



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:03 AM UTC

PDB ID : 1BKE / pdb_00001bke
Title : HUMAN SERUM ALBUMIN IN A COMPLEX WITH MYRISTIC ACID
AND TRI-IODOBENZOIC ACID
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Deposited on : 1998-07-06
Resolution : 3.15 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

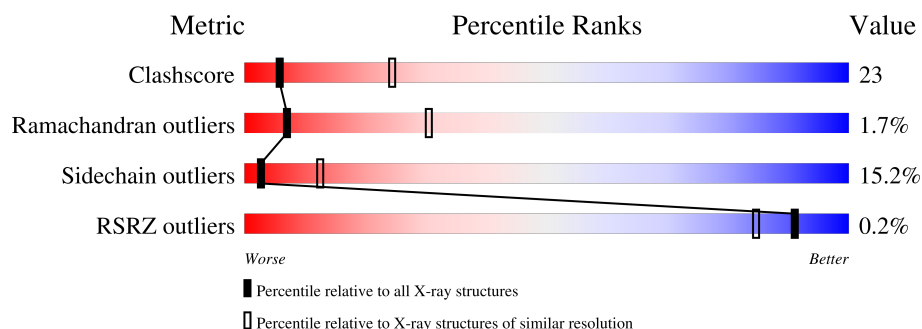
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	581	

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
3	B3I	A	2002[A]	-	-	X	-
3	B3I	A	2002[B]	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4562 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 SERUM ALBUMIN.

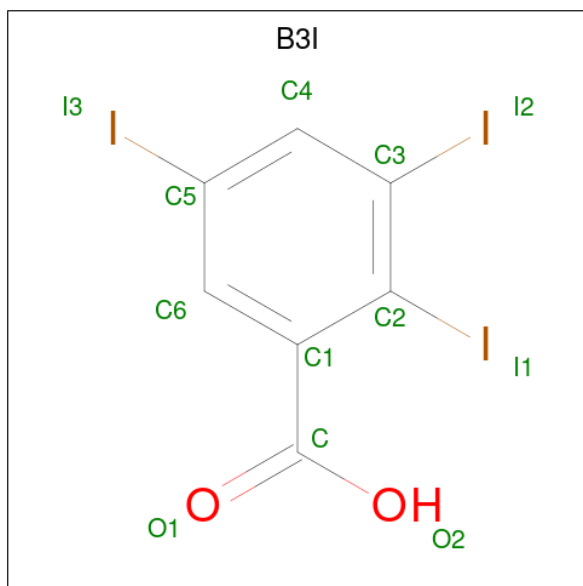
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4445	2811	744	849	41			

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is 2,3,5-TRIODOBENZOIC ACID (CCD ID: B3I) (formula: $C_7H_3I_3O_2$).

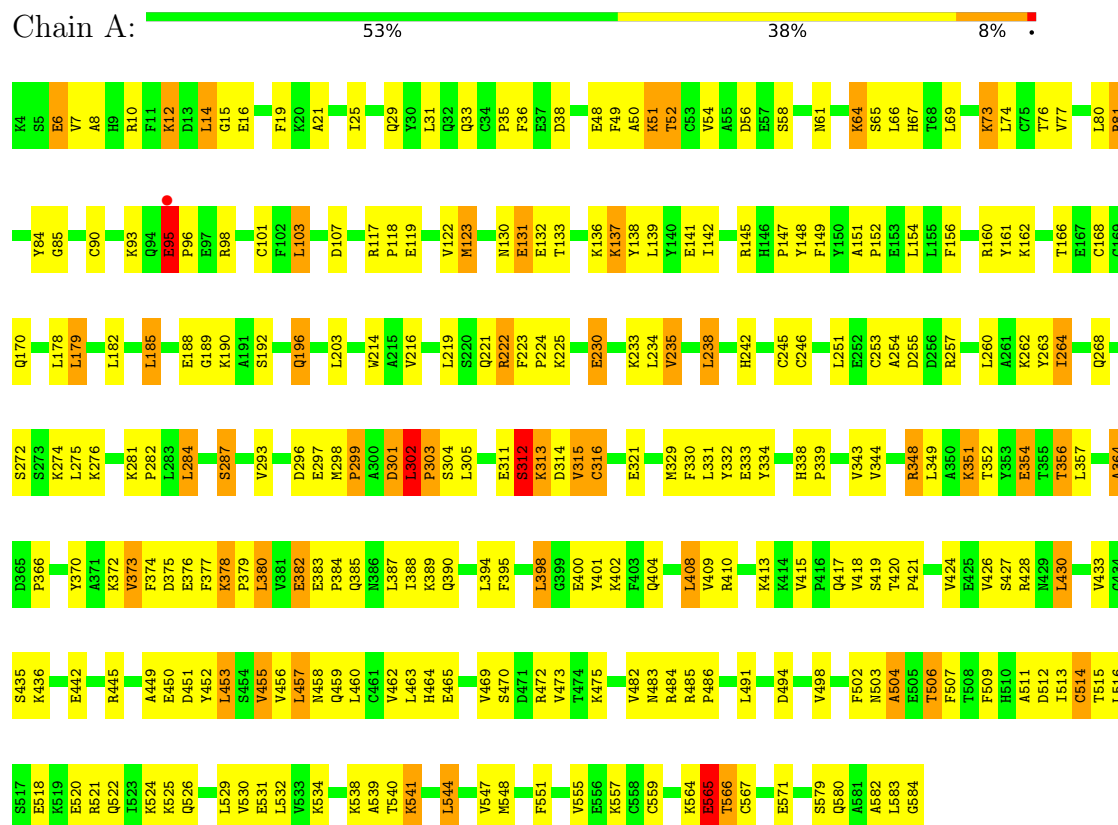


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	I	O	0	1
			24	14	6	4		
3	A	1	Total	C	I	O	0	1
			24	14	6	4		

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: SERUM ALBUMIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.65Å 38.87Å 95.91Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-3.15) 96.9 (20.00-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 3.14Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.177 , 0.248 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 98.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4562	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: B3I, MYR

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	0.41	0/4531	0.93	14/6144 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ASP	N-CA-C	-7.88	103.74	112.72
1	A	541	LYS	N-CA-C	-7.15	103.82	112.54
1	A	178	LEU	N-CA-C	6.75	118.30	111.07
1	A	315	VAL	N-CA-C	-6.53	104.66	111.58
1	A	95	GLU	N-CA-C	6.18	123.47	109.81
1	A	313	LYS	N-CA-C	-5.92	102.67	110.43
1	A	12	LYS	N-CA-C	5.61	117.85	111.11
1	A	139	LEU	N-CA-C	-5.58	105.12	111.14
1	A	316	CYS	N-CA-C	-5.57	105.36	111.82
1	A	298	MET	CA-C-N	5.57	126.80	119.84
1	A	298	MET	C-N-CA	5.57	126.80	119.84
1	A	302	LEU	N-CA-C	5.38	117.42	109.50
1	A	382	GLU	N-CA-C	5.08	117.72	111.82
1	A	566	THR	N-CA-C	-5.01	105.49	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4445	0	4213	203	0
2	A	69	0	101	12	0
3	A	48	0	8	13	0
All	All	4562	0	4322	205	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 23.

