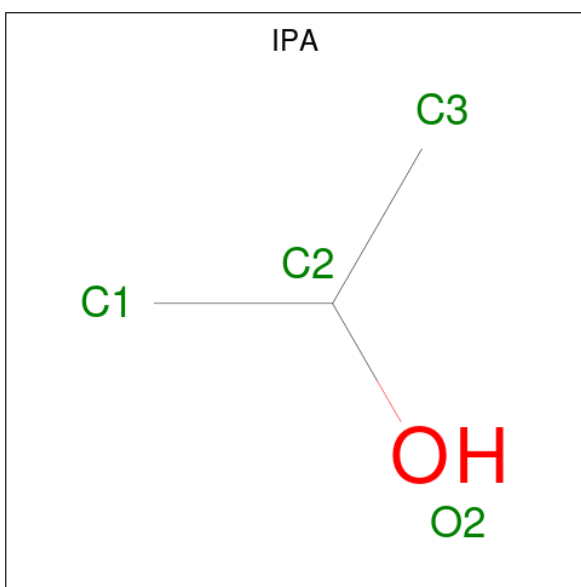
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	cloning artifact	UNP P55055
A	210	SER	-	cloning artifact	UNP P55055
A	211	HIS	-	cloning artifact	UNP P55055
A	212	MET	-	cloning artifact	UNP P55055
B	209	GLY	-	cloning artifact	UNP P55055
B	210	SER	-	cloning artifact	UNP P55055
B	211	HIS	-	cloning artifact	UNP P55055
B	212	MET	-	cloning artifact	UNP P55055
C	209	GLY	-	cloning artifact	UNP P55055
C	210	SER	-	cloning artifact	UNP P55055
C	211	HIS	-	cloning artifact	UNP P55055
C	212	MET	-	cloning artifact	UNP P55055
D	209	GLY	-	cloning artifact	UNP P55055
D	210	SER	-	cloning artifact	UNP P55055
D	211	HIS	-	cloning artifact	UNP P55055
D	212	MET	-	cloning artifact	UNP P55055

- Molecule 2 is [3-(3-{[2-chloro-3-(trifluoromethyl)benzyl](2,2-diphenylethyl)amino}propoxy)phenyl]acetic acid (CCD ID: 965) (formula: C₃₃H₃₁ClF₃NO₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0
2	B	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0
2	D	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: $\text{C}_3\text{H}_8\text{O}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		

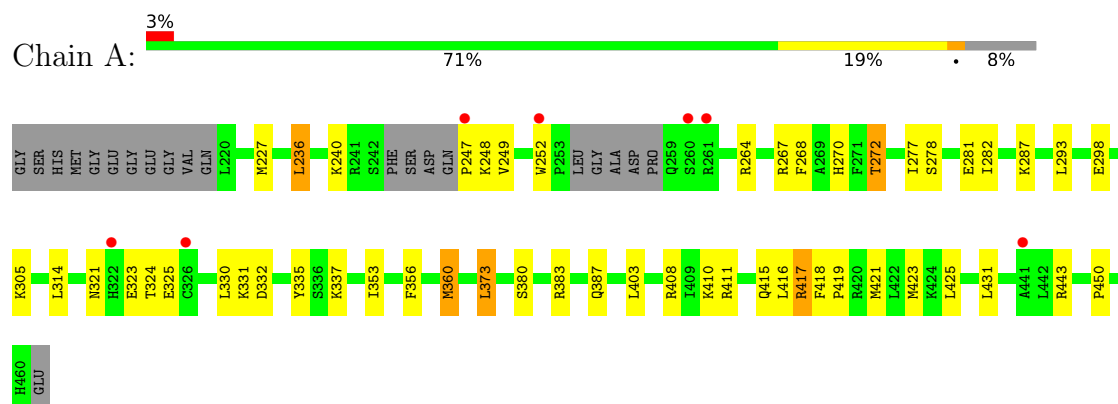
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	69	Total	O	0	0
			69	69		
4	C	19	Total	O	0	0
			19	19		
4	D	28	Total	O	0	0
			28	28		

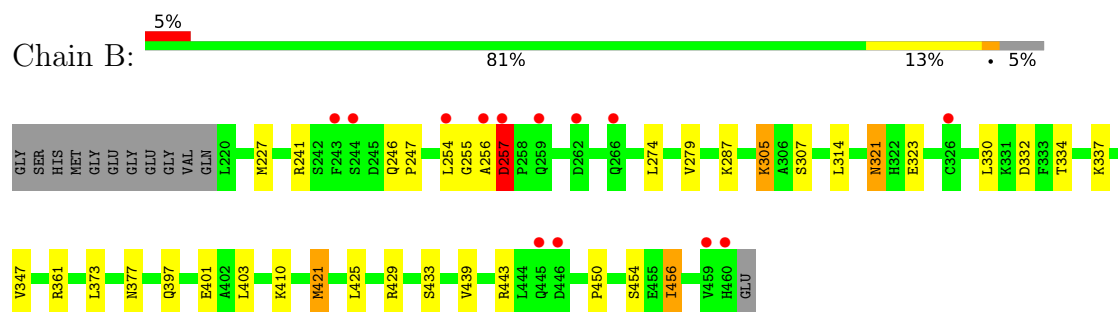
3 Residue-property plots [i](#)

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.

