



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:50 AM UTC

PDB ID : 2Y3P / pdb_00002y3p
Title : Crystal structure of N-terminal domain of GyrA with the antibiotic simocyclinone D8
Authors : Edwards, M.J.; Flatman, R.H.; Mitchenall, L.A.; Stevenson, C.E.M.; Le, T.B.K.; Clarke, T.A.; McKay, A.R.; Fiedler, H.-P.; Buttner, M.J.; Lawson, D.M.; Maxwell, A.
Deposited on : 2010-12-22
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	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

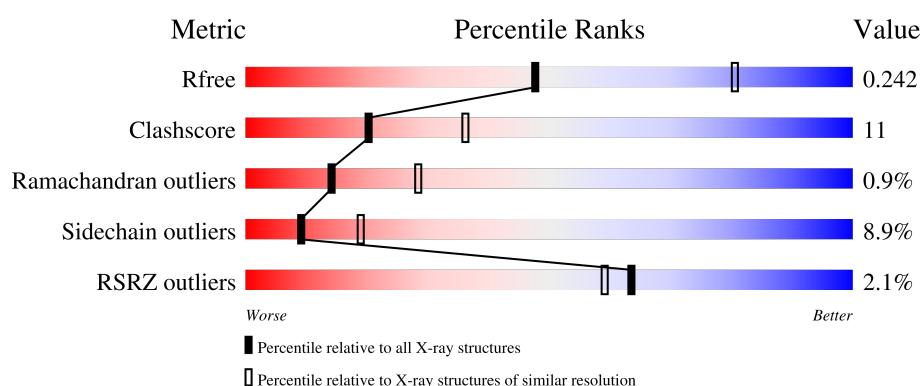
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	522	2% 66% 26% • 5%
1	B	522	2% 73% 21% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7953 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.

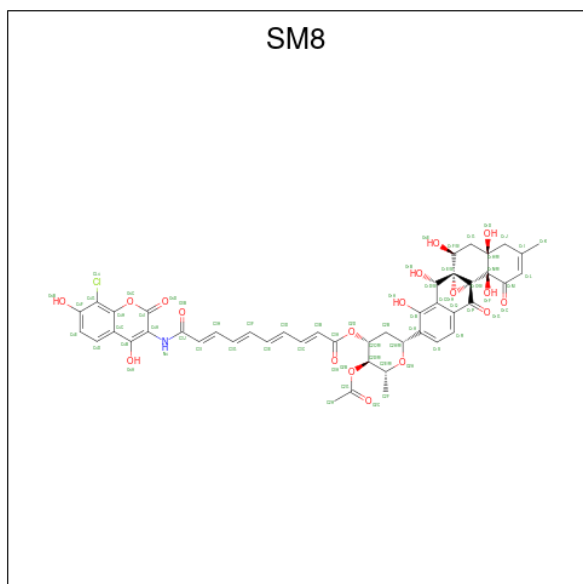
- Molecule 1 is a protein called DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3845	2415	688	727	15			
1	B	506	Total	C	N	O	S	0	0	0
			3876	2436	694	731	15			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SIMOCYCLINONE D8 (CCD ID: SM8) (formula: C₄₆H₄₂ClNO₁₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			66	46	1	1	18		
3	B	1	Total	C	Cl	N	O	0	0
			66	46	1	1	18		

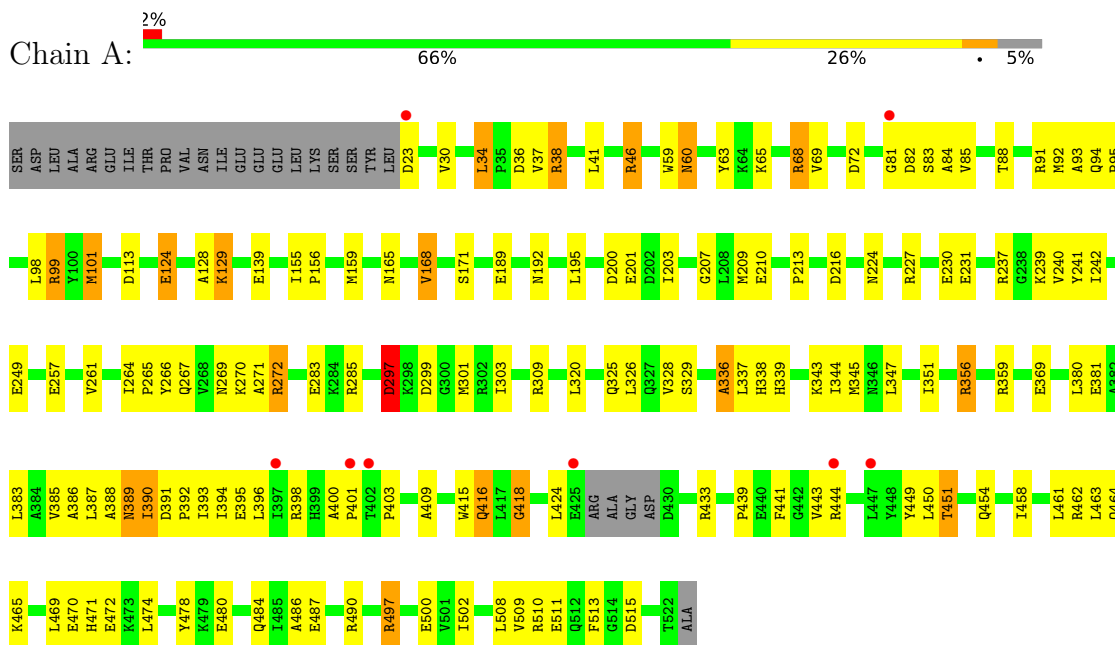
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	50	Total	O	0	0
			50	50		

