



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:24 am BST

PDB ID : 1UHL
Title : Crystal structure of the LXRalpha-RXRbeta LBD heterodimer
Authors : Svensson, S.; Ostberg, T.; Jacobsson, M.; Norstrom, C.; Stefansson, K.;
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Deposited on : 2003-07-03
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

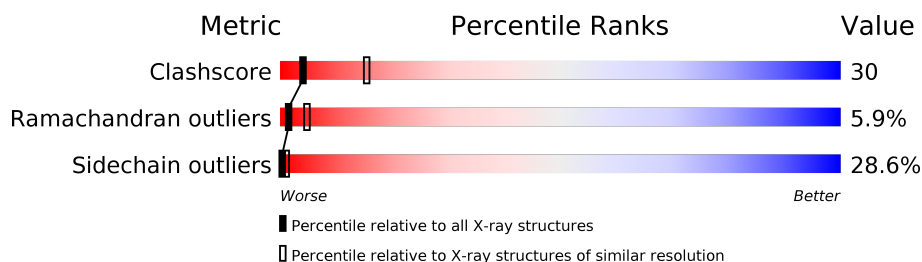
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	
2	B	242	
3	C	10	
3	D	10	

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	MEI	A	1001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3707 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 Retinoic acid receptor RXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1698	1085	294	309	10			

- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1777	1132	311	326	8			

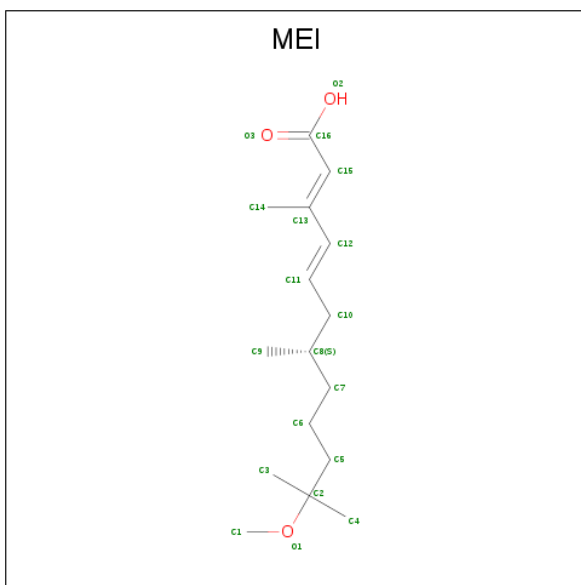
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	MET	-	EXPRESSION TAG	UNP Q13133

- Molecule 3 is a protein called 10-mer peptide from Nuclear receptor coactivator 2.

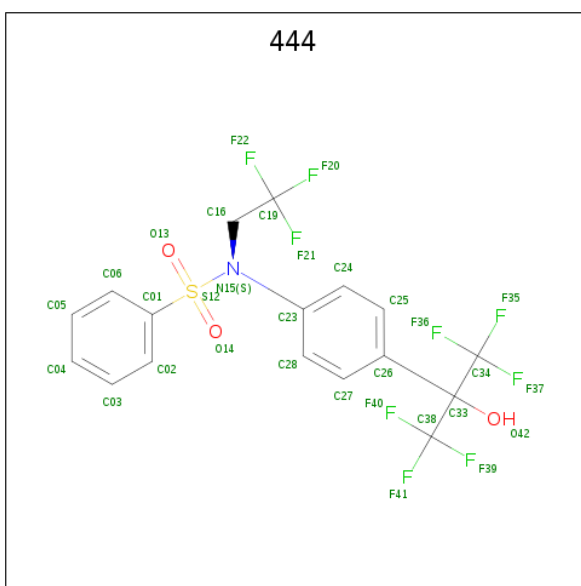
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			81	53	18	10			
3	D	10	Total	C	N	O	0	0	0
			89	57	19	13			

- Molecule 4 is (2E,4E)-11-METHOXY-3,7,11-TRIMETHYLDODECA-2,4-DIENOIC ACID (three-letter code: MEI) (formula: C₁₆H₂₈O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O			0	0
			19	16	3				

- Molecule 5 is N-(2,2,2-TRIFLUOROETHYL)-N-{4-[2,2,2-TRIFLUORO-1-HYDROXY-1-(TRIFLUOROMETHYL)ETHYL]PHENYL}BENZENESULFONAMIDE (three-letter code: 444) (formula: C₁₇H₁₂F₉NO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		

- Molecule 6 is water.

