



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:20 PM UTC

PDB ID : 3VZC / pdb_00003vzc
Title : Crystal structure of Sphingosine Kinase 1 with inhibitor
Authors : Min, X.; Walker, N.P.; Wang, Z.
Deposited on : 2012-10-11
Resolution : 2.30 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

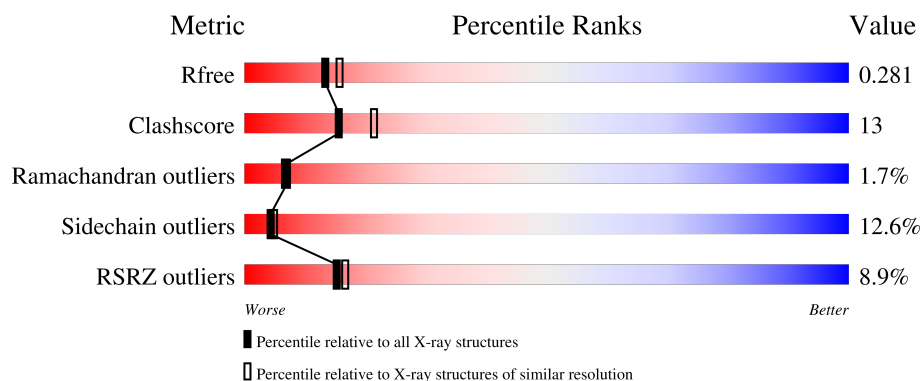
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	361	5% 69% 24% . .
1	B	361	7% 66% 23% 6% 6%
1	C	361	9% 62% 26% 6% . 5%
1	D	361	6% 70% 21% 6% .
1	E	361	6% 66% 24% . . 5%

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Mol	Chain	Length	Quality of chain
1	F	361	17% 62% 30% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16468 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 Sphingosine kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2694	1726	475	472	21			
1	B	340	Total	C	N	O	S	0	0	0
			2653	1702	467	464	20			
1	C	342	Total	C	N	O	S	0	0	0
			2664	1707	469	467	21			
1	D	348	Total	C	N	O	S	0	0	0
			2701	1731	476	473	21			
1	E	342	Total	C	N	O	S	0	0	0
			2663	1707	469	467	20			
1	F	344	Total	C	N	O	S	0	0	0
			2673	1712	471	469	21			

There are 30 discrepancies between the modelled and reference sequences:

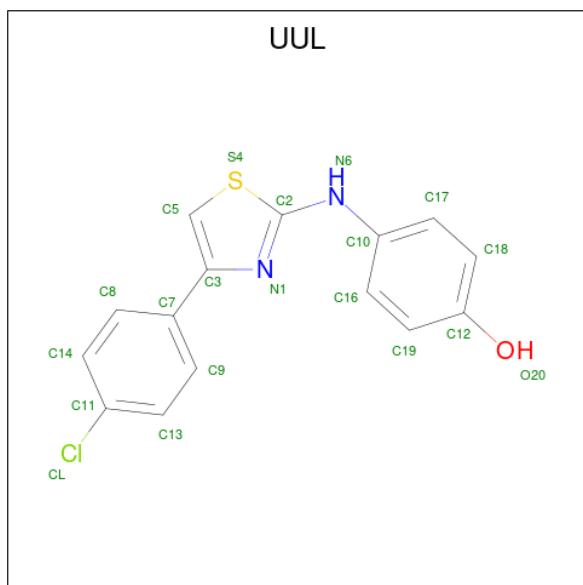
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	expression tag	UNP Q9NYA1
A	5	ALA	-	expression tag	UNP Q9NYA1
A	6	MET	-	expression tag	UNP Q9NYA1
A	7	GLY	-	expression tag	UNP Q9NYA1
A	8	SER	-	expression tag	UNP Q9NYA1
B	4	GLY	-	expression tag	UNP Q9NYA1
B	5	ALA	-	expression tag	UNP Q9NYA1
B	6	MET	-	expression tag	UNP Q9NYA1
B	7	GLY	-	expression tag	UNP Q9NYA1
B	8	SER	-	expression tag	UNP Q9NYA1
C	4	GLY	-	expression tag	UNP Q9NYA1
C	5	ALA	-	expression tag	UNP Q9NYA1
C	6	MET	-	expression tag	UNP Q9NYA1
C	7	GLY	-	expression tag	UNP Q9NYA1
C	8	SER	-	expression tag	UNP Q9NYA1
D	4	GLY	-	expression tag	UNP Q9NYA1
D	5	ALA	-	expression tag	UNP Q9NYA1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	MET	-	expression tag	UNP Q9NYA1
D	7	GLY	-	expression tag	UNP Q9NYA1
D	8	SER	-	expression tag	UNP Q9NYA1
E	4	GLY	-	expression tag	UNP Q9NYA1
E	5	ALA	-	expression tag	UNP Q9NYA1
E	6	MET	-	expression tag	UNP Q9NYA1
E	7	GLY	-	expression tag	UNP Q9NYA1
E	8	SER	-	expression tag	UNP Q9NYA1
F	4	GLY	-	expression tag	UNP Q9NYA1
F	5	ALA	-	expression tag	UNP Q9NYA1
F	6	MET	-	expression tag	UNP Q9NYA1
F	7	GLY	-	expression tag	UNP Q9NYA1
F	8	SER	-	expression tag	UNP Q9NYA1

- Molecule 2 is 4-{[4-(4-chlorophenyl)-1,3-thiazol-2-yl]amino}phenol (CCD ID: UUL) (formula: C₁₅H₁₁ClN₂OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 20	C 15	Cl 1	N 2	O 1	S 1	0	0
2	B	1	Total 20	C 15	Cl 1	N 2	O 1	S 1	0	0
2	C	1	Total 20	C 15	Cl 1	N 2	O 1	S 1	0	0
2	D	1	Total 20	C 15	Cl 1	N 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	53	Total	O	0	0
			53	53		
4	C	62	Total	O	0	0
			62	62		
4	D	35	Total	O	0	0
			35	35		
4	E	46	Total	O	0	0
			46	46		

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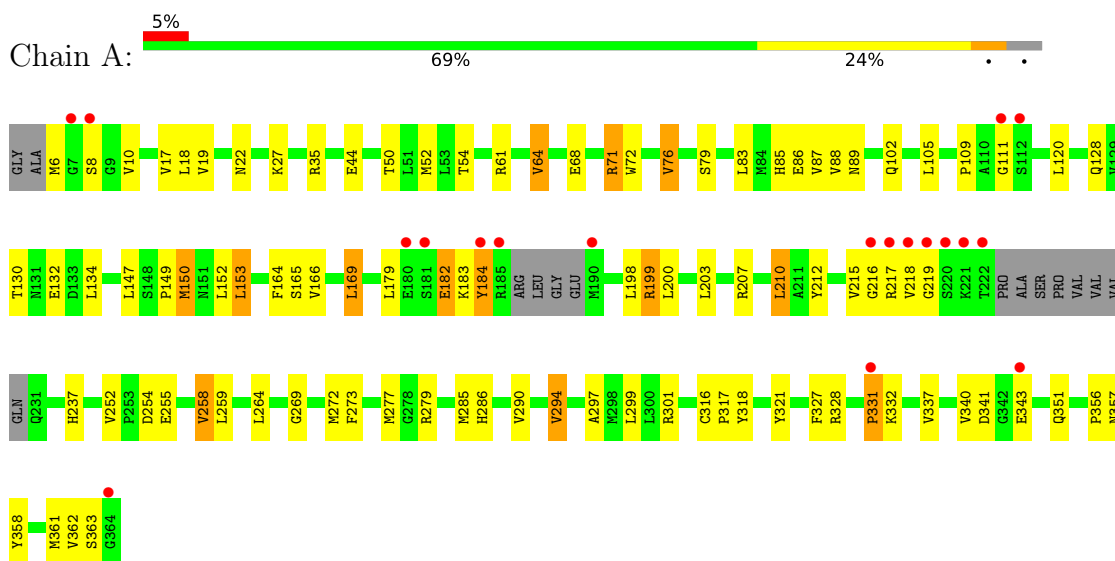
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	36	Total	O	0	0
			36	36		

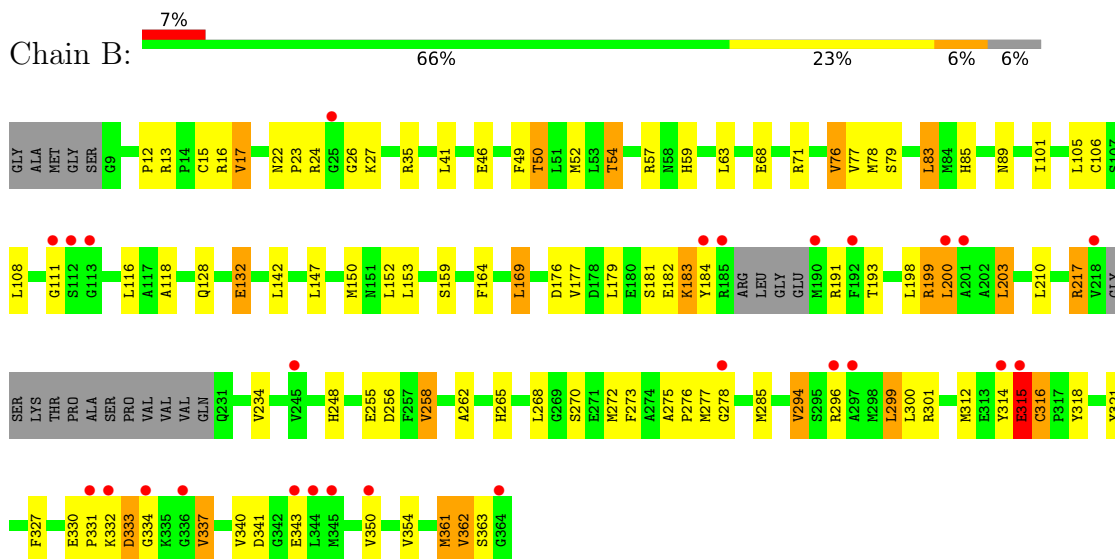
3 Residue-property plots [i](#)

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.