All (205) 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:A:1001:MYR:H21	3:A:2002[A]:B3I:I3	2.40	0.92
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.56	0.85
1:A:12:LYS:HE2	1:A:54:VAL:HG13	1.59	0.84
1:A:10:ARG:O	1:A:14:LEU:HB2	1.79	0.82
1:A:564:LYS:O	1:A:565:GLU:HB2	1.83	0.79
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.66	0.78
1:A:219:LEU:HD21	3:A:2001[A]:B3I:I3	2.53	0.78
1:A:257:ARG:HH21	1:A:287:SER:HB2	1.49	0.76
1:A:225:LYS:HG3	1:A:299:PRO:HD3	1.68	0.75
1:A:567:CYS:O	1:A:571:GLU:HB2	1.87	0.75
1:A:138:TYR:HB3	2:A:1001:MYR:H101	1.69	0.74
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.52	0.73
1:A:424:VAL:O	1:A:428:ARG:HG3	1.90	0.72
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.25	0.72
1:A:356:THR:HG21	1:A:373:VAL:CG2	2.21	0.70
1:A:77:VAL:O	1:A:80:LEU:HB2	1.90	0.70
1:A:149:PHE:CZ	3:A:2002[B]:B3I:I3	3.15	0.70
1:A:149:PHE:CE1	3:A:2002[B]:B3I:I3	3.15	0.69
1:A:530:VAL:HG12	1:A:534:LYS:HE3	1.74	0.69
1:A:462:VAL:O	1:A:465:GLU:HB3	1.93	0.68
1:A:433:VAL:HG22	1:A:452:TYR:HB3	1.76	0.68
1:A:137:LYS:O	1:A:141:GLU:HG2	1.93	0.68
1:A:119:GLU:O	1:A:122:VAL:HG22	1.94	0.67
1:A:260:LEU:O	1:A:264:ILE:HG13	1.95	0.67
1:A:364:ALA:O	1:A:366:PRO:HD3	1.94	0.67
1:A:77:VAL:HB	1:A:80:LEU:HD13	1.76	0.66
1:A:349:LEU:HD23	1:A:380:LEU:HD23	1.77	0.66
1:A:351:LYS:HE3	1:A:354:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:O	1:A:52:THR:HB	1.96	0.65
1:A:25:ILE:O	1:A:29:GLN:HG3	1.96	0.64
1:A:518:GLU:HA	1:A:518:GLU:OE1	1.94	0.64
1:A:221:GLN:HG2	1:A:339:PRO:HA	1.79	0.64
1:A:254:ALA:HB1	2:A:1002:MYR:H51	1.80	0.63
1:A:458:ASN:O	1:A:462:VAL:HG23	1.98	0.63
1:A:141:GLU:O	1:A:145:ARG:HD2	1.99	0.62
1:A:149:PHE:CE2	3:A:2002[B]:B3I:I3	3.23	0.62
1:A:149:PHE:CD1	3:A:2002[B]:B3I:I3	3.23	0.62
2:A:1001:MYR:C2	3:A:2002[A]:B3I:I3	3.15	0.62
1:A:118:PRO:HD2	1:A:123:MET:HE3	1.80	0.61
1:A:272:SER:HB3	1:A:275:LEU:HG	1.82	0.61
1:A:313:LYS:O	1:A:314:ASP:HB2	2.00	0.61
1:A:222:ARG:HG2	1:A:222:ARG:NH1	2.13	0.61
1:A:420:THR:N	1:A:421:PRO:HD2	2.16	0.61
1:A:388:ILE:HD13	2:A:1003:MYR:H72	1.83	0.61
1:A:95:GLU:OE1	1:A:98:ARG:NH2	2.33	0.61
1:A:149:PHE:CD2	1:A:154:LEU:HD13	2.34	0.61
1:A:547:VAL:HG21	1:A:583:LEU:HD21	1.82	0.60
1:A:551:PHE:O	1:A:555:VAL:HG23	2.02	0.60
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.84	0.59
1:A:415:VAL:HG11	1:A:473:VAL:HG23	1.85	0.58
1:A:458:ASN:HA	1:A:484:ARG:HH12	1.68	0.58
1:A:118:PRO:HB2	1:A:122:VAL:CG2	2.34	0.58
1:A:189:GLY:HA3	3:A:2002[A]:B3I:I2	2.74	0.57
1:A:398:LEU:HB3	1:A:402:LYS:HB3	1.86	0.57
1:A:73:LYS:O	1:A:76:THR:HB	2.05	0.57
1:A:48:GLU:HA	1:A:48:GLU:OE1	2.04	0.57
1:A:138:TYR:O	1:A:142:ILE:HG12	2.05	0.57
1:A:452:TYR:O	1:A:455:VAL:HG23	2.06	0.56
1:A:119:GLU:HB2	1:A:122:VAL:HG13	1.86	0.56
1:A:464:HIS:HE1	1:A:470:SER:O	1.89	0.56
1:A:219:LEU:HD21	3:A:2001[B]:B3I:I2	2.76	0.56
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.36	0.56
1:A:299:PRO:C	1:A:301:ASP:H	2.14	0.56
1:A:373:VAL:HG12	1:A:374:PHE:N	2.20	0.55
1:A:8:ALA:O	1:A:12:LYS:HG3	2.06	0.55
1:A:372:LYS:O	1:A:375:ASP:HB2	2.07	0.55
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.88	0.55
1:A:33:GLN:HA	1:A:33:GLN:OE1	2.07	0.55
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD13	1:A:427:SER:CB	2.38	0.54
1:A:35:PRO:O	1:A:38:ASP:HB2	2.07	0.54
1:A:245:CYS:HA	1:A:253:CYS:HB2	1.89	0.54
1:A:415:VAL:HB	1:A:418:VAL:HG23	1.90	0.53
1:A:190:LYS:HG2	3:A:2002[A]:B3I:O1	2.08	0.53
1:A:313:LYS:O	1:A:314:ASP:CB	2.56	0.53
1:A:149:PHE:CD2	3:A:2002[B]:B3I:I3	3.32	0.53
1:A:331:LEU:O	1:A:332:TYR:C	2.51	0.53
1:A:95:GLU:O	1:A:96:PRO:C	2.51	0.53
1:A:149:PHE:CG	3:A:2002[B]:B3I:I3	3.32	0.53
1:A:33:GLN:HB2	1:A:84:TYR:CE2	2.43	0.52
1:A:16:GLU:OE1	1:A:51:LYS:HE2	2.08	0.52
1:A:513:ILE:CD1	1:A:555:VAL:HG13	2.40	0.52
1:A:284:LEU:HG	1:A:284:LEU:O	2.10	0.51
1:A:394:LEU:HD11	1:A:398:LEU:HD11	1.91	0.51
1:A:464:HIS:CE1	1:A:469:VAL:H	2.27	0.51
1:A:21:ALA:O	1:A:25:ILE:HG13	2.10	0.51
1:A:449:ALA:O	1:A:453:LEU:HB2	2.10	0.51
1:A:540:THR:HG22	1:A:541:LYS:H	1.76	0.51
1:A:547:VAL:CG2	1:A:583:LEU:HD21	2.40	0.51
1:A:348:ARG:HG3	1:A:482:VAL:HG13	1.92	0.51
1:A:520:GLU:O	1:A:524:LYS:HG3	2.10	0.51
1:A:398:LEU:CB	1:A:402:LYS:HB3	2.40	0.50
1:A:315:VAL:HG11	1:A:370:TYR:CZ	2.46	0.50
1:A:530:VAL:CG1	1:A:534:LYS:HE3	2.41	0.50
1:A:148:TYR:O	1:A:196:GLN:NE2	2.45	0.50
1:A:539:ALA:HB3	1:A:544:LEU:HD13	1.94	0.49
1:A:520:GLU:HA	1:A:520:GLU:OE1	2.12	0.49
1:A:548:MET:HG2	2:A:1005:MYR:H52	1.95	0.49
1:A:142:ILE:N	1:A:142:ILE:HD13	2.27	0.49
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.94	0.49
1:A:272:SER:HB3	1:A:275:LEU:CG	2.42	0.49
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.94	0.49
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.43	0.49
1:A:518:GLU:O	1:A:522:GLN:HG3	2.12	0.49
