



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:27 PM UTC

PDB ID : 3IIQ / pdb_00003iiq
Title : Crystallographic analysis of bacterial signal peptidase in ternary complex with Arylomycin A2 and a beta-sultam inhibitor
Authors : Paetzel, M.
Deposited on : 2009-08-03
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

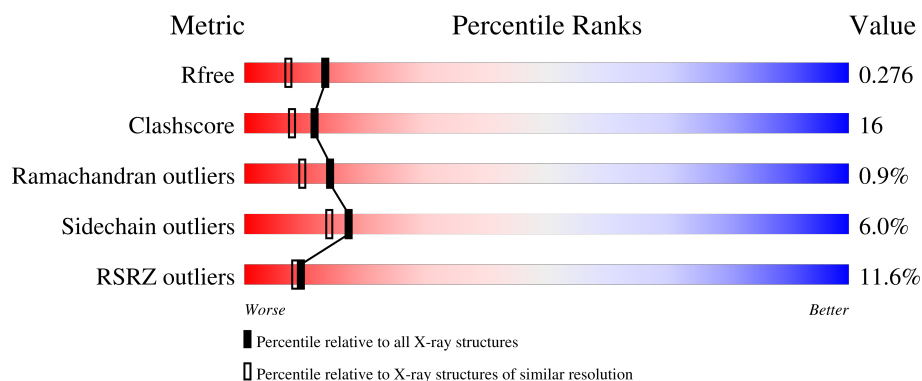
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	249	
1	B	249	
2	C	6	
2	D	6	

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	JZA	B	324	-	-	X	-
5	GOL	A	328	-	-	X	-
6	CCN	A	330	-	-	X	-
6	CCN	A	331	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3933 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 SIGNAL PEPTIDASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1726	1108	286	324	8			
1	B	224	Total	C	N	O	S	0	0	0
			1755	1121	295	331	8			

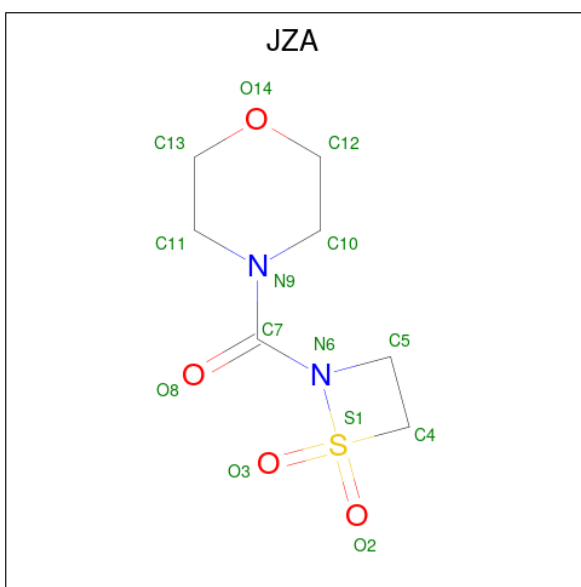
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	initiating methionine	UNP P00803
B	75	MET	-	initiating methionine	UNP P00803

- Molecule 2 is a protein called ARYLOMYCIN A2.

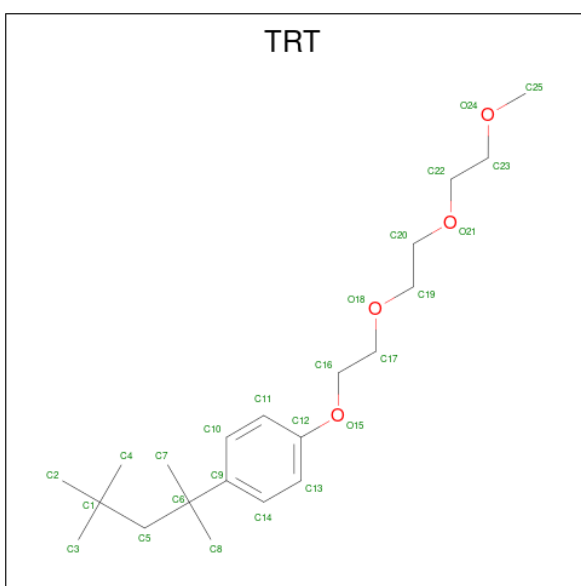
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			46	30	6	10			
2	D	6	Total	C	N	O	0	0	0
			46	30	6	10			

- Molecule 3 is 4-[(1,1-dioxido-1,2-thiazetidin-2-yl)carbonyl]morpholine (CCD ID: JZA) (formula: C₇H₁₂N₂O₄S).



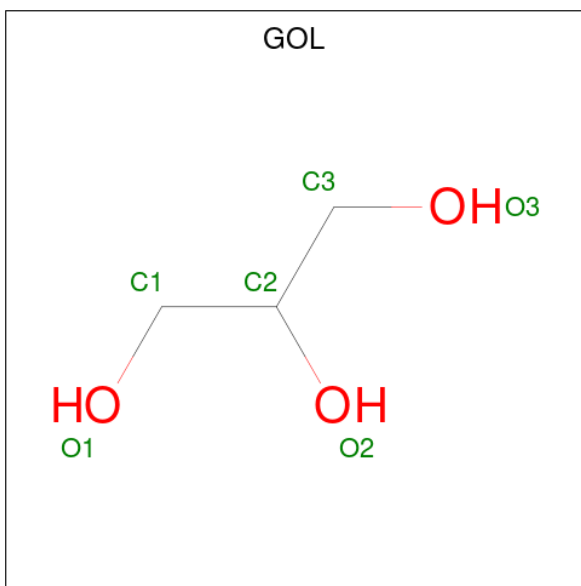
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	7	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	7	2	4	1		

- Molecule 4 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: $C_{21}H_{36}O_4$).