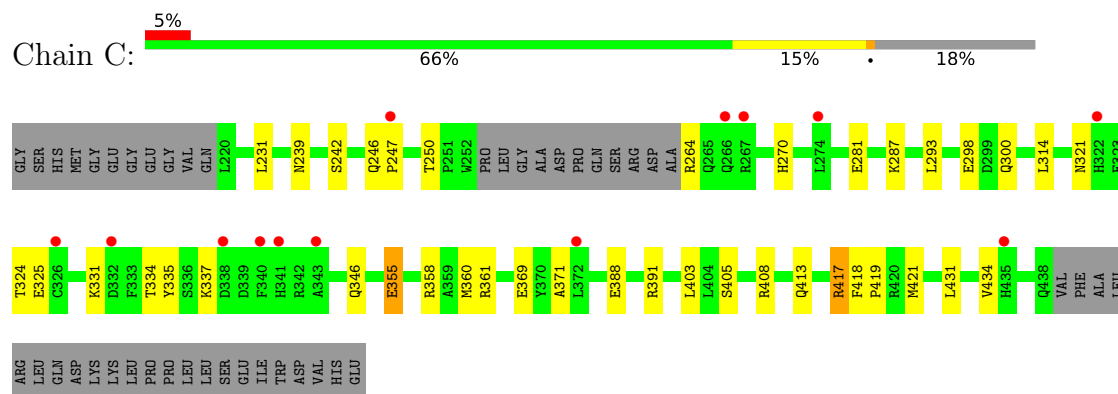
• Molecule 1: Oxysterols receptor LXR-beta



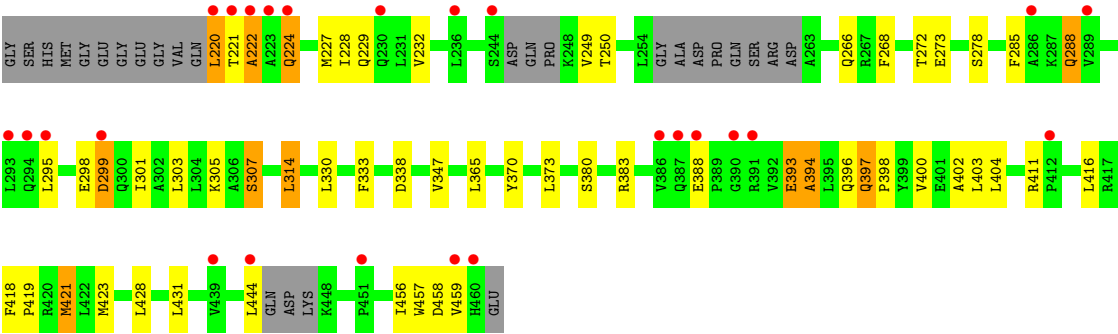
• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.72Å 98.93Å 175.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.40 87.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (87.71-2.40) 98.4 (87.71-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.207 , 0.262 0.289 , 0.331	Depositor DCC
R_{free} test set	2021 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: 965, IPA

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	0.94	2/1914 (0.1%)	0.97	0/2587
1	B	0.89	2/1989 (0.1%)	0.99	2/2693 (0.1%)
1	C	0.75	2/1729 (0.1%)	0.91	0/2334
1	D	1.18	9/1882 (0.5%)	0.96	1/2542 (0.0%)
All	All	0.95	15/7514 (0.2%)	0.96	3/10156 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	ASP	CG-OD2	26.56	1.75	1.25
1	A	360	MET	SD-CE	-13.34	1.46	1.79
1	D	222	ALA	C-O	13.10	1.39	1.24
1	D	299	ASP	CG-OD1	11.55	1.47	1.25
1	D	229	GLN	C-O	9.29	1.35	1.24
1	D	394	ALA	C-O	8.41	1.34	1.24
1	C	325	GLU	C-O	7.07	1.32	1.23
1	B	421	MET	SD-CE	-5.83	1.65	1.79
1	D	421	MET	SD-CE	-5.50	1.65	1.79
1	D	393	GLU	C-O	5.30	1.30	1.24
1	D	299	ASP	CB-CG	5.29	1.65	1.52
1	C	360	MET	SD-CE	-5.11	1.66	1.79
1	A	418	PHE	N-CA	-5.09	1.41	1.46
1	D	266	GLN	CD-OE1	5.08	1.33	1.23
1	B	257	ASP	CA-CB	5.04	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	299	ASP	CB-CG-OD1	-8.29	99.34	118.40
1	B	450	PRO	O-C-N	6.60	124.25	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	LEU	N-CA-C	-6.27	100.87	109.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1879	0	1902	24	0
1	B	1950	0	1968	22	0
1	C	1698	0	1716	12	0
1	D	1848	0	1883	25	0
2	A	41	0	30	1	0
2	B	41	0	30	1	0
2	D	41	0	30	1	0
3	A	4	0	8	2	0
3	B	4	0	8	0	0
4	A	51	0	0	0	0
4	B	69	0	0	1	0
4	C	19	0	0	0	0
4	D	28	0	0	0	0
All	All	7673	0	7575	82	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 5.