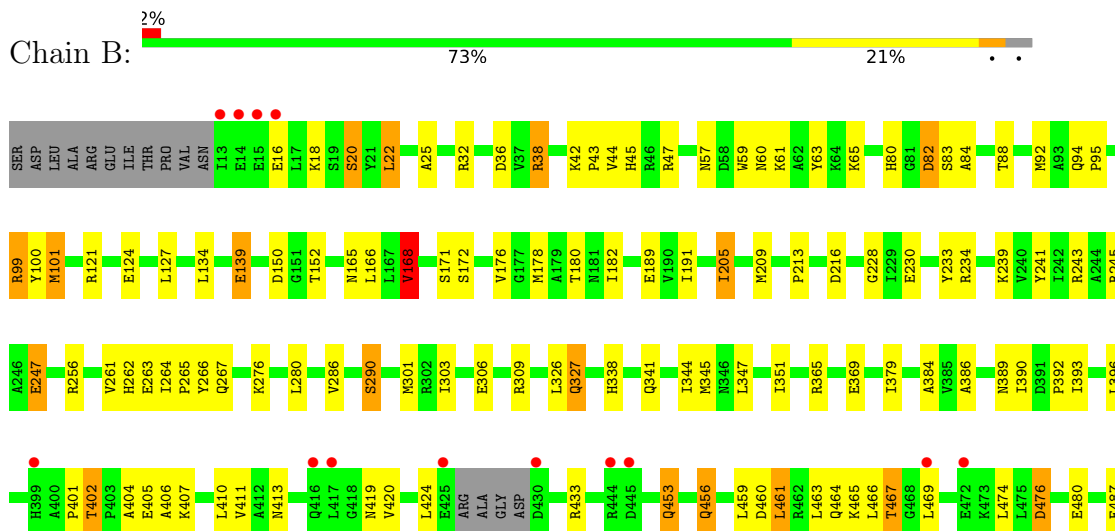
3 Residue-property plots

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: DNA GYRASE SUBUNIT A



• Molecule 1: DNA GYRASE SUBUNIT A





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.91Å 153.09Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.47 – 2.62 27.47 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.47-2.62) 99.6 (27.47-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	2967 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SM8, MG