1:A:219:LEU:CD2	3:A:2001[A]:B3I:I3	3.29	0.48
1:A:315:VAL:HG13	1:A:316:CYS:N	2.28	0.48
1:A:242:HIS:O	1:A:246:CYS:SG	2.72	0.47
1:A:138:TYR:CB	2:A:1001:MYR:H101	2.43	0.47
1:A:64:LYS:HB2	1:A:69:LEU:HG	1.95	0.47
1:A:67:HIS:CE1	1:A:251:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:O	1:A:10:ARG:HG2	2.14	0.47
1:A:117:ARG:HG3	1:A:123:MET:HE1	1.96	0.47
1:A:311:GLU:O	1:A:312:SER:C	2.57	0.47
1:A:118:PRO:HG2	1:A:123:MET:HG3	1.96	0.47
1:A:36:PHE:CE1	1:A:137:LYS:HA	2.49	0.47
1:A:56:ASP:OD1	1:A:58:SER:HB2	2.15	0.47
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.49	0.47
1:A:356:THR:HG21	1:A:373:VAL:HG21	1.96	0.47
1:A:61:ASN:O	1:A:64:LYS:HG3	2.15	0.46
1:A:579:SER:O	1:A:580:GLN:C	2.58	0.46
1:A:540:THR:HG22	1:A:541:LYS:N	2.31	0.46
1:A:507:PHE:CD1	2:A:1005:MYR:H102	2.51	0.46
1:A:514:CYS:HB3	1:A:559:CYS:HB3	1.80	0.45
1:A:400:GLU:O	1:A:404:GLN:HG3	2.16	0.45
1:A:521:ARG:O	1:A:525:LYS:HG3	2.16	0.45
1:A:539:ALA:CB	1:A:544:LEU:HD13	2.46	0.45
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.98	0.45
1:A:453:LEU:O	1:A:457:LEU:HB2	2.18	0.44
1:A:464:HIS:CE1	1:A:470:SER:H	2.34	0.44
1:A:6:GLU:OE1	1:A:66:LEU:HG	2.17	0.44
1:A:409:VAL:O	1:A:413:LYS:HG3	2.15	0.44
1:A:485:ARG:H	1:A:486:PRO:CD	2.30	0.44
1:A:131:GLU:OE2	1:A:162:LYS:HE3	2.17	0.44
1:A:388:ILE:HD13	2:A:1003:MYR:H81	1.98	0.44
1:A:230:GLU:OE1	1:A:263:TYR:OH	2.34	0.44
1:A:12:LYS:CE	1:A:54:VAL:HG13	2.38	0.43
1:A:49:PHE:O	1:A:52:THR:N	2.46	0.43
1:A:234:LEU:O	1:A:238:LEU:HB2	2.18	0.43
1:A:10:ARG:HH22	1:A:255:ASP:CG	2.25	0.43
1:A:299:PRO:C	1:A:301:ASP:N	2.73	0.43
1:A:383:GLU:HB3	1:A:384:PRO:HD3	2.00	0.43
1:A:168:CYS:C	1:A:170:GLN:H	2.26	0.43
1:A:315:VAL:CG1	1:A:316:CYS:N	2.81	0.43
1:A:136:LYS:HD3	1:A:136:LYS:HA	1.82	0.43
1:A:257:ARG:HH21	1:A:287:SER:CB	2.25	0.43
1:A:107:ASP:O	1:A:147:PRO:HG3	2.19	0.43
1:A:219:LEU:HD12	1:A:235:VAL:HG23	1.99	0.43
1:A:303:PRO:HB2	1:A:304:SER:H	1.62	0.43
1:A:512:ASP:O	1:A:515:THR:HG22	2.18	0.43
1:A:394:LEU:CD1	1:A:398:LEU:HD11	2.48	0.43
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.44	0.43
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.86	0.43
1:A:415:VAL:HG11	1:A:473:VAL:CG2	2.49	0.43
1:A:420:THR:HG23	1:A:530:VAL:HG11	2.00	0.43
1:A:502:PHE:HE1	2:A:1005:MYR:H142	1.83	0.43
1:A:160:ARG:HH22	1:A:188:GLU:CD	2.26	0.42
1:A:330:PHE:HZ	1:A:377:PHE:CE2	2.37	0.42
1:A:463:LEU:N	1:A:463:LEU:HD23	2.34	0.42
1:A:503:ASN:O	1:A:504:ALA:C	2.62	0.42
1:A:384:PRO:O	1:A:388:ILE:HG12	2.20	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.87	0.42
1:A:395:PHE:CZ	1:A:435:SER:HA	2.54	0.42
1:A:419:SER:OG	1:A:421:PRO:HD2	2.20	0.42
1:A:98:ARG:O	1:A:101:CYS:HB3	2.20	0.42
1:A:161:TYR:CD1	1:A:185:LEU:HD23	2.55	0.42
1:A:334:TYR:CE1	1:A:338:HIS:HD2	2.38	0.42
1:A:513:ILE:HG13	1:A:514:CYS:N	2.34	0.42
1:A:268:GLN:HG3	1:A:275:LEU:HD12	2.01	0.42
1:A:430:LEU:CD1	1:A:456:VAL:HG11	2.50	0.42
1:A:513:ILE:HD11	1:A:555:VAL:HG13	2.01	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.91	0.42
1:A:299:PRO:HB2	1:A:302:LEU:CD2	2.50	0.42
1:A:485:ARG:N	1:A:486:PRO:CD	2.83	0.42
1:A:344:VAL:HG22	1:A:450:GLU:OE2	2.19	0.42
1:A:382:GLU:HA	1:A:385:GLN:HB2	2.01	0.42
1:A:389:LYS:O	1:A:390:GLN:C	2.62	0.42
1:A:123:MET:HE1	2:A:1001:MYR:H41	2.01	0.42
1:A:408:LEU:HD23	1:A:526:GLN:HG2	2.02	0.42
1:A:458:ASN:CA	1:A:484:ARG:HH12	2.30	0.42
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.50	0.41
1:A:516:LEU:HD22	1:A:520:GLU:CB	2.50	0.41
1:A:582:ALA:C	1:A:584:GLY:H	2.27	0.41
1:A:15:GLY:O	1:A:19:PHE:HB2	2.20	0.41
1:A:296:ASP:OD1	1:A:297:GLU:N	2.54	0.41
1:A:472:ARG:HB3	1:A:491:LEU:HD21	2.02	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.83	0.41
1:A:420:THR:N	1:A:421:PRO:CD	2.82	0.41
1:A:49:PHE:O	1:A:50:ALA:C	2.63	0.41
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.55	0.41
1:A:457:LEU:HA	1:A:457:LEU:HD12	1.85	0.41
1:A:161:TYR:HE1	1:A:182:LEU:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:CYS:O	1:A:98:ARG:HG3	2.21	0.41
1:A:302:LEU:HA	1:A:303:PRO:HD3	1.79	0.41
1:A:417:GLN:HB3	1:A:469:VAL:CG1	2.51	0.41
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.49	0.41
1:A:506:THR:CG2	1:A:531:GLU:HG3	2.51	0.41
1:A:81:ARG:O	1:A:85:GLY:HA2	2.21	0.40
1:A:408:LEU:HD13	1:A:427:SER:HB2	2.02	0.40
1:A:156:PHE:CE2	1:A:160:ARG:HD2	2.57	0.40
1:A:287:SER:OG	2:A:1002:MYR:O2	2.33	0.40
1:A:373:VAL:O	1:A:376:GLU:HB2	2.22	0.40
1:A:532:LEU:O	1:A:532:LEU:HD12	2.21	0.40
1:A:130:ASN:OD1	1:A:133:THR:HG23	2.22	0.40
1:A:483:ASN:C	1:A:486:PRO:HD2	2.46	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	579/581 (100%)	503 (87%)	66 (11%)	10 (2%)	7 30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	303	PRO
1	A	276	LYS
1	A	312	SER
1	A	364	ALA
1	A	511	ALA
1	A	557	LYS
1	A	565	GLU