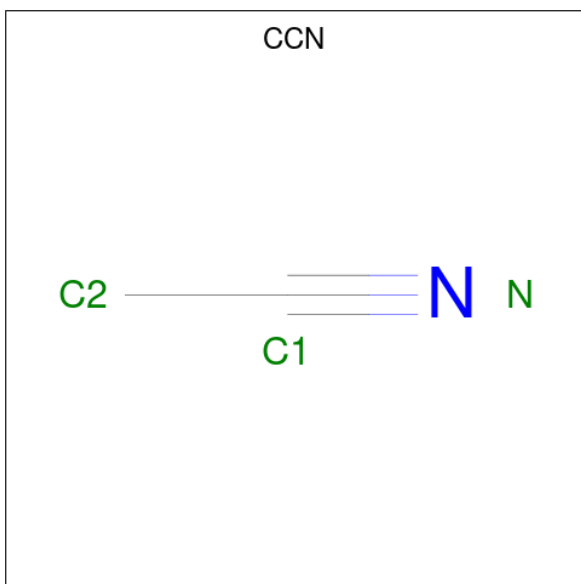
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



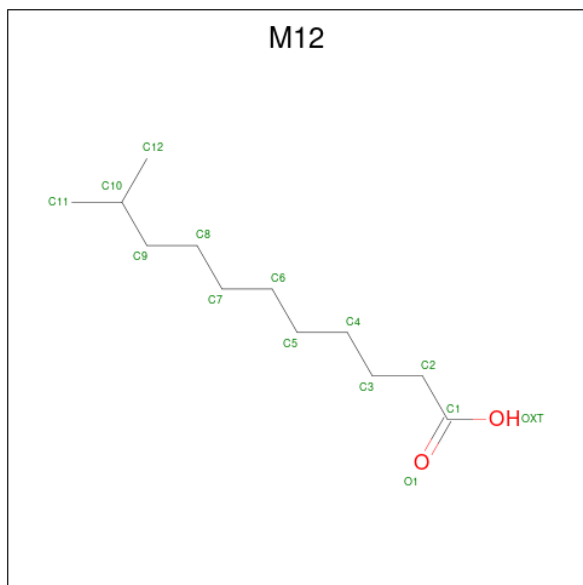
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETONITRILE (CCD ID: CCN) (formula: C_2H_3N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 3 2 1	0	0
6	A	1	Total C N 3 2 1	0	0

- Molecule 7 is 10-METHYLUNDECANOIC ACID (CCD ID: M12) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 12 1	0	0
7	D	1	Total C O 3 2 1	0	0

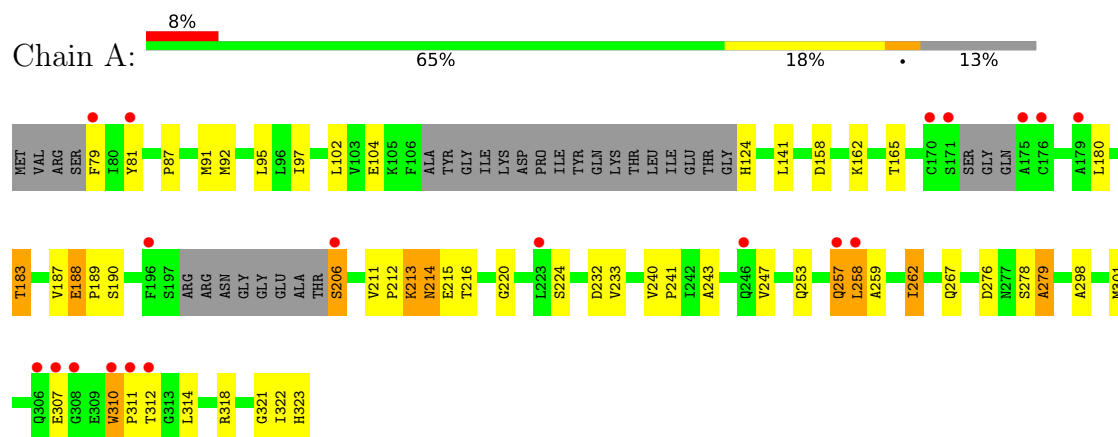
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	128	Total O 128 128	0	0
8	B	111	Total O 111 111	0	0
8	C	2	Total O 2 2	0	0
8	D	5	Total O 5 5	0	0

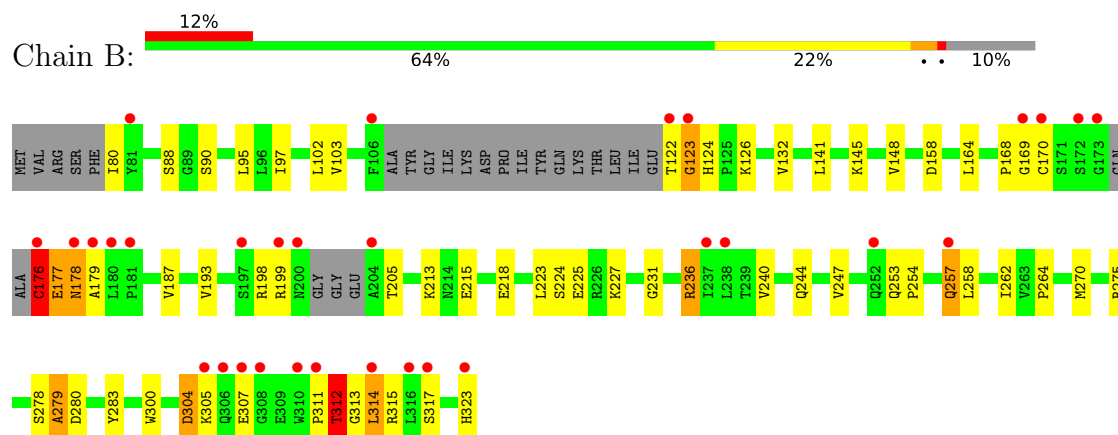
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