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	1.09	4/3906 (0.1%)	1.20	11/5296 (0.2%)
1	B	1.11	4/3938 (0.1%)	1.21	7/5344 (0.1%)
All	All	1.10	8/7844 (0.1%)	1.21	18/10640 (0.2%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	VAL	CA-CB	-6.38	1.47	1.54
1	B	25	ALA	CA-CB	-6.20	1.43	1.53
1	B	247	GLU	N-CA	5.59	1.52	1.45
1	B	80	HIS	C-O	5.44	1.30	1.23
1	A	336	ALA	CA-CB	-5.43	1.45	1.53
1	A	81	GLY	C-O	5.37	1.30	1.23
1	B	521	ILE	CA-CB	5.12	1.60	1.54
1	A	93	ALA	CA-CB	-5.12	1.46	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	SER	N-CA-C	8.42	121.39	108.42
1	A	165	ASN	N-CA-C	6.62	118.50	111.28
1	B	82	ASP	N-CA-CB	6.19	119.28	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	GLU	N-CA-C	6.16	120.27	112.87
1	B	413	ASN	CA-C-N	-6.05	113.45	119.92
1	B	413	ASN	C-N-CA	-6.05	113.45	119.92
1	A	400	ALA	N-CA-C	5.62	118.15	110.01
1	A	46	ARG	N-CA-C	-5.56	105.22	111.28
1	B	168	VAL	CB-CA-C	5.54	119.28	112.02
1	A	497	ARG	N-CA-C	-5.50	105.36	111.36
1	A	94	GLN	N-CA-C	5.48	116.86	109.24
1	A	297	ASP	CB-CA-C	-5.43	99.83	111.78
1	A	385	VAL	N-CA-C	-5.33	105.65	110.82
1	A	69	VAL	N-CA-C	-5.32	105.21	111.00
1	A	433	ARG	CA-C-N	-5.27	114.33	119.76
1	A	433	ARG	C-N-CA	-5.27	114.33	119.76
1	A	168	VAL	N-CA-C	-5.16	105.51	110.72
1	B	165	ASN	N-CA-C	5.14	116.88	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ASP	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	3845	0	3808	97	0
1	B	3876	0	3801	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	66	0	39	3	0
3	B	66	0	38	1	0
4	A	46	0	0	3	0
4	B	50	0	0	0	0
All	All	7953	0	7686	176	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 11.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HG3	1:A:68:ARG:HH11	0.98	1.11
1:A:270:LYS:HD3	1:A:301:MET:HE3	1.40	1.01
1:A:387:LEU:O	1:A:390:ILE:HG13	1.66	0.96
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.30	0.95
1:A:68:ARG:HH11	1:A:68:ARG:CG	1.81	0.94
1:A:68:ARG:HG3	1:A:68:ARG:NH1	1.79	0.93
1:A:297:ASP:HB2	1:A:299:ASP:H	1.35	0.92
1:A:390:ILE:O	1:A:394:ILE:HG12	1.71	0.91
1:B:101:MET:HE3	1:B:101:MET:H	1.33	0.89
1:B:209:MET:HE1	1:B:230:GLU:HG2	1.56	0.86
1:B:99:ARG:NH1	1:B:216:ASP:OD2	2.11	0.83
1:A:444:ARG:HH21	1:A:449:TYR:CB	1.91	0.82
1:A:297:ASP:CB	1:A:299:ASP:H	1.94	0.80
1:A:356:ARG:HD3	1:A:359:ARG:HH12	1.46	0.79
1:B:205:ILE:HD13	1:B:234:ARG:HA	1.65	0.79
1:A:388:ALA:C	1:A:389:ASN:HD22	1.92	0.77
1:A:356:ARG:HD3	1:A:359:ARG:NH1	2.02	0.74
1:B:266:TYR:O	1:B:267:GLN:HB2	1.88	0.73
1:B:101:MET:H	1:B:101:MET:CE	2.01	0.73
1:B:38:ARG:CG	1:B:38:ARG:HH11	2.03	0.71
1:A:68:ARG:CG	1:A:68:ARG:NH1	2.47	0.71
1:A:451:THR:H	1:A:454:GLN:HE21	1.37	0.70
1:B:63:TYR:HB3	1:B:124:GLU:HB3	1.73	0.70
1:A:171:SER:HB2	4:A:2025:HOH:O	1.93	0.68
1:A:34:LEU:HD23	1:A:337:LEU:HB2	1.74	0.67
1:A:200:ASP:O	1:A:203:ILE:HG22	1.95	0.67
1:A:207:GLY:O	1:A:210:GLU:HG2	1.94	0.66
1:A:444:ARG:NH2	1:A:449:TYR:CB	2.59	0.65
1:B:280:LEU:HB3	1:B:286:VAL:HG23	1.76	0.65
1:A:487:GLU:OE1	1:A:490:ARG:NH2	2.30	0.64
1:A:389:ASN:HD22	1:A:389:ASN:N	1.94	0.64
1:A:92:MET:HA	1:A:98:LEU:HD22	1.78	0.64
1:A:113:ASP:OD1	1:A:270:LYS:HB3	1.98	0.64
1:A:386:ALA:HB2	1:A:458:ILE:HG12	1.80	0.64
1:A:386:ALA:HA	1:A:393:ILE:CD1	2.28	0.63