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Mol	Chain	Res	Type
1	A	299	PRO
1	A	504	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	462/508 (91%)	392 (85%)	70 (15%)	3 12

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	VAL
1	A	14	LEU
1	A	31	LEU
1	A	51	LYS
1	A	52	THR
1	A	64	LYS
1	A	65	SER
1	A	73	LYS
1	A	74	LEU
1	A	81	ARG
1	A	93	LYS
1	A	95	GLU
1	A	103	LEU
1	A	123	MET
1	A	131	GLU
1	A	132	GLU
1	A	137	LYS
1	A	166	THR
1	A	179	LEU
1	A	185	LEU
1	A	192	SER
1	A	196	GLN
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	222	ARG
1	A	230	GLU
1	A	233	LYS
1	A	235	VAL
1	A	238	LEU
1	A	262	LYS
1	A	264	ILE
1	A	274	LYS
1	A	284	LEU
1	A	287	SER
1	A	293	VAL
1	A	302	LEU
1	A	312	SER
1	A	321	GLU
1	A	329	MET
1	A	348	ARG
1	A	351	LYS
1	A	352	THR
1	A	354	GLU
1	A	356	THR
1	A	357	LEU
1	A	373	VAL
1	A	378	LYS
1	A	380	LEU
1	A	398	LEU
1	A	408	LEU
1	A	410	ARG
1	A	426	VAL
1	A	430	LEU
1	A	436	LYS
1	A	451	ASP
1	A	453	LEU
1	A	455	VAL
1	A	457	LEU
1	A	459	GLN
1	A	460	LEU
1	A	475	LYS
1	A	498	VAL
1	A	506	THR
1	A	509	PHE
1	A	514	CYS
1	A	529	LEU

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Mol	Chain	Res	Type
1	A	538	LYS
1	A	544	LEU
1	A	565	GLU
1	A	566	THR

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	105	HIS
1	A	196	GLN
1	A	268	GLN
1	A	288	HIS
1	A	295	ASN
1	A	318	ASN
1	A	338	HIS
1	A	391	ASN

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](#)

9 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	B3I	A	2001[A]	-	12,12,12	2.32	4 (33%)	15,17,17	1.08	1 (6%)
3	B3I	A	2002[A]	-	12,12,12	2.16	5 (41%)	15,17,17	1.11	1 (6%)
2	MYR	A	1001	-	13,13,15	0.62	0	13,13,15	0.74	0
2	MYR	A	1002	-	12,12,15	0.73	0	12,12,15	0.69	0
2	MYR	A	1004	-	12,12,15	0.64	0	12,12,15	0.76	0
2	MYR	A	1003	-	12,12,15	0.71	0	12,12,15	0.72	0
3	B3I	A	2001[B]	-	12,12,12	2.18	6 (50%)	15,17,17	1.53	2 (13%)
2	MYR	A	1005	-	15,15,15	0.57	0	15,15,15	0.79	0
3	B3I	A	2002[B]	-	12,12,12	1.99	3 (25%)	15,17,17	1.45	2 (13%)

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
3	B3I	A	2001[A]	-	-	4/4/4/4	0/1/1/1
3	B3I	A	2002[A]	-	-	4/4/4/4	0/1/1/1
2	MYR	A	1001	-	-	5/11/11/13	-
2	MYR	A	1002	-	-	3/10/10/13	-
2	MYR	A	1004	-	-	7/10/10/13	-
2	MYR	A	1003	-	-	7/10/10/13	-
3	B3I	A	2001[B]	-	-	4/4/4/4	0/1/1/1
2	MYR	A	1005	-	-	6/13/13/13	-
3	B3I	A	2002[B]	-	-	4/4/4/4	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001[A]	B3I	C1-C	-4.48	1.40	1.49
3	A	2002[B]	B3I	C1-C	-4.07	1.40	1.49
3	A	2001[B]	B3I	C1-C	-4.05	1.41	1.49
3	A	2001[A]	B3I	C2-I1	-3.80	2.02	2.09
3	A	2002[A]	B3I	C1-C	-3.64	1.41	1.49
3	A	2001[A]	B3I	C5-I3	-3.59	2.00	2.10
3	A	2002[A]	B3I	C2-I1	-3.00	2.04	2.09
3	A	2001[B]	B3I	C2-I1	-2.77	2.04	2.09
3	A	2002[B]	B3I	C2-I1	-2.68	2.04	2.09
3	A	2001[A]	B3I	C2-C3	2.67	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001[B]	B3I	C3-I2	-2.53	2.04	2.10
3	A	2002[A]	B3I	C5-I3	-2.52	2.03	2.10
3	A	2001[B]	B3I	C6-C1	2.44	1.43	1.39
3	A	2001[B]	B3I	C6-C5	2.40	1.43	1.38
3	A	2002[A]	B3I	C1-C2	2.28	1.44	1.40
3	A	2002[A]	B3I	C3-I2	-2.27	2.05	2.10
3	A	2001[B]	B3I	C1-C2	2.07	1.43	1.40
3	A	2002[B]	B3I	C3-I2	-2.05	2.05	2.10

