



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 AM UTC

PDB ID : 3OE8 / pdb_00003oe8
Title : Crystal structure of the CXCR4 chemokine receptor in complex with a small molecule antagonist IT1t in P1 spacegroup
Authors : Wu, B.; Mol, C.D.; Han, G.W.; Katritch, V.; Chien, E.Y.T.; Liu, W.; Cherezov, V.; Stevens, R.C.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D); GPCR Network (GPCR)
Deposited on : 2010-08-12
Resolution : 3.10 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

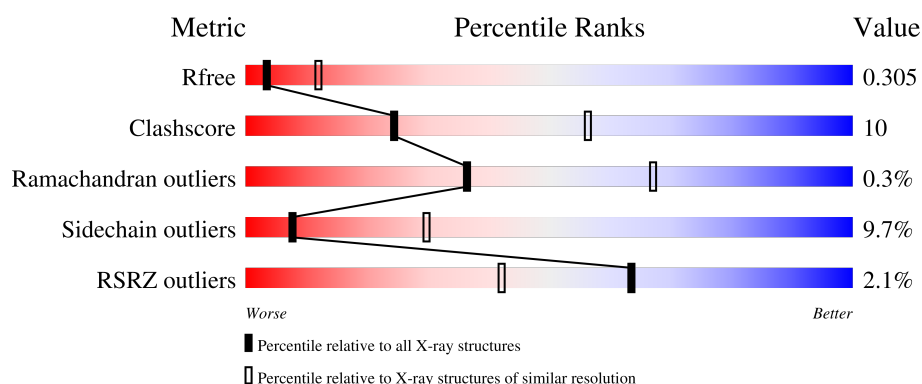
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	502	2% 64% 17% 5% 14%
1	B	502	2% 65% 16% • 15%
1	C	502	2% 69% 14% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10373 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 C-X-C chemokine receptor type 4, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3459	2269	577	597	16			
1	B	426	Total	C	N	O	S	0	0	0
			3404	2240	570	578	16			
1	C	428	Total	C	N	O	S	0	0	0
			3429	2263	567	583	16			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
A	-2	ALA	-	expression tag	UNP P61073
A	-1	GLY	-	expression tag	UNP P61073
A	0	ALA	-	expression tag	UNP P61073
A	1	PRO	-	expression tag	UNP P61073
A	125	TRP	LEU	engineered mutation	UNP P61073
A	900	GLY	-	linker	UNP P61073
A	901	SER	-	linker	UNP P61073
A	1200	GLY	-	linker	UNP P61073
A	1201	SER	-	linker	UNP P61073
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	320	GLY	-	expression tag	UNP P61073
A	321	ARG	-	expression tag	UNP P61073
A	322	PRO	-	expression tag	UNP P61073
A	323	LEU	-	expression tag	UNP P61073
A	324	GLU	-	expression tag	UNP P61073

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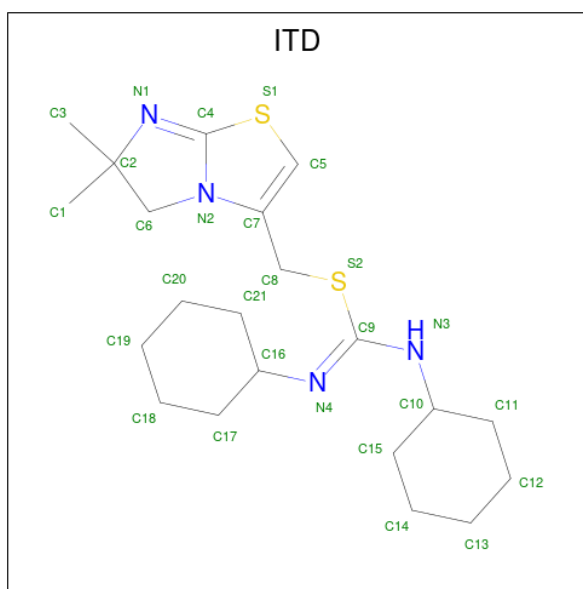
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	VAL	-	expression tag	UNP P61073
A	326	LEU	-	expression tag	UNP P61073
A	327	PHE	-	expression tag	UNP P61073
A	328	GLN	-	expression tag	UNP P61073
B	-9	ASP	-	expression tag	UNP P61073
B	-8	TYR	-	expression tag	UNP P61073
B	-7	LYS	-	expression tag	UNP P61073
B	-6	ASP	-	expression tag	UNP P61073
B	-5	ASP	-	expression tag	UNP P61073
B	-4	ASP	-	expression tag	UNP P61073
B	-3	ASP	-	expression tag	UNP P61073
B	-2	ALA	-	expression tag	UNP P61073
B	-1	GLY	-	expression tag	UNP P61073
B	0	ALA	-	expression tag	UNP P61073
B	1	PRO	-	expression tag	UNP P61073
B	125	TRP	LEU	engineered mutation	UNP P61073
B	900	GLY	-	linker	UNP P61073
B	901	SER	-	linker	UNP P61073
B	1200	GLY	-	linker	UNP P61073
B	1201	SER	-	linker	UNP P61073
B	1054	THR	CYS	engineered mutation	UNP P00720
B	1097	ALA	CYS	engineered mutation	UNP P00720
B	320	GLY	-	expression tag	UNP P61073
B	321	ARG	-	expression tag	UNP P61073
B	322	PRO	-	expression tag	UNP P61073
B	323	LEU	-	expression tag	UNP P61073
B	324	GLU	-	expression tag	UNP P61073
B	325	VAL	-	expression tag	UNP P61073
B	326	LEU	-	expression tag	UNP P61073
B	327	PHE	-	expression tag	UNP P61073
B	328	GLN	-	expression tag	UNP P61073
C	-9	ASP	-	expression tag	UNP P61073
C	-8	TYR	-	expression tag	UNP P61073
C	-7	LYS	-	expression tag	UNP P61073
C	-6	ASP	-	expression tag	UNP P61073
C	-5	ASP	-	expression tag	UNP P61073
C	-4	ASP	-	expression tag	UNP P61073
C	-3	ASP	-	expression tag	UNP P61073
C	-2	ALA	-	expression tag	UNP P61073
C	-1	GLY	-	expression tag	UNP P61073
C	0	ALA	-	expression tag	UNP P61073
C	1	PRO	-	expression tag	UNP P61073

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Chain	Residue	Modelled	Actual	Comment	Reference
C	125	TRP	LEU	engineered mutation	UNP P61073
C	900	GLY	-	linker	UNP P61073
C	901	SER	-	linker	UNP P61073
C	1200	GLY	-	linker	UNP P61073
C	1201	SER	-	linker	UNP P61073
C	1054	THR	CYS	engineered mutation	UNP P00720
C	1097	ALA	CYS	engineered mutation	UNP P00720
C	320	GLY	-	expression tag	UNP P61073
C	321	ARG	-	expression tag	UNP P61073
C	322	PRO	-	expression tag	UNP P61073
C	323	LEU	-	expression tag	UNP P61073
C	324	GLU	-	expression tag	UNP P61073
C	325	VAL	-	expression tag	UNP P61073
C	326	LEU	-	expression tag	UNP P61073
C	327	PHE	-	expression tag	UNP P61073
C	328	GLN	-	expression tag	UNP P61073