1:A:387:LEU:O	1:A:390:ILE:CG1	2.43	0.63
1:B:20:SER:HB3	1:B:22:LEU:H	1.63	0.63
1:A:297:ASP:HB2	1:A:299:ASP:N	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:SER:HB3	1:B:22:LEU:HB2	1.82	0.61
1:A:113:ASP:HB3	1:A:271:ALA:HB2	1.83	0.60
1:B:43:PRO:O	1:B:47:ARG:HG3	2.00	0.60
1:A:325:GLN:HG3	4:A:2034:HOH:O	2.02	0.60
1:A:266:TYR:O	1:A:267:GLN:HB2	2.01	0.59
1:B:59:TRP:CE2	1:B:60:ASN:HB3	2.37	0.59
1:A:403:PRO:HD3	1:B:467:THR:HG21	1.85	0.59
1:A:129:LYS:HZ2	1:A:513:PHE:HZ	1.48	0.59
1:A:451:THR:H	1:A:454:GLN:NE2	2.01	0.58
1:B:338:HIS:HB2	1:B:345:MET:CE	2.34	0.58
1:B:100:TYR:CE2	1:B:168:VAL:HG22	2.38	0.58
1:A:155:ILE:CG2	1:A:156:PRO:HD2	2.34	0.57
1:A:209:MET:HE1	1:A:230:GLU:HG2	1.86	0.57
1:B:189:GLU:OE1	1:B:213:PRO:HD2	2.04	0.57
1:B:36:ASP:OD1	1:B:38:ARG:HG2	2.04	0.57
1:A:486:ALA:O	1:A:490:ARG:HG3	2.05	0.56
1:B:38:ARG:CG	1:B:38:ARG:NH1	2.67	0.56
1:A:99:ARG:NH1	1:A:216:ASP:OD2	2.38	0.56
1:A:416:GLN:HE22	1:A:418:GLY:HA2	1.70	0.56
1:B:150:ASP:OD1	1:B:152:THR:HB	2.06	0.56
1:B:36:ASP:OD2	1:B:38:ARG:NH1	2.39	0.56
1:A:336:ALA:HB3	1:A:345:MET:HE3	1.88	0.55
1:B:42:LYS:HG3	1:B:45:HIS:CE1	2.42	0.54
1:B:38:ARG:HH11	1:B:38:ARG:HG2	1.71	0.54
1:A:463:LEU:HD22	1:B:461:LEU:CD2	2.38	0.54
1:B:338:HIS:HB2	1:B:345:MET:HE1	1.89	0.54
1:A:383:LEU:HD22	1:A:461:LEU:HD13	1.91	0.53
1:B:262:HIS:O	1:B:301:MET:HB3	2.09	0.52
1:B:384:ALA:C	1:B:420:VAL:HG21	2.35	0.52
1:A:88:THR:HG22	1:A:92:MET:HE2	1.92	0.52
1:A:359:ARG:HA	1:A:502:ILE:HD11	1.92	0.51
1:B:365:ARG:O	1:B:369:GLU:HG2	2.10	0.51
1:A:82:ASP:C	1:A:84:ALA:H	2.17	0.51
1:B:38:ARG:NH1	1:B:38:ARG:HG3	2.26	0.51
1:A:231:GLU:HG2	1:A:237:ARG:O	2.12	0.50
1:A:261:VAL:HB	1:A:303:ILE:HB	1.94	0.50
1:B:243:ARG:NH1	1:B:327:GLN:OE1	2.45	0.50
1:B:99:ARG:HG3	1:B:100:TYR:CE2	2.47	0.50
1:B:261:VAL:HB	1:B:303:ILE:HD12	1.94	0.50
1:A:63:TYR:HB3	1:A:124:GLU:HG3	1.92	0.49
1:B:20:SER:C	1:B:22:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASN:O	1:B:392:PRO:HD2	2.11	0.49
1:A:59:TRP:CE3	1:A:129:LYS:HG3	2.47	0.49
1:B:407:LYS:HE2	1:B:456:GLN:HE21	1.77	0.49
1:B:476:ASP:O	1:B:480:GLU:HG3	2.13	0.49
1:B:88:THR:HG22	1:B:92:MET:HE2	1.95	0.49
1:B:402:THR:HG22	1:B:404:ALA:N	2.28	0.49
1:B:233:TYR:CG	1:B:347:LEU:HD22	2.48	0.49
1:A:465:LYS:O	1:A:470:GLU:HB2	2.14	0.48
1:B:384:ALA:O	1:B:420:VAL:HG21	2.14	0.48
1:B:396:LEU:HD12	1:B:396:LEU:O	2.12	0.48
1:B:406:ALA:O	1:B:410:LEU:HG	2.13	0.48
1:B:65:LYS:HD3	1:B:124:GLU:HG3	1.96	0.48
1:A:264:ILE:CG2	1:A:301:MET:HE1	2.44	0.48
1:B:407:LYS:HE2	1:B:456:GLN:NE2	2.28	0.48
1:A:464:GLN:HB3	1:B:459:LEU:HB3	1.94	0.48
1:B:172:SER:HA	1:B:180:THR:O	2.14	0.48
1:A:155:ILE:HG23	1:A:156:PRO:HD2	1.96	0.47
1:B:38:ARG:HH11	1:B:38:ARG:HG3	1.77	0.47
1:A:41:LEU:HB2	1:A:46:ARG:NH1	2.29	0.47
1:A:60:ASN:C	1:A:60:ASN:HD22	2.22	0.47
1:A:497:ARG:NH1	1:A:500:GLU:OE1	2.40	0.47
1:A:269:ASN:HB3	1:A:272:ARG:HB2	1.97	0.47
1:A:387:LEU:C	1:A:390:ILE:HG13	2.38	0.47
1:A:36:ASP:HA	1:A:337:LEU:HB3	1.97	0.47
1:A:91:ARG:HD2	3:A:901:SM8:HN4	1.80	0.47
3:A:901:SM8:H22H	3:A:901:SM8:H2D	1.83	0.47
1:B:290:SER:OG	1:B:306:GLU:HG2	2.14	0.47
1:B:386:ALA:HA	1:B:393:ILE:CD1	2.45	0.46
1:A:95:PRO:HA	1:A:101:MET:SD	2.55	0.46
1:A:470:GLU:O	1:A:471:HIS:C	2.58	0.46
1:B:453:GLN:O	1:B:456:GLN:HB2	2.15	0.46