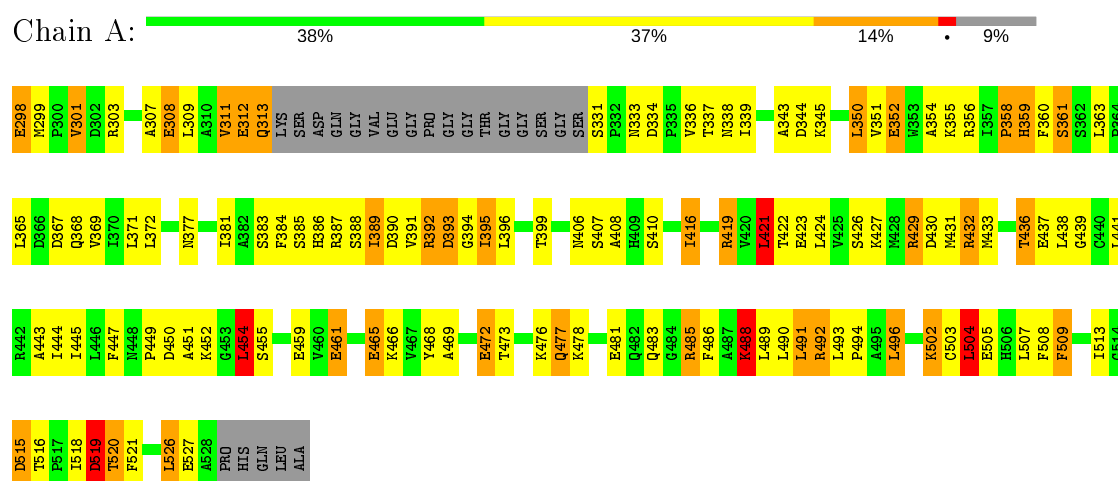
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0
6	B	1	Total 1	O 1	0	0

3 Residue-property plots

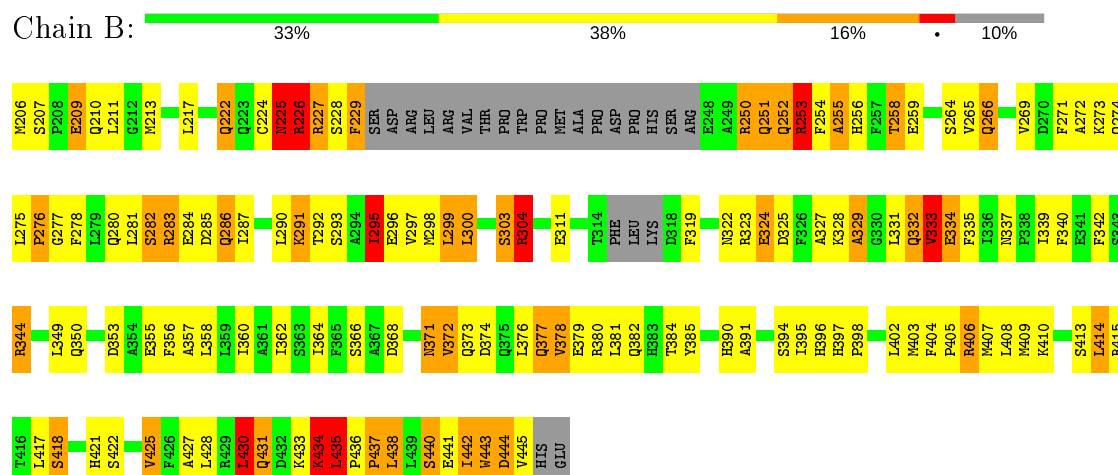
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

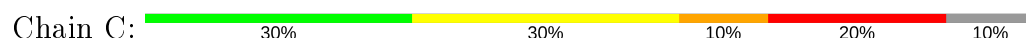
• Molecule 1: Retinoic acid receptor RXR-beta

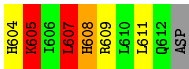


• Molecule 2: Oxysterols receptor LXR-alpha

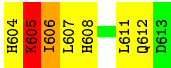


• Molecule 3: 10-mer peptide from Nuclear receptor coactivator 2





- Molecule 3: 10-mer peptide from Nuclear receptor coactivator 2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.63 Å 89.00 Å 90.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.65 – 2.90	Depositor
% Data completeness (in resolution range)	99.9 (19.65-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3707	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEI, 444

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	1.30	6/1729 (0.3%)	1.45	21/2336 (0.9%)
2	B	1.27	6/1810 (0.3%)	1.39	13/2443 (0.5%)
3	C	1.26	0/82	1.39	1/108 (0.9%)
3	D	1.18	0/90	1.21	1/119 (0.8%)
All	All	1.28	12/3711 (0.3%)	1.41	36/5006 (0.7%)

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
2	B	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	GLU	CD-OE1	6.13	1.32	1.25
2	B	340	PHE	CE2-CZ	5.96	1.48	1.37
1	A	426	SER	CB-OG	5.94	1.50	1.42
2	B	443	TRP	CB-CG	5.94	1.60	1.50
1	A	416	ILE	CA-CB	5.87	1.68	1.54
1	A	488	LYS	CD-CE	5.64	1.65	1.51
1	A	477	GLN	CB-CG	5.50	1.67	1.52
2	B	211	LEU	CG-CD2	5.30	1.71	1.51
2	B	333	VAL	CB-CG2	5.29	1.64	1.52
1	A	477	GLN	CG-CD	5.24	1.63	1.51
2	B	324	GLU	CG-CD	5.20	1.59	1.51
2	B	250	ARG	CG-CD	5.09	1.64	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ARG	NE-CZ-NH1	11.38	125.99	120.30
2	B	444	ASP	CB-CG-OD2	10.14	127.43	118.30
1	A	387	ARG	NE-CZ-NH1	-9.49	115.56	120.30
2	B	253	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	491	LEU	CA-CB-CG	-8.23	96.36	115.30
1	A	344	ASP	CB-CG-OD2	8.15	125.63	118.30
1	A	390	ASP	CB-CG-OD1	8.10	125.59	118.30
2	B	430	LEU	CA-CB-CG	7.84	133.34	115.30
2	B	325	ASP	CB-CG-OD2	7.81	125.33	118.30
2	B	344	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	B	253	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	492	ARG	NE-CZ-NH1	7.48	124.04	120.30
2	B	372	VAL	CB-CA-C	-7.40	97.34	111.40
1	A	492	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	504	LEU	CA-CB-CG	7.07	131.55	115.30
2	B	304	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	B	353	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	367	ASP	CB-CG-OD2	6.53	124.17	118.30
2	B	211	LEU	CB-CG-CD2	6.44	121.95	111.00
1	A	429	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	432	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	421	LEU	CB-CG-CD1	6.13	121.42	111.00
3	D	605	LYS	N-CA-C	6.06	127.36	111.00
1	A	371	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	485	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	350	LEU	CB-CG-CD2	5.64	120.59	111.00
3	C	607	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	454	LEU	CB-CA-C	-5.50	99.76	110.20
1	A	519	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	295	ILE	CB-CA-C	-5.31	100.98	111.60
1	A	526	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	515	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	435	LEU	CB-CA-C	5.19	120.06	110.20
1	A	416	ILE	N-CA-CB	5.04	122.39	110.80
2	B	378	VAL	CB-CA-C	5.04	120.97	111.40
1	A	344	ASP	CB-CG-OD1	-5.03	113.77	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	ARG	Peptide
2	B	334	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	431	GLN	Peptide
2	B	434	LYS	Peptide
2	B	435	LEU	Peptide