All (82) 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:D:299:ASP:OD2	1:D:299:ASP:CG	1.75	1.30
1:C:242:SER:OG	1:C:281:GLU:OE2	1.97	0.82
1:A:415:GLN:NE2	1:B:401:GLU:OE1	2.20	0.73
1:A:356:PHE:CZ	1:A:360:MET:CE	2.72	0.73
1:B:403:LEU:HD11	1:B:421:MET:HE1	1.74	0.70
1:D:303:LEU:O	1:D:307:SER:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:HD22	1:B:321:ASN:C	2.04	0.66
1:A:419:PRO:O	1:A:423:MET:HG2	1.94	0.65
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.25	0.65
1:D:403:LEU:HD11	1:D:421:MET:HE1	1.79	0.65
1:A:423:MET:HA	1:A:423:MET:HE2	1.80	0.63
1:A:356:PHE:CZ	1:A:360:MET:HE2	2.34	0.61
1:D:228:ILE:O	1:D:232:VAL:HG23	2.02	0.58
1:D:419:PRO:O	1:D:423:MET:HG2	2.03	0.58
1:B:279:VAL:HG11	1:B:456:ILE:HD11	1.85	0.58
1:A:278:SER:HB2	2:A:1500:965:C32	2.35	0.57
1:A:321:ASN:HD22	1:A:324:THR:H	1.53	0.56
1:C:369:GLU:OE1	1:C:417:ARG:NH2	2.38	0.56
1:A:272:THR:HG23	1:A:450:PRO:HG3	1.87	0.55
1:B:307:SER:HB2	1:B:377:ASN:ND2	2.22	0.54
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.89	0.54
1:D:224:GLN:HG2	1:D:402:ALA:HB2	1.88	0.54
1:A:423:MET:HE1	1:B:425:LEU:HD12	1.89	0.54
1:B:255:GLY:C	1:B:257:ASP:N	2.66	0.53
1:B:321:ASN:ND2	1:B:323:GLU:H	2.06	0.53
1:C:250:THR:O	1:C:270:HIS:ND1	2.42	0.53
1:D:268:PHE:O	1:D:272:THR:HG23	2.10	0.52
1:A:380:SER:O	1:A:383:ARG:HG2	2.10	0.52
1:B:321:ASN:HD22	1:B:323:GLU:H	1.57	0.51
1:B:274:LEU:HD22	1:B:330:LEU:HD11	1.93	0.51
1:C:388:GLU:OE1	1:C:391:ARG:HD2	2.11	0.51
1:D:314:LEU:HD13	1:D:428:LEU:HD11	1.93	0.50
1:A:403:LEU:HD11	1:A:421:MET:HE1	1.93	0.50
1:B:255:GLY:C	1:B:257:ASP:H	2.19	0.50
1:C:403:LEU:HD11	1:C:421:MET:HE1	1.93	0.50
1:B:257:ASP:CG	1:B:257:ASP:O	2.56	0.49
1:D:299:ASP:OD2	1:D:388:GLU:OE1	2.31	0.49
1:C:231:LEU:HB3	1:C:371:ALA:HB1	1.96	0.48
1:D:394:ALA:O	1:D:398:PRO:CD	2.61	0.48
1:A:281:GLU:HB3	3:A:1501:IPA:H31	1.96	0.48
1:A:287:LYS:HD2	1:A:293:LEU:HD21	1.96	0.47
1:D:220:LEU:HD22	1:D:224:GLN:HB2	1.96	0.46
1:D:394:ALA:O	1:D:398:PRO:HD3	2.15	0.46
1:A:277:ILE:HG21	1:A:330:LEU:HD21	1.99	0.45
1:D:285:PHE:O	1:D:288:GLN:HG2	2.17	0.44
1:B:373:LEU:HD22	1:B:425:LEU:HD21	1.98	0.44
1:C:246:GLN:N	1:C:247:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:HE22	1:B:332:ASP:HB2	1.83	0.44
1:B:321:ASN:C	1:B:321:ASN:ND2	2.75	0.44
1:A:287:LYS:CD	1:A:293:LEU:HD21	2.47	0.44
2:B:2500:965:H251	2:B:2500:965:H161	1.87	0.44
1:D:397:GLN:HB3	1:D:398:PRO:HD3	1.99	0.44
1:D:404:LEU:HD13	1:D:418:PHE:CD2	2.53	0.43
1:C:270:HIS:NE2	1:C:335:TYR:OH	2.51	0.43
1:B:307:SER:HB2	1:B:377:ASN:HD22	1.84	0.43
1:A:282:ILE:HA	3:A:1501:IPA:H33	2.00	0.43
1:A:411:ARG:HD3	1:A:417:ARG:HG3	2.00	0.43
1:D:330:LEU:HD12	1:D:333:PHE:CE1	2.54	0.43
1:B:403:LEU:HD21	1:B:421:MET:HE2	2.00	0.43
1:D:416:LEU:C	1:D:419:PRO:HD2	2.43	0.43
1:D:250:THR:OG1	1:D:273:GLU:OE2	2.28	0.42
1:D:365:LEU:HB2	1:D:370:TYR:CE1	2.54	0.42
1:D:298:GLU:HA	1:D:301:ILE:HD12	2.02	0.42
1:A:236:LEU:HD12	1:A:236:LEU:O	2.20	0.42
1:B:257:ASP:O	1:B:257:ASP:OD2	2.38	0.42
1:D:418:PHE:HB3	1:D:419:PRO:HD3	2.01	0.42
1:B:305:LYS:NZ	4:B:57:HOH:O	2.52	0.41
1:D:456:ILE:HG22	1:D:457:TRP:CD1	2.55	0.41
2:D:3500:965:F42	2:D:3500:965:CL4	2.65	0.41
1:C:293:LEU:HA	1:C:300:GLN:NE2	2.36	0.41
1:C:355:GLU:HG3	1:C:358:ARG:NH1	2.36	0.41
1:A:416:LEU:CD1	1:B:397:GLN:HG3	2.51	0.41
1:D:396:GLN:O	1:D:400:VAL:HG23	2.21	0.41
1:A:268:PHE:O	1:A:272:THR:HB	2.21	0.41
1:C:321:ASN:ND2	1:C:324:THR:HG23	2.36	0.41
1:A:247:PRO:HD2	1:A:277:ILE:HD12	2.03	0.40
1:D:222:ALA:C	1:D:224:GLN:H	2.29	0.40
1:A:373:LEU:HD22	1:A:425:LEU:HD21	2.03	0.40
1:D:380:SER:O	1:D:383:ARG:HG2	2.21	0.40
1:A:252:TRP:CH2	1:A:267:ARG:HD3	2.56	0.40
1:B:246:GLN:N	1:B:247:PRO:CD	2.83	0.40
1:B:429:ARG:HD3	1:B:429:ARG:HA	1.92	0.40

There are no symmetry-related clashes.