3:A:901:SM8:O1A	3:A:901:SM8:O1B	2.28	0.46
1:B:487:GLU:OE1	1:B:490:ARG:NH2	2.35	0.46
1:B:386:ALA:HA	1:B:393:ILE:HD11	1.97	0.46
1:A:272:ARG:HD3	1:A:272:ARG:HA	1.69	0.45
1:A:23:ASP:OD1	1:A:23:ASP:C	2.59	0.45
1:A:242:ILE:HB	1:A:265:PRO:HB3	1.99	0.45
1:A:309:ARG:HA	1:A:309:ARG:HD2	1.65	0.45
1:A:320:LEU:HB3	1:A:326:LEU:HD12	1.98	0.45
1:B:256:ARG:HD2	1:B:309:ARG:HD3	1.98	0.45
1:A:128:ALA:O	1:A:129:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:HB3	1:B:263:GLU:HB2	1.99	0.45
1:A:387:LEU:O	1:A:390:ILE:CD1	2.65	0.45
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.10	0.44
1:B:59:TRP:HA	1:B:127:LEU:O	2.16	0.44
1:A:396:LEU:HD21	1:A:409:ALA:HB1	1.99	0.44
1:A:189:GLU:OE1	1:A:213:PRO:HD2	2.16	0.44
1:B:379:ILE:HD11	1:B:453:GLN:NE2	2.32	0.44
1:A:415:TRP:HA	4:A:2039:HOH:O	2.17	0.44
1:A:480:GLU:O	1:A:484:GLN:HG3	2.16	0.44
1:A:239:LYS:HE3	1:A:329:SER:CB	2.48	0.44
1:B:166:LEU:HD11	1:B:182:ILE:HD12	1.98	0.44
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.87	0.43
1:B:178:MET:HE3	1:B:178:MET:HB2	1.88	0.43
1:B:228:GLY:HA3	1:B:239:LYS:O	2.18	0.43
1:A:391:ASP:HB2	1:A:392:PRO:HD3	2.00	0.43
1:B:209:MET:CE	1:B:230:GLU:HG2	2.37	0.43
1:A:439:PRO:C	1:A:441:PHE:H	2.27	0.43
1:A:338:HIS:HB2	1:A:345:MET:CE	2.49	0.43
1:B:82:ASP:C	1:B:84:ALA:N	2.76	0.43
1:B:99:ARG:NH2	1:B:515:ASP:OD2	2.51	0.43
1:A:155:ILE:HG22	1:A:156:PRO:HD2	2.00	0.43
1:A:462:ARG:HG2	1:B:460:ASP:O	2.19	0.43
1:A:347:LEU:O	1:A:351:ILE:HG12	2.18	0.43
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.81	0.43
1:B:82:ASP:C	1:B:84:ALA:H	2.26	0.43
1:B:139:GLU:CD	1:B:139:GLU:H	2.27	0.43
1:B:465:LYS:C	1:B:467:THR:H	2.27	0.43
1:A:249:GLU:O	1:A:257:GLU:HA	2.18	0.42
1:B:389:ASN:O	1:B:390:ILE:C	2.62	0.42
1:B:402:THR:HG22	1:B:405:GLU:H	1.83	0.42
1:B:396:LEU:HD12	1:B:396:LEU:C	2.44	0.42
1:A:469:LEU:O	1:A:469:LEU:HG	2.19	0.42
1:A:82:ASP:C	1:A:84:ALA:N	2.75	0.42
1:A:386:ALA:HA	1:A:393:ILE:HD11	2.01	0.42
1:A:192:ASN:HA	1:A:195:LEU:HD12	2.01	0.42
1:A:283:GLU:C	1:A:285:ARG:H	2.28	0.41
1:A:338:HIS:O	1:A:339:HIS:C	2.62	0.41
3:B:901:SM8:H22H	3:B:901:SM8:H2D	1.87	0.41
1:A:490:ARG:HB3	1:A:490:ARG:NH1	2.35	0.41
1:A:46:ARG:HG3	1:A:159:MET:HE2	2.03	0.41
1:B:402:THR:CG2	1:B:404:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ALA:CB	1:A:458:ILE:HG12	2.48	0.41
1:B:94:GLN:HA	1:B:95:PRO:HD3	1.96	0.41
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.93	0.41
1:B:338:HIS:HB2	1:B:345:MET:HE2	2.03	0.41
1:A:37:VAL:HG13	1:A:38:ARG:N	2.35	0.41
1:B:379:ILE:HD11	1:B:453:GLN:HE21	1.86	0.41
1:B:401:PRO:HD2	1:B:405:GLU:CB	2.49	0.41
1:A:395:GLU:HA	1:A:395:GLU:OE1	2.21	0.41
1:B:59:TRP:CZ2	1:B:60:ASN:HB3	2.56	0.41
1:B:264:ILE:HB	1:B:265:PRO:CD	2.51	0.41
1:B:241:TYR:CD1	1:B:241:TYR:N	2.89	0.40
1:A:381:GLU:HG3	1:A:478:TYR:HE2	1.87	0.40
1:A:240:VAL:CG1	1:A:241:TYR:N	2.83	0.40
1:A:99:ARG:NH2	1:A:515:ASP:OD1	2.54	0.40
1:B:419:ASN:H	1:B:419:ASN:HD22	1.70	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	492/522 (94%)	452 (92%)	36 (7%)	4 (1%)	16	31
1	B	502/522 (96%)	466 (93%)	31 (6%)	5 (1%)	12	26
All	All	994/1044 (95%)	918 (92%)	67 (7%)	9 (1%)	14	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	GLY
1	A	401	PRO
1	B	83	SER