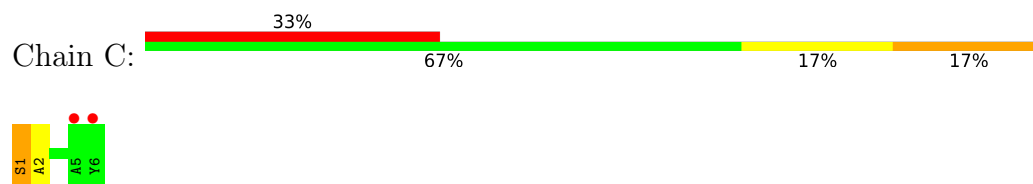
• Molecule 1: SIGNAL PEPTIDASE I



• Molecule 1: SIGNAL PEPTIDASE I



• Molecule 2: ARYLOMYCIN A2



• Molecule 2: ARYLOMYCIN A2



S1	A2	G3	G4	A5	Y6
----	----	----	----	----	----

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.01Å 70.01Å 259.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.40 – 2.00 67.40 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.1 (67.40-2.00) 95.1 (67.40-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.250 0.236 , 0.276	Depositor DCC
R_{free} test set	2035 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3933	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: JZA, TRT, DSE, DAL, GOL, M12, CCN, 5PG

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	1.40	10/1772 (0.6%)	1.26	10/2402 (0.4%)
1	B	1.54	19/1800 (1.1%)	1.17	13/2440 (0.5%)
2	C	1.50	0/21	1.88	0/24
2	D	1.30	0/21	1.40	0/24
All	All	1.47	29/3614 (0.8%)	1.22	23/4890 (0.5%)

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
1	B	0	3
2	C	0	1
2	D	0	1
All	All	0	6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	CYS	C-N	18.78	1.59	1.33
1	A	216	THR	C-N	15.18	1.54	1.33
1	B	177	GLU	C-N	13.52	1.52	1.34
1	B	170	CYS	C-N	11.72	1.49	1.33
1	B	257	GLN	CD-NE2	10.05	1.54	1.33
1	B	177	GLU	CD-OE1	9.47	1.43	1.25
1	B	170	CYS	C-O	8.88	1.34	1.23
1	B	177	GLU	C-O	8.65	1.40	1.23
1	B	257	GLN	CD-OE1	8.45	1.39	1.23
1	B	178	ASN	CA-C	-8.31	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ALA	CA-CB	7.86	1.62	1.52
1	A	211	VAL	CA-CB	6.88	1.63	1.54
1	B	279	ALA	CA-CB	6.70	1.61	1.52
1	B	323	HIS	CE1-NE2	6.53	1.39	1.32
1	B	236	ARG	CZ-NH1	5.78	1.40	1.32
1	B	177	GLU	CG-CD	-5.78	1.37	1.52
1	B	323	HIS	C-OXT	5.74	1.35	1.23
1	A	262	ILE	CA-CB	5.69	1.61	1.53
1	A	220	GLY	N-CA	5.62	1.50	1.44
1	A	92	MET	CA-C	5.58	1.58	1.53
1	B	275	ARG	CG-CD	-5.36	1.36	1.52
1	A	243	ALA	CA-CB	5.34	1.62	1.53
1	A	206	SER	CB-OG	5.25	1.52	1.42
1	A	232	ASP	N-CA	5.17	1.52	1.46
1	B	158	ASP	C-O	-5.10	1.17	1.24
1	B	323	HIS	CG-ND1	5.05	1.43	1.38
1	B	199	ARG	C-O	5.01	1.29	1.24
1	A	298	ALA	CA-CB	5.01	1.62	1.53
1	B	193	VAL	CA-CB	5.00	1.60	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	TRP	CA-C-N	16.39	140.33	119.84
1	A	310	TRP	C-N-CA	16.39	140.33	119.84
1	B	177	GLU	CA-C-N	-10.16	107.10	121.33
1	B	177	GLU	C-N-CA	-10.16	107.10	121.33
1	A	213	LYS	CA-C-N	8.94	132.06	120.44
1	A	213	LYS	C-N-CA	8.94	132.06	120.44
1	A	312	THR	N-CA-C	8.59	120.26	111.07
1	B	179	ALA	N-CA-C	7.07	120.63	110.24
1	A	214	ASN	N-CA-CB	-6.57	100.49	110.01
1	B	257	GLN	OE1-CD-NE2	6.08	128.68	122.60
1	B	170	CYS	CA-C-N	-5.70	112.57	120.38
1	B	170	CYS	C-N-CA	-5.70	112.57	120.38
1	B	178	ASN	CB-CA-C	5.62	118.40	111.43
1	B	177	GLU	CA-CB-CG	-5.32	103.47	114.10
1	B	264	PRO	CA-C-N	-5.23	114.57	119.85
1	B	264	PRO	C-N-CA	-5.23	114.57	119.85
1	A	310	TRP	N-CA-C	5.18	118.52	107.91
1	A	213	LYS	CA-C-O	5.16	125.61	119.10
1	B	213	LYS	CG-CD-CE	-5.13	99.50	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLU	N-CA-C	-5.02	103.70	108.22
1	A	259	ALA	N-CA-C	5.01	118.51	111.90
1	B	205	THR	N-CA-C	5.01	117.47	109.81
1	B	177	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	TRP	Peptide
1	B	123	GLY	Peptide
1	B	176	CYS	Mainchain
1	B	198	ARG	Peptide
2	C	2	DAL	Mainchain
2	D	2	DAL	Mainchain

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	1726	0	1676	46	0
1	B	1755	0	1698	53	0
2	C	46	0	37	1	0
2	D	46	0	37	2	0
3	A	14	0	12	3	0
3	B	14	0	12	7	0
4	A	20	0	27	2	0
4	B	20	0	27	9	0
5	A	24	0	32	14	0
6	A	6	0	6	7	0
7	C	13	0	23	1	0
7	D	3	0	0	0	0
8	A	128	0	0	6	0
8	B	111	0	0	5	0
8	C	2	0	0	0	0
8	D	5	0	0	0	0
All	All	3933	0	3587	116	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 16.