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001[B]	B3I	C2-C3-I2	-3.95	119.42	122.87
3	A	2002[B]	B3I	C2-C3-I2	-3.62	119.71	122.87
3	A	2001[B]	B3I	C3-C2-I1	-2.69	118.80	121.17
3	A	2001[A]	B3I	C4-C3-C2	-2.20	119.46	121.10
3	A	2002[A]	B3I	C2-C3-I2	-2.19	120.96	122.87
3	A	2002[B]	B3I	O2-C-O1	-2.02	119.01	123.35

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	MYR	C1-C2-C3-C4
2	A	1002	MYR	C2-C3-C4-C5
2	A	1004	MYR	C1-C2-C3-C4
2	A	1003	MYR	C6-C7-C8-C9
2	A	1003	MYR	C5-C6-C7-C8
2	A	1005	MYR	C1-C2-C3-C4
2	A	1001	MYR	C4-C5-C6-C7
3	A	2002[A]	B3I	O2-C-C1-C2
3	A	2002[B]	B3I	O2-C-C1-C2
2	A	1001	MYR	C2-C3-C4-C5
2	A	1005	MYR	C10-C11-C12-C13
3	A	2001[A]	B3I	O1-C-C1-C2
3	A	2002[A]	B3I	O1-C-C1-C2
2	A	1005	MYR	C4-C5-C6-C7
2	A	1004	MYR	C2-C3-C4-C5
3	A	2002[B]	B3I	O1-C-C1-C2
2	A	1003	MYR	C11-C10-C9-C8
2	A	1004	MYR	C4-C5-C6-C7
3	A	2001[A]	B3I	O2-C-C1-C2

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Mol	Chain	Res	Type	Atoms
2	A	1001	MYR	C5-C6-C7-C8
3	A	2001[B]	B3I	O1-C-C1-C2
2	A	1005	MYR	C6-C7-C8-C9
2	A	1004	MYR	C6-C7-C8-C9
3	A	2001[B]	B3I	O2-C-C1-C2
3	A	2001[B]	B3I	O2-C-C1-C6
2	A	1004	MYR	C11-C10-C9-C8
3	A	2001[B]	B3I	O1-C-C1-C6
3	A	2001[A]	B3I	O1-C-C1-C6
3	A	2001[A]	B3I	O2-C-C1-C6
3	A	2002[B]	B3I	O2-C-C1-C6
2	A	1003	MYR	C4-C5-C6-C7
2	A	1005	MYR	C11-C10-C9-C8
2	A	1003	MYR	O1-C1-C2-C3
2	A	1003	MYR	O2-C1-C2-C3
2	A	1002	MYR	O2-C1-C2-C3
3	A	2002[A]	B3I	O2-C-C1-C6
2	A	1004	MYR	O2-C1-C2-C3
3	A	2002[B]	B3I	O1-C-C1-C6
2	A	1002	MYR	O1-C1-C2-C3
2	A	1004	MYR	O1-C1-C2-C3
2	A	1001	MYR	O2-C1-C2-C3
3	A	2002[A]	B3I	O1-C-C1-C6
2	A	1001	MYR	O1-C1-C2-C3
2	A	1005	MYR	C2-C3-C4-C5

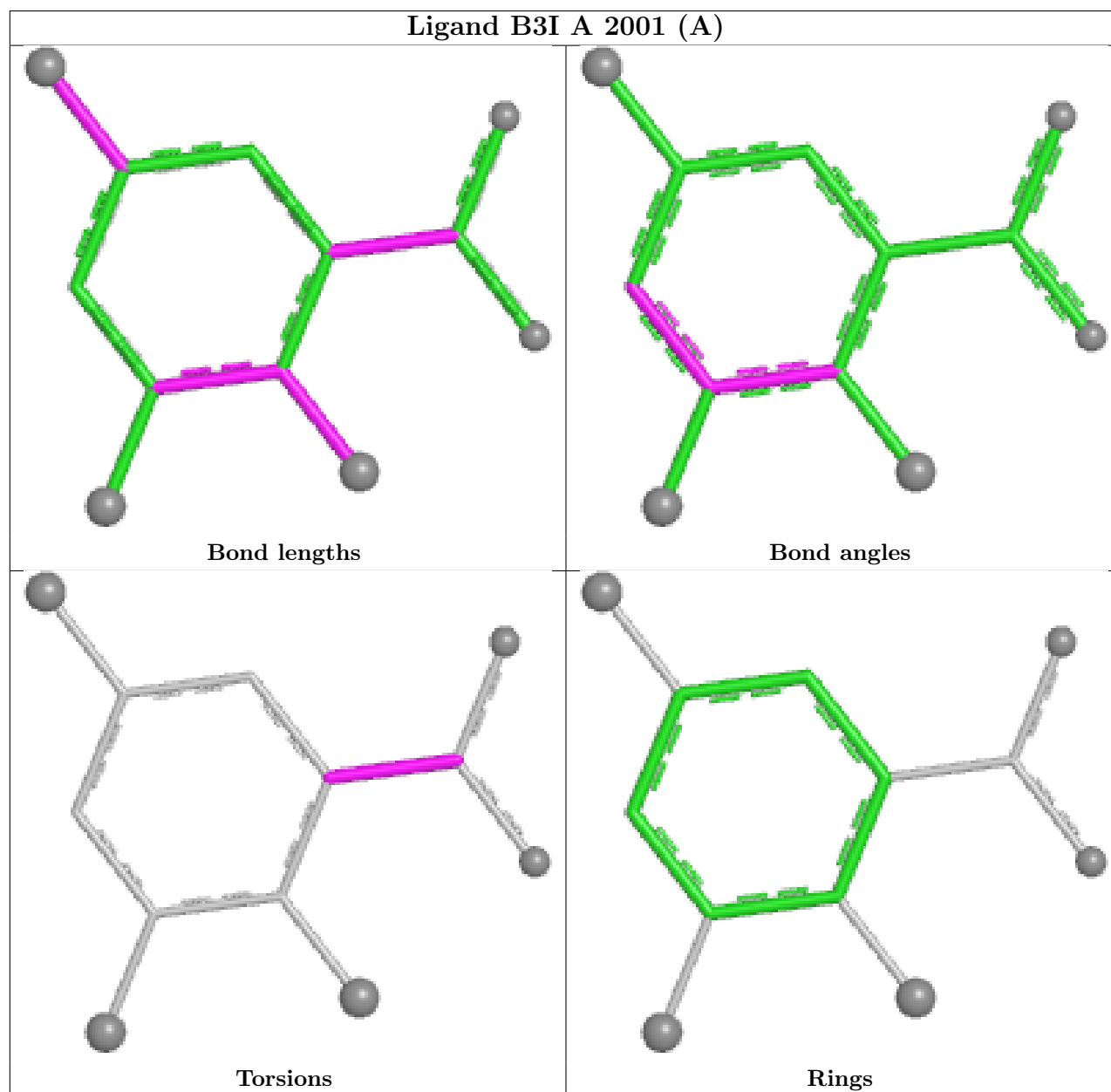
There are no ring outliers.