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Mol	Chain	Res	Type
1	A	83	SER
1	B	464	GLN
1	B	466	LEU
1	B	469	LEU
1	B	18	LYS
1	A	390	ILE

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	396/437 (91%)	361 (91%)	35 (9%)	9	19
1	B	392/437 (90%)	357 (91%)	35 (9%)	9	19
All	All	788/874 (90%)	718 (91%)	70 (9%)	9	19

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

Mol	Chain	Res	Type
1	A	30	VAL
1	A	34	LEU
1	A	38	ARG
1	A	60	ASN
1	A	65	LYS
1	A	68	ARG
1	A	72	ASP
1	A	99	ARG
1	A	101	MET
1	A	124	GLU
1	A	129	LYS
1	A	139	GLU
1	A	168	VAL
1	A	201	GLU
1	A	224	ASN
1	A	227	ARG
1	A	272	ARG

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Mol	Chain	Res	Type
1	A	328	VAL
1	A	343	LYS
1	A	344	ILE
1	A	356	ARG
1	A	369	GLU
1	A	380	LEU
1	A	389	ASN
1	A	398	ARG
1	A	416	GLN
1	A	424	LEU
1	A	443	VAL
1	A	450	LEU
1	A	451	THR
1	A	472	GLU
1	A	474	LEU
1	A	509	VAL
1	A	510	ARG
1	A	511	GLU
1	B	20	SER
1	B	22	LEU
1	B	32	ARG
1	B	38	ARG
1	B	44	VAL
1	B	57	ASN
1	B	61	LYS
1	B	99	ARG
1	B	101	MET
1	B	121	ARG
1	B	134	LEU
1	B	139	GLU
1	B	168	VAL
1	B	176	VAL
1	B	191	ILE
1	B	205	ILE
1	B	247	GLU
1	B	276	LYS
1	B	290	SER
1	B	327	GLN
1	B	341	GLN
1	B	344	ILE
1	B	351	ILE
1	B	402	THR

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Mol	Chain	Res	Type
1	B	411	VAL
1	B	424	LEU
1	B	433	ARG
1	B	453	GLN
1	B	456	GLN
1	B	461	LEU
1	B	463	LEU
1	B	467	THR
1	B	474	LEU
1	B	476	ASP
1	B	510	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	262	HIS
1	A	333	ASN
1	A	389	ASN
1	A	416	GLN
1	A	419	ASN
1	A	454	GLN
1	B	319	ASN
1	B	323	GLN
1	B	339	HIS
1	B	419	ASN
1	B	453	GLN
1	B	456	GLN
1	B	471	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	SM8	B	901	2	69,73,73	2.40	14 (20%)	79,115,115	1.78	21 (26%)
3	SM8	A	901	2	69,73,73	2.37	14 (20%)	79,115,115	1.92	18 (22%)

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	SM8	B	901	2	-	2/27/119/119	0/8/8/8
3	SM8	A	901	2	-	2/27/119/119	0/8/8/8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	SM8	C4A-C4B	12.03	1.49	1.37
3	A	901	SM8	C4A-C4B	11.49	1.48	1.37
3	A	901	SM8	C3I-C3J	-6.66	1.34	1.48
3	B	901	SM8	C3I-C3J	-6.58	1.34	1.48
3	B	901	SM8	C3B-C3A	-6.20	1.34	1.48
3	A	901	SM8	C3B-C3A	-6.14	1.34	1.48
3	B	901	SM8	O2D-C3A	5.32	1.45	1.34
3	A	901	SM8	C1C-C1D	-5.19	1.47	1.51
3	A	901	SM8	O2D-C3A	5.11	1.45	1.34
3	B	901	SM8	O2B-C2G	4.82	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	SM8	O2B-C2G	4.82	1.45	1.35
3	B	901	SM8	C1C-C1D	-4.62	1.48	1.51
3	A	901	SM8	C3E-C3F	-3.45	1.33	1.44
3	A	901	SM8	C3C-C3D	-3.45	1.33	1.44
3	B	901	SM8	C3G-C3H	-3.43	1.33	1.44
3	B	901	SM8	C3C-C3D	-3.43	1.33	1.44
3	A	901	SM8	C3G-C3H	-3.41	1.33	1.44
3	B	901	SM8	C3E-C3F	-3.41	1.33	1.44
3	A	901	SM8	C4G-CL4	3.27	1.79	1.72
3	B	901	SM8	C4G-CL4	3.17	1.79	1.72
3	B	901	SM8	C3J-N4	-2.50	1.32	1.38
3	A	901	SM8	C3J-N4	-2.34	1.33	1.38
3	A	901	SM8	C4C-C4B	2.33	1.49	1.45
3	B	901	SM8	C4C-C4B	2.32	1.49	1.45
3	A	901	SM8	C1N-C1H	-2.26	1.52	1.56
3	B	901	SM8	C1N-C1H	-2.20	1.53	1.56
3	B	901	SM8	O4D-C4I	2.13	1.25	1.21
3	A	901	SM8	O2D-C2C	-2.04	1.42	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	SM8	C2C-O2D-C3A	-5.64	109.19	117.50
3	B	901	SM8	O2B-C2G-C2H	5.02	120.03	111.09
3	A	901	SM8	O2B-C2G-C2H	5.00	120.01	111.09
3	B	901	SM8	C2D-O2B-C2G	-4.85	110.18	117.72
3	A	901	SM8	C2D-O2B-C2G	-4.23	111.14	117.72
3	A	901	SM8	C3G-C3H-C3I	-4.19	114.75	124.65
3	B	901	SM8	O1H-C1E-C1O	-3.94	57.83	60.09
3	A	901	SM8	C3E-C3F-C3G	-3.85	115.82	124.72
3	A	901	SM8	O1H-C1E-C1O	-3.81	57.90	60.09
3	A	901	SM8	O2D-C3A-C3B	3.77	119.60	111.39
3	A	901	SM8	O4A-C4B-C4C	3.52	122.66	115.69
3	A	901	SM8	C3C-C3D-C3E	-3.43	116.80	124.72
3	A	901	SM8	O2D-C3A-O3A	-3.33	118.01	123.34
3	B	901	SM8	C3E-C3F-C3G	-3.24	117.23	124.72
3	B	901	SM8	O2D-C3A-C3B	3.11	118.16	111.39
3	B	901	SM8	C3G-C3H-C3I	-3.09	117.34	124.65
3	B	901	SM8	O4C-C4H-C4C	3.07	124.61	121.25
3	A	901	SM8	O4C-C4I-O4D	2.96	120.13	116.22
3	B	901	SM8	O4A-C4B-C4C	2.87	121.38	115.69
3	B	901	SM8	O4C-C4I-O4D	2.85	119.98	116.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	SM8	O2B-C2G-O2C	-2.82	117.55	122.99
3	A	901	SM8	C4C-C4B-C4A	-2.81	116.26	121.30
3	B	901	SM8	C2C-O2D-C3A	-2.77	113.42	117.50
3	B	901	SM8	C3D-C3C-C3B	-2.73	118.18	124.65
3	B	901	SM8	O2B-C2G-O2C	-2.72	117.74	122.99
3	B	901	SM8	C4C-C4B-C4A	-2.68	116.49	121.30
3	A	901	SM8	O1B-C1D-C1C	2.58	114.67	110.05
3	B	901	SM8	O4C-C4H-C4G	-2.57	114.66	117.63
3	B	901	SM8	C1H-C1G-C1F	-2.57	111.59	113.82
3	A	901	SM8	O4C-C4H-C4C	2.55	124.05	121.25
3	A	901	SM8	C1S-C1A-C1B	2.46	120.95	117.91
3	B	901	SM8	C1K-C1I-C1J	2.44	121.72	115.15
3	B	901	SM8	C3C-C3D-C3E	-2.38	119.21	124.72
3	A	901	SM8	O4C-C4H-C4G	-2.33	114.93	117.63
3	B	901	SM8	C1S-C1A-C1B	2.30	120.77	117.91
3	B	901	SM8	O1B-C1D-C1C	2.27	114.12	110.05
3	A	901	SM8	C1Q-C1C-C1B	2.20	120.11	118.44
3	B	901	SM8	C4F-C4G-CL4	2.05	123.25	118.60
3	B	901	SM8	C4I-C4A-N4	2.04	116.69	112.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	SM8	C2H-C2G-O2B-C2D
3	A	901	SM8	O2C-C2G-O2B-C2D
3	B	901	SM8	C2H-C2G-O2B-C2D
3	B	901	SM8	O2C-C2G-O2B-C2D