All (116) 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:B:176:CYS:N	1:B:177:GLU:CG	1.75	1.46
1:B:168:PRO:HD2	1:B:178:ASN:O	1.30	1.23
1:B:176:CYS:N	1:B:177:GLU:HG2	0.86	1.18
4:B:325:TRT:H3C3	4:B:325:TRT:H8C2	1.34	1.07
1:B:123:GLY:HA2	1:B:124:HIS:CG	1.90	1.06
4:B:325:TRT:H3C3	4:B:325:TRT:C8	1.85	1.06
6:A:330:CCN:H21	6:A:331:CCN:H21	1.40	1.03
1:B:317:SER:HB3	8:B:2106:HOH:O	1.60	1.02
1:A:323:HIS:CD2	5:A:328:GOL:H32	2.01	0.95
1:A:183:THR:HG23	8:A:2044:HOH:O	1.64	0.95
1:A:253:GLN:HE22	1:A:262:ILE:H	1.13	0.94
1:B:314:LEU:N	1:B:314:LEU:CD1	2.30	0.94
1:B:313:GLY:C	1:B:314:LEU:HD12	1.95	0.92
1:B:312:THR:HG22	1:B:313:GLY:N	1.86	0.91
6:A:330:CCN:H21	6:A:331:CCN:C2	2.02	0.90
1:A:323:HIS:HD2	5:A:328:GOL:C3	1.85	0.90
1:A:323:HIS:HD2	5:A:328:GOL:H32	1.37	0.87
1:A:323:HIS:CD2	5:A:328:GOL:C3	2.58	0.87
1:A:241:PRO:HA	8:A:2035:HOH:O	1.76	0.84
1:A:323:HIS:CD2	5:A:328:GOL:H12	2.14	0.82
1:B:314:LEU:N	1:B:314:LEU:HD12	1.95	0.82
1:B:123:GLY:HA2	1:B:124:HIS:CD2	2.16	0.80
1:B:278:SER:HA	3:B:324:JZA:H4	1.65	0.79
1:B:168:PRO:CD	1:B:178:ASN:O	2.24	0.79
1:A:323:HIS:HD2	5:A:328:GOL:H12	1.46	0.79
1:A:79:PHE:HA	8:A:2001:HOH:O	1.82	0.78
1:A:257:GLN:HB2	8:A:2053:HOH:O	1.86	0.76
1:A:323:HIS:HD2	5:A:328:GOL:C1	2.00	0.74
1:B:253:GLN:HE22	1:B:262:ILE:H	1.32	0.73
1:B:314:LEU:N	1:B:314:LEU:HD13	2.01	0.73
4:B:325:TRT:C8	4:B:325:TRT:C3	2.63	0.73
4:B:325:TRT:H8C2	4:B:325:TRT:C3	2.15	0.73
1:A:323:HIS:OXT	6:A:331:CCN:H22	1.88	0.72
1:A:278:SER:HA	3:A:324:JZA:H4	1.72	0.69
1:B:313:GLY:C	1:B:314:LEU:CD1	2.63	0.69
1:B:176:CYS:N	1:B:177:GLU:CB	2.55	0.68
1:A:301:MET:HE1	1:A:314:LEU:HD22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:330:CCN:C2	6:A:331:CCN:H21	2.21	0.67
1:B:187:VAL:CG1	1:B:224:SER:HB3	2.25	0.67
1:A:124:HIS:N	8:A:2011:HOH:O	2.27	0.67
3:B:324:JZA:H11A	2:D:6:TYR:HB3	1.76	0.67
1:B:123:GLY:HA2	1:B:124:HIS:ND1	2.08	0.66
1:A:323:HIS:CD2	5:A:328:GOL:C1	2.77	0.65
1:B:97:ILE:O	1:B:315:ARG:NH1	2.31	0.63
1:B:304:ASP:O	1:B:311:PRO:CB	2.47	0.62
1:B:176:CYS:HB2	1:B:177:GLU:HA	1.82	0.62
1:A:187:VAL:CG1	1:A:224:SER:HB3	2.31	0.61
4:B:325:TRT:H3C3	4:B:325:TRT:H8C1	1.77	0.60
5:A:328:GOL:O3	6:A:330:CCN:H22	2.01	0.60
1:A:253:GLN:HE22	1:A:262:ILE:N	1.93	0.60
1:B:145:LYS:HE3	1:B:280:ASP:HB3	1.84	0.60
1:B:148:VAL:HG11	1:B:164:LEU:HD13	1.83	0.59
1:A:189:PRO:HG2	1:A:213:LYS:HE3	1.85	0.58
1:B:123:GLY:CA	1:B:124:HIS:CG	2.78	0.58
1:B:279:ALA:H	3:B:324:JZA:C4	2.17	0.58
1:A:247:VAL:HG12	1:A:258:LEU:HG	1.86	0.57
1:A:323:HIS:CD2	5:A:328:GOL:H31	2.39	0.57
1:A:97:ILE:HD13	1:A:307:GLU:HB2	1.87	0.57
1:B:225:GLU:OE2	1:B:236:ARG:HD2	2.06	0.56
1:A:322:ILE:HA	6:A:330:CCN:H23	1.87	0.56
4:B:325:TRT:H8C1	4:B:325:TRT:H4C2	1.89	0.55
1:B:123:GLY:HA2	1:B:124:HIS:CE1	2.42	0.54
