



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:12 AM UTC

PDB ID : 3OE9 / pdb_00003oe9
Title : Crystal structure of the chemokine CXCR4 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

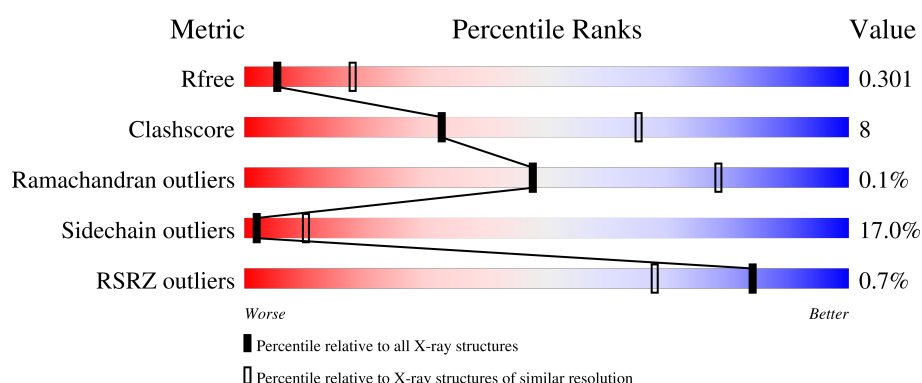
1 Overall quality at a glance

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	499	% 60% 21% •• 16%
1	B	499	% 57% 19% 6% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6780 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	420	Total	C	N	O	S	0	0	0
			3383	2229	563	575	16			
1	B	415	Total	C	N	O	S	0	0	0
			3343	2202	553	573	15			

There are 54 discrepancies between the modelled and reference sequences:

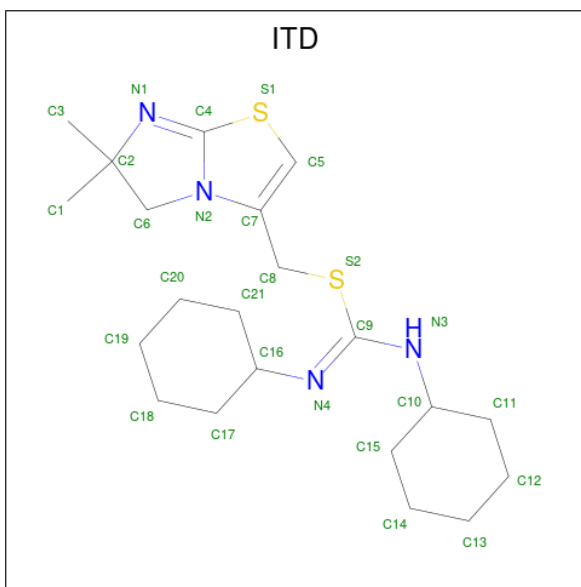
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
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	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	1200	SER	-	linker	UNP P61073
A	1201	GLY	-	linker	UNP P61073
A	1202	SER	-	linker	UNP P61073
A	240	PRO	THR	engineered mutation	UNP P61073
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
A	325	VAL	-	expression tag	UNP P61073
A	326	LEU	-	expression tag	UNP P61073

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1054	THR	CYS	engineered mutation	UNP P00720
B	1097	ALA	CYS	engineered mutation	UNP P00720
B	1200	SER	-	linker	UNP P61073
B	1201	GLY	-	linker	UNP P61073
B	1202	SER	-	linker	UNP P61073
B	240	PRO	THR	engineered mutation	UNP P61073
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

- 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).