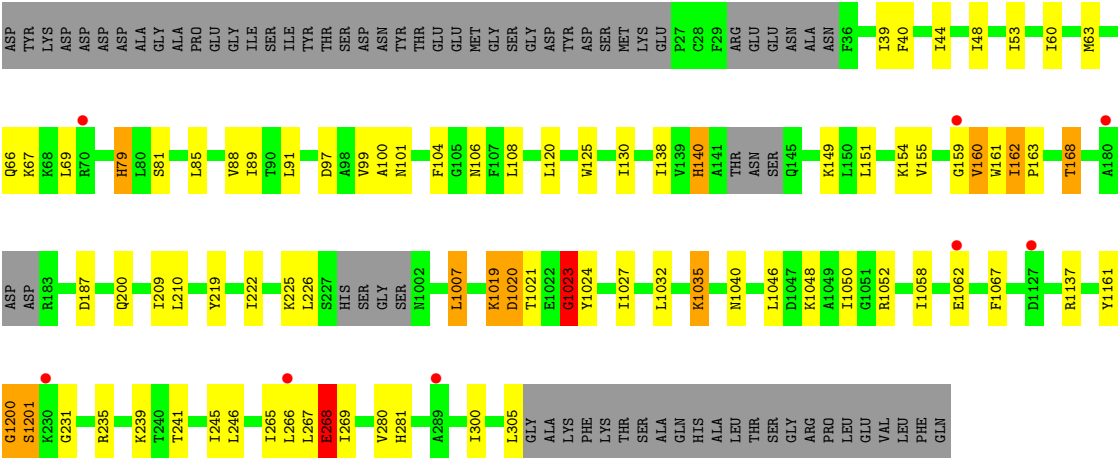
- Molecule 2 is (6,6-dimethyl-5,6-dihydroimidazo[2,1-b][1,3]thiazol-3-yl)methyl N,N'-dicyclohexylimidothiocarbamate (CCD ID: ITD) (formula: C₂₁H₃₄N₄S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			27	21	4	2		
2	B	1	Total	C	N	S	0	0
			27	21	4	2		
2	C	1	Total	C	N	S	0	0
			27	21	4	2		

ALA
LEU
THR
SER
GLY
ARG
PRO
LEU
GLU
VAL
PHE
GLN

● Molecule 1: C-X-C chemokine receptor type 4, Lysozyme Chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.37Å 76.60Å 91.72Å 96.00° 97.78° 97.38°	Depositor
Resolution (Å)	19.97 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.97-3.10) 85.9 (19.97-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.09Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.250 , 0.295 0.251 , 0.305	Depositor DCC
R_{free} test set	1441 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10373	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: ITD

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	0.81	2/3543 (0.1%)	1.67	47/4814 (1.0%)
1	B	0.79	0/3485	1.54	35/4731 (0.7%)
1	C	0.85	5/3511 (0.1%)	1.67	36/4767 (0.8%)
All	All	0.82	7/10539 (0.1%)	1.63	118/14312 (0.8%)

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	C	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1201	SER	CA-C	-12.37	1.32	1.52
1	C	1201	SER	C-O	11.62	1.42	1.23
1	C	1200	GLY	CA-C	-7.28	1.41	1.51
1	C	1200	GLY	C-O	5.61	1.31	1.23
1	C	162	ILE	CA-CB	5.45	1.57	1.54
1	A	169	ILE	CA-CB	5.41	1.57	1.54
1	A	173	ILE	CA-CB	-5.26	1.49	1.55

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1201	SER	N-CA-C	24.87	146.55	112.72
1	B	1201	SER	N-CA-C	22.63	148.71	111.37
1	C	1201	SER	CB-CA-C	-21.69	84.54	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	MET	N-CA-C	-17.31	90.23	112.90
1	A	173	ILE	N-CA-C	17.02	127.84	111.67
1	A	173	ILE	CB-CA-C	-16.23	92.65	111.80
1	C	1201	SER	CA-C-N	16.10	146.97	122.17
1	C	1201	SER	C-N-CA	16.10	146.97	122.17
1	C	268	GLU	N-CA-C	16.02	133.37	111.74
1	C	269	ILE	N-CA-C	15.35	133.99	112.35
1	A	229	SER	O-C-N	-15.00	102.64	122.59
1	C	101	ASN	N-CA-CB	-14.89	89.84	110.38
1	A	1115	THR	N-CA-C	13.84	128.28	111.40
1	A	267	LEU	N-CA-C	-13.71	96.59	113.18
1	B	208	LEU	N-CA-C	13.48	129.97	113.12
1	A	232	HIS	N-CA-CB	-13.34	87.82	110.50
1	A	138	ILE	N-CA-C	13.31	124.31	111.67
1	A	99	VAL	N-CA-C	13.10	125.28	111.00
1	C	1200	GLY	CA-C-N	12.57	146.99	122.61
1	C	1200	GLY	C-N-CA	12.57	146.99	122.61
1	A	141	ALA	N-CA-C	12.34	125.92	111.11
1	A	99	VAL	CB-CA-C	-12.34	95.70	112.24
1	A	900	GLY	N-CA-C	12.01	141.65	113.18
1	B	231	GLY	N-CA-C	-11.98	93.33	111.42
1	B	261	ILE	CB-CA-C	-11.83	96.55	112.04
1	A	233	GLN	N-CA-C	-11.80	99.36	113.88
1	C	160	VAL	N-CA-C	11.71	122.79	111.67
1	C	1023	GLY	N-CA-C	11.51	140.45	113.18
1	C	1201	SER	O-C-N	-11.35	103.37	121.53
1	B	257	ILE	CB-CA-C	-10.93	95.22	112.16
1	A	232	HIS	N-CA-C	10.71	140.99	111.00
1	B	1201	SER	CB-CA-C	-10.68	93.02	110.74
1	A	1005	GLU	CB-CA-C	-10.57	90.81	110.36
1	A	101	ASN	N-CA-C	10.39	125.97	109.86
1	B	259	ILE	N-CA-C	-10.37	100.67	110.42
1	B	1105	GLN	N-CA-C	10.25	122.41	111.03
1	A	100	ALA	N-CA-C	-10.01	94.20	109.41
1	B	259	ILE	CB-CA-C	-9.86	99.15	111.87
1	A	103	TYR	N-CA-C	-9.70	102.24	114.56
1	A	1003	ILE	N-CA-C	-9.64	104.55	113.71
1	A	268	GLU	N-CA-C	9.50	124.57	111.74
1	C	1201	SER	CA-C-O	-8.46	105.19	120.42
1	A	139	VAL	CB-CA-C	8.39	125.16	112.16
1	C	101	ASN	N-CA-C	8.31	121.82	110.35
1	A	101	ASN	N-CA-CB	-8.26	97.26	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ILE	N-CA-CB	-8.23	99.08	110.68
1	C	168	THR	CA-C-N	7.96	126.70	120.33
1	C	168	THR	C-N-CA	7.96	126.70	120.33
1	A	183	ARG	N-CA-CB	7.93	123.61	111.56
1	C	1019	LYS	N-CA-C	-7.91	97.19	109.76
1	B	1161	TYR	O-C-N	-7.72	113.31	122.27
1	A	1116	ASN	N-CA-C	-7.64	102.29	111.69
1	C	100	ALA	N-CA-C	-7.63	94.55	110.80
1	B	260	SER	CB-CA-C	-7.62	95.25	110.42
1	A	266	LEU	N-CA-C	7.61	121.49	111.75
1	B	230	LYS	N-CA-C	-7.57	97.90	109.85
1	C	100	ALA	CB-CA-C	-7.56	95.37	110.42
1	A	100	ALA	CB-CA-C	-7.51	95.42	110.30
1	A	229	SER	CA-C-N	7.50	136.12	121.41
1	A	229	SER	C-N-CA	7.50	136.12	121.41
1	B	208	LEU	N-CA-CB	-7.47	99.00	110.42
1	A	103	TYR	N-CA-CB	7.28	120.68	111.00
1	A	266	LEU	CB-CA-C	-7.24	96.41	110.46
1	A	1115	THR	CB-CA-C	-7.09	98.88	110.79
1	A	137	ALA	CB-CA-C	7.07	123.72	110.63
1	B	1161	TYR	N-CA-C	-6.92	104.50	114.12
1	B	260	SER	N-CA-C	6.86	125.42	110.80
1	A	184	TYR	N-CA-C	-6.84	100.40	110.52
1	A	182	ASP	CB-CA-C	-6.81	96.87	110.42
1	A	140	HIS	N-CA-CB	-6.75	95.48	111.74
1	A	141	ALA	CB-CA-C	-6.74	100.02	110.81
1	B	68	LYS	CA-C-N	-6.53	113.83	123.11
1	B	68	LYS	C-N-CA	-6.53	113.83	123.11
1	B	65	TYR	N-CA-C	6.46	120.99	112.13
1	C	268	GLU	CB-CA-C	-6.45	102.57	111.73
1	C	269	ILE	N-CA-CB	-6.45	98.08	111.24
1	A	65	TYR	N-CA-C	6.43	120.95	112.13
1	C	140	HIS	N-CA-C	6.25	117.67	107.23
1	B	168	THR	CA-C-N	6.18	125.27	120.33
1	B	168	THR	C-N-CA	6.18	125.27	120.33
1	C	209	ILE	N-CA-C	6.15	116.27	110.30
1	B	233	GLN	N-CA-C	-6.13	104.71	111.82
1	C	1200	GLY	N-CA-C	6.11	127.65	113.18
1	B	154	LYS	N-CA-C	6.08	122.28	114.56
1	A	252	TRP	N-CA-C	5.87	119.63	112.23
1	B	174	PHE	N-CA-C	5.81	119.55	112.23
1	B	106	ASN	N-CA-C	5.80	117.68	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	LYS	CB-CA-C	5.79	121.95	110.42
1	A	144	SER	N-CA-CB	-5.77	101.68	111.20
1	A	67	LYS	N-CA-C	5.76	118.54	109.96
1	C	104	PHE	N-CA-C	5.76	119.78	112.87
1	B	67	LYS	N-CA-C	5.62	118.48	110.10
1	B	126	ILE	N-CA-C	-5.58	104.92	111.00
1	C	1019	LYS	CB-CA-C	5.51	118.82	109.84
1	C	67	LYS	N-CA-C	5.49	122.50	110.80
1	B	161	TRP	N-CA-C	5.48	116.93	111.07
1	C	154	LYS	CB-CA-C	-5.47	100.59	109.13
1	B	154	LYS	CB-CA-C	-5.47	100.60	109.13
1	A	168	THR	CA-C-N	5.42	124.67	120.33
1	A	168	THR	C-N-CA	5.42	124.67	120.33
1	B	168	THR	CB-CA-C	5.40	119.04	109.65
1	B	239	LYS	CA-C-N	5.39	127.45	120.44
1	B	239	LYS	C-N-CA	5.39	127.45	120.44
1	A	198	VAL	N-CA-CB	5.36	116.82	110.55
1	C	154	LYS	N-CA-C	5.35	121.36	114.56
1	C	101	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	1091	LEU	N-CA-C	5.30	118.46	109.76
1	C	219	TYR	N-CA-C	5.30	117.97	111.82
1	B	214	VAL	CA-C-N	5.19	127.10	120.56
1	B	214	VAL	C-N-CA	5.19	127.10	120.56
1	B	285	SER	CA-C-N	5.19	127.10	120.56
1	B	285	SER	C-N-CA	5.19	127.10	120.56
1	C	79	HIS	CA-C-N	5.18	127.47	120.38
1	C	79	HIS	C-N-CA	5.18	127.47	120.38
1	C	1040	ASN	N-CA-C	5.16	116.90	111.28
1	C	280	VAL	N-CA-CB	5.11	117.11	110.57
1	A	1026	THR	CA-C-N	5.03	127.74	122.11
1	A	1026	THR	C-N-CA	5.03	127.74	122.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1200	GLY	Peptide,Mainchain
1	C	1201	SER	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	3459	0	3494	110	0
1	B	3404	0	3454	70	0
1	C	3429	0	3496	29	0
2	A	27	0	34	2	0
2	B	27	0	34	4	0
2	C	27	0	34	3	0
All	All	10373	0	10546	206	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 10.