1:B:223:LEU:HD22	1:B:240:VAL:HG22	1.90	0.54
1:A:81:TYR:CE2	1:A:104:GLU:HG2	2.43	0.54
1:B:304:ASP:O	1:B:311:PRO:CA	2.56	0.54
1:B:304:ASP:O	1:B:311:PRO:HB3	2.07	0.53
3:B:324:JZA:H11A	2:D:6:TYR:CB	2.39	0.53
1:B:223:LEU:CD2	1:B:240:VAL:HG22	2.39	0.53
1:B:307:GLU:HA	8:B:2004:HOH:O	2.08	0.53
1:A:279:ALA:H	3:A:324:JZA:H4A	1.72	0.52
1:A:253:GLN:NE2	1:A:262:ILE:H	1.94	0.52
1:A:214:ASN:HD22	1:A:215:GLU:HG3	1.74	0.52
1:B:176:CYS:N	1:B:177:GLU:CA	2.73	0.52
1:B:187:VAL:HG13	1:B:224:SER:HB3	1.91	0.52
1:A:190:SER:HB2	8:A:2072:HOH:O	2.09	0.51
1:B:304:ASP:O	1:B:311:PRO:HA	2.10	0.51
4:A:325:TRT:H2C3	4:A:325:TRT:H8C2	1.92	0.51
1:B:315:ARG:NH2	8:B:2103:HOH:O	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:325:TRT:C14	4:A:325:TRT:H2C2	2.42	0.50
1:B:283:TYR:CE2	4:B:325:TRT:H3C1	2.47	0.49
1:A:187:VAL:HG13	1:A:224:SER:HB3	1.95	0.48
1:A:212:PRO:C	1:A:214:ASN:H	2.21	0.48
1:B:247:VAL:HG12	1:B:258:LEU:HD23	1.96	0.48
1:B:145:LYS:HB2	1:B:270:MET:HB3	1.96	0.47
5:A:327:GOL:H32	5:A:329:GOL:O1	2.14	0.47
1:A:322:ILE:CA	6:A:330:CCN:H23	2.44	0.47
1:A:247:VAL:HG11	1:A:258:LEU:HB3	1.96	0.47
1:B:218:GLU:H	1:B:218:GLU:CD	2.23	0.46
1:A:323:HIS:HD2	5:A:328:GOL:C2	2.29	0.46
1:B:244:GLN:NE2	8:B:2077:HOH:O	2.49	0.46
1:A:279:ALA:H	3:A:324:JZA:C4	2.29	0.45
1:B:88:SER:HB3	3:B:324:JZA:H11	1.99	0.45
1:A:321:GLY:C	5:A:328:GOL:H2	2.41	0.45
1:B:148:VAL:HG11	1:B:164:LEU:CD1	2.46	0.44
1:A:81:TYR:HB3	1:A:102:LEU:HD11	1.99	0.44
1:A:183:THR:HG21	8:B:2075:HOH:O	2.17	0.44
1:B:103:VAL:HG21	1:B:132:VAL:HG21	1.99	0.44
1:B:176:CYS:N	1:B:177:GLU:HG3	2.10	0.43
1:A:240:VAL:HG23	1:A:276:ASP:HB2	2.00	0.43
1:A:158:ASP:O	1:A:162:LYS:N	2.52	0.42
1:B:148:VAL:CG1	1:B:164:LEU:HD13	2.48	0.42
1:A:247:VAL:CG1	1:A:258:LEU:HB3	2.49	0.42
1:B:88:SER:CB	3:B:324:JZA:H11	2.49	0.42
1:A:212:PRO:C	1:A:214:ASN:N	2.77	0.42
1:B:283:TYR:CZ	4:B:325:TRT:H3C1	2.55	0.42
1:B:169:GLY:O	1:B:176:CYS:O	2.38	0.42
1:B:253:GLN:HE22	1:B:262:ILE:N	2.09	0.42
2:C:1:DSE:HN1	7:C:0:M12:H21C	1.51	0.42
1:A:318:ARG:HA	5:A:329:GOL:H2	2.02	0.41
1:B:300:TRP:CD1	1:B:300:TRP:C	2.96	0.41
1:B:90:SER:HB3	3:B:324:JZA:O2	2.20	0.41
1:B:227:LYS:HG2	1:B:236:ARG:HG2	2.01	0.41
1:A:214:ASN:ND2	1:A:215:GLU:HG3	2.34	0.41
1:A:91:MET:HE3	1:A:91:MET:HB3	1.98	0.41
4:B:325:TRT:H11	4:B:325:TRT:H161	1.94	0.41
1:A:188:GLU:HB2	1:A:189:PRO:HD2	2.03	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	209/249 (84%)	203 (97%)	5 (2%)	1 (0%)	24	21
1	B	216/249 (87%)	205 (95%)	8 (4%)	3 (1%)	9	4
2	C	2/6 (33%)	2 (100%)	0	0	100	100
2	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	429/510 (84%)	412 (96%)	13 (3%)	4 (1%)	14	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
1	B	312	THR
1	B	254	PRO
1	B	231	GLY