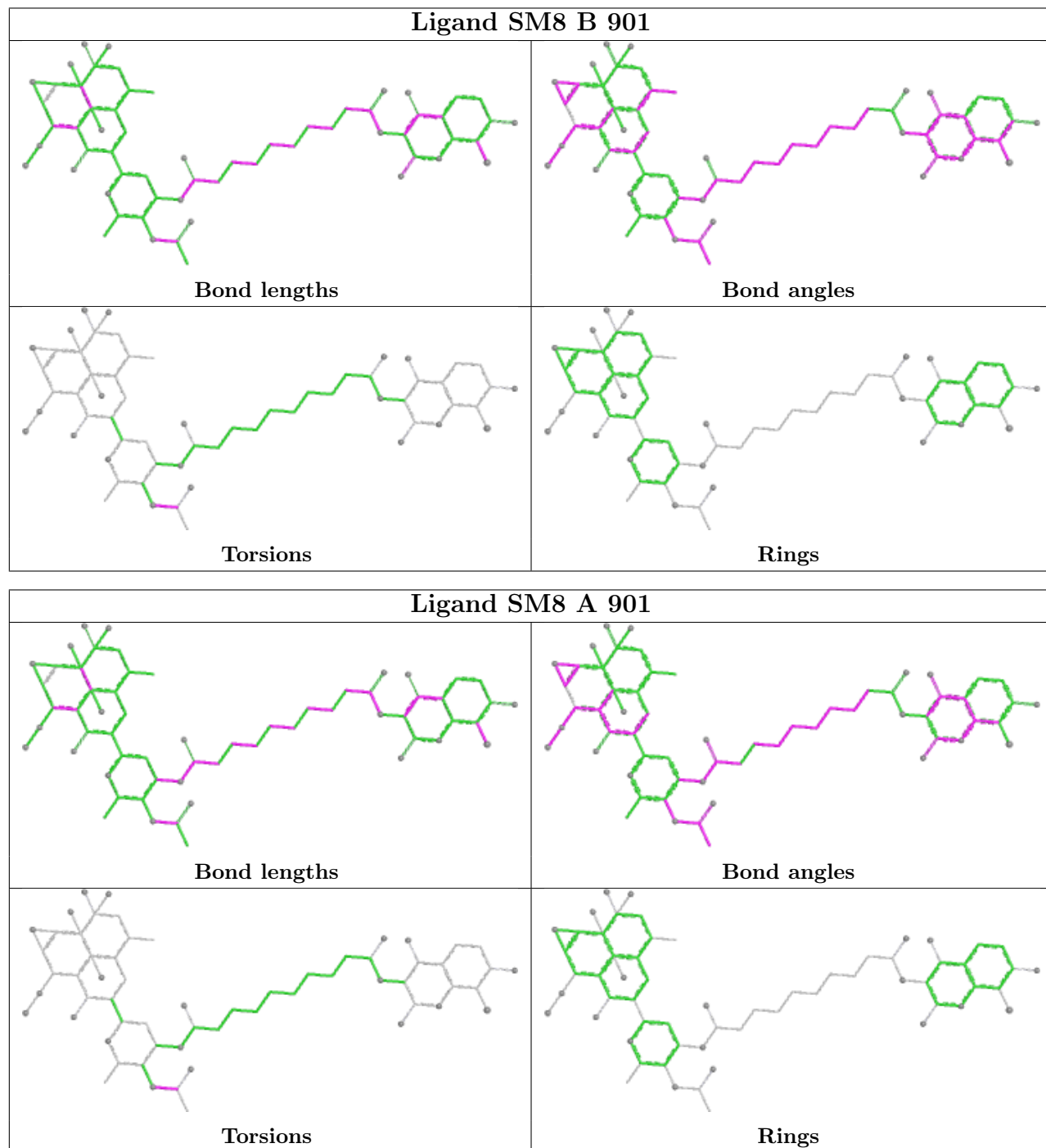
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	SM8	1	0
3	A	901	SM8	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/522 (95%)	-0.51	8 (1%) 70 67	29, 48, 92, 106	0
1	B	506/522 (96%)	-0.44	13 (2%) 57 52	28, 47, 90, 113	0
All	All	1002/1044 (95%)	-0.48	21 (2%) 63 59	28, 48, 91, 113	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	GLU	5.4
1	B	425	GLU	5.0
1	B	13	ILE	4.1
1	B	445	ASP	4.0
1	A	425	GLU	3.7
1	B	416	GLN	3.7
1	B	14	GLU	3.5
1	A	444	ARG	3.1
1	A	402	THR	3.0
1	B	444	ARG	2.8
1	B	469	LEU	2.8
1	A	23	ASP	2.8
1	A	81	GLY	2.7
1	B	16	GLU	2.4
1	B	472	GLU	2.4
1	A	447	LEU	2.3
1	B	399	HIS	2.3
1	A	397	ILE	2.2
1	A	401	PRO	2.1
1	B	417	LEU	2.1
1	B	430	ASP	2.0