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	1698	0	1734	88	0
2	B	1777	0	1776	132	0
3	C	81	0	91	4	0
3	D	89	0	95	8	0
4	A	19	0	27	11	0
5	B	31	0	12	3	0
6	A	11	0	0	0	0
6	B	1	0	0	0	0
All	All	3707	0	3735	223	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 30.

All (223) 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:295:ILE:CD1	2:B:295:ILE:H	1.54	1.20
1:A:419:ARG:HG2	1:A:419:ARG:HH11	1.05	1.13
2:B:295:ILE:HD12	2:B:295:ILE:H	1.22	1.01
2:B:406:ARG:HH11	2:B:406:ARG:HG3	1.29	0.97
2:B:349:LEU:HD21	2:B:406:ARG:HD2	1.47	0.95
1:A:419:ARG:NH1	1:A:419:ARG:HG2	1.77	0.95
2:B:295:ILE:N	2:B:295:ILE:HD13	1.81	0.93
2:B:295:ILE:N	2:B:295:ILE:CD1	2.23	0.92
2:B:278:PHE:CZ	2:B:286:GLN:HB2	2.05	0.91
1:A:351:VAL:O	1:A:355:LYS:HG3	1.73	0.88
1:A:468:TYR:OH	2:B:409:MET:HG3	1.74	0.86
1:A:358:PRO:O	1:A:359:HIS:HB2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ILE:H	2:B:295:ILE:HD13	1.35	0.84
2:B:331:LEU:O	2:B:333:VAL:N	2.12	0.83
2:B:278:PHE:CE2	2:B:286:GLN:HB2	2.15	0.82
1:A:298:GLU:HG3	1:A:466:LYS:HE3	1.62	0.82
2:B:300:LEU:HD13	2:B:414:LEU:HD21	1.61	0.81
1:A:343:ALA:HA	4:A:1001:MEI:H142	1.62	0.79
2:B:295:ILE:HD12	2:B:443:TRP:CH2	2.18	0.78
2:B:295:ILE:HD12	2:B:443:TRP:HH2	1.50	0.77
1:A:392:ARG:NH1	1:A:392:ARG:HB2	2.00	0.75
1:A:298:GLU:OE1	1:A:298:GLU:HA	1.87	0.75
1:A:431:MET:O	1:A:432:ARG:HB2	1.87	0.73
2:B:376:LEU:O	2:B:380:ARG:HB2	1.89	0.73
1:A:504:LEU:HD22	1:A:508:PHE:CE2	2.24	0.73
2:B:335:PHE:HE1	2:B:421:HIS:HB2	1.52	0.73
2:B:377:GLN:HA	2:B:377:GLN:NE2	2.04	0.73
2:B:349:LEU:CD2	2:B:406:ARG:HD2	2.19	0.72
2:B:402:LEU:O	2:B:406:ARG:HB2	1.90	0.72
1:A:465:GLU:OE1	2:B:406:ARG:HG3	1.90	0.71
2:B:269:VAL:HG12	2:B:290:LEU:HD13	1.72	0.71
1:A:339:ILE:HD13	4:A:1001:MEI:H32	1.73	0.70
1:A:465:GLU:OE2	2:B:406:ARG:NH1	2.25	0.70
2:B:355:GLU:HB3	2:B:407:MET:HE1	1.75	0.69
2:B:355:GLU:HB3	2:B:407:MET:CE	2.24	0.68
1:A:333:ASN:HB3	1:A:338:ASN:HD21	1.59	0.67
2:B:295:ILE:HG12	2:B:418:SER:HB2	1.76	0.66
2:B:295:ILE:HA	2:B:298:MET:HG2	1.77	0.66
1:A:336:VAL:HG12	1:A:516:THR:HG21	1.79	0.64
2:B:228:SER:C	2:B:229:PHE:HD1	2.00	0.64
2:B:440:SER:HB3	2:B:445:VAL:HB	1.79	0.63
1:A:358:PRO:O	1:A:359:HIS:CB	2.46	0.63
2:B:283:ARG:HA	2:B:286:GLN:NE2	2.14	0.63
2:B:298:MET:HB2	5:B:1002:444:H03	1.80	0.62
3:D:604:HIS:O	3:D:605:LYS:HB2	2.00	0.62
2:B:335:PHE:CE1	2:B:421:HIS:HA	2.35	0.62
2:B:206:MET:HB3	2:B:210:GLN:OE1	2.00	0.62
1:A:336:VAL:HG12	1:A:516:THR:CG2	2.30	0.61
1:A:496:LEU:O	1:A:496:LEU:HD22	1.99	0.61
1:A:419:ARG:CG	1:A:419:ARG:HH11	1.90	0.61
1:A:309:LEU:O	1:A:312:GLU:CB	2.49	0.60
2:B:335:PHE:CE1	2:B:421:HIS:HB2	2.35	0.60