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	226/253 (89%)	221 (98%)	5 (2%)	0	100	100
1	B	239/253 (94%)	232 (97%)	6 (2%)	1 (0%)	30	43
1	C	204/253 (81%)	199 (98%)	5 (2%)	0	100	100
1	D	219/253 (87%)	209 (95%)	10 (5%)	0	100	100
All	All	888/1012 (88%)	861 (97%)	26 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ALA

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	203/222 (91%)	180 (89%)	23 (11%)	5	8
1	B	212/222 (96%)	195 (92%)	17 (8%)	11	19
1	C	185/222 (83%)	168 (91%)	17 (9%)	8	14
1	D	201/222 (90%)	180 (90%)	21 (10%)	7	10
All	All	801/888 (90%)	723 (90%)	78 (10%)	8	12

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	MET
1	A	236	LEU
1	A	240	LYS
1	A	248	LYS
1	A	249	VAL
1	A	264	ARG
1	A	272	THR
1	A	298	GLU
1	A	305	LYS
1	A	314	LEU
1	A	323	GLU
1	A	325	GLU
1	A	331	LYS
1	A	332	ASP
1	A	337	LYS
1	A	353	ILE
1	A	373	LEU
1	A	387	GLN
1	A	408	ARG
1	A	410	LYS
1	A	417	ARG
1	A	431	LEU
1	A	443	ARG
1	B	227	MET
1	B	241	ARG
1	B	257	ASP
1	B	287	LYS
1	B	305	LYS
1	B	314	LEU
1	B	321	ASN
1	B	334	THR
1	B	337	LYS
1	B	347	VAL
1	B	361	ARG
1	B	410	LYS
1	B	433	SER
1	B	439	VAL
1	B	443	ARG
1	B	454	SER
1	B	456	ILE
1	C	239	ASN
1	C	264	ARG
1	C	287	LYS

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Mol	Chain	Res	Type
1	C	298	GLU
1	C	314	LEU
1	C	331	LYS
1	C	334	THR
1	C	337	LYS
1	C	346	GLN
1	C	355	GLU
1	C	361	ARG
1	C	405	SER
1	C	408	ARG
1	C	413	GLN
1	C	417	ARG
1	C	431	LEU
1	C	434	VAL
1	D	220	LEU
1	D	221	THR
1	D	224	GLN
1	D	227	MET
1	D	249	VAL
1	D	278	SER
1	D	288	GLN
1	D	295	LEU
1	D	305	LYS
1	D	307	SER
1	D	314	LEU
1	D	338	ASP
1	D	347	VAL
1	D	373	LEU
1	D	393	GLU
1	D	397	GLN
1	D	411	ARG
1	D	431	LEU
1	D	444	LEU
1	D	458	ASP
1	D	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	300	GLN
1	A	321	ASN

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Mol	Chain	Res	Type
1	A	377	ASN
1	A	396	GLN
1	A	397	GLN
1	A	415	GLN
1	B	266	GLN
1	B	321	ASN
1	B	346	GLN
1	B	396	GLN
1	B	445	GLN
1	C	265	GLN
1	C	266	GLN
1	C	294	GLN
1	C	300	GLN
1	C	341	HIS
1	C	377	ASN
1	C	397	GLN
1	C	435	HIS
1	C	438	GLN
1	D	294	GLN
1	D	300	GLN
1	D	341	HIS
1	D	377	ASN
1	D	396	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](#)

5 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	IPA	A	1501	-	3,3,3	0.42	0	3,3,3	0.41	0
3	IPA	B	2501	-	3,3,3	0.34	0	3,3,3	0.41	0
2	965	B	2500	-	43,44,44	1.53	2 (4%)	57,60,60	1.51	11 (19%)
2	965	A	1500	-	43,44,44	1.41	3 (6%)	57,60,60	1.48	10 (17%)
2	965	D	3500	-	43,44,44	1.38	4 (9%)	57,60,60	1.60	7 (12%)

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	965	A	1500	-	-	8/33/33/33	0/4/4/4
2	965	B	2500	-	-	7/33/33/33	0/4/4/4
2	965	D	3500	-	-	11/33/33/33	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2500	965	C19-C18	8.40	1.48	1.39
2	A	1500	965	C19-C18	7.47	1.47	1.39
2	D	3500	965	C19-C18	7.23	1.46	1.39
2	B	2500	965	C19-CL4	3.91	1.81	1.72
2	A	1500	965	C19-CL4	2.85	1.78	1.72
2	D	3500	965	C19-CL4	2.68	1.78	1.72
2	D	3500	965	O37-C35	-2.14	1.23	1.30
2	A	1500	965	O37-C35	-2.10	1.23	1.30
2	D	3500	965	C10-C07	-2.08	1.47	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3500	965	C17-N09-C08	5.64	125.06	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3500	965	C39-C20-C19	-4.48	118.57	121.80
2	B	2500	965	C18-C16-N09	4.33	120.43	112.75
2	A	1500	965	C39-C20-C19	-4.12	118.83	121.80
2	D	3500	965	F41-C39-C20	-3.86	105.81	112.65
2	A	1500	965	C17-N09-C08	3.60	120.30	111.89
2	B	2500	965	C16-N09-C08	3.55	119.88	110.78
2	B	2500	965	C39-C20-C19	-3.44	119.32	121.80
2	D	3500	965	C16-N09-C08	3.38	119.46	110.78
2	A	1500	965	C16-N09-C17	3.34	118.23	111.28
2	A	1500	965	C16-N09-C08	3.31	119.27	110.78
2	B	2500	965	O36-C35-C34	-3.09	113.63	122.94
2	A	1500	965	F41-C39-C20	-3.07	107.20	112.65
2	B	2500	965	F41-C39-C20	-2.97	107.38	112.65
2	B	2500	965	C17-N09-C08	2.78	118.38	111.89
2	A	1500	965	O36-C35-C34	-2.77	114.58	122.94
2	A	1500	965	C21-C20-C39	2.76	123.98	118.06
2	B	2500	965	C16-N09-C17	2.72	116.94	111.28
2	D	3500	965	C25-C17-N09	-2.72	106.30	113.93
2	D	3500	965	C21-C20-C39	2.67	123.79	118.06
2	A	1500	965	C23-C18-C19	2.65	119.41	117.33
2	A	1500	965	O37-C35-C34	2.46	123.36	113.98
2	B	2500	965	O37-C35-C34	2.39	123.11	113.98
2	B	2500	965	C21-C20-C19	2.38	119.14	116.54
2	B	2500	965	C32-C34-C35	-2.30	107.17	113.71
2	D	3500	965	C16-C18-C19	-2.30	117.91	121.67
2	B	2500	965	F42-C39-C20	-2.25	108.66	112.65
2	A	1500	965	C16-C18-C19	-2.20	118.07	121.67