All (206) 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:265:ILE:HG22	1:A:266:LEU:N	1.55	1.12
1:C:1024:TYR:HE2	1:C:1035:LYS:HB3	1.19	1.06
1:C:267:LEU:O	1:C:268:GLU:HG3	1.59	1.01
1:C:1024:TYR:CE2	1:C:1035:LYS:HB3	1.96	1.01
1:C:66:GLN:HG2	1:C:66:GLN:O	1.60	1.00
1:A:146:ARG:N	1:A:147:PRO:HD2	1.72	1.00
1:B:261:ILE:HG22	1:B:262:ASP:N	1.77	0.99
1:A:137:ALA:HB2	1:A:148:ARG:CZ	1.92	0.98
1:A:143:ASN:H	1:A:143:ASN:ND2	1.52	0.95
1:B:208:LEU:HD22	1:B:256:TYR:CZ	2.01	0.94
1:A:1002:ASN:O	1:A:1158:TRP:CZ3	2.21	0.93
1:A:140:HIS:O	1:A:144:SER:HB3	1.68	0.93
1:A:265:ILE:CG2	1:A:266:LEU:N	2.31	0.93
1:B:259:ILE:HG22	1:B:260:SER:N	1.81	0.93
1:A:1004:PHE:CZ	1:A:1064:GLU:HG3	2.04	0.93
1:A:143:ASN:HD22	1:A:143:ASN:N	1.62	0.92
1:A:173:ILE:HG22	1:A:174:PHE:N	1.80	0.92
1:C:267:LEU:C	1:C:268:GLU:HG3	1.94	0.92
1:A:265:ILE:O	1:A:268:GLU:HA	1.73	0.89
1:B:1050:ILE:HD12	1:B:1062:GLU:HG2	1.56	0.88
1:B:259:ILE:O	1:B:263:SER:CB	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASP:HB2	1:B:280:VAL:HG11	1.56	0.86
1:A:174:PHE:O	1:A:188:ARG:HA	1.74	0.86
1:B:60:ILE:HD12	1:B:85:LEU:HD22	1.56	0.86
1:C:66:GLN:O	1:C:66:GLN:CG	2.24	0.85
1:A:146:ARG:H	1:A:147:PRO:HD2	1.42	0.84
1:A:1006:MET:HE3	1:A:1161:TYR:CE2	2.13	0.83
1:B:265:ILE:O	1:B:266:LEU:HG	1.77	0.82
1:A:181:ASP:O	1:A:182:ASP:CB	2.30	0.80
1:B:232:HIS:H	1:B:232:HIS:CD2	1.95	0.80
1:B:265:ILE:O	1:B:266:LEU:CG	2.30	0.80
1:A:265:ILE:O	1:A:268:GLU:CA	2.30	0.80
1:A:1004:PHE:CE1	1:A:1064:GLU:HG3	2.17	0.79
1:B:1050:ILE:HG23	1:B:1062:GLU:HG2	1.64	0.79
1:A:137:ALA:HB2	1:A:148:ARG:NE	1.97	0.78
1:A:265:ILE:HG22	1:A:266:LEU:H	1.49	0.76
1:A:267:LEU:O	1:A:268:GLU:HG2	1.84	0.76
1:A:137:ALA:CB	1:A:148:ARG:CZ	2.64	0.75
1:A:146:ARG:N	1:A:147:PRO:CD	2.50	0.75
1:A:1006:MET:CE	1:A:1161:TYR:CZ	2.70	0.75
1:A:144:SER:HA	1:A:147:PRO:HG3	1.69	0.74
1:A:267:LEU:C	1:A:268:GLU:HG2	2.13	0.73
1:B:60:ILE:CD1	1:B:85:LEU:HD22	2.17	0.73
1:B:79:HIS:HD2	1:B:161:TRP:HE1	1.35	0.73
1:B:208:LEU:HD22	1:B:256:TYR:CE1	2.23	0.72
1:B:266:LEU:C	1:B:266:LEU:HD12	2.14	0.72
1:A:1005:GLU:HA	1:A:1008:ARG:CB	2.20	0.72
1:B:262:ASP:HB2	1:B:280:VAL:CG1	2.20	0.71
1:B:1050:ILE:HG23	1:B:1062:GLU:CG	2.21	0.70
1:A:143:ASN:H	1:A:143:ASN:HD22	0.77	0.69
1:B:1005:GLU:OE2	1:B:230:LYS:HE2	1.91	0.69
1:B:259:ILE:O	1:B:263:SER:N	2.26	0.69
2:B:1500:ITD:S2	2:B:1500:ITD:H17	2.33	0.69
1:A:1006:MET:CE	1:A:1161:TYR:CE2	2.76	0.68
1:A:180:ALA:HB2	1:A:185:ILE:HD12	1.76	0.68
1:B:265:ILE:O	1:B:266:LEU:CB	2.40	0.68
1:A:1006:MET:HE3	1:A:1161:TYR:CZ	2.31	0.66
1:A:70:ARG:HH21	1:A:75:LYS:HD3	1.59	0.65
1:A:63:MET:HE1	1:A:302:TYR:OH	1.96	0.65
1:A:265:ILE:O	1:A:268:GLU:N	2.30	0.64
1:C:63:MET:HE3	1:C:66:GLN:HE22	1.63	0.64
1:B:265:ILE:O	1:B:265:ILE:HG22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:SER:C	1:A:147:PRO:HD2	2.23	0.64
1:B:1023:GLY:O	1:B:1024:TYR:CD2	2.51	0.64
1:A:180:ALA:CB	1:A:185:ILE:HD12	2.28	0.63
1:A:272:GLN:HG3	1:A:276:PHE:CD2	2.33	0.63
1:A:276:PHE:O	1:A:280:VAL:HG23	1.99	0.63
1:A:174:PHE:CD1	1:A:190:TYR:CE2	2.87	0.63
1:A:142:THR:OG1	1:A:143:ASN:N	2.30	0.62
1:A:179:GLU:HG3	1:A:184:TYR:CE1	2.34	0.62
1:A:1005:GLU:HA	1:A:1008:ARG:HB2	1.80	0.62
1:B:232:HIS:CD2	1:B:232:HIS:N	2.67	0.62
1:A:1006:MET:HE2	1:A:1161:TYR:OH	2.00	0.61
1:A:101:ASN:HD22	1:A:184:TYR:H	1.46	0.61
1:A:101:ASN:HB2	1:A:183:ARG:HB2	1.81	0.61
1:A:65:TYR:CD1	1:A:65:TYR:N	2.69	0.60
1:A:63:MET:CE	1:A:302:TYR:OH	2.49	0.60
1:A:1004:PHE:CE1	1:A:1064:GLU:HA	2.37	0.59
1:A:225:LYS:HA	1:A:228:HIS:CE1	2.36	0.59
1:A:173:ILE:HG22	1:A:174:PHE:CA	2.32	0.58
1:B:1050:ILE:HD12	1:B:1062:GLU:CG	2.32	0.58
1:B:65:TYR:CD1	1:B:65:TYR:N	2.69	0.58
1:A:264:PHE:O	1:A:268:GLU:N	2.37	0.58
1:A:267:LEU:O	1:A:268:GLU:CG	2.52	0.57
1:A:144:SER:HA	1:A:147:PRO:CG	2.34	0.57
1:B:1006:MET:HG3	1:B:1161:TYR:CZ	2.39	0.57
1:A:1004:PHE:CE1	1:A:1064:GLU:CG	2.87	0.56
1:B:1022:GLU:HA	1:B:1022:GLU:OE1	2.04	0.56
1:C:40:PHE:CE2	1:C:44:ILE:HD11	2.40	0.56
1:A:144:SER:CA	1:A:147:PRO:HG3	2.35	0.56
1:A:1005:GLU:HA	1:A:1008:ARG:HB3	1.87	0.56
1:A:1006:MET:HE2	1:A:1161:TYR:CZ	2.39	0.56
1:A:273:GLY:O	1:A:274:CYS:C	2.49	0.55
1:B:1005:GLU:HG3	1:B:230:LYS:NZ	2.20	0.55
1:A:144:SER:O	1:A:147:PRO:HG2	2.07	0.55
1:C:1050:ILE:HD12	1:C:1062:GLU:HB3	1.89	0.54
1:B:1050:ILE:CG2	1:B:1062:GLU:HG2	2.36	0.54
1:A:66:GLN:HE22	1:B:224:SER:HB3	1.73	0.54
1:B:1061:ASP:N	1:B:1061:ASP:OD1	2.42	0.53
1:C:267:LEU:C	1:C:268:GLU:CG	2.75	0.53
1:A:101:ASN:CB	1:A:183:ARG:HB2	2.37	0.53
1:C:1019:LYS:HE3	1:C:1023:GLY:HA2	1.90	0.53
1:A:273:GLY:O	1:A:275:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:MET:HE1	1:B:1098:ALA:HA	1.92	0.52
1:A:39:ILE:HG12	1:B:261:ILE:HD13	1.91	0.52
1:A:62:VAL:HG21	1:B:223:ILE:HD12	1.91	0.52