2:B:434:LYS:HG3	2:B:435:LEU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:PRO:O	2:B:437:PRO:C	2.37	0.59
2:B:217:LEU:HD21	2:B:275:LEU:CD2	2.32	0.59
2:B:297:VAL:HG13	2:B:360:ILE:HG23	1.85	0.59
2:B:207:SER:HB2	2:B:209:GLU:HG3	1.85	0.58
1:A:336:VAL:CG1	1:A:516:THR:HG21	2.33	0.58
2:B:281:LEU:O	2:B:286:GLN:NE2	2.37	0.58
1:A:381:ILE:HA	1:A:384:PHE:CE2	2.39	0.58
2:B:442:ILE:HD12	2:B:443:TRP:CE2	2.38	0.58
1:A:451:ALA:O	1:A:454:LEU:HD22	2.04	0.58
2:B:283:ARG:NH2	3:D:608:HIS:HE1	2.02	0.58
2:B:362:ILE:HG23	2:B:382:GLN:NE2	2.18	0.57
1:A:309:LEU:O	1:A:312:GLU:HB3	2.03	0.57
1:A:343:ALA:CA	4:A:1001:MEI:H142	2.32	0.57
2:B:228:SER:O	2:B:229:PHE:HD1	1.87	0.57
1:A:333:ASN:HB3	1:A:338:ASN:ND2	2.19	0.56
2:B:342:PHE:HB2	2:B:417:LEU:HD11	1.88	0.56
2:B:406:ARG:HH11	2:B:406:ARG:CG	2.12	0.56
2:B:303:SER:C	2:B:304:ARG:O	2.42	0.56
2:B:297:VAL:HG13	2:B:360:ILE:CG2	2.36	0.56
1:A:469:ALA:HB2	2:B:402:LEU:HD21	1.88	0.56
1:A:459:GLU:HA	1:A:459:GLU:OE2	2.04	0.55
1:A:368:GLN:HB3	3:C:611:LEU:HD13	1.88	0.55
2:B:277:GLY:O	2:B:280:GLN:HB3	2.06	0.55
2:B:355:GLU:OE1	2:B:397:HIS:HE1	1.89	0.55
2:B:253:ARG:O	2:B:256:HIS:CB	2.55	0.55
2:B:390:HIS:HB2	2:B:404:PHE:CZ	2.42	0.55
1:A:384:PHE:CD1	1:A:395:ILE:HG12	2.41	0.55
2:B:339:ILE:HD13	2:B:339:ILE:N	2.20	0.55
2:B:300:LEU:HD13	2:B:414:LEU:CD2	2.36	0.54
2:B:251:GLN:O	2:B:253:ARG:N	2.40	0.54
2:B:293:SER:O	2:B:297:VAL:HG23	2.07	0.54
2:B:276:PRO:HG2	2:B:385:TYR:OH	2.07	0.54
1:A:308:GLU:HG2	1:A:439:GLY:CA	2.38	0.54
1:A:419:ARG:NH1	1:A:419:ARG:CG	2.54	0.54
2:B:295:ILE:O	2:B:299:LEU:HD12	2.08	0.53
2:B:396:HIS:C	2:B:398:PRO:CD	2.77	0.53
2:B:404:PHE:HB3	2:B:405:PRO:CD	2.39	0.53
2:B:406:ARG:NH1	2:B:406:ARG:HG3	2.06	0.53
2:B:434:LYS:O	2:B:435:LEU:C	2.46	0.53
1:A:333:ASN:CB	1:A:338:ASN:HD21	2.22	0.52
1:A:352:GLU:O	1:A:356:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:THR:O	1:A:518:ILE:HD12	2.09	0.52
3:D:604:HIS:CD2	3:D:604:HIS:O	2.62	0.52
1:A:486:PHE:O	1:A:489:LEU:HB2	2.10	0.52
1:A:360:PHE:CE2	1:A:368:GLN:HG2	2.44	0.52
2:B:273:LYS:CE	3:D:611:LEU:HA	2.39	0.52
2:B:206:MET:HB2	2:B:391:ALA:HB1	1.91	0.52
1:A:461:GLU:O	1:A:465:GLU:HG3	2.09	0.52
2:B:206:MET:HA	2:B:395:ILE:HD11	1.92	0.51
2:B:441:GLU:OE1	3:D:605:LYS:N	2.43	0.51
1:A:407:SER:O	1:A:408:ALA:C	2.49	0.51
2:B:334:GLU:HG2	2:B:337:ASN:OD1	2.11	0.51
2:B:207:SER:OG	2:B:210:GLN:HG3	2.11	0.51
1:A:437:GLU:OE2	1:A:485:ARG:HD3	2.11	0.51
1:A:392:ARG:HB2	1:A:392:ARG:HH11	1.75	0.50
2:B:378:VAL:C	2:B:380:ARG:H	2.13	0.50
1:A:386:HIS:CG	1:A:438:LEU:HD22	2.47	0.50
2:B:427:ALA:O	2:B:430:LEU:HD12	2.12	0.50
2:B:253:ARG:O	2:B:256:HIS:HB3	2.11	0.50
2:B:282:SER:O	2:B:285:ASP:HB2	2.12	0.50