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3500	965	C07-C08-N09-C17
2	D	3500	965	C19-C20-C39-F40
2	D	3500	965	C19-C20-C39-F42
2	A	1500	965	C33-C28-O27-C26
2	A	1500	965	C29-C28-O27-C26
2	D	3500	965	C33-C28-O27-C26
2	D	3500	965	C29-C28-O27-C26
2	D	3500	965	C25-C17-N09-C08
2	A	1500	965	N09-C17-C25-C26
2	A	1500	965	C07-C08-N09-C17

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Mol	Chain	Res	Type	Atoms
2	D	3500	965	C19-C20-C39-F41
2	D	3500	965	C25-C26-O27-C28
2	D	3500	965	C18-C16-N09-C17
2	B	2500	965	C19-C20-C39-F40
2	B	2500	965	C19-C20-C39-F42
2	B	2500	965	C17-C25-C26-O27
2	A	1500	965	C18-C16-N09-C17
2	A	1500	965	C25-C17-N09-C16
2	B	2500	965	C25-C17-N09-C16
2	B	2500	965	C32-C34-C35-O37
2	B	2500	965	C19-C20-C39-F41
2	D	3500	965	C32-C34-C35-O37
2	B	2500	965	C32-C34-C35-O36
2	D	3500	965	C32-C34-C35-O36
2	A	1500	965	C32-C34-C35-O37
2	A	1500	965	C32-C34-C35-O36

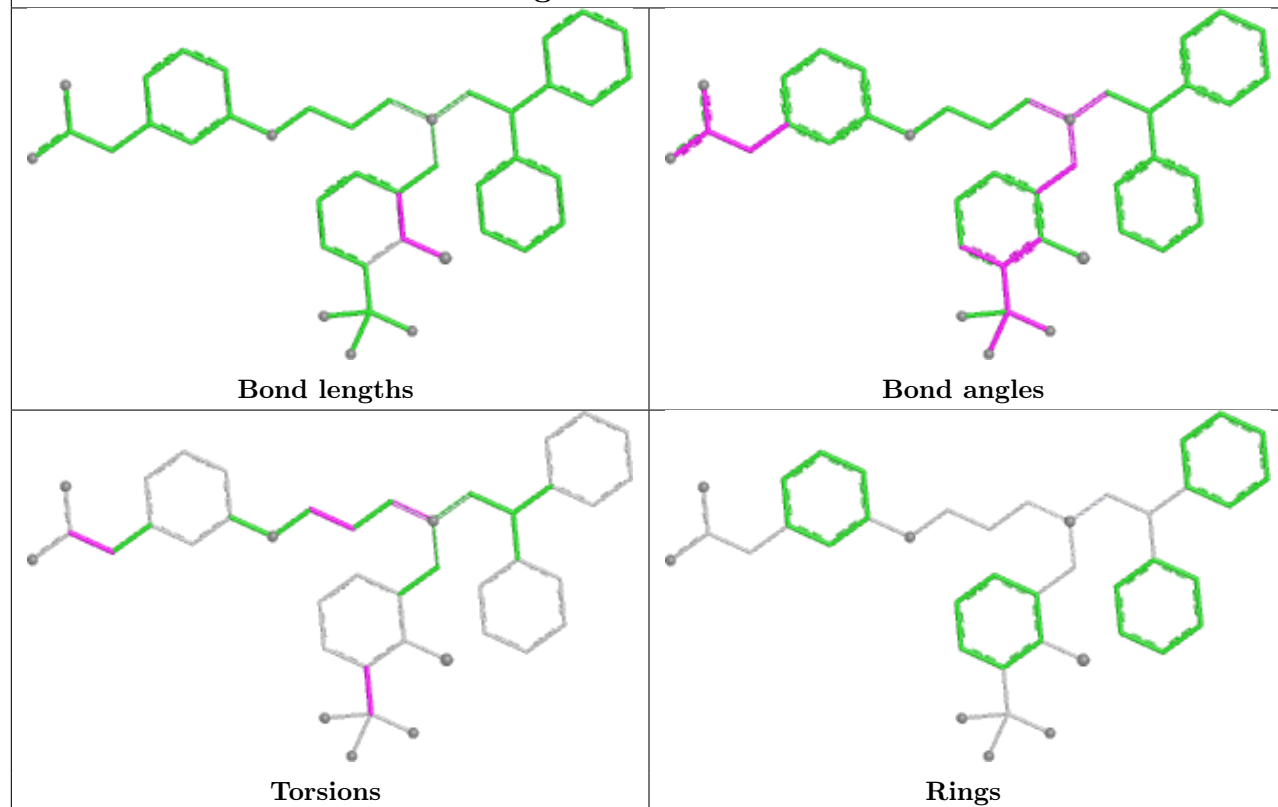
There are no ring outliers.