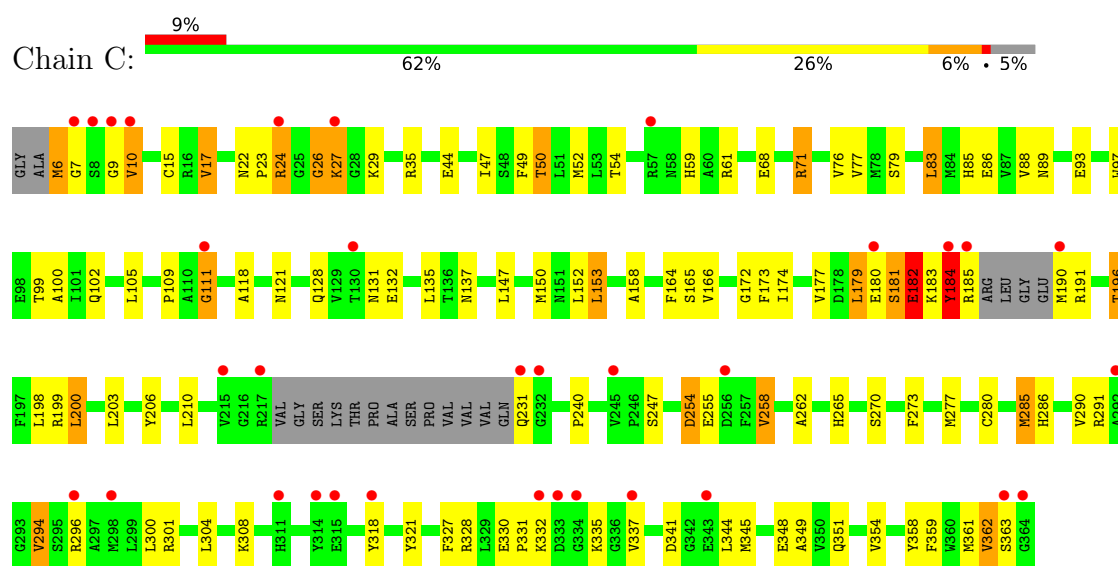
• Molecule 1: Sphingosine kinase 1



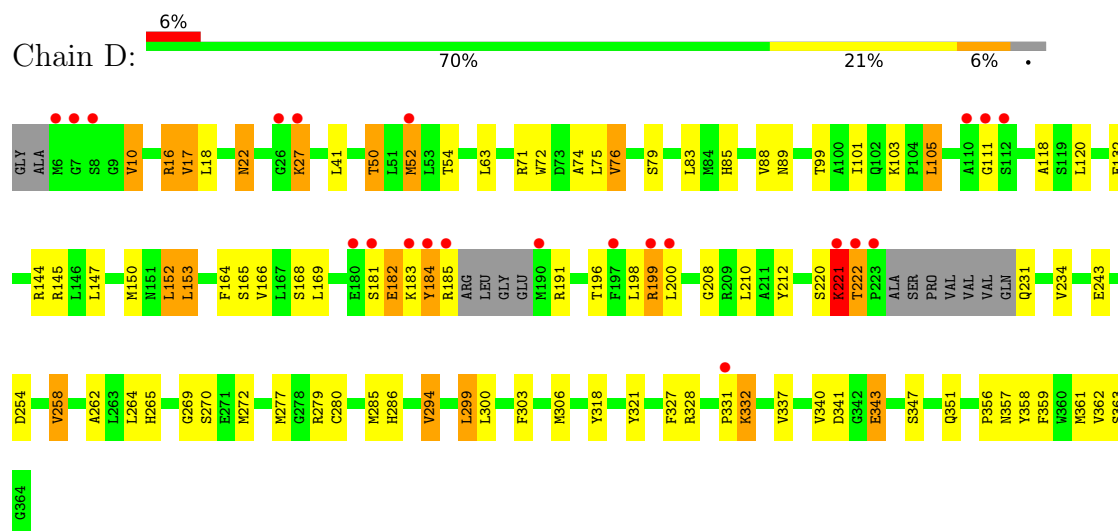
• Molecule 1: Sphingosine kinase 1



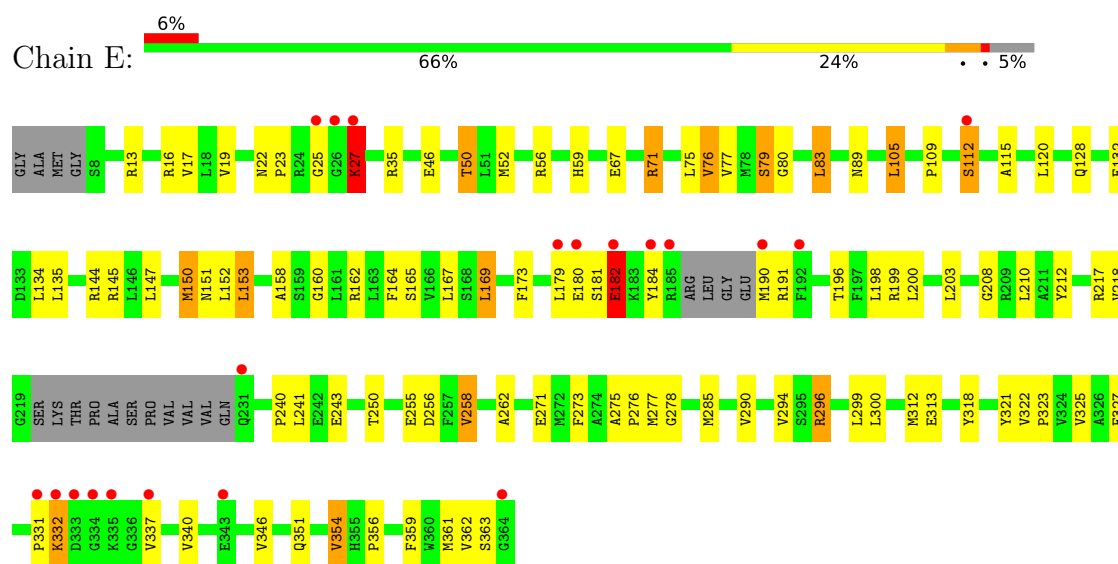
• Molecule 1: Sphingosine kinase 1



• Molecule 1: Sphingosine kinase 1

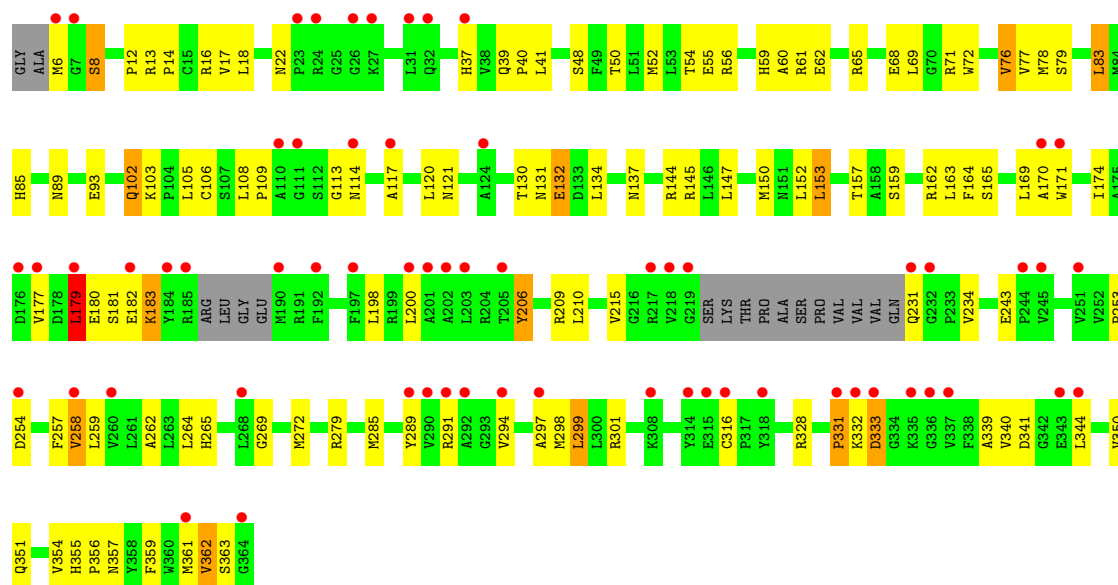


• Molecule 1: Sphingosine kinase 1



● Molecule 1: Sphingosine kinase 1

Chain F:  17% 62% 30% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.22Å 106.61Å 226.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.30) 92.0 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.285 0.227 , 0.281	Depositor DCC
R_{free} test set	5084 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16468	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4545e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UUL, EDO

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	0.76	0/2755	0.92	2/3735 (0.1%)
1	B	0.76	0/2714	0.94	1/3682 (0.0%)
1	C	0.75	0/2725	0.91	1/3695 (0.0%)
1	D	0.74	0/2763	0.91	4/3747 (0.1%)
1	E	0.73	0/2724	0.92	0/3695
1	F	0.74	0/2734	0.92	2/3707 (0.1%)
All	All	0.75	0/16415	0.92	10/22261 (0.0%)

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	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	MET	N-CA-C	-9.49	98.00	110.53
1	B	316	CYS	N-CA-C	-7.89	92.36	109.81
1	F	355	HIS	CA-C-N	6.51	126.86	119.83
1	F	355	HIS	C-N-CA	6.51	126.86	119.83
1	A	184	TYR	N-CA-C	-6.29	104.66	112.72
1	D	277	MET	N-CA-C	-6.04	102.98	110.41
1	C	131	ASN	CB-CA-C	-5.26	110.53	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	SER	N-CA-C	5.21	116.45	108.42
1	D	243	GLU	CA-C-N	-5.03	115.05	120.03
1	D	243	GLU	C-N-CA	-5.03	115.05	120.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	PRO	Peptide
1	B	315	GLU	Peptide
1	C	26	GLY	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	2694	0	2716	63	0
1	B	2653	0	2679	86	0
1	C	2664	0	2687	74	0
1	D	2701	0	2723	74	0
1	E	2663	0	2687	79	0
1	F	2673	0	2692	78	0
2	A	20	0	10	0	0
2	B	20	0	11	1	0
2	C	20	0	10	1	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	11	0	0
3	D	4	0	6	0	0
3	F	4	0	6	2	0
4	A	60	0	0	7	0
4	B	53	0	0	7	0
4	C	62	0	0	6	0
4	D	35	0	0	1	0
4	E	46	0	0	2	0
4	F	36	0	0	2	0
All	All	16468	0	16258	435	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 13.