2:B:291:LYS:HA	2:B:442:ILE:HG22	1.94	0.50
1:A:503:CYS:HB3	4:A:1001:MEI:H62	1.95	0.49
1:A:386:HIS:O	1:A:389:ILE:HG13	2.13	0.49
1:A:447:PHE:O	1:A:449:PRO:HD3	2.12	0.49
2:B:283:ARG:HA	2:B:286:GLN:HG2	1.95	0.49
2:B:327:ALA:O	2:B:332:GLN:CG	2.60	0.49
2:B:422:SER:O	2:B:425:VAL:HG12	2.13	0.49
2:B:335:PHE:HE1	2:B:421:HIS:CB	2.22	0.49
1:A:504:LEU:HD13	1:A:508:PHE:HE2	1.78	0.48
2:B:443:TRP:HA	2:B:443:TRP:HE3	1.78	0.48
4:A:1001:MEI:H101	4:A:1001:MEI:H52	1.95	0.48
2:B:266:GLN:O	2:B:269:VAL:HG22	2.14	0.48
2:B:355:GLU:OE1	2:B:397:HIS:CE1	2.67	0.47
1:A:465:GLU:HB3	2:B:402:LEU:HD13	1.95	0.47
2:B:295:ILE:HB	2:B:299:LEU:HD12	1.95	0.47
2:B:295:ILE:HD13	2:B:296:GLU:H	1.79	0.47
3:C:607:LEU:O	3:C:608:HIS:C	2.52	0.47
1:A:392:ARG:HB2	1:A:392:ARG:CZ	2.44	0.47
1:A:307:ALA:O	1:A:308:GLU:C	2.53	0.47
2:B:295:ILE:HD12	2:B:295:ILE:N	2.05	0.47
2:B:406:ARG:NH1	2:B:406:ARG:CG	2.74	0.47
2:B:409:MET:HA	2:B:409:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PHE:C	1:A:509:PHE:CD2	2.89	0.46
1:A:427:LYS:HE2	2:B:379:GLU:OE2	2.16	0.46
2:B:381:LEU:O	2:B:385:TYR:HD1	1.97	0.46
1:A:431:MET:O	1:A:432:ARG:CB	2.54	0.46
2:B:404:PHE:HB3	2:B:405:PRO:HD3	1.98	0.46
2:B:339:ILE:H	2:B:339:ILE:HD13	1.81	0.46
1:A:388:SER:OG	1:A:395:ILE:HA	2.15	0.46
2:B:357:ALA:O	2:B:358:LEU:C	2.53	0.46
1:A:509:PHE:O	1:A:513:ILE:HG12	2.15	0.46
2:B:228:SER:O	2:B:229:PHE:O	2.34	0.46
1:A:339:ILE:HG23	4:A:1001:MEI:H12	1.98	0.46
2:B:327:ALA:O	2:B:332:GLN:HG2	2.16	0.45
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.77	0.45
2:B:283:ARG:HA	2:B:286:GLN:CD	2.36	0.45
2:B:355:GLU:HB3	2:B:407:MET:HE3	1.98	0.45
2:B:283:ARG:N	2:B:283:ARG:HD3	2.31	0.45
2:B:443:TRP:CE3	2:B:443:TRP:HA	2.52	0.45
1:A:431:MET:CE	1:A:488:LYS:HB3	2.46	0.45
2:B:258:THR:HG23	2:B:436:PRO:HG2	1.98	0.45
1:A:301:VAL:HG13	1:A:436:THR:HG21	1.99	0.45
1:A:384:PHE:CE1	1:A:395:ILE:HG12	2.51	0.45
2:B:417:LEU:HD23	2:B:417:LEU:HA	1.61	0.45
2:B:217:LEU:HD21	2:B:275:LEU:HD23	1.98	0.45
1:A:472:GLU:OE2	2:B:390:HIS:HE1	2.00	0.44
2:B:273:LYS:HE3	3:D:611:LEU:HA	1.99	0.44
2:B:409:MET:HA	2:B:409:MET:CE	2.48	0.44
1:A:334:ASP:HB3	1:A:337:THR:HB	1.99	0.44
1:A:343:ALA:HA	4:A:1001:MEI:C14	2.42	0.44
1:A:502:LYS:HE3	1:A:502:LYS:HB2	1.66	0.44
5:B:1002:444:F39	5:B:1002:444:F36	2.13	0.44
2:B:433:LYS:HA	2:B:433:LYS:HD3	1.71	0.44
1:A:343:ALA:CB	4:A:1001:MEI:H142	2.47	0.44
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.89	0.44
2:B:254:PHE:HA	2:B:329:ALA:HB1	1.99	0.44
2:B:271:PHE:O	2:B:272:ALA:C	2.56	0.44
1:A:354:ALA:HB2	1:A:372:LEU:HD21	2.00	0.43
2:B:304:ARG:HG3	2:B:356:PHE:CE2	2.53	0.43
2:B:328:LYS:C	2:B:329:ALA:O	2.53	0.43