1:C:1007:LEU:HD13	1:C:1067:PHE:HZ	1.75	0.51
1:A:63:MET:O	1:A:64:GLY:C	2.53	0.51
1:A:219:TYR:O	1:A:223:ILE:HG12	2.10	0.51
1:C:97:ASP:CG	2:C:1500:ITD:H21	2.36	0.51
1:C:231:GLY:O	1:C:235:ARG:NH1	2.44	0.51
1:B:111:ALA:HA	1:B:114:VAL:HG22	1.93	0.51
1:B:1005:GLU:HG3	1:B:230:LYS:HZ1	1.75	0.51
1:A:1002:ASN:O	1:A:1158:TRP:CH2	2.63	0.50
1:C:187:ASP:HB3	2:C:1500:ITD:S2	2.52	0.50
1:C:159:GLY:O	1:C:163:PRO:HG2	2.11	0.50
1:C:63:MET:HE3	1:C:66:GLN:NE2	2.26	0.50
1:A:146:ARG:H	1:A:147:PRO:CD	2.14	0.50
1:A:1004:PHE:HE1	1:A:1064:GLU:HA	1.77	0.50
1:B:63:MET:O	1:B:64:GLY:C	2.54	0.49
1:A:70:ARG:NH2	1:A:75:LYS:HD3	2.25	0.49
1:A:181:ASP:OD1	1:A:181:ASP:N	2.45	0.49
1:B:116:TYR:CE2	2:B:1500:ITD:H3B	2.47	0.49
1:C:138:ILE:HG21	1:C:222:ILE:HG23	1.94	0.49
1:A:215:ILE:HG21	1:A:245:ILE:HG21	1.94	0.49
1:B:1005:GLU:OE2	1:B:230:LYS:CE	2.60	0.48
1:B:294:HIS:HA	1:B:297:LEU:HD12	1.95	0.48
1:C:151:LEU:HA	1:C:155:VAL:HB	1.95	0.48
1:A:134:ARG:O	1:A:138:ILE:HG13	2.14	0.48
1:A:174:PHE:CD1	1:A:190:TYR:HE2	2.30	0.48
1:B:1050:ILE:HG23	1:B:1062:GLU:CD	2.38	0.48
1:B:1157:THR:HA	1:B:232:HIS:CE1	2.48	0.48
1:C:1050:ILE:HG23	1:C:1062:GLU:HG2	1.95	0.48
1:A:63:MET:HE2	1:A:302:TYR:CZ	2.49	0.47
1:B:88:VAL:HA	1:B:91:LEU:HD12	1.96	0.47
1:B:1091:LEU:HD22	1:B:1095:ARG:HB3	1.97	0.47
1:A:144:SER:C	1:A:147:PRO:CD	2.87	0.47
1:C:1161:TYR:CD2	1:C:1161:TYR:N	2.82	0.47
1:A:39:ILE:HG12	1:B:261:ILE:CD1	2.44	0.47
1:A:901:SER:C	1:A:1003:ILE:H	2.23	0.47
1:C:1020:ASP:OD2	1:C:1024:TYR:O	2.32	0.47
1:A:174:PHE:CD1	1:A:190:TYR:CD2	3.02	0.47
1:B:200:GLN:O	1:B:204:ILE:HG12	2.15	0.47
1:B:265:ILE:O	1:B:266:LEU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:NH2	2:B:1500:ITD:H13A	2.31	0.46
1:A:174:PHE:HD1	1:A:190:TYR:HE2	1.64	0.46
1:A:273:GLY:C	1:A:275:GLU:N	2.74	0.46
1:B:1006:MET:HG3	1:B:1161:TYR:CE1	2.50	0.46
1:B:266:LEU:C	1:B:266:LEU:CD1	2.85	0.46
1:A:163:PRO:HA	1:A:166:LEU:HD12	1.97	0.46
1:A:144:SER:CA	1:A:147:PRO:CG	2.93	0.46
1:B:151:LEU:HA	1:B:155:VAL:HB	1.98	0.46
1:B:1021:THR:O	1:B:1021:THR:HG22	2.16	0.46
1:A:1006:MET:CE	1:A:1161:TYR:OH	2.63	0.45
1:A:114:VAL:HG11	1:A:172:PHE:CE2	2.52	0.45
1:A:60:ILE:HD12	1:A:85:LEU:HD22	1.99	0.45
1:B:187:ASP:HB3	2:B:1500:ITD:S2	2.56	0.45
1:B:259:ILE:C	1:B:263:SER:CB	2.90	0.45
1:B:259:ILE:CG2	1:B:260:SER:N	2.49	0.45
1:A:97:ASP:OD1	2:A:1500:ITD:H15	2.17	0.44
1:A:1125:ARG:HB3	1:A:1128:GLU:HB2	1.98	0.44
1:A:173:ILE:CG2	1:A:174:PHE:N	2.51	0.44
1:A:143:ASN:ND2	1:A:143:ASN:N	2.30	0.44
1:A:266:LEU:C	1:A:268:GLU:N	2.71	0.44
1:A:114:VAL:HG11	1:A:172:PHE:CD2	2.53	0.44
1:B:262:ASP:O	1:B:262:ASP:OD1	2.35	0.44
1:B:1054:THR:HG21	1:B:1058:ILE:HG22	2.00	0.43
1:A:1005:GLU:H	1:A:1005:GLU:HG2	1.55	0.43
1:A:228:HIS:O	1:A:228:HIS:CG	2.70	0.43
1:A:1016:LYS:HG3	1:A:1057:VAL:HG22	2.01	0.43
1:C:125:TRP:HB3	1:C:160:VAL:HG22	2.01	0.43
1:B:1157:THR:HA	1:B:232:HIS:NE2	2.34	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.82	0.43
1:A:901:SER:C	1:A:1003:ILE:N	2.76	0.43
1:C:130:ILE:HG22	1:C:241:THR:HG23	2.01	0.42
1:A:65:TYR:N	1:A:65:TYR:HD1	2.16	0.42
1:A:144:SER:O	1:A:147:PRO:CG	2.67	0.42
1:B:210:LEU:HD21	1:C:210:LEU:HD11	2.01	0.42
2:C:1500:ITD:S2	2:C:1500:ITD:C17	3.07	0.42
1:B:261:ILE:HG22	1:B:262:ASP:CA	2.48	0.42
1:A:262:ASP:O	1:A:266:LEU:HD12	2.19	0.42
1:B:259:ILE:HG23	1:B:263:SER:CB	2.50	0.42
1:A:265:ILE:HG22	1:A:266:LEU:CA	2.42	0.42
1:B:64:GLY:C	1:B:65:TYR:CD1	2.98	0.41
1:B:1034:THR:HB	1:B:1045:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1027:ILE:HG21	1:C:1046:LEU:HD13	2.01	0.41
1:A:102:TRP:HE1	1:A:109:CYS:HB2	1.84	0.41
1:A:190:TYR:HB3	1:A:195:TRP:HB2	2.02	0.41
1:A:1002:ASN:O	1:A:1158:TRP:CE3	2.69	0.41
1:B:70:ARG:CZ	1:B:78:LEU:HD21	2.50	0.41
1:C:88:VAL:HA	1:C:91:LEU:HD12	2.02	0.41
1:B:132:LEU:HA	1:B:218:CYS:SG	2.60	0.41
1:A:145:GLN:H	1:A:145:GLN:HG3	1.55	0.41
1:A:64:GLY:C	1:A:65:TYR:CD1	2.98	0.41
1:A:102:TRP:CH2	2:A:1500:ITD:H20	2.55	0.41
1:A:264:PHE:O	1:A:265:ILE:C	2.62	0.41
1:A:265:ILE:C	1:A:268:GLU:H	2.29	0.41
1:B:58:LEU:O	1:B:59:VAL:C	2.64	0.41
1:A:1094:VAL:HG22	1:A:1158:TRP:HE1	1.86	0.41
1:B:262:ASP:HA	1:B:265:ILE:HB	2.03	0.41
1:B:1124:LYS:HD3	1:B:1126:TRP:HZ2	1.86	0.41
1:A:272:GLN:HG3	1:A:276:PHE:HD2	1.80	0.40
1:B:65:TYR:N	1:B:65:TYR:HD1	2.15	0.40
1:C:79:HIS:HD2	1:C:161:TRP:HE1	1.68	0.40
1:C:85:LEU:HA	1:C:88:VAL:HG22	2.04	0.40
1:B:167:LEU:HD21	1:B:206:VAL:HG11	2.04	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	427/502 (85%)	395 (92%)	29 (7%)	3 (1%)	18	49
1	B	416/502 (83%)	394 (95%)	22 (5%)	0	100	100
1	C	418/502 (83%)	402 (96%)	15 (4%)	1 (0%)	43	73
All	All	1261/1506 (84%)	1191 (94%)	66 (5%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1023	GLY
1	A	182	ASP
1	A	274	CYS
1	A	1077	GLY