5.3.2 Protein sidechains [i](#)

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	189/214 (88%)	178 (94%)	11 (6%)	18	15
1	B	190/214 (89%)	178 (94%)	12 (6%)	16	13
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	381/430 (89%)	358 (94%)	23 (6%)	17	14

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	PRO
1	A	95	LEU
1	A	141	LEU
1	A	165	THR
1	A	180	LEU
1	A	183	THR
1	A	206	SER
1	A	233	VAL
1	A	257	GLN
1	A	258	LEU
1	A	267	GLN
1	B	80	ILE
1	B	95	LEU
1	B	102	LEU
1	B	122	THR
1	B	126	LYS
1	B	141	LEU
1	B	215	GLU
1	B	257	GLN
1	B	304	ASP
1	B	305	LYS
1	B	312	THR
1	B	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	214	ASN
1	A	244	GLN
1	A	253	GLN
1	A	257	GLN
1	A	267	GLN
1	A	291	ASN
1	A	323	HIS
1	B	178	ASN
1	B	235	HIS
1	B	244	GLN
1	B	252	GLN
1	B	253	GLN
1	B	291	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	323	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5PG	C	4	2	11,12,13	1.32	0	10,15,17	1.22	0
2	5PG	D	4	2	11,12,13	2.03	3 (27%)	10,15,17	1.10	1 (10%)
2	DSE	D	1	2,7	5,6,7	1.33	0	5,6,8	2.52	3 (60%)
2	DSE	C	1	2,7	5,6,7	0.83	0	5,6,8	1.90	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5PG	C	4	2	-	5/5/8/10	0/1/1/1
2	5PG	D	4	2	-	5/5/8/10	0/1/1/1
2	DSE	D	1	2,7	-	0/3/6/8	-
2	DSE	C	1	2,7	-	0/3/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	5PG	CB-CA	3.52	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	5PG	CD1-CC1	3.37	1.44	1.38
2	D	4	5PG	CN-N	2.82	1.53	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	DSE	CN-N-CA	4.07	125.86	113.70
2	D	1	DSE	O-C-CA	-2.73	117.76	124.77
2	C	1	DSE	CN-N-CA	2.65	121.62	113.70
2	D	1	DSE	OG-CB-CA	-2.46	104.36	111.13
2	D	4	5PG	CC2-CB-CC1	2.26	121.11	118.30
2	C	1	DSE	OG-CB-CA	-2.15	105.20	111.13

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	5PG	CB-CA-N-CN
2	C	4	5PG	N-CA-CB-CC1
2	C	4	5PG	N-CA-CB-CC2
2	C	4	5PG	C-CA-CB-CC2
2	D	4	5PG	CB-CA-N-CN
2	D	4	5PG	N-CA-CB-CC1
2	D	4	5PG	C-CA-CB-CC1
2	D	4	5PG	C-CA-CB-CC2
2	C	4	5PG	C-CA-CB-CC1
2	D	4	5PG	N-CA-CB-CC2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	DSE	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
6	CCN	A	331	-	2,2,2	1.86	1 (50%)	1,1,1	0.37	0
6	CCN	A	330	-	2,2,2	1.25	0	1,1,1	0.43	0
3	JZA	B	324	-	11,15,15	4.22	3 (27%)	11,22,22	1.51	2 (18%)
5	GOL	A	328	-	5,5,5	0.88	0	5,5,5	1.07	0
4	TRT	A	325	-	20,20,25	1.13	1 (5%)	28,28,33	0.67	0
5	GOL	A	326	-	5,5,5	0.19	0	5,5,5	0.60	0
3	JZA	A	324	-	11,15,15	4.00	3 (27%)	11,22,22	1.42	2 (18%)
5	GOL	A	327	-	5,5,5	0.49	0	5,5,5	1.33	0
7	M12	C	0	2	11,12,13	1.10	0	11,12,14	0.55	0
5	GOL	A	329	-	5,5,5	0.55	0	5,5,5	0.98	0
7	M12	D	0	2	1,2,13	0.96	0	0,1,14	-	-
4	TRT	B	325	-	20,20,25	1.53	3 (15%)	28,28,33	1.15	2 (7%)

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	JZA	B	324	-	-	0/4/28/28	0/2/2/2
5	GOL	A	328	-	-	0/4/4/4	-
4	TRT	A	325	-	-	9/18/18/23	0/1/1/1
5	GOL	A	326	-	-	0/4/4/4	-
3	JZA	A	324	-	-	4/4/28/28	0/2/2/2
5	GOL	A	327	-	-	3/4/4/4	-
7	M12	C	0	2	-	5/10/10/11	-
5	GOL	A	329	-	-	4/4/4/4	-
4	TRT	B	325	-	-	11/18/18/23	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	324	JZA	O3-S1	8.31	1.52	1.43
3	B	324	JZA	O2-S1	7.73	1.52	1.43
3	A	324	JZA	O2-S1	7.58	1.52	1.43
3	A	324	JZA	C7-N9	7.43	1.52	1.35
3	B	324	JZA	C7-N9	7.10	1.51	1.35
3	A	324	JZA	O3-S1	6.99	1.51	1.43
4	B	325	TRT	C6-C9	3.59	1.59	1.53
4	A	325	TRT	C6-C9	3.09	1.58	1.53
4	B	325	TRT	O18-C17	2.61	1.53	1.42
6	A	331	CCN	C2-C1	2.44	1.61	1.44
4	B	325	TRT	O15-C16	2.17	1.51	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	325	TRT	O15-C16-C17	3.53	120.55	108.71
4	B	325	TRT	O18-C17-C16	3.08	124.37	110.35
3	A	324	JZA	C10-N9-C7	-2.63	110.86	121.53
3	B	324	JZA	O14-C12-C10	2.36	116.86	111.77
3	B	324	JZA	O14-C13-C11	2.26	116.64	111.77
3	A	324	JZA	C13-C11-N9	2.06	114.15	109.82