1:A:493:LEU:N	1:A:494:PRO:CD	2.81	0.43
1:A:311:VAL:O	1:A:313:GLN:NE2	2.50	0.43
1:A:443:ALA:O	1:A:444:ILE:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ALA:HA	2:B:258:THR:HB	2.00	0.43
2:B:209:GLU:H	2:B:209:GLU:HG2	1.19	0.43
1:A:299:MET:SD	1:A:358:PRO:HG2	2.59	0.43
1:A:389:ILE:O	1:A:429:ARG:NH1	2.33	0.43
2:B:396:HIS:C	2:B:398:PRO:HD3	2.39	0.43
2:B:264:SER:O	2:B:265:VAL:C	2.57	0.43
2:B:397:HIS:N	2:B:398:PRO:CD	2.80	0.43
2:B:436:PRO:O	2:B:438:LEU:N	2.52	0.43
1:A:391:VAL:HG12	1:A:392:ARG:N	2.34	0.42
1:A:394:GLY:O	1:A:421:LEU:HD11	2.19	0.42
2:B:374:ASP:CG	2:B:377:GLN:HB2	2.39	0.42
2:B:251:GLN:O	2:B:254:PHE:N	2.52	0.42
2:B:349:LEU:O	2:B:350:GLN:HB2	2.19	0.42
2:B:396:HIS:O	2:B:398:PRO:HD2	2.19	0.42
1:A:369:VAL:HG22	3:C:607:LEU:HD13	2.00	0.42
2:B:337:ASN:HD22	2:B:337:ASN:HA	1.65	0.42
2:B:335:PHE:CE1	2:B:421:HIS:CB	2.99	0.42
1:A:354:ALA:HB1	1:A:360:PHE:CE2	2.54	0.42
5:B:1002:444:C27	5:B:1002:444:F40	2.57	0.42
1:A:441:LEU:O	1:A:445:ILE:HG13	2.20	0.42
2:B:258:THR:HG22	2:B:259:GLU:N	2.35	0.42
1:A:381:ILE:HA	1:A:384:PHE:CD2	2.55	0.42
1:A:429:ARG:O	1:A:430:ASP:C	2.58	0.42
1:A:518:ILE:HG22	1:A:519:ASP:N	2.35	0.42
1:A:369:VAL:CG1	1:A:369:VAL:O	2.68	0.41
2:B:368:ASP:CG	2:B:415:ARG:HH22	2.22	0.41
1:A:396:LEU:O	1:A:396:LEU:HG	2.19	0.41
2:B:335:PHE:CE1	2:B:421:HIS:CA	3.01	0.41
3:D:605:LYS:N	3:D:608:HIS:HD2	2.18	0.41
1:A:504:LEU:HD22	1:A:508:PHE:CZ	2.54	0.41
2:B:442:ILE:HD12	2:B:443:TRP:CD2	2.55	0.41
1:A:343:ALA:HB2	4:A:1001:MEI:C11	2.51	0.41
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.83	0.41
2:B:349:LEU:HD22	2:B:403:MET:SD	2.60	0.41
2:B:378:VAL:C	2:B:380:ARG:N	2.74	0.41
1:A:492:ARG:NE	1:A:492:ARG:HA	2.35	0.41
2:B:441:GLU:OE2	3:D:606:ILE:HB	2.21	0.41
4:A:1001:MEI:H62	4:A:1001:MEI:H43	1.75	0.41
2:B:224:CYS:C	2:B:226:ARG:H	2.24	0.41
2:B:225:ASN:O	2:B:226:ARG:HB3	2.21	0.41
1:A:395:ILE:HD12	1:A:421:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:OD1	1:A:407:SER:N	2.52	0.41
2:B:258:THR:O	2:B:259:GLU:C	2.59	0.41
3:C:604:HIS:HB3	3:C:605:LYS:H	1.65	0.40
2:B:227:ARG:H	2:B:227:ARG:HG2	1.62	0.40
2:B:390:HIS:CD2	2:B:390:HIS:C	2.94	0.40
4:A:1001:MEI:H143	4:A:1001:MEI:H11	1.44	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	210/236 (89%)	181 (86%)	21 (10%)	8 (4%)	3	13
2	B	213/242 (88%)	166 (78%)	31 (15%)	16 (8%)	1	2
3	C	7/10 (70%)	4 (57%)	2 (29%)	1 (14%)	0	0
3	D	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	438/498 (88%)	356 (81%)	56 (13%)	26 (6%)	1	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	520	THR
2	B	225	ASN
2	B	252	GLN
2	B	311	GLU
2	B	332	GLN
2	B	371	ASN
2	B	434	LYS
2	B	435	LEU