8 monomers are involved in 23 short contacts:

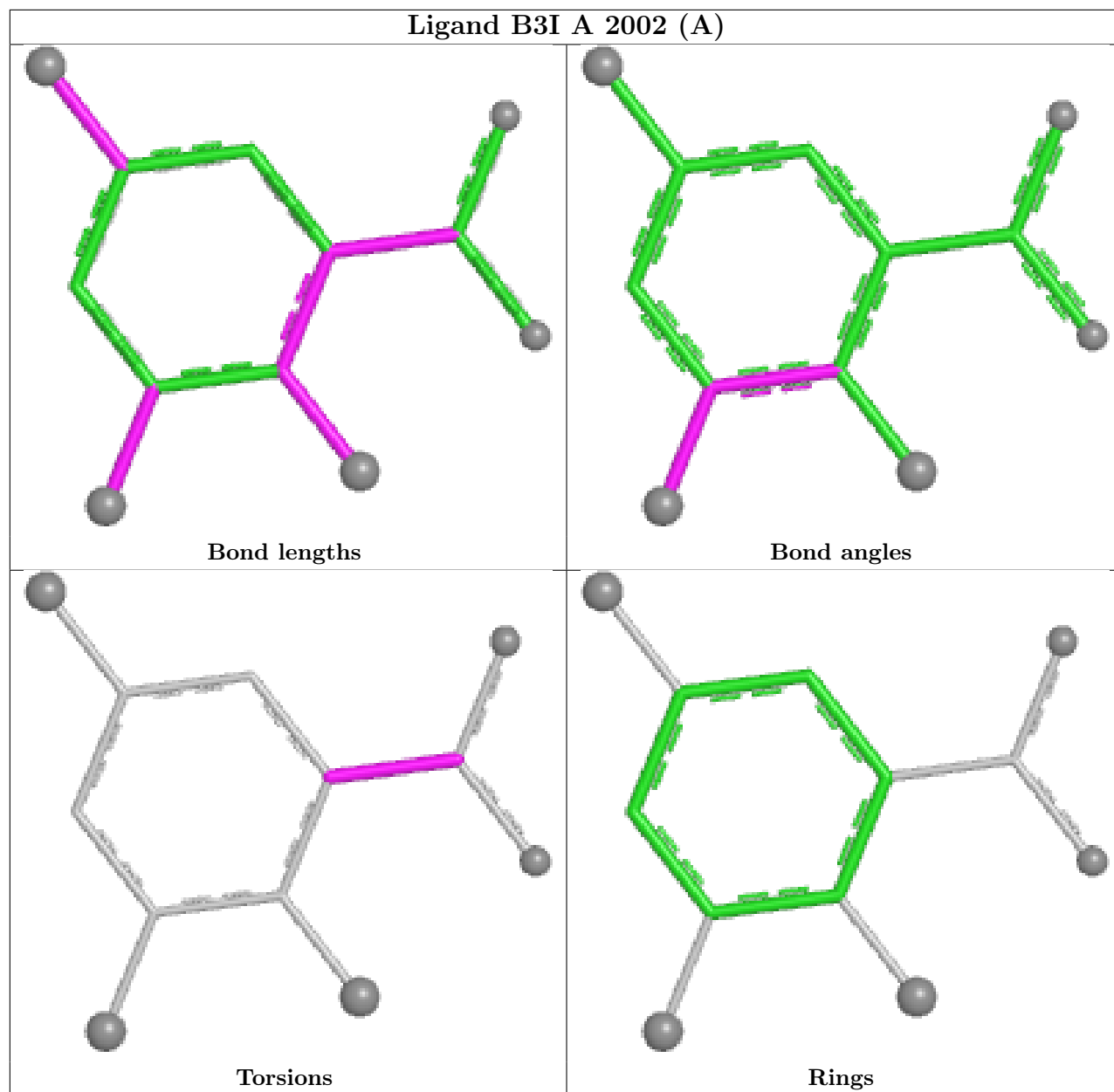
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001[A]	B3I	2	0
3	A	2002[A]	B3I	4	0
2	A	1001	MYR	5	0
2	A	1002	MYR	2	0
2	A	1003	MYR	2	0
3	A	2001[B]	B3I	1	0
2	A	1005	MYR	3	0
3	A	2002[B]	B3I	6	0

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

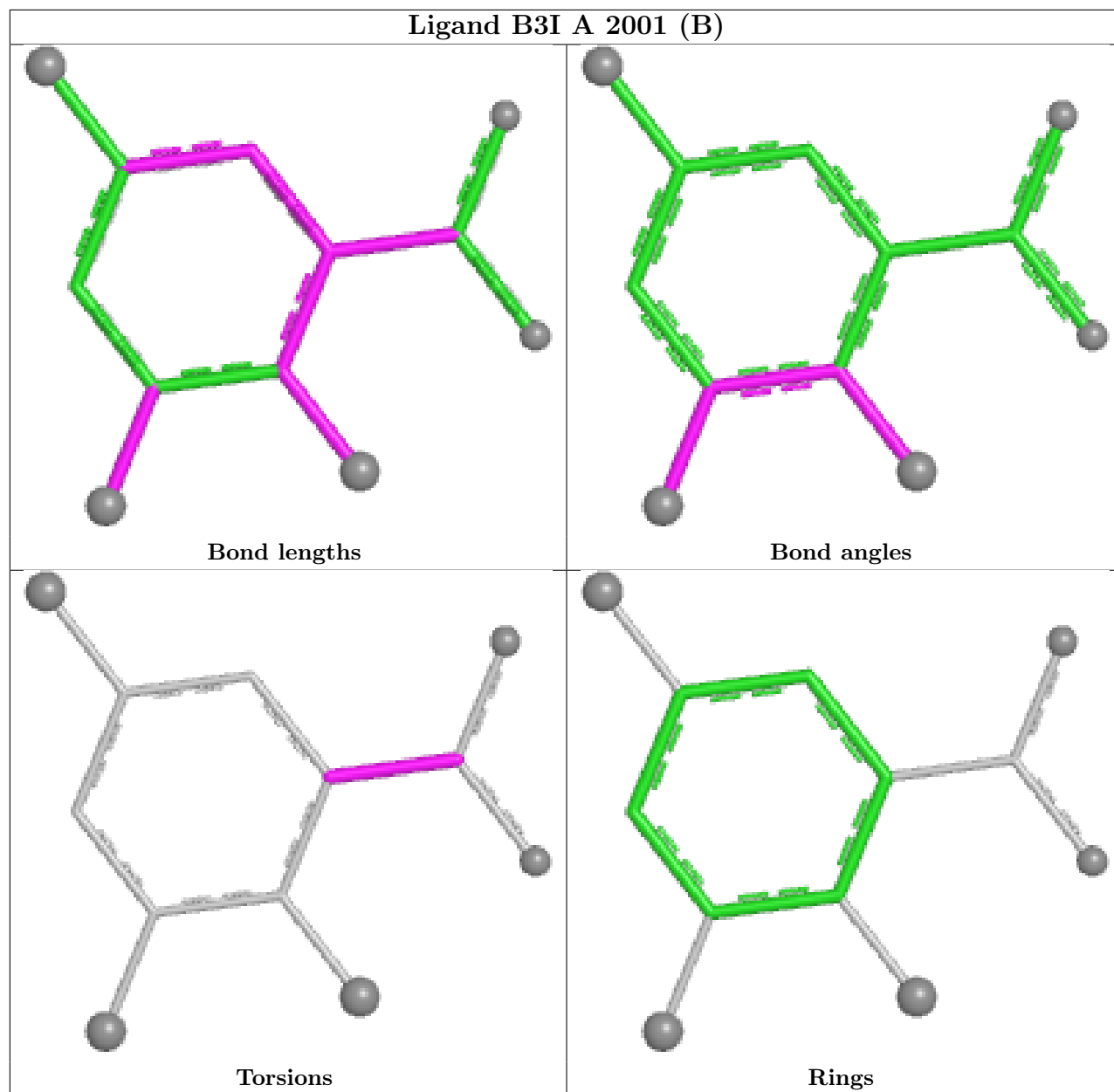
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