All (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:PRO:HA	1:D:332:LYS:HB2	1.17	1.15
1:B:52:MET:HE2	1:C:52:MET:HE2	1.30	1.13
1:B:52:MET:HE2	1:C:52:MET:CE	1.81	1.11
1:F:150:MET:HE2	1:F:265:HIS:HE1	1.18	1.07
1:C:262:ALA:HB1	1:C:285:MET:HE3	1.40	1.03
1:A:18:LEU:HD11	1:A:52:MET:HE3	1.39	1.02
1:B:262:ALA:HB1	1:B:285:MET:CE	1.91	1.00
1:B:315:GLU:HB2	1:D:10:VAL:HG23	1.43	0.97
1:F:17:VAL:HG11	1:F:76:VAL:HG12	1.46	0.96
1:E:52:MET:HE2	1:F:52:MET:HE2	1.46	0.96
1:B:89:ASN:HD21	1:B:164:PHE:H	1.11	0.96
1:F:150:MET:CE	1:F:265:HIS:HE1	1.79	0.95
1:C:9:GLY:HA2	1:C:10:VAL:HG22	1.50	0.94
1:E:52:MET:HE2	1:F:52:MET:CE	1.96	0.94
1:B:150:MET:HE2	1:B:265:HIS:HE1	1.32	0.93
1:E:89:ASN:HD21	1:E:164:PHE:H	1.01	0.92
1:F:17:VAL:CG1	1:F:76:VAL:HG12	2.01	0.91
1:D:89:ASN:HD21	1:D:164:PHE:H	1.18	0.91
1:D:18:LEU:HD11	1:D:52:MET:HE3	1.53	0.90
1:E:52:MET:CE	1:F:52:MET:HE2	2.03	0.88
1:C:9:GLY:HA2	1:C:10:VAL:CG2	2.03	0.88
1:D:343:GLU:HB2	4:D:1125:HOH:O	1.72	0.88
1:F:359:PHE:HE2	1:F:361:MET:HE2	1.37	0.88
1:B:150:MET:HE2	1:B:265:HIS:CE1	2.09	0.87
1:F:150:MET:HE2	1:F:265:HIS:CE1	2.09	0.86
1:F:17:VAL:HG11	1:F:76:VAL:CG1	2.06	0.85
1:B:116:LEU:HD21	1:B:361:MET:HE1	1.57	0.85
1:C:89:ASN:HD21	1:C:164:PHE:H	1.21	0.84
1:F:89:ASN:HD21	1:F:164:PHE:H	1.24	0.83
1:D:16:ARG:HG2	1:D:16:ARG:HH11	1.43	0.83
1:A:264:LEU:CD1	1:A:285:MET:HE3	2.10	0.82
1:D:199:ARG:HG3	1:D:199:ARG:HH11	1.44	0.82
1:A:182:GLU:O	1:A:182:GLU:HG2	1.79	0.81
1:F:264:LEU:CD1	1:F:285:MET:HE3	2.10	0.81
1:F:177:VAL:O	1:F:181:SER:HB2	1.81	0.81
1:B:52:MET:CE	1:C:52:MET:HE2	2.10	0.80
1:D:264:LEU:HD12	1:D:285:MET:HE3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:O	1:B:181:SER:HB2	1.82	0.79
1:C:285:MET:SD	1:C:354:VAL:HG22	2.22	0.79
1:D:221:LYS:O	1:D:222:THR:CB	2.30	0.78
1:F:169:LEU:HD12	1:F:340:VAL:HG22	1.66	0.78
1:F:17:VAL:CG1	1:F:76:VAL:CG1	2.62	0.77
1:C:150:MET:HE2	1:C:265:HIS:HE1	1.47	0.77
1:E:296:ARG:HH21	1:E:296:ARG:HB2	1.49	0.77
1:A:89:ASN:HD21	1:A:164:PHE:H	1.32	0.77
1:B:52:MET:HE2	1:C:52:MET:HE1	1.65	0.76
1:C:121:ASN:HD21	1:C:137:ASN:HD22	1.32	0.76
1:E:262:ALA:HB1	1:E:285:MET:HE2	1.69	0.75
1:C:182:GLU:OE1	1:C:182:GLU:O	2.05	0.75
1:F:269:GLY:HA3	1:F:272:MET:HE3	1.69	0.74
1:F:264:LEU:HD12	1:F:285:MET:HE3	1.69	0.73
1:D:199:ARG:HH11	1:D:199:ARG:CG	2.01	0.73
1:D:18:LEU:CD1	1:D:52:MET:HE3	2.18	0.73
1:F:150:MET:CE	1:F:265:HIS:CE1	2.68	0.73
1:C:262:ALA:HB1	1:C:285:MET:CE	2.17	0.72
1:E:89:ASN:ND2	1:E:164:PHE:H	1.84	0.72
1:D:17:VAL:HG13	1:D:76:VAL:HG13	1.72	0.71
1:E:217:ARG:NH2	1:E:250:THR:OG1	2.21	0.71
1:C:150:MET:HE2	1:C:265:HIS:CE1	2.26	0.71
1:A:18:LEU:CD1	1:A:52:MET:HE3	2.19	0.71
1:D:331:PRO:CA	1:D:332:LYS:HB2	2.07	0.71
1:B:296:ARG:HD3	4:B:1151:HOH:O	1.89	0.70
1:C:9:GLY:CA	1:C:10:VAL:HG22	2.21	0.70
1:D:328:ARG:HH21	1:D:351:GLN:HE22	1.40	0.69
1:F:121:ASN:HD21	1:F:137:ASN:HD22	1.40	0.69
1:F:298:MET:HE3	1:F:316:CYS:HB2	1.73	0.69
1:C:177:VAL:O	1:C:181:SER:HB2	1.91	0.69
1:A:10:VAL:HG11	1:E:313:GLU:O	1.91	0.69
1:B:262:ALA:HB1	1:B:285:MET:HE3	1.73	0.69
1:C:331:PRO:HA	1:C:332:LYS:HB3	1.74	0.69
1:F:55:GLU:H	1:F:59:HIS:HD1	1.40	0.69
1:B:150:MET:CE	1:B:265:HIS:HE1	2.03	0.68
1:E:181:SER:HB3	1:E:191:ARG:HD2	1.74	0.68
1:E:217:ARG:HH21	1:E:250:THR:HG1	1.42	0.67
1:C:22:ASN:C	1:C:22:ASN:HD22	2.02	0.67
1:E:331:PRO:HA	1:E:332:LYS:CB	2.23	0.67
1:F:113:GLY:HA3	4:F:1115:HOH:O	1.93	0.67
1:A:264:LEU:HD11	1:A:285:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:PRO:HA	1:D:332:LYS:CB	2.07	0.66
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.07	0.66
1:D:220:SER:C	1:D:221:LYS:HG2	2.20	0.66
1:A:264:LEU:HD12	1:A:285:MET:HE3	1.77	0.66
1:F:264:LEU:HD11	1:F:285:MET:HE3	1.78	0.66
1:B:315:GLU:CB	1:D:10:VAL:HG23	2.24	0.65
1:B:184:TYR:HA	1:B:191:ARG:HD3	1.78	0.65
1:A:216:GLY:HA2	4:A:1150:HOH:O	1.96	0.65
1:F:169:LEU:CD1	1:F:340:VAL:HG22	2.26	0.65
1:F:262:ALA:HB1	1:F:285:MET:HE2	1.78	0.65
1:E:277:MET:HE1	1:E:312:MET:HE2	1.79	0.65
1:A:120:LEU:HD22	1:A:363:SER:HB3	1.77	0.64
1:F:359:PHE:CE2	1:F:361:MET:HE2	2.27	0.64
1:A:316:CYS:HA	4:A:1131:HOH:O	1.97	0.64
1:A:297:ALA:O	1:A:301:ARG:HG3	1.97	0.64
1:D:16:ARG:HG2	1:D:16:ARG:NH1	2.08	0.64
1:D:262:ALA:HB1	1:D:285:MET:CE	2.27	0.64
1:A:331:PRO:HA	1:A:332:LYS:HB3	1.80	0.64
1:B:217:ARG:NH2	1:B:248:HIS:O	2.31	0.64
1:B:268:LEU:HB3	1:B:272:MET:HE3	1.80	0.64
1:E:22:ASN:C	1:E:22:ASN:HD22	2.06	0.63
1:F:328:ARG:HE	1:F:351:GLN:NE2	1.97	0.63
1:A:286:HIS:HD2	1:A:321:TYR:OH	1.81	0.63
1:D:258:VAL:HG21	1:D:299:LEU:HD11	1.81	0.62
4:A:1137:HOH:O	1:E:278:GLY:HA3	1.99	0.62
1:C:26:GLY:H	1:C:111:GLY:HA2	1.64	0.62
1:A:18:LEU:HD11	1:A:52:MET:CE	2.23	0.62
1:B:315:GLU:HB2	1:D:10:VAL:CG2	2.24	0.62
1:B:331:PRO:HA	1:B:332:LYS:CB	2.30	0.62
1:C:86:GLU:HG3	4:C:1160:HOH:O	1.98	0.62
1:D:200:LEU:HD21	1:D:300:LEU:HB2	1.82	0.62
1:B:22:ASN:C	1:B:22:ASN:HD22	2.07	0.61
1:E:56:ARG:HG2	1:E:59:HIS:HB2	1.82	0.61
1:E:112:SER:HB3	1:E:191:ARG:HH21	1.66	0.61
1:B:59:HIS:NE2	1:C:50:THR:HG22	2.16	0.61
1:B:285:MET:SD	1:B:354:VAL:HG22	2.41	0.61
1:E:296:ARG:HB2	1:E:296:ARG:NH2	2.16	0.61
1:C:88:VAL:HG21	1:C:166:VAL:HG11	1.83	0.61
1:B:89:ASN:ND2	1:B:164:PHE:H	1.92	0.61
1:D:181:SER:HB3	1:D:191:ARG:HH11	1.65	0.61
1:C:150:MET:HG3	1:C:361:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:LEU:HD21	1:E:351:GLN:HG2	1.83	0.60
1:C:362:VAL:HG22	4:C:1101:HOH:O	2.00	0.60
1:D:22:ASN:C	1:D:22:ASN:HD22	2.07	0.60
1:B:169:LEU:HD12	1:B:340:VAL:HG22	1.83	0.60
1:C:359:PHE:HE2	1:C:361:MET:HE2	1.66	0.60
1:B:17:VAL:HG13	1:B:76:VAL:HG13	1.83	0.59
1:B:116:LEU:CD2	1:B:361:MET:HE1	2.31	0.59
1:D:50:THR:HG23	1:D:72:TRP:CH2	2.37	0.59
1:A:328:ARG:HH21	1:A:351:GLN:HE22	1.50	0.59
1:A:264:LEU:CD1	1:A:285:MET:CE	2.79	0.59
1:E:17:VAL:CG1	1:E:76:VAL:HG13	2.33	0.58
1:A:182:GLU:O	1:A:182:GLU:CG	2.52	0.58
1:C:68:GLU:O	1:C:71:ARG:HG3	2.04	0.58
1:C:254:ASP:CG	1:C:291:ARG:HD2	2.28	0.58
1:A:153:LEU:HB3	1:A:165:SER:HB3	1.85	0.58
1:B:50:THR:CG2	1:C:59:HIS:HE2	2.16	0.58
1:E:25:GLY:HA2	1:E:27:LYS:NZ	2.18	0.58
1:F:253:PRO:HA	4:F:1133:HOH:O	2.03	0.58
1:A:150:MET:HE1	1:A:279:ARG:NH2	2.19	0.58
1:C:359:PHE:CE2	1:C:361:MET:HE2	2.39	0.57
1:D:262:ALA:HB1	1:D:285:MET:HE2	1.86	0.57
1:F:62:GLU:HG2	1:F:65:ARG:NH2	2.19	0.57
1:A:331:PRO:HA	1:A:332:LYS:CB	2.34	0.57
1:A:255:GLU:OE1	1:A:332:LYS:NZ	2.37	0.57
1:E:173:PHE:CE1	1:E:196:THR:HG23	2.40	0.57
1:E:17:VAL:HG13	1:E:76:VAL:HG13	1.87	0.57
1:F:22:ASN:C	1:F:22:ASN:HD22	2.11	0.57
1:D:17:VAL:HG22	1:D:74:ALA:HB3	1.86	0.57
1:A:150:MET:HE1	1:A:279:ARG:HH21	1.70	0.56
1:E:52:MET:CE	1:F:52:MET:CE	2.72	0.56
1:C:285:MET:SD	1:C:354:VAL:CG2	2.93	0.56
1:C:196:THR:HG23	1:C:200:LEU:HD23	1.88	0.56
1:E:153:LEU:HB3	1:E:165:SER:HB3	1.86	0.56
1:E:182:GLU:HG2	1:E:182:GLU:O	2.04	0.56
1:B:116:LEU:HD21	1:B:361:MET:CE	2.32	0.56
1:B:13:ARG:NH1	1:B:46:GLU:OE2	2.40	0.55
1:B:315:GLU:HG3	1:B:316:CYS:H	1.71	0.55
1:A:264:LEU:HD11	1:A:285:MET:CE	2.37	0.55
1:E:89:ASN:HD21	1:E:164:PHE:N	1.86	0.55
1:D:150:MET:HE3	1:D:150:MET:HA	1.87	0.55
1:B:128:GLN:HE22	1:B:273:PHE:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:LEU:HD13	1:F:180:GLU:N	2.22	0.55
1:F:262:ALA:HB1	1:F:285:MET:CE	2.37	0.55
1:A:264:LEU:HD12	1:A:285:MET:CE	2.36	0.55
1:B:332:LYS:O	1:B:333:ASP:HB3	2.06	0.55
1:E:150:MET:HG3	1:E:361:MET:HE3	1.89	0.54
1:D:89:ASN:HD21	1:D:164:PHE:N	1.96	0.54
1:C:300:LEU:O	1:C:304:LEU:HG	2.07	0.54
1:B:16:ARG:HD2	1:B:71:ARG:O	2.08	0.54
1:B:276:PRO:HG3	1:B:312:MET:HG3	1.88	0.54
1:A:19:VAL:HG22	1:A:76:VAL:HG22	1.90	0.54
1:A:149:PRO:O	1:A:150:MET:HE3	2.06	0.54
1:A:150:MET:HG3	1:A:361:MET:HE2	1.87	0.54
1:D:54:THR:HG23	1:D:54:THR:O	2.09	0.53
1:C:328:ARG:HE	1:C:351:GLN:NE2	2.05	0.53
1:E:363:SER:HB2	4:E:1107:HOH:O	2.08	0.53
1:F:114:ASN:HB3	1:F:117:ALA:HB3	1.89	0.53
1:B:22:ASN:HD21	1:B:24:ARG:HB2	1.73	0.53
1:B:50:THR:HG22	1:C:59:HIS:HE2	1.73	0.53
1:D:328:ARG:HE	1:D:351:GLN:NE2	2.05	0.53
1:F:37:HIS:CE1	1:F:132:GLU:HB3	2.43	0.53
1:F:279:ARG:HG3	3:F:1002:EDO:O2	2.09	0.53
1:D:294:VAL:HG13	1:D:318:TYR:CB	2.38	0.53
1:E:120:LEU:HD22	1:E:363:SER:HB3	1.90	0.52
1:E:169:LEU:HD12	1:E:340:VAL:HG22	1.91	0.52
1:B:301:ARG:HD3	1:B:314:TYR:CE2	2.44	0.52
1:F:89:ASN:HD21	1:F:164:PHE:N	2.02	0.52
1:F:206:TYR:CD1	1:F:206:TYR:N	2.77	0.52
1:B:262:ALA:HB1	1:B:285:MET:HE2	1.83	0.52
1:B:22:ASN:ND2	1:B:24:ARG:H	2.07	0.52
1:D:264:LEU:CD1	1:D:285:MET:HE3	2.36	0.52
1:C:88:VAL:HG21	1:C:166:VAL:CG1	2.39	0.52
1:C:179:LEU:HG	1:C:344:LEU:HD13	1.91	0.52
1:F:254:ASP:OD1	1:F:291:ARG:HD2	2.10	0.52
1:A:54:THR:HG23	1:A:54:THR:O	2.10	0.52
1:C:22:ASN:HD21	1:C:24:ARG:HB2	1.75	0.52
1:E:181:SER:HB3	1:E:191:ARG:HH11	1.74	0.52
1:B:314:TYR:O	1:B:315:GLU:O	2.27	0.52
1:E:77:VAL:CG1	1:E:83:LEU:HB3	2.40	0.51
1:C:331:PRO:HA	1:C:332:LYS:CB	2.38	0.51
1:D:208:GLY:HA2	1:D:332:LYS:HG3	1.92	0.51
1:E:200:LEU:HD21	1:E:300:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ALA:HB2	1:D:270:SER:HA	1.93	0.51
1:D:280:CYS:SG	1:D:286:HIS:CE1	3.04	0.51
1:D:152:LEU:CD2	1:D:164:PHE:HB3	2.40	0.51
1:E:359:PHE:CE2	1:E:361:MET:HE2	2.46	0.51
1:F:144:ARG:O	1:F:145:ARG:HB2	2.11	0.51
1:C:301:ARG:HD3	4:C:1159:HOH:O	2.10	0.51
1:D:286:HIS:HD2	1:D:321:TYR:OH	1.94	0.51
1:C:128:GLN:HE22	1:C:273:PHE:HB2	1.76	0.51
1:D:120:LEU:HD21	1:D:361:MET:HE3	1.93	0.50
1:F:356:PRO:O	1:F:357:ASN:C	2.54	0.50
1:C:173:PHE:CE2	1:C:199:ARG:HB3	2.46	0.50
1:F:106:CYS:HB2	1:F:362:VAL:HG13	1.92	0.50
1:F:264:LEU:HD11	1:F:285:MET:CE	2.42	0.50
1:A:68:GLU:O	1:A:71:ARG:HG3	2.11	0.50
1:A:269:GLY:HA3	1:A:272:MET:HE3	1.93	0.50
1:B:150:MET:HG3	1:B:361:MET:HG3	1.94	0.50
1:F:150:MET:HG3	1:F:361:MET:HE3	1.93	0.50
1:D:120:LEU:HD22	1:D:363:SER:HB3	1.94	0.50
1:B:277:MET:HE2	1:B:321:TYR:CE2	2.47	0.50
1:B:277:MET:HE1	1:B:312:MET:HE2	1.93	0.50