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Mol	Chain	Res	Type
2	B	444	ASP
3	C	605	LYS
3	D	605	LYS
1	A	359	HIS
1	A	473	THR
2	B	222	GLN
2	B	226	ARG
1	A	393	ASP
1	A	472	GLU
1	A	477	GLN
2	B	255	ALA
2	B	329	ALA
2	B	373	GLN
2	B	304	ARG
2	B	437	PRO
2	B	276	PRO
1	A	358	PRO

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	187/201 (93%)	134 (72%)	53 (28%)	0	1
2	B	196/219 (90%)	142 (72%)	54 (28%)	0	1
3	C	9/10 (90%)	5 (56%)	4 (44%)	0	0
3	D	10/10 (100%)	6 (60%)	4 (40%)	0	0
All	All	402/440 (91%)	287 (71%)	115 (29%)	0	1

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	301	VAL
1	A	303	ARG
1	A	308	GLU

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Mol	Chain	Res	Type
1	A	311	VAL
1	A	312	GLU
1	A	313	GLN
1	A	331	SER
1	A	345	LYS
1	A	350	LEU
1	A	352	GLU
1	A	361	SER
1	A	363	LEU
1	A	377	ASN
1	A	383	SER
1	A	385	SER
1	A	389	ILE
1	A	392	ARG
1	A	393	ASP
1	A	395	ILE
1	A	399	THR
1	A	410	SER
1	A	416	ILE
1	A	419	ARG
1	A	421	LEU
1	A	422	THR
1	A	423	GLU
1	A	424	LEU
1	A	433	MET
1	A	436	THR
1	A	450	ASP
1	A	452	LYS
1	A	454	LEU
1	A	455	SER
1	A	461	GLU
1	A	476	LYS
1	A	478	LYS
1	A	481	GLU
1	A	483	GLN
1	A	488	LYS
1	A	490	LEU
1	A	496	LEU
1	A	502	LYS
1	A	504	LEU
1	A	505	GLU
1	A	507	LEU

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Mol	Chain	Res	Type
1	A	509	PHE
1	A	515	ASP
1	A	519	ASP
1	A	520	THR
1	A	521	PHE
1	A	526	LEU
1	A	527	GLU
2	B	209	GLU
2	B	213	MET
2	B	222	GLN
2	B	225	ASN
2	B	226	ARG
2	B	227	ARG
2	B	229	PHE
2	B	250	ARG
2	B	251	GLN
2	B	252	GLN
2	B	253	ARG
2	B	258	THR
2	B	266	GLN
2	B	274	GLN
2	B	282	SER
2	B	283	ARG
2	B	284	GLU
2	B	286	GLN
2	B	287	ILE
2	B	291	LYS
2	B	292	THR
2	B	295	ILE
2	B	299	LEU
2	B	300	LEU
2	B	303	SER
2	B	304	ARG
2	B	319	PHE
2	B	322	ASN
2	B	323	ARG
2	B	324	GLU
2	B	333	VAL
2	B	344	ARG
2	B	364	ILE
2	B	366	SER
2	B	371	ASN

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Mol	Chain	Res	Type
2	B	372	VAL
2	B	377	GLN
2	B	384	THR
2	B	394	SER
2	B	406	ARG
2	B	408	LEU
2	B	410	LYS
2	B	413	SER
2	B	414	LEU
2	B	418	SER
2	B	425	VAL
2	B	428	LEU
2	B	430	LEU
2	B	431	GLN
2	B	434	LYS
2	B	435	LEU
2	B	438	LEU
2	B	440	SER
2	B	442	ILE
3	C	605	LYS
3	C	607	LEU
3	C	608	HIS
3	C	609	ARG
3	D	605	LYS
3	D	606	ILE
3	D	607	LEU
3	D	612	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	338	ASN
1	A	368	GLN
1	A	409	HIS
2	B	225	ASN
2	B	252	GLN
2	B	280	GLN
2	B	377	GLN
2	B	382	GLN
2	B	390	HIS
2	B	397	HIS

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Mol	Chain	Res	Type
3	D	604	HIS
3	D	608	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	$\# Z > 2$
5	444	B	1002	-	31,32,32	2.48	5 (16%)	52,52,52	3.24	16 (30%)
4	MEI	A	1001	-	15,18,18	0.53	0	17,23,23	3.67	4 (23%)

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
5	444	B	1002	-	-	7/45/45/45	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MEI	A	1001	-	-	8/18/20/20	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	444	C01-S12	-10.09	1.62	1.76
5	B	1002	444	C16-C19	5.77	1.58	1.50
5	B	1002	444	O13-S12	4.36	1.48	1.43
5	B	1002	444	C34-C33	-2.37	1.50	1.54
5	B	1002	444	C27-C26	2.03	1.42	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	MEI	C11-C12-C13	-13.42	105.61	125.89
5	B	1002	444	O14-S12-O13	-10.10	103.16	119.52
5	B	1002	444	O14-S12-N15	8.20	116.41	106.71
5	B	1002	444	C16-N15-S12	7.47	127.41	117.00
5	B	1002	444	C19-C16-N15	7.10	119.04	112.14
5	B	1002	444	O13-S12-N15	6.92	114.90	106.71
5	B	1002	444	C38-C33-C34	-6.17	102.55	110.28
5	B	1002	444	C34-C33-C26	5.57	119.81	110.34
5	B	1002	444	O14-S12-C01	-5.50	101.08	108.05
5	B	1002	444	C01-S12-N15	4.87	113.56	106.92
4	A	1001	MEI	C14-C13-C12	-4.31	111.29	118.08
5	B	1002	444	C38-C33-C26	-4.04	103.46	110.34
5	B	1002	444	F41-C38-C33	4.04	119.57	111.85
4	A	1001	MEI	C12-C13-C15	3.48	128.41	119.11
5	B	1002	444	F40-C38-C33	-3.07	105.99	111.85
5	B	1002	444	F36-C34-C33	-3.07	106.00	111.85
5	B	1002	444	F37-C34-F36	2.48	115.12	107.53
5	B	1002	444	F35-C34-F36	-2.26	100.62	107.53
4	A	1001	MEI	C14-C13-C15	-2.10	120.25	124.64
5	B	1002	444	F20-C19-F22	-2.02	99.02	106.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	MEI	C3-C2-C5-C6
4	A	1001	MEI	C4-C2-C5-C6