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](#)

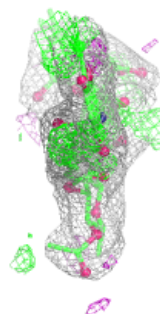
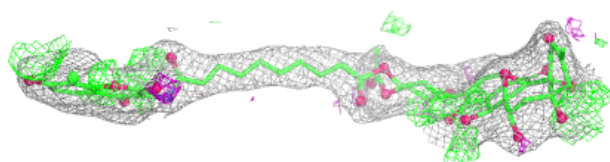
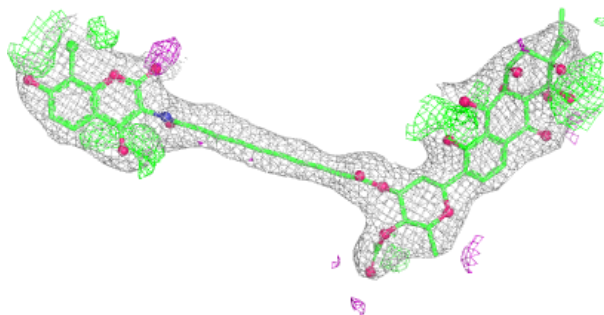
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	951	1/1	0.86	0.21	60,60,60,60	0
2	MG	A	951	1/1	0.87	0.20	58,58,58,58	0
3	SM8	A	901	66/66	0.92	0.10	34,51,61,67	0
3	SM8	B	901	66/66	0.92	0.10	33,51,57,63	0
2	MG	A	952	1/1	0.95	0.17	37,37,37,37	0
2	MG	B	952	1/1	0.95	0.20	31,31,31,31	0

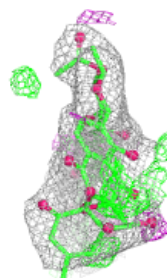
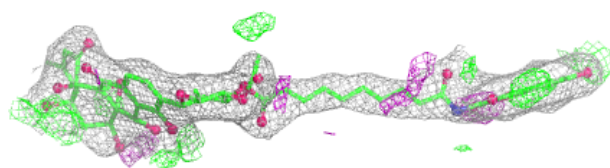
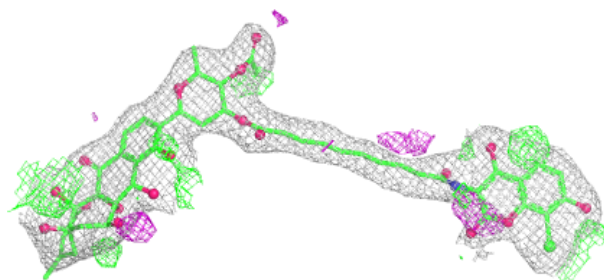
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SM8 A 901:

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

**Electron density around SM8 B 901:**

$2mF_o-DF_c$ (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.