1:D:75:LEU:HB2	1:D:105:LEU:HD12	1.92	0.50
1:F:258:VAL:HG21	1:F:299:LEU:HD11	1.93	0.50
1:E:240:PRO:HG2	1:E:243:GLU:HG3	1.93	0.49
1:B:57:ARG:HA	4:B:1129:HOH:O	2.12	0.49
1:F:297:ALA:HB1	1:F:301:ARG:HH12	1.77	0.49
1:C:185:ARG:HA	1:C:190:MET:SD	2.51	0.49
1:C:290:VAL:CG1	1:C:294:VAL:HG21	2.42	0.49
1:F:16:ARG:HB3	1:F:48:SER:HB2	1.93	0.49
1:D:196:THR:O	1:D:200:LEU:HB2	2.12	0.49
1:D:294:VAL:HG13	1:D:318:TYR:HB2	1.95	0.49
1:E:275:ALA:O	1:E:277:MET:O	2.30	0.49
1:A:237:HIS:HD2	4:A:1107:HOH:O	1.95	0.49
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.75	0.49
1:A:258:VAL:HG22	1:A:290:VAL:HB	1.94	0.49
1:A:128:GLN:HE22	1:A:273:PHE:HB2	1.78	0.49
1:C:196:THR:HG23	1:C:200:LEU:CD2	2.42	0.49
1:C:335:LYS:HG3	1:C:348:GLU:HG3	1.94	0.49
1:F:12:PRO:O	1:F:145:ARG:NE	2.41	0.49
1:A:149:PRO:HB2	1:A:357:ASN:HB3	1.95	0.48
1:B:150:MET:CE	1:B:265:HIS:CE1	2.86	0.48
1:F:153:LEU:HB3	1:F:165:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ALA:CB	1:D:270:SER:HA	2.43	0.48
1:D:85:HIS:HD2	1:D:341:ASP:OD2	1.96	0.48
1:F:174:ILE:HD13	1:F:259:LEU:HD22	1.93	0.48
1:E:27:LYS:HE3	1:E:27:LYS:HA	1.96	0.48
1:A:85:HIS:HD2	1:A:341:ASP:OD2	1.96	0.48
1:B:331:PRO:HA	1:B:332:LYS:HB2	1.96	0.48
1:C:172:GLY:HA2	1:C:206:TYR:CE1	2.50	0.47
1:D:182:GLU:O	1:D:182:GLU:HG2	2.14	0.47
1:E:359:PHE:HE2	1:E:361:MET:HE2	1.79	0.47
1:D:200:LEU:HD11	1:D:299:LEU:HB3	1.96	0.47
1:A:216:GLY:CA	4:A:1150:HOH:O	2.57	0.47
1:B:150:MET:HE3	1:B:150:MET:HA	1.95	0.47
1:F:120:LEU:HD22	1:F:363:SER:HB3	1.97	0.47
1:B:183:LYS:H	1:B:183:LYS:HD3	1.80	0.47
1:E:83:LEU:HD23	1:E:83:LEU:HA	1.73	0.47
1:E:150:MET:HE3	1:E:150:MET:HA	1.97	0.47
1:F:269:GLY:H	1:F:272:MET:HB2	1.79	0.47
1:B:77:VAL:CG1	1:B:83:LEU:HB3	2.45	0.47
1:D:169:LEU:HD12	1:D:340:VAL:HG22	1.96	0.47
1:A:8:SER:O	1:E:312:MET:HE3	2.14	0.47
1:A:61:ARG:HD3	1:A:86:GLU:OE2	2.14	0.47
1:D:150:MET:HE2	1:D:265:HIS:HE1	1.78	0.47
1:D:184:TYR:O	1:D:185:ARG:C	2.56	0.47
1:D:303:PHE:O	1:D:306:MET:HB3	2.15	0.47
1:F:39:GLN:N	1:F:40:PRO:HD2	2.30	0.47
1:F:157:THR:HG22	1:F:350:VAL:HG22	1.95	0.47
1:F:109:PRO:HG3	1:F:134:LEU:HG	1.97	0.47
1:C:182:GLU:O	1:C:182:GLU:CG	2.62	0.47
1:C:285:MET:HE1	1:C:327:PHE:CE2	2.50	0.47
1:E:19:VAL:HG22	1:E:76:VAL:HG22	1.97	0.47
1:E:173:PHE:HE1	1:E:196:THR:HG23	1.77	0.46
1:F:171:TRP:CZ2	1:F:331:PRO:HG3	2.50	0.46
1:A:71:ARG:HD3	1:A:72:TRP:CE2	2.50	0.46
1:D:17:VAL:CG1	1:D:76:VAL:HG13	2.43	0.46
1:E:25:GLY:HA2	1:E:27:LYS:HZ1	1.79	0.46
1:E:109:PRO:HG3	1:E:134:LEU:HG	1.98	0.46
1:E:158:ALA:C	1:E:160:GLY:H	2.24	0.46
1:A:217:ARG:H	1:A:217:ARG:HD3	1.80	0.46
1:A:219:GLY:HA2	1:E:356:PRO:O	2.16	0.46
1:E:285:MET:SD	1:E:354:VAL:HG22	2.54	0.46
1:E:294:VAL:HG22	1:E:318:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ASN:HD22	1:B:24:ARG:H	1.62	0.46
1:B:54:THR:HG23	1:B:54:THR:O	2.16	0.46
1:C:85:HIS:HD2	1:C:341:ASP:OD2	1.99	0.46
1:F:78:MET:HA	1:F:108:LEU:O	2.15	0.46
1:F:85:HIS:HD2	1:F:341:ASP:OD2	1.99	0.46
1:B:22:ASN:HD22	1:B:23:PRO:N	2.14	0.46
1:B:77:VAL:HG13	1:B:83:LEU:HD13	1.97	0.46
1:B:85:HIS:HD2	1:B:341:ASP:OD2	1.98	0.46
1:C:286:HIS:HD2	1:C:321:TYR:OH	1.98	0.46
1:A:207:ARG:O	1:A:332:LYS:HB3	2.16	0.46
1:B:118:ALA:CB	1:B:270:SER:HA	2.45	0.46
1:B:181:SER:HB3	1:B:191:ARG:HH11	1.81	0.46
1:C:6:MET:HE3	1:C:358:TYR:HA	1.96	0.46
1:E:77:VAL:HG13	1:E:83:LEU:HD13	1.98	0.46
1:F:68:GLU:HB3	1:F:71:ARG:HD2	1.98	0.46
1:A:6:MET:HB3	4:A:1129:HOH:O	2.15	0.45
1:D:262:ALA:HB1	1:D:285:MET:HE1	1.98	0.45
1:E:331:PRO:HA	1:E:332:LYS:HB3	1.98	0.45
1:F:183:LYS:O	1:F:183:LYS:HG2	2.16	0.45
1:F:289:TYR:HE1	1:F:291:ARG:HG2	1.81	0.45
1:B:150:MET:HE3	4:B:1137:HOH:O	2.16	0.45
1:E:262:ALA:HB1	1:E:285:MET:CE	2.45	0.45
1:B:363:SER:HB2	4:B:1102:HOH:O	2.15	0.45
1:C:27:LYS:CD	1:C:184:TYR:HB3	2.46	0.45
1:D:27:LYS:HE3	1:D:27:LYS:O	2.17	0.45
1:D:101:ILE:HG13	1:D:359:PHE:HB3	1.98	0.45
1:D:199:ARG:CG	1:D:199:ARG:NH1	2.70	0.45
1:D:212:TYR:HA	1:D:327:PHE:HA	1.99	0.45
1:A:294:VAL:HG13	1:A:318:TYR:HB2	1.98	0.45
1:B:181:SER:HB3	1:B:191:ARG:NH1	2.32	0.45
1:B:277:MET:HE2	1:B:321:TYR:CZ	2.51	0.45
1:D:152:LEU:HD21	1:D:164:PHE:HB3	1.99	0.45
1:E:150:MET:HE2	4:E:1110:HOH:O	2.16	0.45
1:F:17:VAL:HG12	1:F:76:VAL:CG1	2.47	0.45
1:A:259:LEU:HD12	1:A:259:LEU:C	2.42	0.44
1:B:68:GLU:HB3	1:B:71:ARG:HD2	1.99	0.44
1:C:24:ARG:O	1:C:27:LYS:HA	2.16	0.44
1:C:258:VAL:HG22	1:C:290:VAL:HB	1.98	0.44
1:E:208:GLY:HA2	1:E:332:LYS:HB3	1.99	0.44
1:B:142:LEU:HA	1:B:362:VAL:HG21	1.98	0.44
1:E:50:THR:HG22	1:F:59:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:VAL:HG22	1:E:318:TYR:CB	2.47	0.44
1:A:328:ARG:HE	1:A:351:GLN:NE2	2.15	0.44
1:D:153:LEU:HB3	1:D:165:SER:HB3	2.00	0.44
1:E:23:PRO:C	1:E:25:GLY:H	2.25	0.44
1:F:22:ASN:C	1:F:22:ASN:ND2	2.74	0.44
1:B:12:PRO:O	1:B:15:CYS:HB3	2.17	0.44
1:C:109:PRO:O	1:C:135:LEU:HD13	2.18	0.44
1:A:64:VAL:HG21	1:A:87:VAL:HG13	1.99	0.44
1:B:176:ASP:OD2	1:B:199:ARG:NH1	2.51	0.44
1:C:286:HIS:HE1	4:C:1112:HOH:O	2.00	0.44
1:E:75:LEU:HB2	1:E:105:LEU:HD12	1.99	0.44
1:E:321:TYR:CE2	1:E:323:PRO:HD3	2.53	0.44
1:A:71:ARG:HD3	1:A:72:TRP:NE1	2.33	0.44
1:B:78:MET:HA	1:B:108:LEU:O	2.18	0.44
1:F:61:ARG:NH2	1:F:93:GLU:OE2	2.44	0.44
1:F:18:LEU:HB2	1:F:72:TRP:CE2	2.52	0.44
1:A:343:GLU:HB3	4:A:1157:HOH:O	2.18	0.43
1:B:26:GLY:H	1:B:111:GLY:HA2	1.83	0.43
1:C:118:ALA:CB	1:C:270:SER:HA	2.48	0.43
1:D:50:THR:HG23	1:D:72:TRP:CZ3	2.53	0.43
1:E:22:ASN:C	1:E:22:ASN:ND2	2.74	0.43
1:A:210:LEU:HD13	1:A:252:VAL:HG21	2.01	0.43
1:C:150:MET:HE3	4:C:1107:HOH:O	2.18	0.43
1:E:115:ALA:HB3	1:E:167:LEU:HD21	1.99	0.43
1:E:331:PRO:HA	1:E:332:LYS:HB2	1.97	0.43
1:A:182:GLU:OE1	1:A:183:LYS:HE2	2.19	0.43
1:B:272:MET:HE1	2:B:1001:UUL:H2	2.00	0.43
1:C:109:PRO:HD2	1:C:135:LEU:HD12	1.99	0.43
1:D:16:ARG:HH11	1:D:16:ARG:CG	2.20	0.43
1:F:54:THR:HG21	1:F:60:ALA:HB2	2.00	0.43
1:A:27:LYS:HG3	1:A:27:LYS:O	2.18	0.43
1:C:29:LYS:HA	4:C:1104:HOH:O	2.19	0.43
1:E:128:GLN:HE22	1:E:273:PHE:HB2	1.84	0.43
1:E:109:PRO:HD2	1:E:135:LEU:HA	2.01	0.43
1:E:150:MET:HA	1:E:150:MET:CE	2.48	0.43
1:F:130:THR:OG1	1:F:131:ASN:N	2.52	0.43
1:B:17:VAL:O	1:B:49:PHE:HA	2.19	0.42
1:C:77:VAL:CG1	1:C:83:LEU:HB3	2.50	0.42
1:C:158:ALA:HB2	1:C:349:ALA:HB3	2.01	0.42
1:D:182:GLU:OE1	1:D:183:LYS:HG2	2.18	0.42
1:D:356:PRO:O	1:D:357:ASN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD21	1:B:300:LEU:HB2	2.01	0.42
1:B:275:ALA:O	1:B:277:MET:O	2.37	0.42
1:F:332:LYS:O	1:F:333:ASP:HB2	2.18	0.42
1:A:109:PRO:HG3	1:A:134:LEU:HG	2.01	0.42
1:A:88:VAL:HG21	1:A:166:VAL:HG11	2.02	0.42
1:C:22:ASN:HD22	1:C:23:PRO:N	2.16	0.42
1:C:174:ILE:HG23	2:C:1001:UUL:C12	2.50	0.42
1:C:181:SER:HB3	1:C:191:ARG:NH1	2.34	0.42
1:C:17:VAL:O	1:C:49:PHE:HA	2.20	0.42
1:E:67:GLU:OE2	1:E:71:ARG:NH1	2.48	0.42
1:A:316:CYS:HA	1:A:317:PRO:HD3	1.92	0.42
1:B:132:GLU:H	1:B:132:GLU:HG2	1.54	0.42
1:F:77:VAL:HG13	1:F:83:LEU:HB3	2.01	0.42
1:A:22:ASN:C	1:A:22:ASN:HD22	2.28	0.42
1:B:54:THR:O	1:B:54:THR:CG2	2.68	0.42
1:B:278:GLY:HA3	4:B:1146:HOH:O	2.18	0.42
1:B:337:VAL:HG13	4:B:1111:HOH:O	2.20	0.42
1:D:88:VAL:HG21	1:D:166:VAL:HG11	2.01	0.42
1:E:13:ARG:NH1	1:E:46:GLU:OE2	2.53	0.42
1:A:212:TYR:HA	1:A:327:PHE:HA	2.01	0.41
1:C:294:VAL:HG22	1:C:318:TYR:CB	2.50	0.41
1:C:97:TRP:HA	1:C:100:ALA:HB3	2.02	0.41
1:D:294:VAL:HG13	1:D:318:TYR:CG	2.55	0.41
1:E:144:ARG:O	1:E:145:ARG:HB2	2.20	0.41
1:F:6:MET:HG3	1:F:102:GLN:HE21	1.85	0.41
1:C:280:CYS:SG	1:C:286:HIS:CE1	3.13	0.41
1:D:150:MET:HE2	1:D:265:HIS:CE1	2.55	0.41
1:D:150:MET:HG3	1:D:361:MET:HE2	2.03	0.41
1:F:69:LEU:HB3	1:F:103:LYS:HE3	2.02	0.41
1:B:294:VAL:HG22	1:B:318:TYR:CB	2.51	0.41
1:C:150:MET:HE3	1:C:150:MET:HA	2.01	0.41
1:F:150:MET:HE3	3:F:1002:EDO:O1	2.21	0.41
1:B:258:VAL:HG21	1:B:299:LEU:HD11	2.03	0.41
1:D:144:ARG:O	1:D:145:ARG:HB2	2.20	0.41
1:B:262:ALA:HB1	1:B:285:MET:HE1	1.93	0.41
1:E:212:TYR:HA	1:E:327:PHE:HA	2.03	0.41
1:F:170:ALA:HB3	1:F:339:ALA:HB3	2.02	0.41
1:B:362:VAL:HG22	4:B:1105:HOH:O	2.20	0.41
1:E:181:SER:CB	1:E:191:ARG:HH11	2.33	0.41
1:B:106:CYS:HB2	1:B:362:VAL:HG13	2.03	0.41
1:B:169:LEU:HD22	1:B:327:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:CG	1:B:312:MET:HG3	2.51	0.41
1:E:150:MET:HG3	1:E:361:MET:CE	2.50	0.41
1:F:289:TYR:CE1	1:F:291:ARG:HG2	2.56	0.41
1:B:68:GLU:HG3	1:B:71:ARG:HG3	2.01	0.41
1:B:203:LEU:HD12	1:B:296:ARG:HG3	2.02	0.41
1:D:50:THR:HG23	1:D:72:TRP:HH2	1.84	0.41
1:D:150:MET:HE1	1:D:279:ARG:HH21	1.86	0.41
1:D:269:GLY:HA3	1:D:272:MET:HE3	2.01	0.41
1:E:325:VAL:O	1:E:354:VAL:HG23	2.21	0.41
1:F:174:ILE:CD1	1:F:259:LEU:HD22	2.51	0.41
1:E:79:SER:OG	1:E:80:GLY:N	2.49	0.41
1:E:25:GLY:C	1:E:27:LYS:N	2.75	0.40
1:E:258:VAL:HG13	1:E:290:VAL:HG12	2.04	0.40
1:E:276:PRO:HG3	1:E:312:MET:HG3	2.04	0.40
1:D:328:ARG:NH2	1:D:351:GLN:HE22	2.14	0.40
1:E:277:MET:HE2	1:E:321:TYR:CZ	2.57	0.40
1:B:63:LEU:HD21	1:C:50:THR:HG21	2.03	0.40
1:C:15:CYS:SG	1:C:47:ILE:HG12	2.62	0.40
1:F:206:TYR:HD1	1:F:257:PHE:O	2.05	0.40
1:A:169:LEU:HD12	1:A:340:VAL:HG22	2.03	0.40
1:C:61:ARG:NH2	1:C:93:GLU:OE2	2.44	0.40
1:C:153:LEU:HB3	1:C:165:SER:HB3	2.03	0.40
1:D:50:THR:CG2	1:D:72:TRP:HH2	2.35	0.40
1:E:151:ASN:OD1	1:E:356:PRO:HA	2.21	0.40
1:A:199:ARG:HH11	1:A:199:ARG:HG2	1.84	0.40
1:A:356:PRO:O	1:A:357:ASN:C	2.62	0.40
1:B:22:ASN:C	1:B:22:ASN:ND2	2.75	0.40
1:D:103:LYS:O	1:D:105:LEU:HD13	2.20	0.40
1:F:13:ARG:HA	1:F:14:PRO:HA	1.88	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	341/361 (94%)	319 (94%)	19 (6%)	3 (1%)	14	17
1	B	334/361 (92%)	311 (93%)	18 (5%)	5 (2%)	8	8
1	C	336/361 (93%)	308 (92%)	18 (5%)	10 (3%)	3	2
1	D	342/361 (95%)	322 (94%)	15 (4%)	5 (2%)	8	8
1	E	336/361 (93%)	317 (94%)	14 (4%)	5 (2%)	8	8
1	F	338/361 (94%)	308 (91%)	24 (7%)	6 (2%)	6	6
All	All	2027/2166 (94%)	1885 (93%)	108 (5%)	34 (2%)	7	7