4 monomers are involved in 5 short contacts:

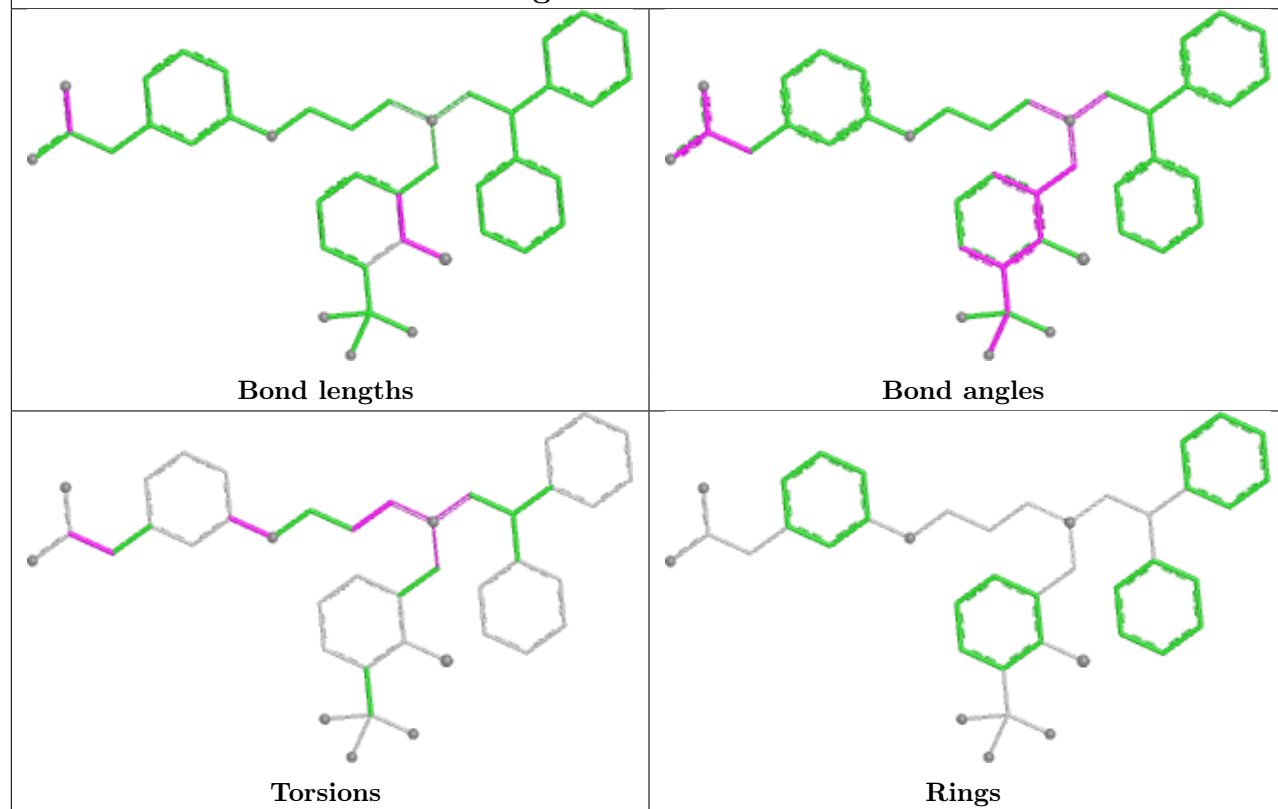
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	IPA	2	0
2	B	2500	965	1	0
2	A	1500	965	1	0
2	D	3500	965	1	0

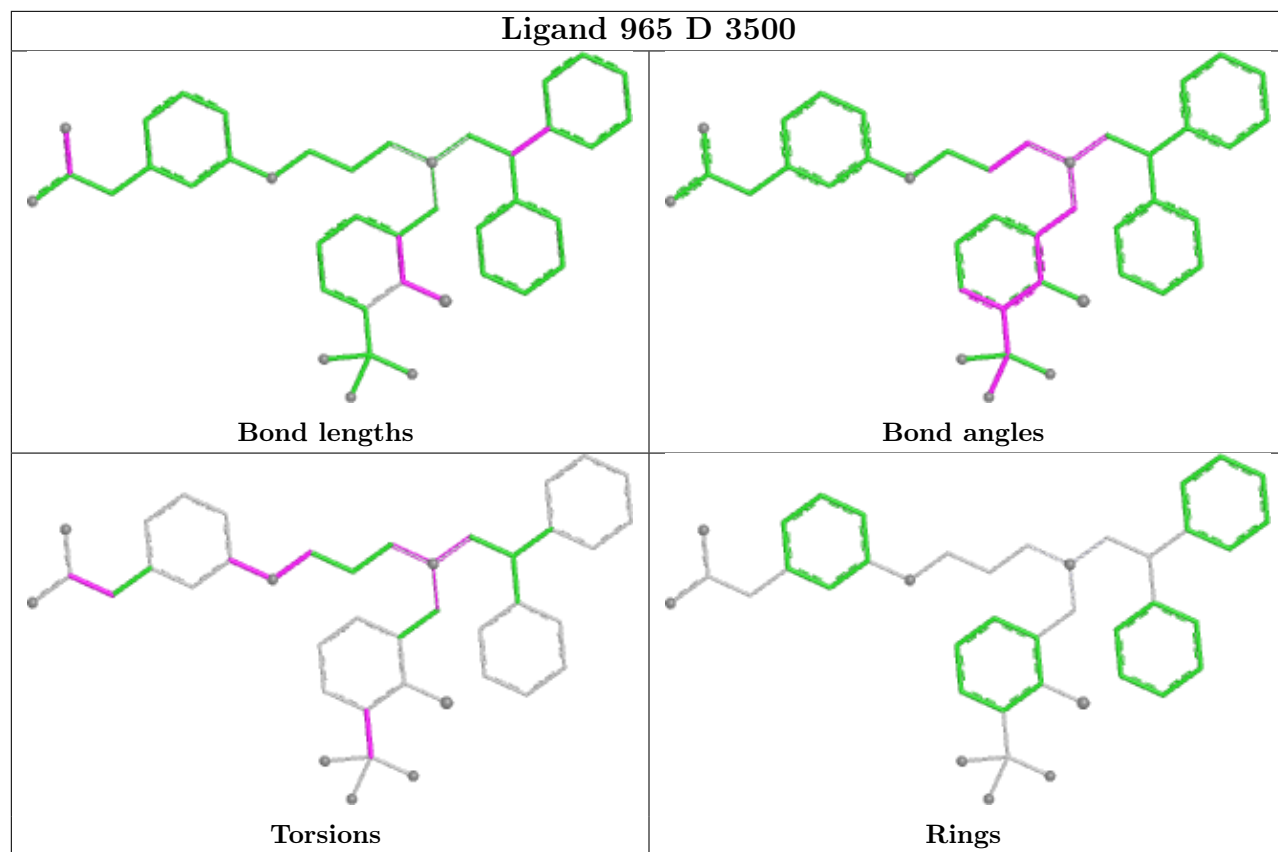
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 965 B 2500