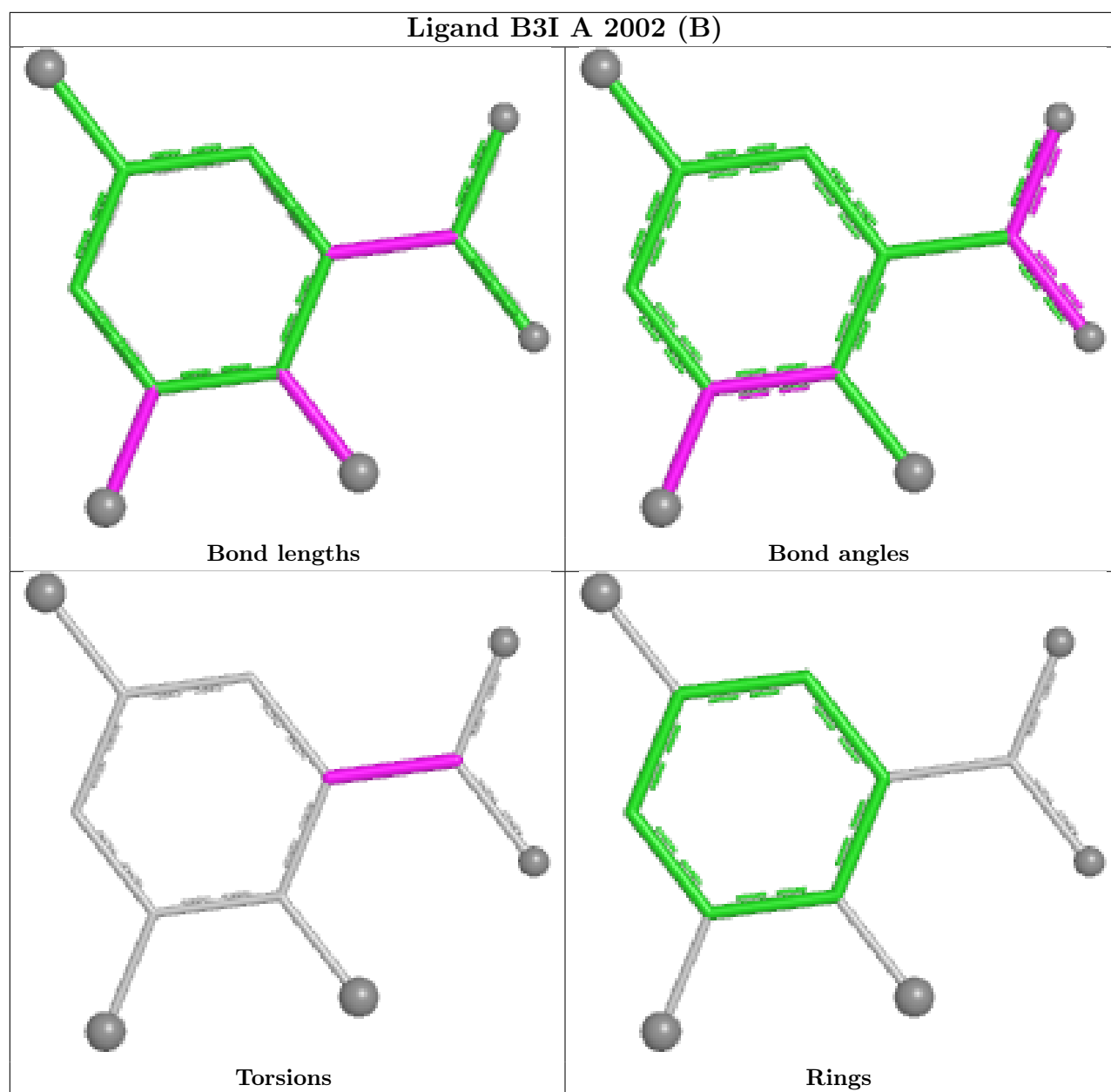


Ligand B3I A 2002 (A)



Ligand B3I A 2001 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/581 (100%)	-0.51	1 (0%) 91 84	17, 53, 98, 136	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	B3I	A	2002[A]	12/12	0.87	0.13	50,50,50,50	12
3	B3I	A	2002[B]	12/12	0.87	0.13	50,50,50,50	12
2	MYR	A	1001	14/16	0.88	0.11	60,60,60,60	0
2	MYR	A	1002	13/16	0.88	0.12	61,61,61,61	0
2	MYR	A	1004	13/16	0.90	0.09	51,51,51,51	0
2	MYR	A	1003	13/16	0.91	0.09	48,48,48,48	0

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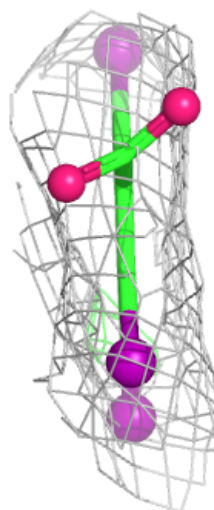
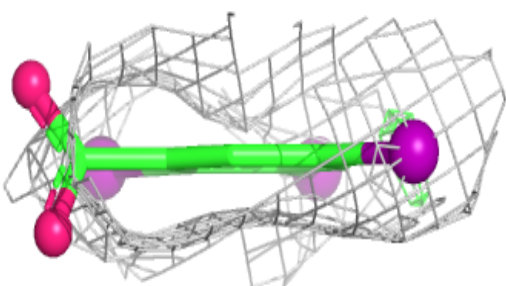
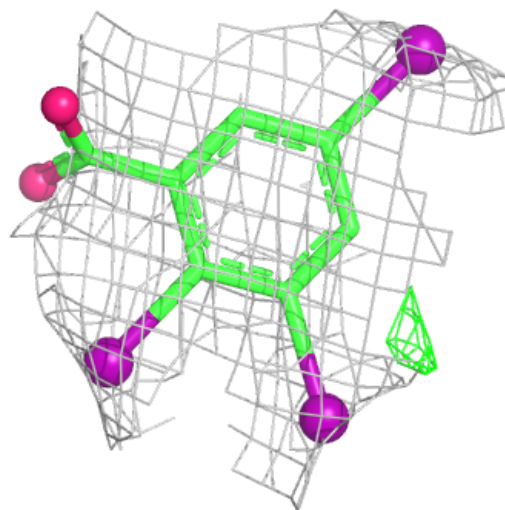
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MYR	A	1005	16/16	0.91	0.10	52,52,52,52	0
3	B3I	A	2001[A]	12/12	0.98	0.07	50,50,50,50	12
3	B3I	A	2001[B]	12/12	0.98	0.07	50,50,50,50	12

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.