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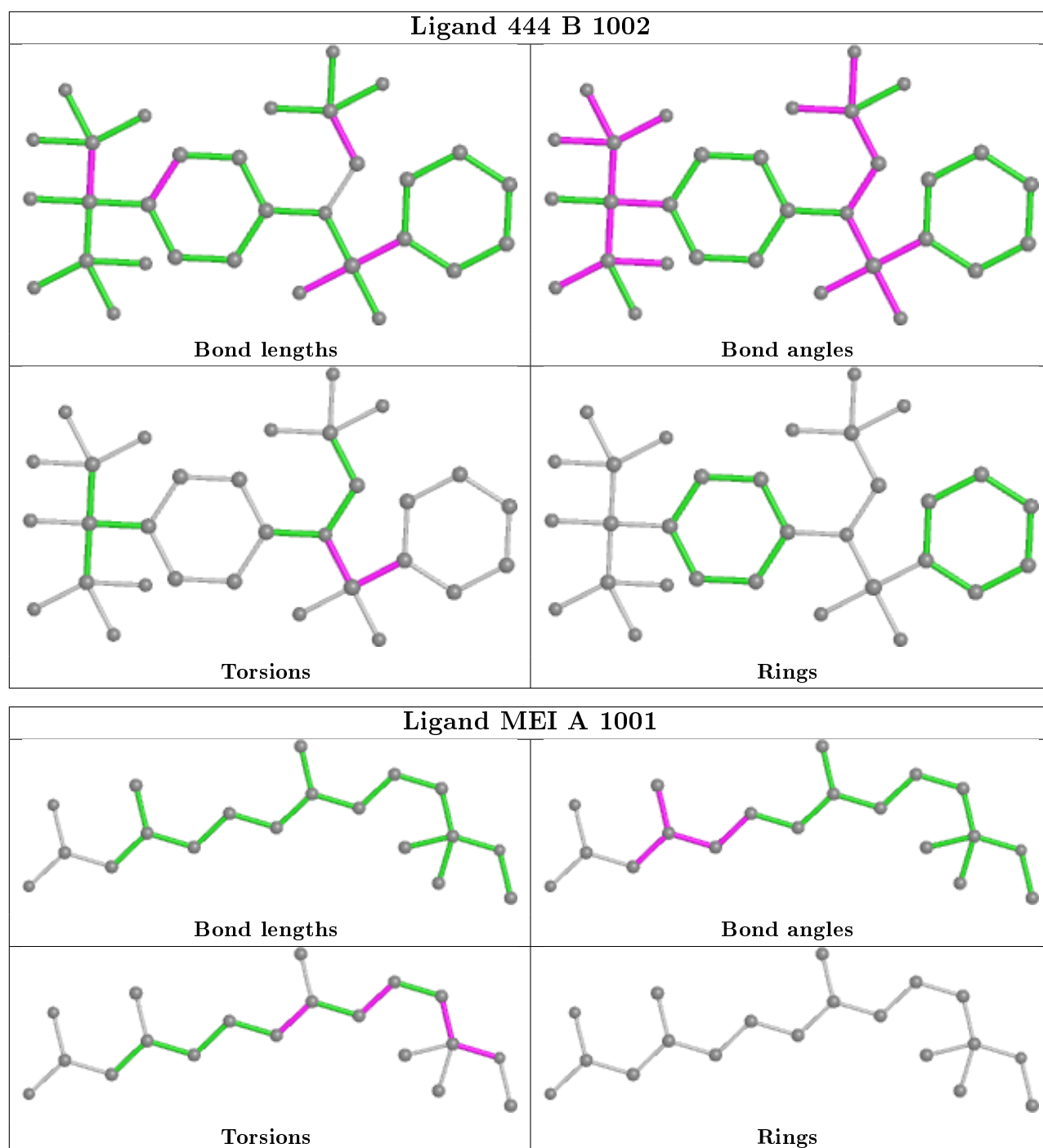
Mol	Chain	Res	Type	Atoms
4	A	1001	MEI	C11-C10-C8-C9
4	A	1001	MEI	C5-C6-C7-C8
5	B	1002	444	C23-N15-S12-C01
5	B	1002	444	C02-C01-S12-O14
5	B	1002	444	C02-C01-S12-N15
5	B	1002	444	C06-C01-S12-O14
5	B	1002	444	C06-C01-S12-N15
4	A	1001	MEI	C4-C2-O1-C1
5	B	1002	444	C23-N15-S12-O13
5	B	1002	444	C23-N15-S12-O14
4	A	1001	MEI	C11-C10-C8-C7
4	A	1001	MEI	C3-C2-O1-C1
4	A	1001	MEI	C5-C2-O1-C1

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1002	444	3	0
4	A	1001	MEI	11	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.