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	324	JZA	O8-C7-N9-C11
3	A	324	JZA	N6-C7-N9-C11
3	A	324	JZA	O8-C7-N9-C10
3	A	324	JZA	N6-C7-N9-C10
5	A	327	GOL	C1-C2-C3-O3
5	A	329	GOL	O1-C1-C2-C3
7	C	0	M12	O1-C1-C2-C3
4	B	325	TRT	C1-C5-C6-C8
4	B	325	TRT	C1-C5-C6-C9
4	A	325	TRT	C2-C1-C5-C6
4	A	325	TRT	C4-C1-C5-C6
4	A	325	TRT	C3-C1-C5-C6
4	B	325	TRT	C1-C5-C6-C7
4	A	325	TRT	C13-C12-O15-C16
4	A	325	TRT	C11-C12-O15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	329	GOL	O1-C1-C2-O2
5	A	327	GOL	O1-C1-C2-O2
5	A	329	GOL	O2-C2-C3-O3
4	B	325	TRT	C13-C12-O15-C16
4	B	325	TRT	O15-C16-C17-O18
4	B	325	TRT	C11-C12-O15-C16
5	A	327	GOL	O2-C2-C3-O3
4	B	325	TRT	C20-C19-O18-C17
4	A	325	TRT	C16-C17-O18-C19
4	B	325	TRT	C17-C16-O15-C12
7	C	0	M12	C1-C2-C3-C4
4	A	325	TRT	C17-C16-O15-C12
7	C	0	M12	C11-C10-C9-C8
7	C	0	M12	C7-C8-C9-C10
4	A	325	TRT	O15-C16-C17-O18
5	A	329	GOL	C1-C2-C3-O3
4	B	325	TRT	C7-C6-C9-C14
4	A	325	TRT	C20-C19-O18-C17
7	C	0	M12	C12-C10-C9-C8
4	B	325	TRT	C8-C6-C9-C14
4	B	325	TRT	C7-C6-C9-C10

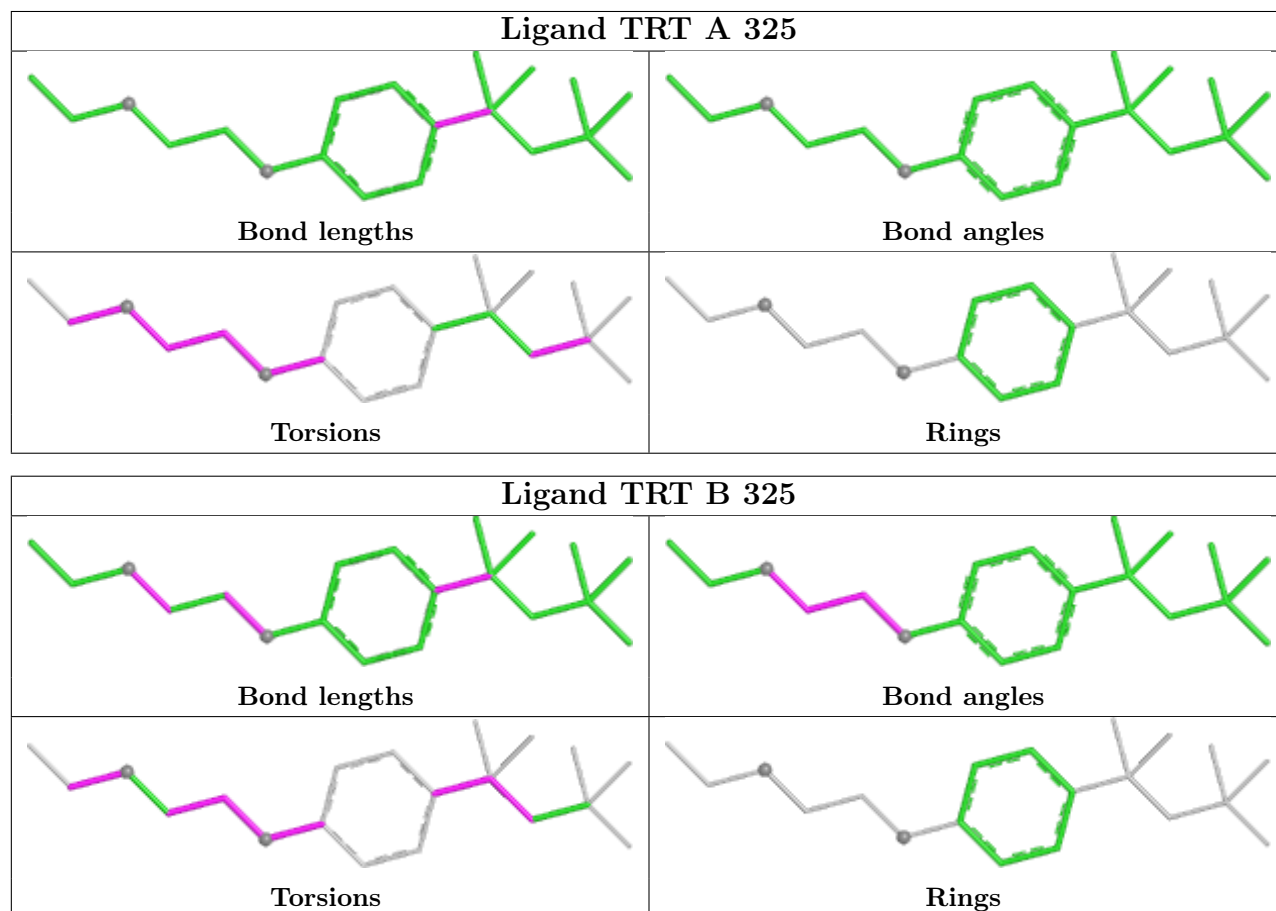
There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	331	CCN	4	0
6	A	330	CCN	6	0
3	B	324	JZA	7	0
5	A	328	GOL	12	0
4	A	325	TRT	2	0
3	A	324	JZA	3	0
5	A	327	GOL	1	0
7	C	0	M12	1	0
5	A	329	GOL	2	0
4	B	325	TRT	9	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	217/249 (87%)	0.69	19 (8%) 15 14	19, 35, 51, 71	0
1	B	224/249 (89%)	0.80	31 (13%) 6 6	20, 36, 69, 78	0
2	C	3/6 (50%)	2.45	2 (66%) 0 0	0, 0, 0, 33	0
2	D	3/6 (50%)	0.68	0 100 100	34, 34, 37, 38	0
All	All	447/510 (87%)	0.76	52 (11%) 9 8	0, 35, 63, 78	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	THR	7.4
1	B	123	GLY	7.2
1	B	200	ASN	6.4
1	A	310	TRP	5.3
1	B	179	ALA	4.7
1	B	176	CYS	4.2
1	B	172	SER	3.9
1	B	170	CYS	3.8
1	B	178	ASN	3.7
1	A	175	ALA	3.7
1	A	196	PHE	3.7
1	B	310	TRP	3.6
1	A	79	PHE	3.5
2	C	5	ALA	3.5
1	B	81	TYR	3.3
1	B	305	LYS	3.3
1	B	257	GLN	3.1
1	A	258	LEU	3.1
1	B	323	HIS	3.0
1	A	81	TYR	2.9
1	B	199	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	2.9
1	B	106	PHE	2.9
1	B	173	GLY	2.9
1	B	314	LEU	2.8
1	B	204	ALA	2.8
1	A	176	CYS	2.8
1	A	312	THR	2.8
2	C	6	TYR	2.8
1	B	237	ILE	2.7
1	B	307	GLU	2.7
1	B	306	GLN	2.7
1	A	179	ALA	2.6
1	A	171	SER	2.6
1	B	308	GLY	2.6
1	B	180	LEU	2.6
1	B	316	LEU	2.6
1	A	306	GLN	2.6
1	A	206	SER	2.6
1	A	246	GLN	2.5
1	B	252	GLN	2.5
1	A	308	GLY	2.5
1	A	170	CYS	2.4
1	A	307	GLU	2.3
1	B	317	SER	2.2
1	B	238	LEU	2.2
1	B	311	PRO	2.1
1	A	223	LEU	2.1
1	B	197	SER	2.1
1	B	181	PRO	2.1
1	A	311	PRO	2.0
1	B	169	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DSE	D	1	7/8	0.67	0.20	59,62,66,69	5
2	DSE	C	1	7/8	0.82	0.17	42,49,56,57	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5PG	C	4	12/13	0.87	0.16	0,0,0,0	0
2	DAL	C	2	5/6	0.89	0.17	33,37,39,39	5
2	DAL	D	2	5/6	0.91	0.13	42,43,46,52	5
2	5PG	D	4	12/13	0.94	0.08	31,33,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