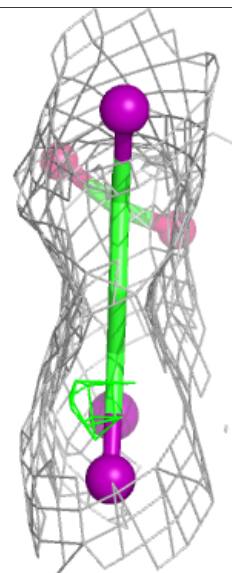
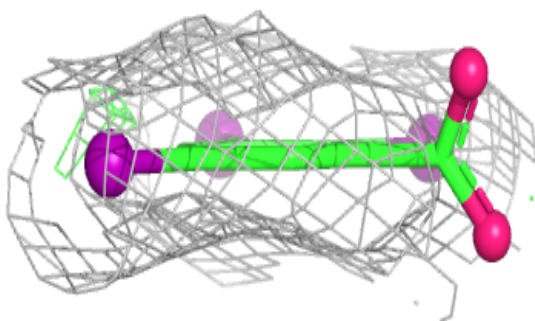
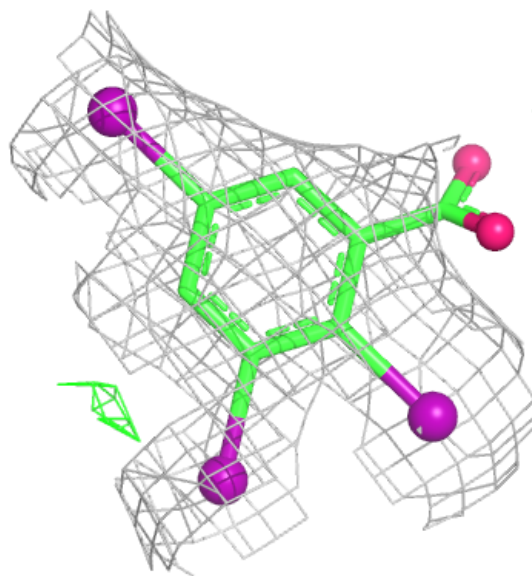
Electron density around B3I A 2002 (A):

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



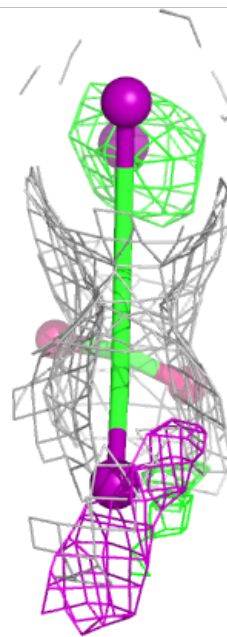
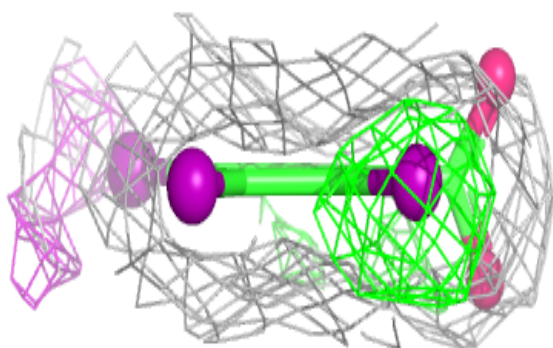
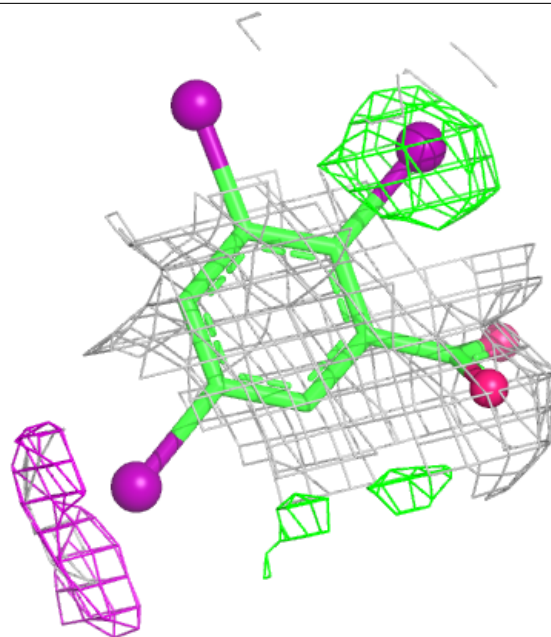
Electron density around B3I A 2002 (B):

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



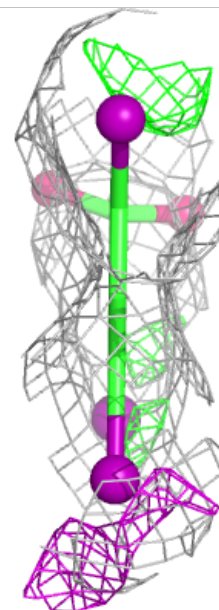
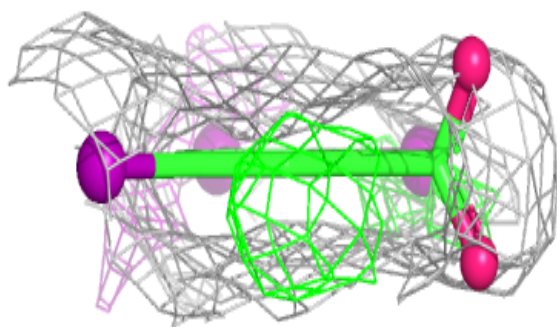
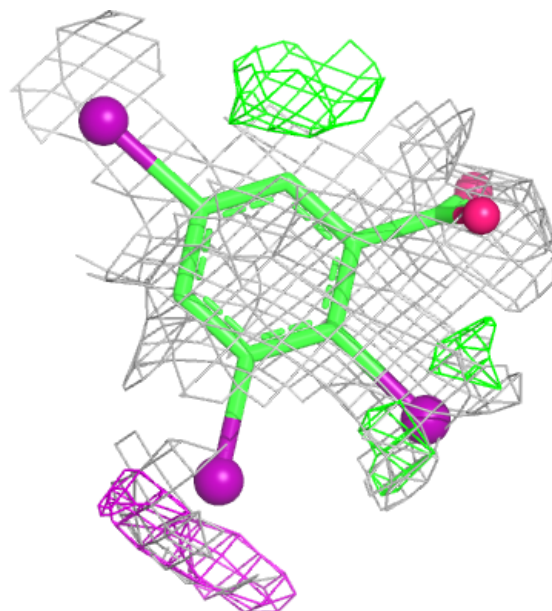
Electron density around B3I A 2001 (A):

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



Electron density around B3I A 2001 (B):

$2mF_o-DF_c$ (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.