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	368/432 (85%)	333 (90%)	35 (10%)	8	30
1	B	359/432 (83%)	324 (90%)	35 (10%)	8	30
1	C	365/432 (84%)	329 (90%)	36 (10%)	7	29
All	All	1092/1296 (84%)	986 (90%)	106 (10%)	8	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	61	LEU
1	A	102	TRP
1	A	132	LEU
1	A	138	ILE
1	A	143	ASN
1	A	144	SER
1	A	145	GLN
1	A	146	ARG
1	A	150	LEU
1	A	156	VAL
1	A	158	VAL
1	A	162	ILE
1	A	165	LEU
1	A	168	THR
1	A	181	ASP
1	A	187	ASP

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	228	HIS
1	A	901	SER
1	A	1005	GLU
1	A	1006	MET
1	A	1007	LEU
1	A	1022	GLU
1	A	1026	THR
1	A	1083	LYS
1	A	1091	LEU
1	A	1132	ASN
1	A	1137	ARG
1	A	1141	GLN
1	A	232	HIS
1	A	253	LEU
1	A	265	ILE
1	A	269	ILE
1	A	277	GLU
1	B	38	LYS
1	B	39	ILE
1	B	44	ILE
1	B	53	ILE
1	B	69	LEU
1	B	70	ARG
1	B	79	HIS
1	B	86	LEU
1	B	106	ASN
1	B	145	GLN
1	B	150	LEU
1	B	167	LEU
1	B	168	THR
1	B	186	CYS
1	B	197	VAL
1	B	205	MET
1	B	210	LEU
1	B	213	ILE
1	B	223	ILE
1	B	1016	LYS
1	B	1019	LYS
1	B	1062	GLU
1	B	1076	ARG
1	B	1085	LYS

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Mol	Chain	Res	Type
1	B	1106	MET
1	B	1201	SER
1	B	230	LYS
1	B	232	HIS
1	B	238	LEU
1	B	259	ILE
1	B	261	ILE
1	B	265	ILE
1	B	266	LEU
1	B	282	LYS
1	B	301	LEU
1	C	39	ILE
1	C	48	ILE
1	C	53	ILE
1	C	60	ILE
1	C	69	LEU
1	C	81	SER
1	C	89	ILE
1	C	99	VAL
1	C	106	ASN
1	C	108	LEU
1	C	120	LEU
1	C	140	HIS
1	C	149	LYS
1	C	162	ILE
1	C	168	THR
1	C	200	GLN
1	C	225	LYS
1	C	226	LEU
1	C	1007	LEU
1	C	1020	ASP
1	C	1021	THR
1	C	1032	LEU
1	C	1035	LYS
1	C	1048	LYS
1	C	1052	ARG
1	C	1058	ILE
1	C	1137	ARG
1	C	239	LYS
1	C	245	ILE
1	C	246	LEU
1	C	265	ILE