Ligand 965 A 1500





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	232/253 (91%)	0.50	7 (3%) 52 48	11, 22, 34, 47	0
1	B	241/253 (95%)	0.63	13 (5%) 31 28	14, 23, 36, 49	0
1	C	208/253 (82%)	0.62	13 (6%) 26 22	12, 21, 38, 42	0
1	D	227/253 (89%)	0.76	25 (11%) 10 8	10, 24, 39, 50	0
All	All	908/1012 (89%)	0.63	58 (6%) 25 22	10, 23, 37, 50	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	ALA	5.1
1	C	267	ARG	3.9
1	D	230	GLN	3.8
1	D	295	LEU	3.5
1	B	257	ASP	3.5
1	A	261	ARG	3.4
1	D	412	PRO	3.4
1	B	459	VAL	3.3
1	A	322	HIS	3.1
1	B	256	ALA	3.1
1	B	262	ASP	3.0
1	B	460	HIS	2.9
1	D	460	HIS	2.8
1	D	386	VAL	2.7
1	D	459	VAL	2.7
1	B	446	ASP	2.7
1	D	299	ASP	2.7
1	D	289	VAL	2.7
1	D	451	PRO	2.6
1	C	343	ALA	2.6
1	D	236	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	254	LEU	2.5
1	D	220	LEU	2.5
1	B	259	GLN	2.5
1	D	439	VAL	2.5
1	B	326	CYS	2.5
1	B	445	GLN	2.5
1	A	252	TRP	2.5
1	D	293	LEU	2.5
1	A	326	CYS	2.5
1	D	294	GLN	2.4
1	D	388	GLU	2.4
1	C	266	GLN	2.4
1	D	224	GLN	2.4
1	C	338	ASP	2.3
1	A	260	SER	2.3
1	B	266	GLN	2.2
1	C	341	HIS	2.2
1	D	286	ALA	2.2
1	C	322	HIS	2.2
1	C	340	PHE	2.2
1	D	222	ALA	2.1
1	D	391	ARG	2.1
1	C	372	LEU	2.1
1	D	390	GLY	2.1
1	D	444	LEU	2.1
1	C	332	ASP	2.1
1	A	441	ALA	2.1
1	C	326	CYS	2.1
1	D	244	SER	2.1
1	B	243	PHE	2.1
1	B	244	SER	2.1
1	C	435	HIS	2.1
1	A	247	PRO	2.0
1	C	247	PRO	2.0
1	D	387	GLN	2.0
1	C	274	LEU	2.0
1	D	221	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