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	GLU
1	C	182	GLU
1	C	183	LYS
1	C	277	MET
1	D	79	SER
1	D	222	THR
1	F	333	ASP
1	A	79	SER
1	A	111	GLY
1	B	79	SER
1	B	333	ASP
1	C	7	GLY
1	C	79	SER
1	C	184	TYR
1	D	111	GLY
1	E	27	LYS
1	E	218	VAL
1	F	79	SER
1	C	27	LYS
1	C	240	PRO
1	D	332	LYS
1	E	79	SER
1	E	184	TYR
1	F	8	SER
1	F	183	LYS
1	D	221	LYS
1	E	182	GLU
1	F	179	LEU
1	F	331	PRO
1	C	10	VAL

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Mol	Chain	Res	Type
1	B	217	ARG
1	B	334	GLY
1	C	111	GLY
1	A	215	VAL

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	286/299 (96%)	253 (88%)	33 (12%)	5	6
1	B	283/299 (95%)	245 (87%)	38 (13%)	4	4
1	C	284/299 (95%)	243 (86%)	41 (14%)	3	3
1	D	287/299 (96%)	252 (88%)	35 (12%)	5	5
1	E	284/299 (95%)	248 (87%)	36 (13%)	4	5
1	F	284/299 (95%)	252 (89%)	32 (11%)	5	7
All	All	1708/1794 (95%)	1493 (87%)	215 (13%)	4	5

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	35	ARG
1	A	44	GLU
1	A	50	THR
1	A	64	VAL
1	A	71	ARG
1	A	76	VAL
1	A	83	LEU
1	A	102	GLN
1	A	105	LEU
1	A	130	THR
1	A	132	GLU
1	A	147	LEU
1	A	150	MET

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	153	LEU
1	A	169	LEU
1	A	179	LEU
1	A	182	GLU
1	A	184	TYR
1	A	198	LEU
1	A	199	ARG
1	A	200	LEU
1	A	203	LEU
1	A	210	LEU
1	A	218	VAL
1	A	254	ASP
1	A	258	VAL
1	A	294	VAL
1	A	299	LEU
1	A	337	VAL
1	A	358	TYR
1	A	362	VAL
1	B	17	VAL
1	B	27	LYS
1	B	35	ARG
1	B	41	LEU
1	B	50	THR
1	B	54	THR
1	B	76	VAL
1	B	83	LEU
1	B	101	ILE
1	B	105	LEU
1	B	132	GLU
1	B	147	LEU
1	B	152	LEU
1	B	153	LEU
1	B	159	SER
1	B	169	LEU
1	B	179	LEU
1	B	182	GLU
1	B	183	LYS
1	B	193	THR
1	B	198	LEU
1	B	199	ARG
1	B	200	LEU

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	210	LEU
1	B	234	VAL
1	B	255	GLU
1	B	256	ASP
1	B	258	VAL
1	B	294	VAL
1	B	299	LEU
1	B	315	GLU
1	B	330	GLU
1	B	337	VAL
1	B	343	GLU
1	B	350	VAL
1	B	361	MET
1	B	362	VAL
1	C	6	MET
1	C	17	VAL
1	C	24	ARG
1	C	35	ARG
1	C	44	GLU
1	C	50	THR
1	C	54	THR
1	C	71	ARG
1	C	76	VAL
1	C	83	LEU
1	C	99	THR
1	C	102	GLN
1	C	105	LEU
1	C	132	GLU
1	C	147	LEU
1	C	152	LEU
1	C	153	LEU
1	C	179	LEU
1	C	180	GLU
1	C	181	SER
1	C	182	GLU
1	C	184	TYR
1	C	196	THR
1	C	198	LEU
1	C	200	LEU
1	C	203	LEU
1	C	210	LEU