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Mol	Chain	Res	Type
1	C	266	LEU
1	C	268	GLU
1	C	281	HIS
1	C	300	ILE
1	C	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	66	GLN
1	A	101	ASN
1	A	143	ASN
1	A	176	ASN
1	A	1053	ASN
1	A	1122	GLN
1	A	233	GLN
1	A	272	GLN
1	B	37	ASN
1	B	79	HIS
1	B	1081	ASN
1	B	1116	ASN
1	B	232	HIS
1	C	66	GLN
1	C	79	HIS
1	C	1101	ASN
1	C	1122	GLN
1	C	1132	ASN
1	C	294	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	ITD	A	1500	-	28,30,30	2.46	6 (21%)	30,42,42	2.15	8 (26%)
2	ITD	C	1500	-	28,30,30	2.52	6 (21%)	30,42,42	1.79	9 (30%)
2	ITD	B	1500	-	28,30,30	2.51	6 (21%)	30,42,42	2.02	10 (33%)

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	ITD	A	1500	-	-	3/12/39/39	0/4/4/4
2	ITD	C	1500	-	-	4/12/39/39	0/4/4/4
2	ITD	B	1500	-	-	4/12/39/39	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1500	ITD	C4-N1	7.22	1.34	1.28
2	B	1500	ITD	C4-N1	6.96	1.34	1.28
2	A	1500	ITD	C4-N1	6.95	1.34	1.28
2	B	1500	ITD	C5-C7	6.76	1.42	1.34
2	C	1500	ITD	C5-C7	6.73	1.42	1.34
2	C	1500	ITD	C9-S2	-6.65	1.66	1.75
2	B	1500	ITD	C9-S2	-6.56	1.66	1.75
2	A	1500	ITD	C5-C7	6.43	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C9-S2	-6.25	1.67	1.75
2	A	1500	ITD	C4-N2	-3.94	1.30	1.38
2	C	1500	ITD	C4-N2	-3.83	1.31	1.38
2	B	1500	ITD	C4-N2	-3.76	1.31	1.38
2	A	1500	ITD	C2-N1	-3.40	1.46	1.49
2	B	1500	ITD	C2-N1	-3.12	1.46	1.49
2	C	1500	ITD	C2-N1	-2.63	1.47	1.49
2	A	1500	ITD	C8-S2	-2.58	1.76	1.80
2	C	1500	ITD	C8-S2	-2.54	1.76	1.80
2	B	1500	ITD	C8-S2	-2.51	1.76	1.80

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ITD	C17-C16-N4	4.60	116.46	109.34
2	A	1500	ITD	C10-N3-C9	4.29	132.02	124.48
2	A	1500	ITD	C8-S2-C9	4.19	110.25	100.98
2	B	1500	ITD	N2-C4-N1	-4.11	111.16	116.95
2	A	1500	ITD	C15-C10-N3	4.07	118.70	110.57
2	B	1500	ITD	C15-C10-N3	4.04	118.64	110.57
2	A	1500	ITD	S1-C4-N2	3.96	115.17	109.31
2	C	1500	ITD	N2-C4-N1	-3.95	111.39	116.95
2	C	1500	ITD	S1-C4-N2	3.84	114.99	109.31
2	C	1500	ITD	C6-C2-N1	3.83	105.96	102.83
2	B	1500	ITD	S1-C4-N2	3.72	114.81	109.31
2	B	1500	ITD	C6-C2-N1	3.69	105.84	102.83
2	A	1500	ITD	C6-C2-N1	3.64	105.80	102.83
2	B	1500	ITD	C10-N3-C9	3.55	130.71	124.48
2	A	1500	ITD	N2-C4-N1	-3.55	111.96	116.95
2	B	1500	ITD	C17-C16-N4	3.31	114.47	109.34
2	A	1500	ITD	C7-C5-S1	-3.19	108.64	113.11
2	C	1500	ITD	C7-C5-S1	-3.05	108.84	113.11
2	B	1500	ITD	C7-C5-S1	-2.91	109.03	113.11
2	C	1500	ITD	C10-N3-C9	2.76	129.33	124.48
2	B	1500	ITD	C3-C2-C6	-2.48	108.68	112.09
2	C	1500	ITD	C8-S2-C9	2.45	106.40	100.98
2	C	1500	ITD	C17-C16-N4	2.44	113.11	109.34
2	B	1500	ITD	C8-S2-C9	2.29	106.04	100.98
2	C	1500	ITD	C11-C10-N3	2.05	114.66	110.57
2	B	1500	ITD	C11-C10-N3	2.02	114.61	110.57
2	C	1500	ITD	C3-C2-C6	-2.00	109.33	112.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

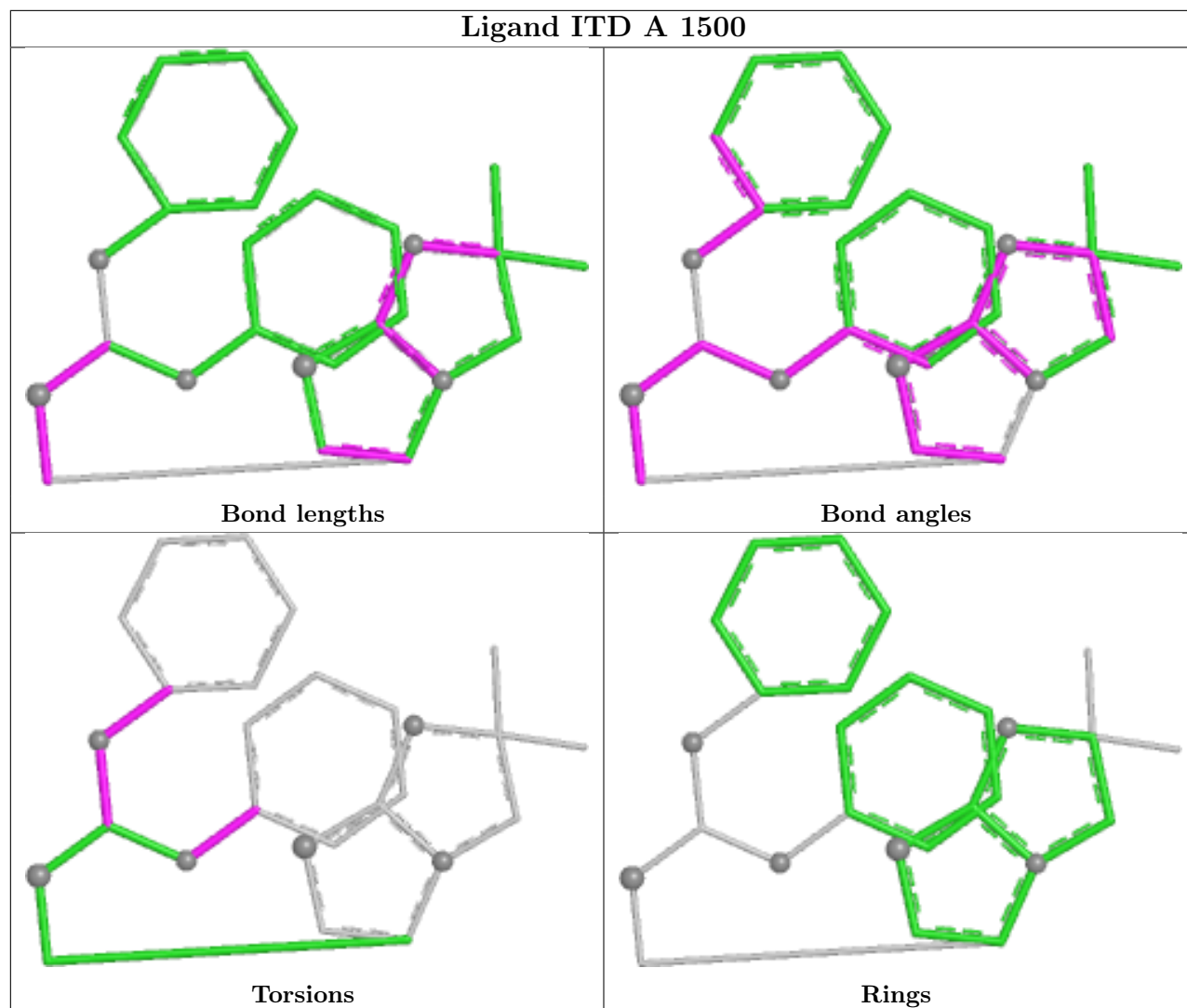
Mol	Chain	Res	Type	Atoms
2	A	1500	ITD	S2-C9-N4-C16
2	A	1500	ITD	C17-C16-N4-C9
2	B	1500	ITD	N3-C9-S2-C8
2	B	1500	ITD	C15-C10-N3-C9
2	B	1500	ITD	C17-C16-N4-C9
2	C	1500	ITD	S2-C9-N4-C16
2	C	1500	ITD	C17-C16-N4-C9
2	A	1500	ITD	C15-C10-N3-C9
2	C	1500	ITD	N3-C9-S2-C8
2	B	1500	ITD	C5-C7-C8-S2
2	C	1500	ITD	C15-C10-N3-C9