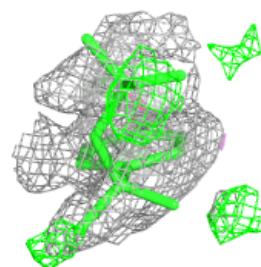
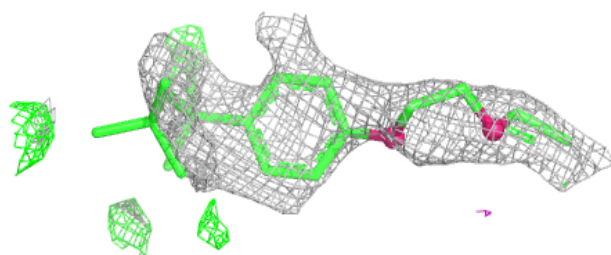
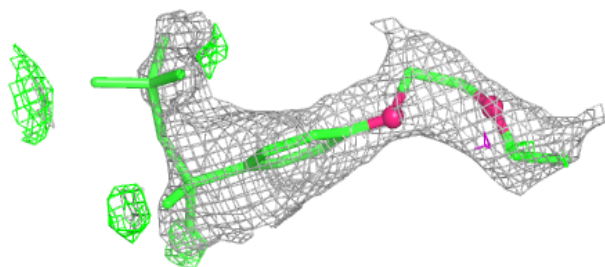
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JZA	B	324	14/14	0.57	0.28	135,138,141,142	0
3	JZA	A	324	14/14	0.63	0.36	161,162,163,163	0
7	M12	D	0	3/14	0.63	0.26	66,66,66,66	3
5	GOL	A	327	6/6	0.65	0.17	83,86,88,88	0
4	TRT	A	325	20/25	0.66	0.31	121,133,137,138	0
5	GOL	A	328	6/6	0.71	0.17	52,59,64,66	0
7	M12	C	0	13/14	0.73	0.27	60,77,83,85	3
4	TRT	B	325	20/25	0.76	0.29	92,97,101,101	0
5	GOL	A	329	6/6	0.78	0.13	64,68,69,70	0
6	CCN	A	331	3/3	0.80	0.23	26,26,35,48	0
6	CCN	A	330	3/3	0.85	0.18	27,27,30,37	0
5	GOL	A	326	6/6	0.88	0.20	82,83,83,86	0

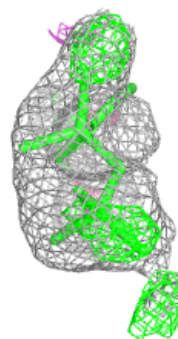
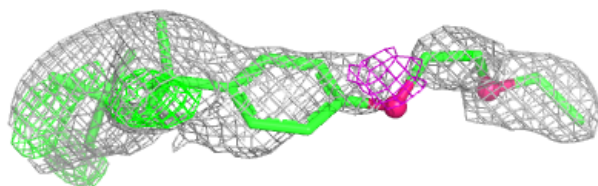
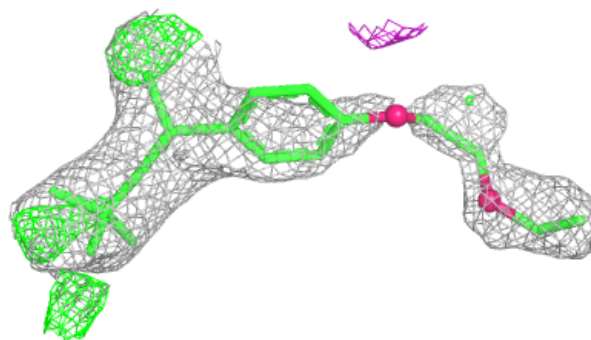
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRT A 325:

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

**Electron density around TRT B 325:**

$2mF_o-DF_c$ (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.