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Mol	Chain	Res	Type
1	C	231	GLN
1	C	247	SER
1	C	254	ASP
1	C	255	GLU
1	C	258	VAL
1	C	285	MET
1	C	294	VAL
1	C	296	ARG
1	C	308	LYS
1	C	330	GLU
1	C	337	VAL
1	C	345	MET
1	C	362	VAL
1	C	363	SER
1	D	10	VAL
1	D	16	ARG
1	D	17	VAL
1	D	22	ASN
1	D	27	LYS
1	D	41	LEU
1	D	50	THR
1	D	52	MET
1	D	63	LEU
1	D	71	ARG
1	D	76	VAL
1	D	83	LEU
1	D	99	THR
1	D	105	LEU
1	D	132	GLU
1	D	147	LEU
1	D	152	LEU
1	D	153	LEU
1	D	182	GLU
1	D	184	TYR
1	D	198	LEU
1	D	199	ARG
1	D	210	LEU
1	D	221	LYS
1	D	231	GLN
1	D	234	VAL
1	D	254	ASP
1	D	258	VAL

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Mol	Chain	Res	Type
1	D	294	VAL
1	D	299	LEU
1	D	337	VAL
1	D	343	GLU
1	D	347	SER
1	D	358	TYR
1	D	362	VAL
1	E	16	ARG
1	E	27	LYS
1	E	35	ARG
1	E	50	THR
1	E	71	ARG
1	E	76	VAL
1	E	83	LEU
1	E	105	LEU
1	E	112	SER
1	E	132	GLU
1	E	147	LEU
1	E	150	MET
1	E	152	LEU
1	E	153	LEU
1	E	162	ARG
1	E	169	LEU
1	E	179	LEU
1	E	180	GLU
1	E	182	GLU
1	E	190	MET
1	E	198	LEU
1	E	199	ARG
1	E	203	LEU
1	E	210	LEU
1	E	255	GLU
1	E	256	ASP
1	E	258	VAL
1	E	271	GLU
1	E	296	ARG
1	E	299	LEU
1	E	322	VAL
1	E	332	LYS
1	E	337	VAL
1	E	346	VAL
1	E	354	VAL

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Mol	Chain	Res	Type
1	E	362	VAL
1	F	8	SER
1	F	41	LEU
1	F	50	THR
1	F	56	ARG
1	F	76	VAL
1	F	83	LEU
1	F	102	GLN
1	F	105	LEU
1	F	132	GLU
1	F	147	LEU
1	F	152	LEU
1	F	153	LEU
1	F	159	SER
1	F	162	ARG
1	F	163	LEU
1	F	179	LEU
1	F	182	GLU
1	F	198	LEU
1	F	200	LEU
1	F	206	TYR
1	F	209	ARG
1	F	210	LEU
1	F	215	VAL
1	F	231	GLN
1	F	234	VAL
1	F	243	GLU
1	F	258	VAL
1	F	294	VAL
1	F	299	LEU
1	F	344	LEU
1	F	354	VAL
1	F	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	85	HIS
1	A	89	ASN
1	A	121	ASN
1	A	122	HIS

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	231	GLN
1	A	237	HIS
1	A	286	HIS
1	A	351	GLN
1	B	22	ASN
1	B	32	GLN
1	B	85	HIS
1	B	89	ASN
1	B	114	ASN
1	B	121	ASN
1	B	122	HIS
1	B	128	GLN
1	B	286	HIS
1	B	351	GLN
1	C	22	ASN
1	C	85	HIS
1	C	89	ASN
1	C	114	ASN
1	C	121	ASN
1	C	128	GLN
1	C	231	GLN
1	C	286	HIS
1	C	351	GLN
1	D	22	ASN
1	D	85	HIS
1	D	89	ASN
1	D	114	ASN
1	D	121	ASN
1	D	122	HIS
1	D	128	GLN
1	D	231	GLN
1	D	237	HIS
1	D	286	HIS
1	D	351	GLN
1	E	22	ASN
1	E	85	HIS
1	E	89	ASN
1	E	121	ASN
1	E	128	GLN
1	E	237	HIS
1	E	286	HIS

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Mol	Chain	Res	Type
1	E	351	GLN
1	F	22	ASN
1	F	85	HIS
1	F	89	ASN
1	F	102	GLN
1	F	121	ASN
1	F	265	HIS
1	F	286	HIS
1	F	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	UUL	A	1001	-	22,22,22	1.46	2 (9%)	30,30,30	2.65	4 (13%)
2	UUL	B	1001	-	22,22,22	1.82	3 (13%)	30,30,30	2.69	6 (20%)
3	EDO	D	1002	-	3,3,3	0.45	0	2,2,2	0.25	0
2	UUL	C	1001	-	22,22,22	1.75	3 (13%)	30,30,30	2.66	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UUL	F	1001	-	22,22,22	1.65	3 (13%)	30,30,30	2.31	4 (13%)
3	EDO	F	1002	-	3,3,3	0.32	0	2,2,2	0.82	0
2	UUL	D	1001	-	22,22,22	1.71	4 (18%)	30,30,30	2.40	5 (16%)
2	UUL	E	1001	-	22,22,22	1.92	3 (13%)	30,30,30	2.57	4 (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
2	UUL	A	1001	-	-	0/8/8/8	0/3/3/3
2	UUL	B	1001	-	-	0/8/8/8	0/3/3/3
3	EDO	D	1002	-	-	0/1/1/1	-
2	UUL	C	1001	-	-	0/8/8/8	0/3/3/3
2	UUL	F	1001	-	-	4/8/8/8	0/3/3/3
3	EDO	F	1002	-	-	0/1/1/1	-
2	UUL	D	1001	-	-	0/8/8/8	0/3/3/3
2	UUL	E	1001	-	-	0/8/8/8	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	UUL	C2-S4	-5.34	1.66	1.74
2	C	1001	UUL	C7-C3	-5.05	1.40	1.47
2	B	1001	UUL	C7-C3	-4.96	1.40	1.47
2	E	1001	UUL	C7-C3	-4.91	1.40	1.47
2	A	1001	UUL	C7-C3	-4.90	1.40	1.47
2	D	1001	UUL	C7-C3	-4.76	1.40	1.47
2	F	1001	UUL	C7-C3	-4.74	1.40	1.47
2	B	1001	UUL	C2-S4	-4.59	1.67	1.74
2	C	1001	UUL	C2-S4	-4.04	1.68	1.74
2	D	1001	UUL	C2-S4	-4.01	1.68	1.74
2	B	1001	UUL	C10-N6	-3.65	1.34	1.41
2	D	1001	UUL	C10-N6	-3.48	1.34	1.41
2	F	1001	UUL	C10-N6	-3.38	1.34	1.41
2	C	1001	UUL	C10-N6	-3.35	1.34	1.41
2	E	1001	UUL	C10-N6	-3.31	1.35	1.41
2	F	1001	UUL	C2-S4	-2.92	1.70	1.74
2	A	1001	UUL	C10-N6	-2.91	1.35	1.41
2	D	1001	UUL	C2-N1	2.02	1.34	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	UUL	C5-S4-C2	8.44	94.96	88.40
2	B	1001	UUL	C5-S4-C2	8.42	94.95	88.40
2	E	1001	UUL	C5-S4-C2	8.22	94.79	88.40
2	A	1001	UUL	C5-S4-C2	7.93	94.57	88.40
2	A	1001	UUL	S4-C2-N1	-7.86	107.43	115.69
2	C	1001	UUL	S4-C2-N1	-7.65	107.65	115.69
2	B	1001	UUL	S4-C2-N1	-7.54	107.77	115.69
2	D	1001	UUL	C5-S4-C2	7.42	94.17	88.40
2	A	1001	UUL	C2-N1-C3	7.25	115.81	109.96
2	E	1001	UUL	S4-C2-N1	-7.19	108.14	115.69
2	E	1001	UUL	C2-N1-C3	7.15	115.74	109.96
2	C	1001	UUL	C2-N1-C3	7.03	115.64	109.96
2	B	1001	UUL	C2-N1-C3	6.98	115.60	109.96
2	F	1001	UUL	C5-S4-C2	6.89	93.76	88.40
2	D	1001	UUL	C2-N1-C3	6.77	115.42	109.96
2	F	1001	UUL	S4-C2-N1	-6.77	108.58	115.69
2	D	1001	UUL	S4-C2-N1	-6.76	108.59	115.69
2	F	1001	UUL	C2-N1-C3	6.74	115.40	109.96
2	C	1001	UUL	C3-C5-S4	-2.90	107.65	111.16
2	E	1001	UUL	C3-C5-S4	-2.81	107.75	111.16
2	A	1001	UUL	C3-C5-S4	-2.78	107.79	111.16
2	B	1001	UUL	C3-C5-S4	-2.67	107.92	111.16
2	B	1001	UUL	C8-C7-C3	-2.58	117.98	120.87
2	D	1001	UUL	C3-C5-S4	-2.44	108.20	111.16
2	F	1001	UUL	C3-C5-S4	-2.43	108.22	111.16
2	D	1001	UUL	C7-C3-C5	-2.34	123.76	126.54
2	C	1001	UUL	C7-C3-C5	-2.13	124.01	126.54
2	C	1001	UUL	C8-C7-C3	-2.08	118.54	120.87
2	B	1001	UUL	C7-C3-C5	-2.02	124.14	126.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

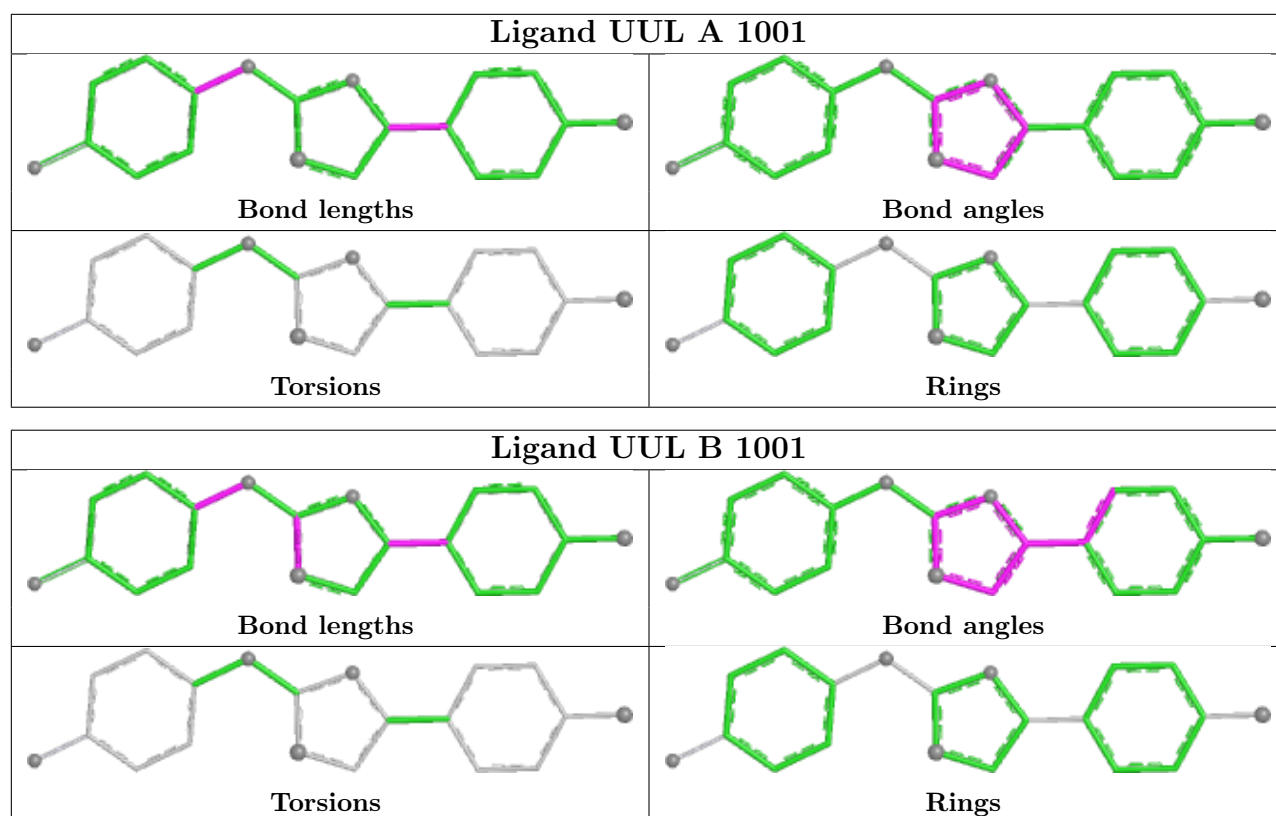
Mol	Chain	Res	Type	Atoms
2	F	1001	UUL	N1-C3-C7-C9
2	F	1001	UUL	N1-C3-C7-C8
2	F	1001	UUL	C5-C3-C7-C9
2	F	1001	UUL	C5-C3-C7-C8