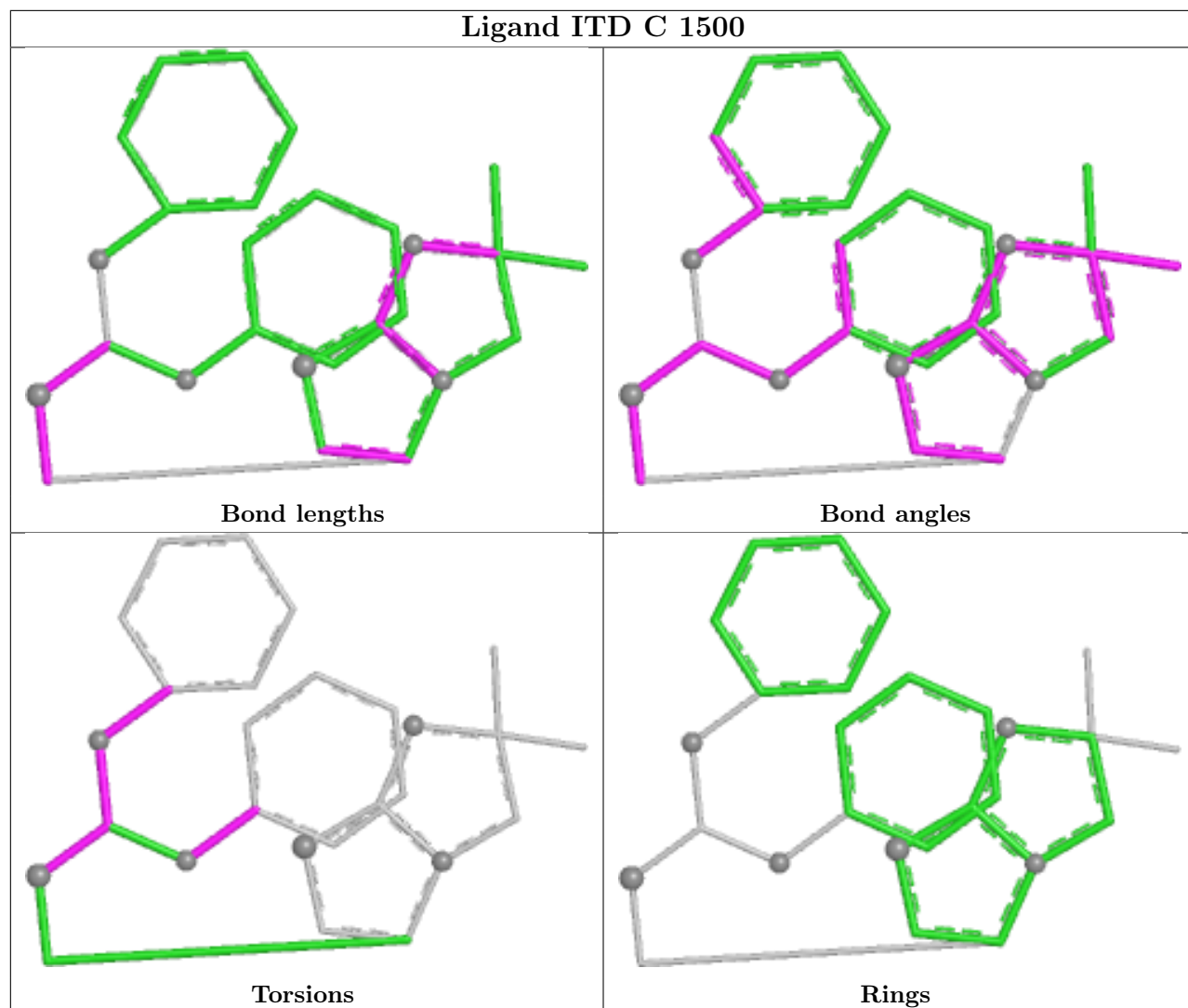
There are no ring outliers.

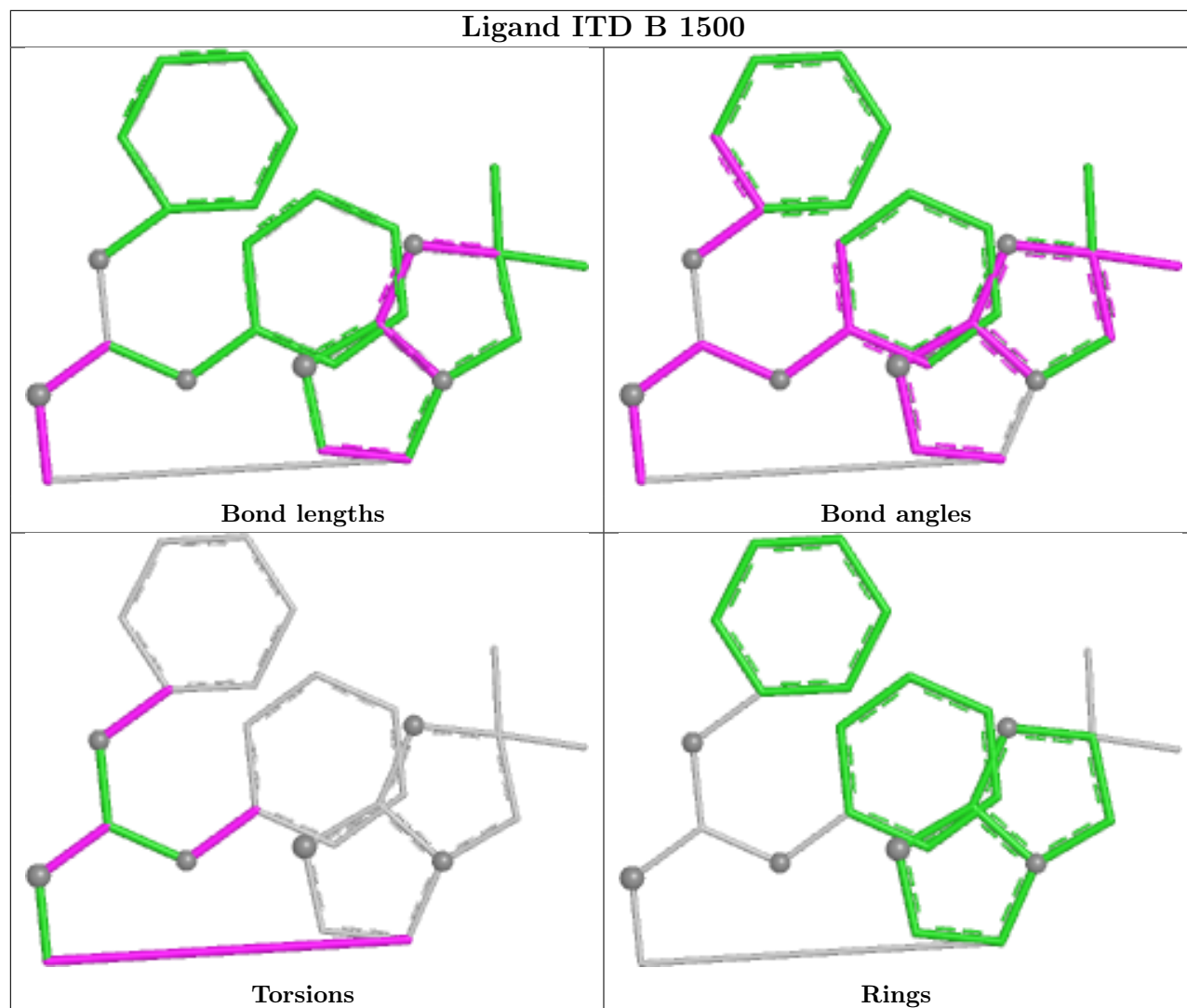
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ITD	2	0
2	C	1500	ITD	3	0
2	B	1500	ITD	4	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	433/502 (86%)	0.05	9 (2%) 63 42	68, 89, 125, 161	0
1	B	426/502 (84%)	0.20	10 (2%) 61 39	63, 100, 181, 198	0
1	C	428/502 (85%)	0.10	8 (1%) 66 45	72, 98, 169, 207	0
All	All	1287/1506 (85%)	0.12	27 (2%) 63 42	63, 94, 169, 207	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	CYS	4.1
1	A	1114	PHE	3.5
1	B	224	SER	3.5
1	A	84	ASP	3.1
1	B	65	TYR	3.1
1	C	230	LYS	2.9
1	C	289	ALA	2.9
1	A	100	ALA	2.8
1	B	63	MET	2.8
1	A	66	GLN	2.6
1	B	262	ASP	2.5
1	A	1003	ILE	2.5
1	A	901	SER	2.5
1	C	180	ALA	2.5
1	C	1127	ASP	2.4
1	B	207	GLY	2.3
1	C	266	LEU	2.2
1	B	84	ASP	2.2
1	B	60	ILE	2.1
1	A	63	MET	2.1
1	B	123	SER	2.1
1	A	147	PRO	2.0
1	B	1201	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	159	GLY	2.0
1	A	275	GLU	2.0
1	C	1062	GLU	2.0
1	C	70	ARG	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](#)