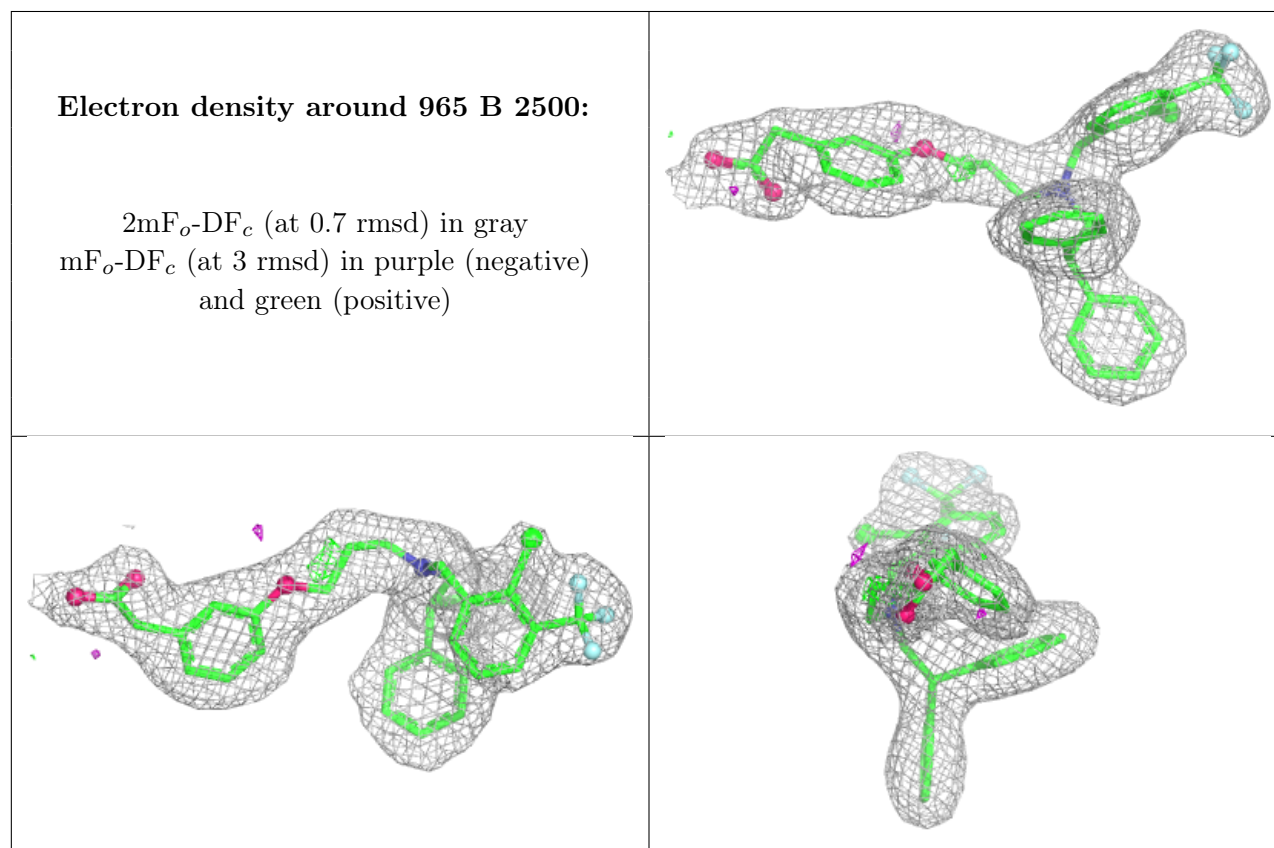
There are no oligosaccharides in this entry.

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.

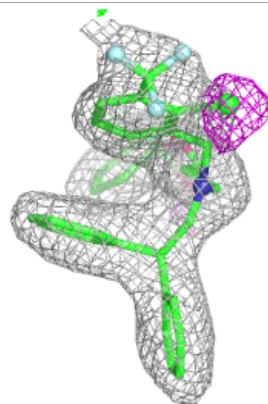
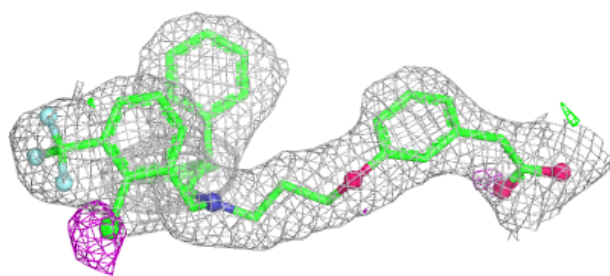
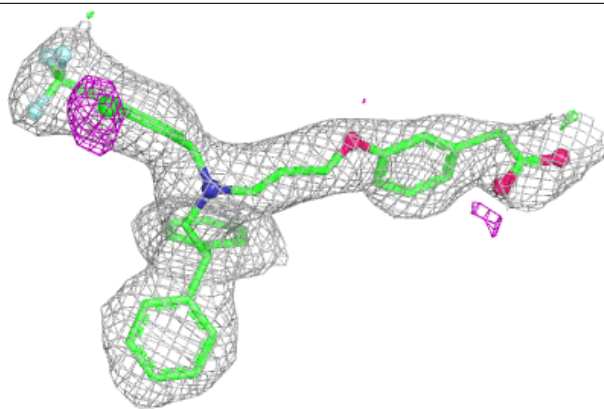
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	965	B	2500	41/41	0.84	0.13	13,21,43,52	0
2	965	D	3500	41/41	0.84	0.11	9,17,39,47	0
2	965	A	1500	41/41	0.85	0.11	16,23,41,48	0
3	IPA	A	1501	4/4	0.89	0.17	45,45,46,47	0
3	IPA	B	2501	4/4	0.92	0.20	37,38,39,41	0

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.

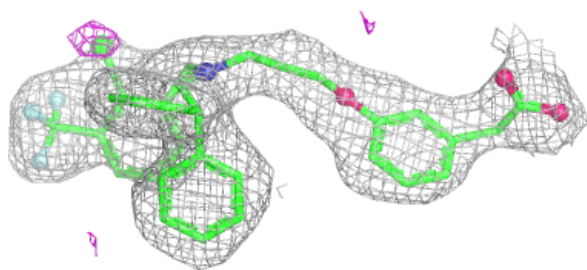
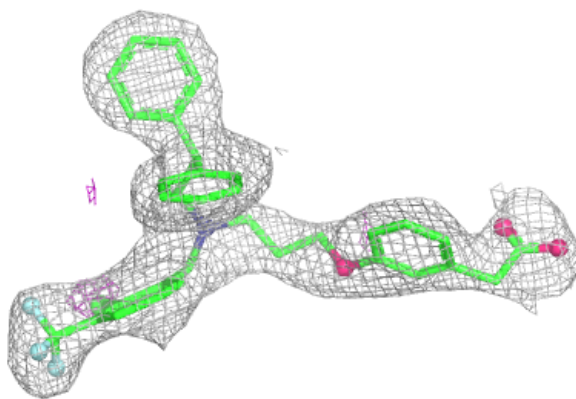


Electron density around 965 D 3500:

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

**Electron density around 965 A 1500:**

$2mF_o-DF_c$ (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.