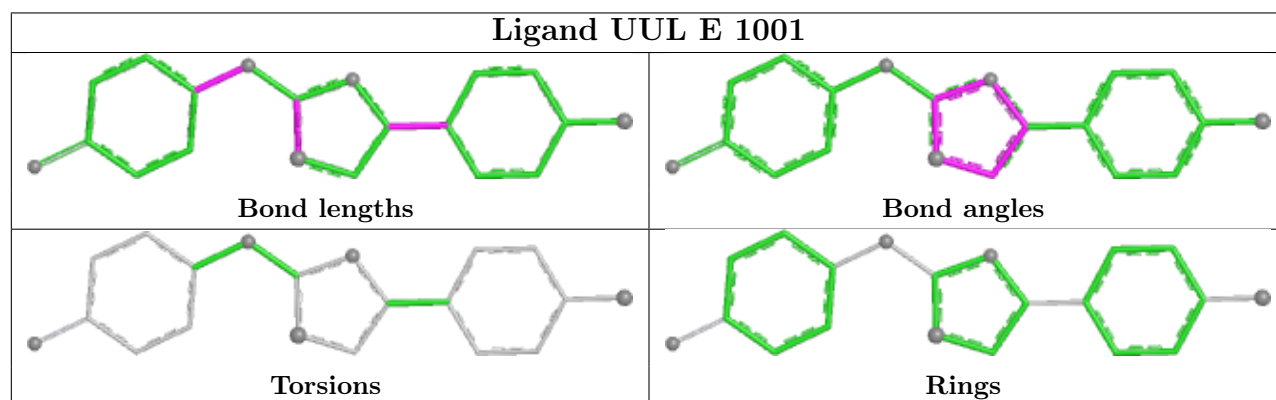
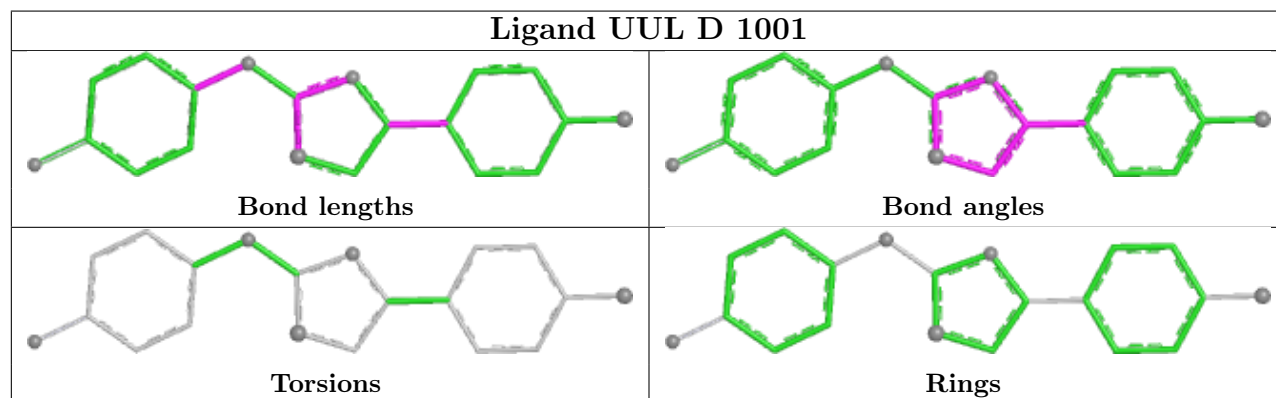
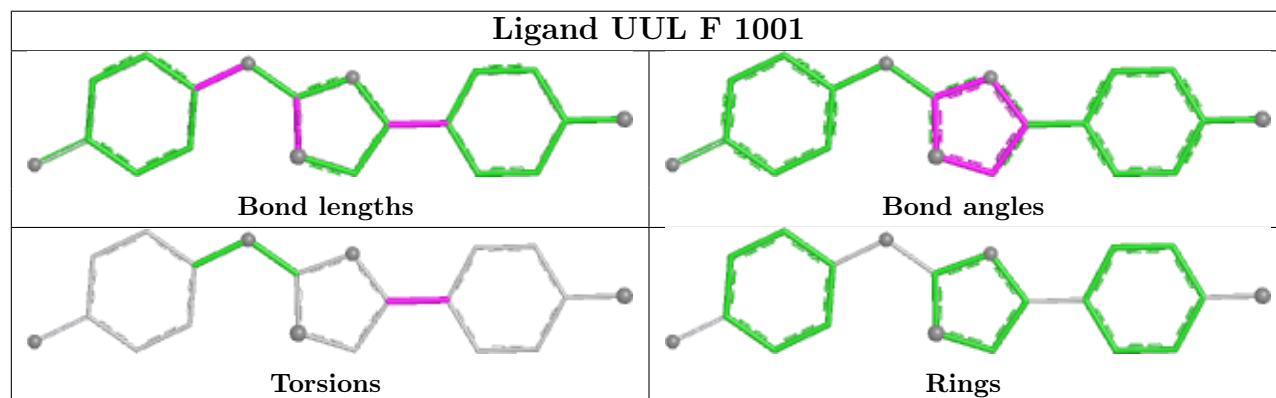
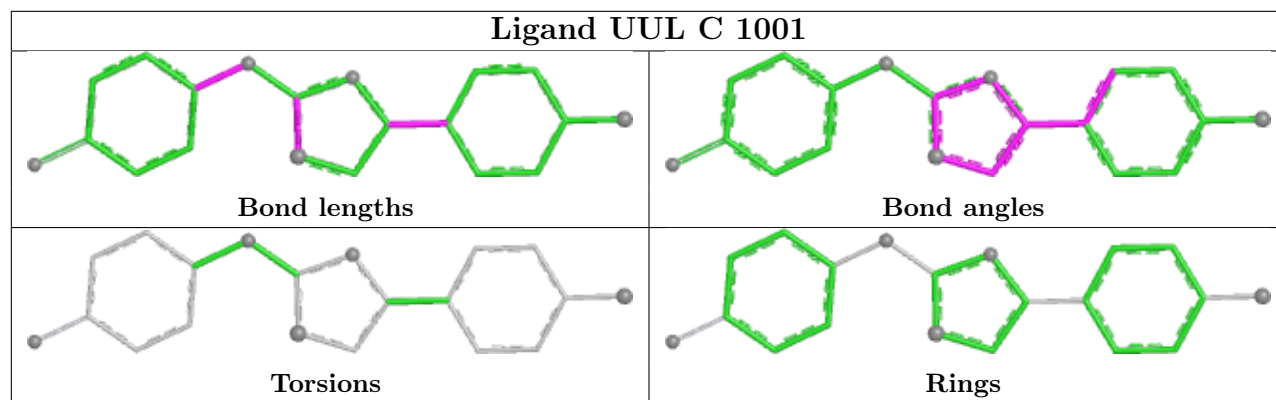
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	UUL	1	0
2	C	1001	UUL	1	0
3	F	1002	EDO	2	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	347/361 (96%)	0.10	19 (5%)	30	32	22, 34, 63, 87	1 (0%)
1	B	340/361 (94%)	0.46	26 (7%)	20	21	22, 39, 75, 116	1 (0%)
1	C	342/361 (94%)	0.57	33 (9%)	13	15	24, 41, 71, 97	1 (0%)
1	D	348/361 (96%)	0.26	22 (6%)	26	28	24, 37, 66, 104	1 (0%)
1	E	342/361 (94%)	0.52	20 (5%)	29	31	25, 41, 73, 110	1 (0%)
1	F	344/361 (95%)	1.17	63 (18%)	3	4	27, 49, 80, 114	1 (0%)
All	All	2063/2166 (95%)	0.51	183 (8%)	15	17	22, 40, 74, 116	6 (0%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	VAL	6.9
1	A	222	THR	5.9
1	E	185	ARG	5.8
1	F	200	LEU	5.6
1	D	223	PRO	5.2
1	B	201	ALA	4.9
1	B	344	LEU	4.9
1	F	110	ALA	4.7
1	D	184	TYR	4.6
1	A	216	GLY	4.5
1	F	251	VAL	4.5
1	A	218	VAL	4.5
1	E	190	MET	4.5
1	C	27	LYS	4.4
1	A	217	ARG	4.4
1	E	184	TYR	4.4
1	A	184	TYR	4.3
1	F	185	ARG	4.2
1	E	364	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	184	TYR	4.1
1	F	219	GLY	4.0
1	F	170	ALA	4.0
1	D	197	PHE	4.0
1	D	112	SER	3.9
1	F	184	TYR	3.9
1	B	185	ARG	3.9
1	B	184	TYR	3.9
1	B	343	GLU	3.9
1	E	343	GLU	3.9
1	F	337	VAL	3.9
1	E	179	LEU	3.8
1	F	364	GLY	3.7
1	F	218	VAL	3.6
1	C	190	MET	3.6
1	F	202	ALA	3.5
1	F	344	LEU	3.5
1	A	185	ARG	3.5
1	E	26	GLY	3.5
1	F	332	LYS	3.4
1	F	26	GLY	3.4
1	F	291	ARG	3.4
1	E	25	GLY	3.4
1	F	6	MET	3.3
1	F	260	VAL	3.3
1	F	290	VAL	3.3
1	B	111	GLY	3.3
1	C	343	GLU	3.3
1	C	315	GLU	3.2
1	D	6	MET	3.2
1	A	8	SER	3.1
1	A	111	GLY	3.1
1	B	364	GLY	3.1
1	D	8	SER	3.1
1	E	112	SER	3.1
1	F	111	GLY	3.1
1	D	222	THR	3.1
1	D	7	GLY	3.0
1	A	220	SER	3.0
1	B	297	ALA	3.0
1	B	112	SER	3.0
1	F	292	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	111	GLY	2.9
1	F	258	VAL	2.9
1	B	332	LYS	2.9
1	D	180	GLU	2.9
1	F	297	ALA	2.9
1	B	334	GLY	2.8
1	E	334	GLY	2.8
1	F	7	GLY	2.8
1	C	185	ARG	2.8
1	B	350	VAL	2.8
1	D	221	LYS	2.8
1	C	256	ASP	2.8
1	A	112	SER	2.8
1	C	364	GLY	2.8
1	C	215	VAL	2.8
1	A	219	GLY	2.8
1	B	200	LEU	2.8
1	E	332	LYS	2.8
1	F	190	MET	2.8
1	F	314	TYR	2.8
1	B	190	MET	2.8
1	F	117	ALA	2.7
1	D	111	GLY	2.7
1	D	52	MET	2.7
1	D	185	ARG	2.7
1	F	316	CYS	2.7
1	F	203	LEU	2.7
1	F	289	TYR	2.6
1	C	333	ASP	2.6
1	F	231	GLN	2.6
1	F	192	PHE	2.6
1	C	318	TYR	2.6
1	C	311	HIS	2.6
1	E	333	ASP	2.6
1	A	331	PRO	2.6
1	E	335	LYS	2.6
1	A	343	GLU	2.5
1	C	57	ARG	2.5
1	B	245	VAL	2.5
1	C	296	ARG	2.5
1	F	24	ARG	2.5
1	A	190	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	2.5
1	D	26	GLY	2.5
1	C	180	GLU	2.5
1	E	182	GLU	2.5
1	B	25	GLY	2.5
1	C	231	GLN	2.5
1	F	182	GLU	2.5
1	B	315	GLU	2.4
1	C	314	TYR	2.4
1	F	27	LYS	2.4
1	B	331	PRO	2.4
1	F	179	LEU	2.4
1	C	7	GLY	2.4
1	C	334	GLY	2.4
1	F	124	ALA	2.4
1	C	130	THR	2.4
1	F	177	VAL	2.4
1	F	268	LEU	2.4
1	F	343	GLU	2.4
1	F	201	ALA	2.4
1	D	181	SER	2.4
1	E	192	PHE	2.3
1	F	294	VAL	2.3
1	B	314	TYR	2.3
1	F	244	PRO	2.3
1	F	331	PRO	2.3
1	B	296	ARG	2.3
1	E	337	VAL	2.3
1	E	27	LYS	2.3
1	B	336	GLY	2.3
1	D	190	MET	2.3
1	F	333	ASP	2.3
1	D	331	PRO	2.3
1	E	331	PRO	2.3
1	C	217	ARG	2.3
1	C	9	GLY	2.2
1	E	180	GLU	2.2
1	A	181	SER	2.2
1	F	32	GLN	2.2
1	C	292	ALA	2.2
1	D	27	LYS	2.2
1	F	318	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	10	VAL	2.2
1	F	232	GLY	2.2
1	D	183	LYS	2.2
1	F	335	LYS	2.2
1	C	337	VAL	2.2
1	F	245	VAL	2.2
1	F	37	HIS	2.2
1	F	254	ASP	2.1
1	F	197	PHE	2.1
1	C	8	SER	2.1
1	F	205	THR	2.1
1	C	24	ARG	2.1
1	F	217	ARG	2.1
1	C	332	LYS	2.1
1	F	336	GLY	2.1
1	D	199	ARG	2.1
1	F	308	LYS	2.1
1	A	180	GLU	2.1
1	F	31	LEU	2.1
1	F	176	ASP	2.1
1	B	192	PHE	2.1
1	B	278	GLY	2.1
1	F	361	MET	2.1
1	A	7	GLY	2.1
1	C	232	GLY	2.1
1	B	345	MET	2.0
1	C	298	MET	2.0
1	D	110	ALA	2.0
1	F	315	GLU	2.0
1	F	114	ASN	2.0
1	C	245	VAL	2.0
1	A	364	GLY	2.0
1	A	221	LYS	2.0
1	F	171	TRP	2.0
1	C	363	SER	2.0
1	E	231	GLN	2.0
1	D	200	LEU	2.0
1	F	23	PRO	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