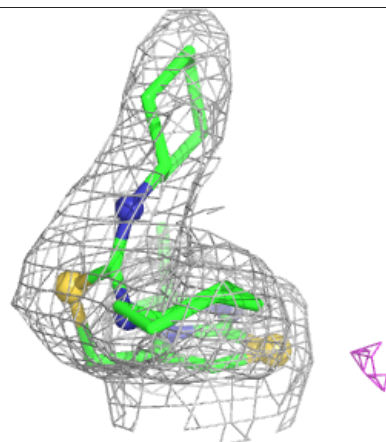
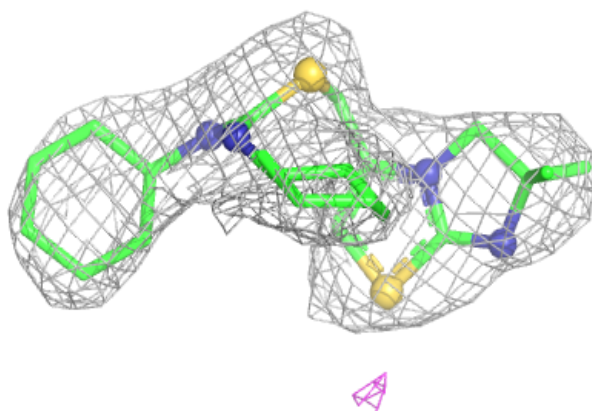
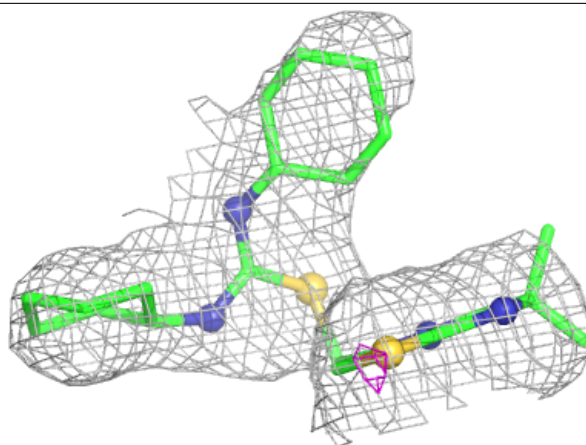
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ITD	A	1500	27/27	0.92	0.11	37,105,187,191	0
2	ITD	C	1500	27/27	0.92	0.10	35,105,168,218	0
2	ITD	B	1500	27/27	0.96	0.09	24,89,203,224	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.

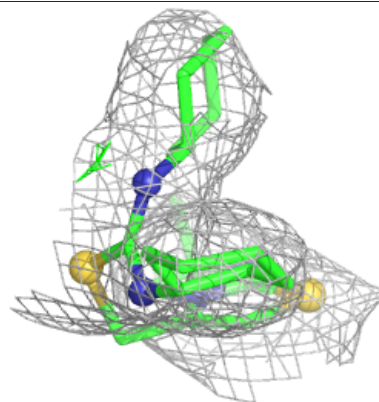
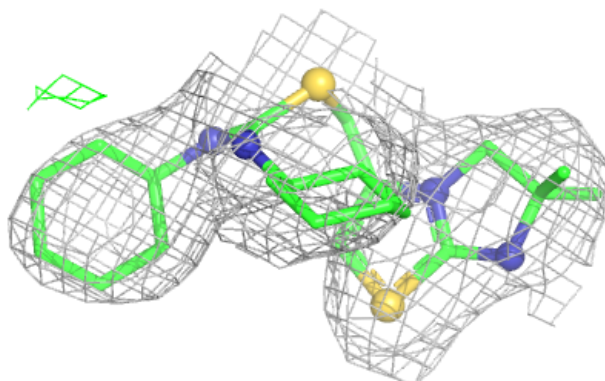
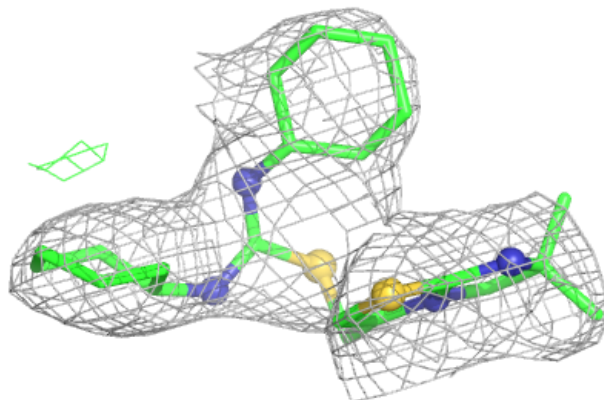
Electron density around ITD A 1500:

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

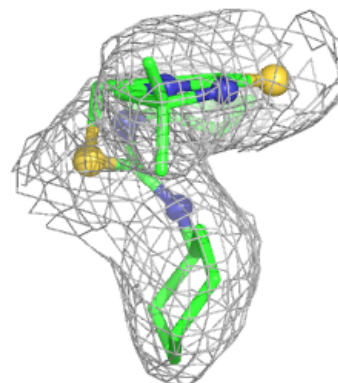
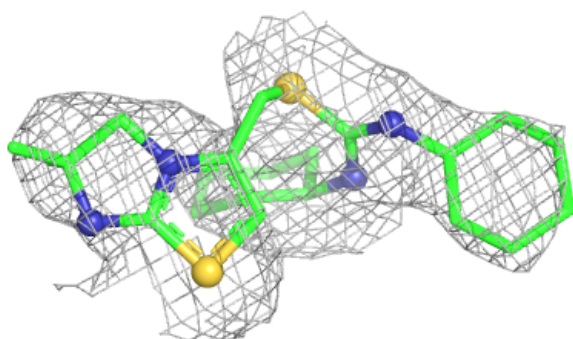
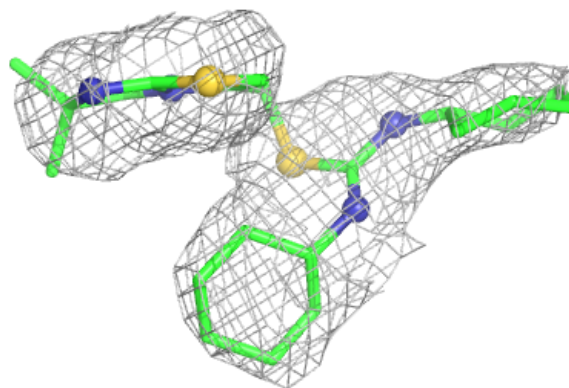


Electron density around ITD C 1500:

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

**Electron density around ITD B 1500:**

$2mF_o-DF_c$ (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.