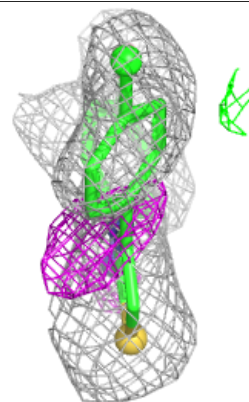
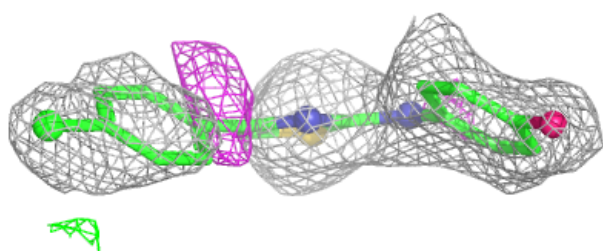
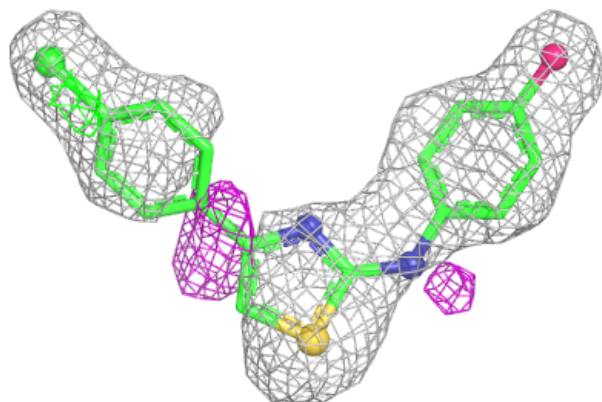
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	F	1002	4/4	0.85	0.13	35,38,42,44	0
2	UUL	F	1001	20/20	0.88	0.16	43,62,77,77	0
3	EDO	D	1002	4/4	0.90	0.12	36,39,43,47	0
2	UUL	C	1001	20/20	0.91	0.13	51,66,73,75	0
2	UUL	B	1001	20/20	0.93	0.11	52,57,63,64	0
2	UUL	E	1001	20/20	0.95	0.08	41,46,51,52	0
2	UUL	D	1001	20/20	0.96	0.07	35,41,45,46	0
2	UUL	A	1001	20/20	0.98	0.05	28,31,38,40	0

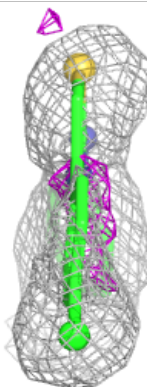
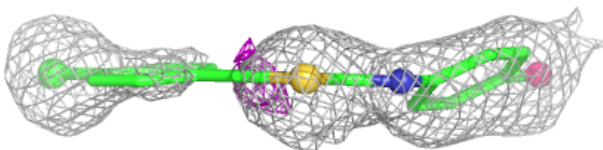
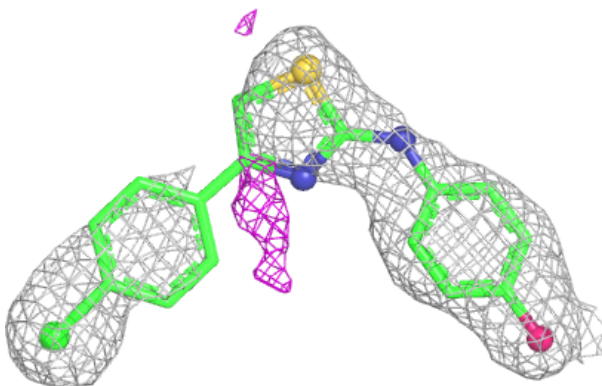
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UUL F 1001:

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

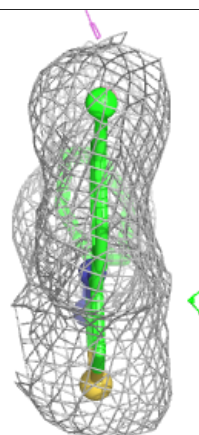
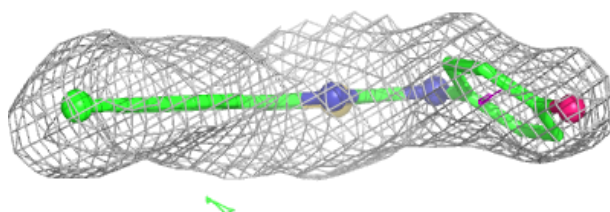
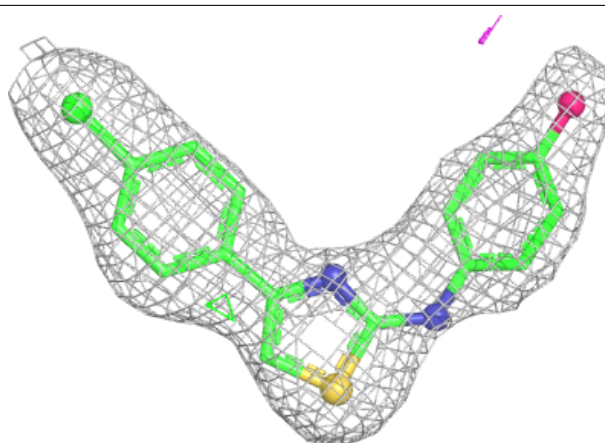
**Electron density around UUL C 1001:**

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

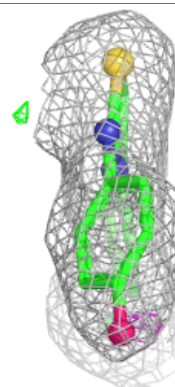
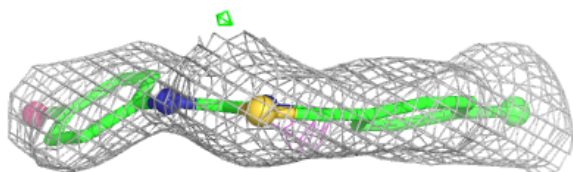
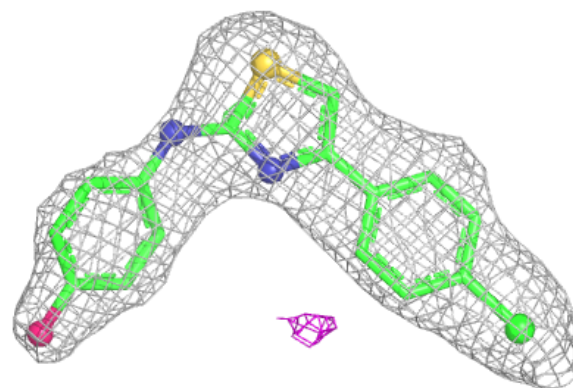


Electron density around UUL B 1001:

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

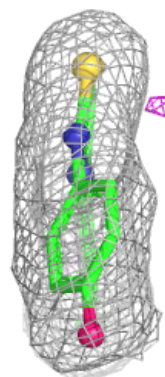
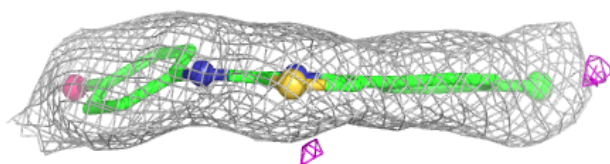
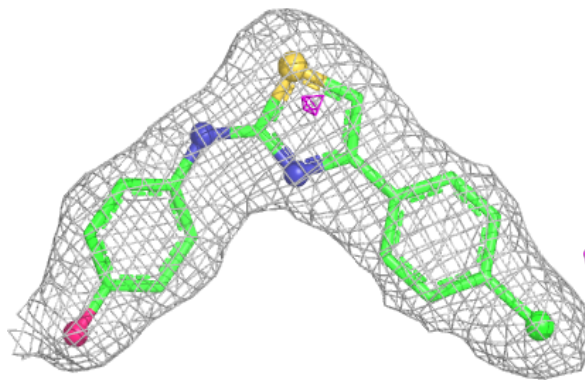
**Electron density around UUL E 1001:**

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

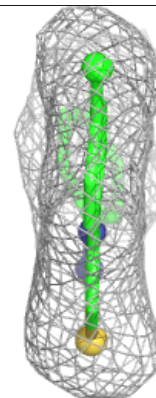
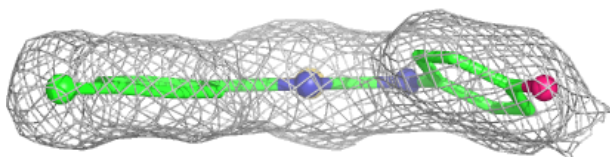
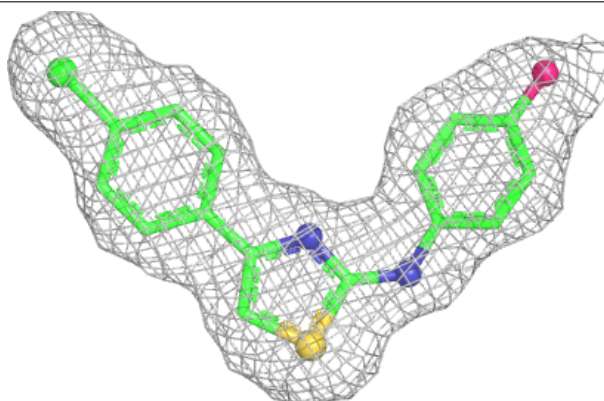


Electron density around UUL D 1001:

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

**Electron density around UUL A 1001:**

$2mF_o-DF_c$ (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.