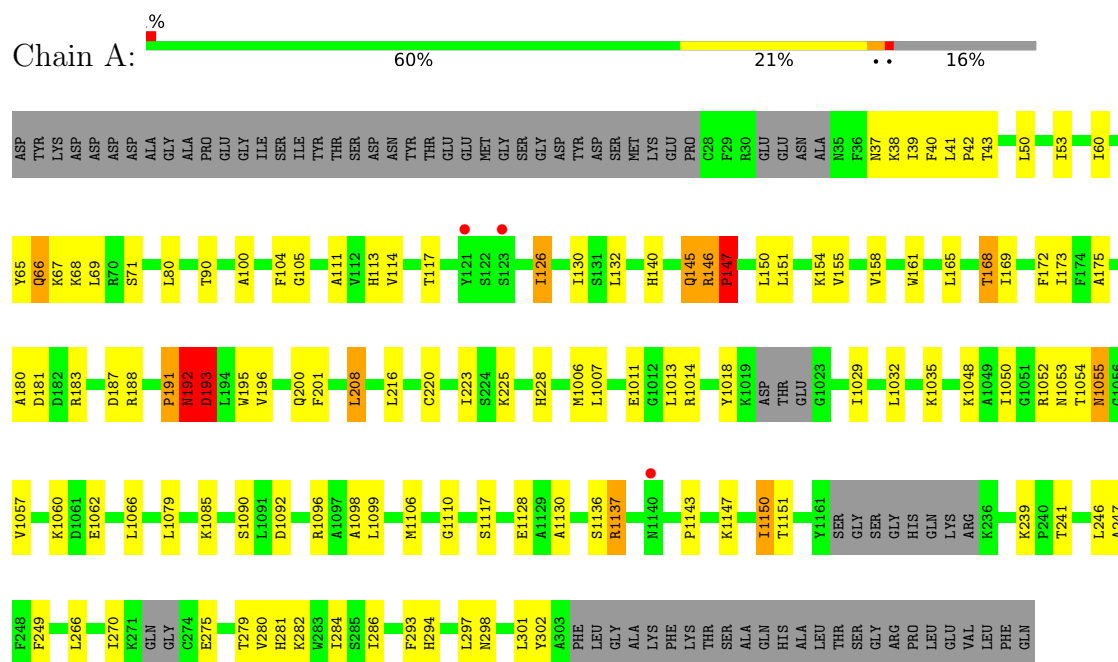


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			27	21	4	2		
2	B	1	Total	C	N	S	0	0
			27	21	4	2		

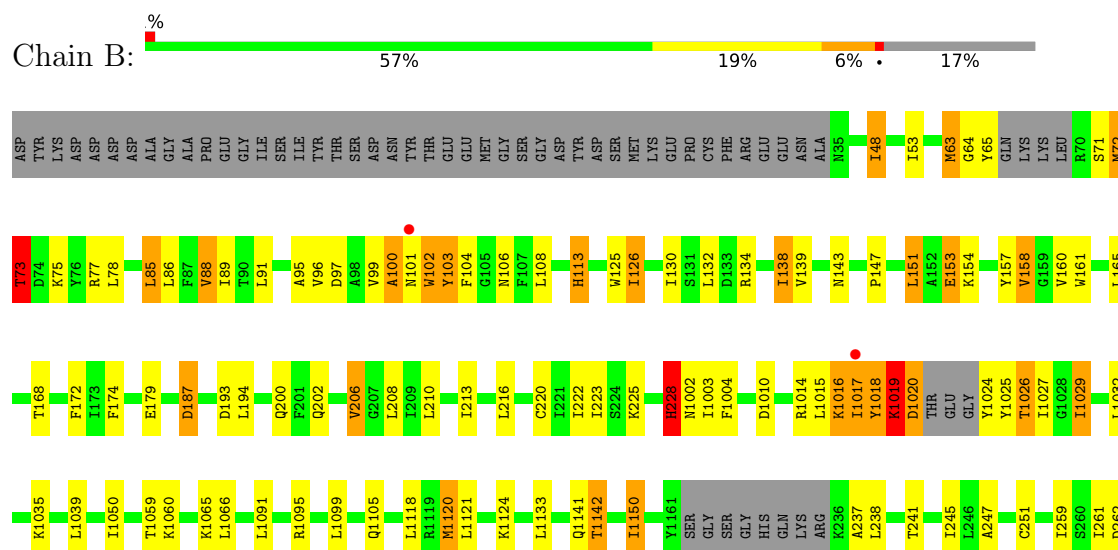
3 Residue-property plots

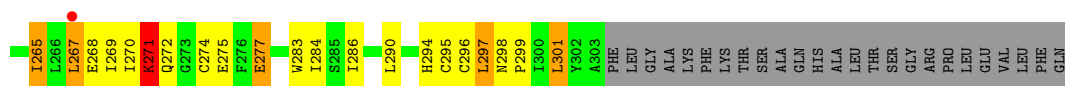
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



- 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	72.50Å 72.74Å 84.27Å 64.66° 73.93° 61.31°	Depositor
Resolution (Å)	19.92 – 3.10 19.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.92-3.10) 98.1 (19.92-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.09Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.252 , 0.284 0.269 , 0.301	Depositor DCC
R_{free} test set	1238 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h+k,k,k-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6780	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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	3/3464 (0.1%)	1.71	53/4704 (1.1%)
1	B	0.84	3/3424 (0.1%)	1.63	44/4655 (0.9%)
All	All	0.82	6/6888 (0.1%)	1.67	97/9359 (1.0%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	HIS	C-N	15.57	1.55	1.33
1	A	147	PRO	N-CD	6.23	1.56	1.47
1	A	294	HIS	ND1-CE1	5.81	1.38	1.32
1	A	169	ILE	CA-CB	5.74	1.57	1.54
1	B	294	HIS	ND1-CE1	5.42	1.38	1.32
1	B	113	HIS	ND1-CE1	5.16	1.37	1.32

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LYS	N-CA-C	32.72	146.08	111.07
1	B	100	ALA	N-CA-C	20.87	140.94	113.18
1	A	192	ASN	N-CA-C	-19.66	83.67	108.45
1	B	268	GLU	N-CA-C	14.54	130.97	113.23
1	B	228	HIS	CA-C-N	12.42	145.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	HIS	C-N-CA	12.42	145.26	121.54
1	B	102	TRP	N-CA-C	-12.16	89.49	109.07
1	A	191	PRO	N-CA-C	11.99	135.14	114.75
1	A	146	ARG	CB-CA-C	11.90	127.70	109.50
1	A	100	ALA	N-CA-C	11.83	128.92	113.18
1	B	153	GLU	CB-CA-C	11.77	127.59	109.34
1	A	191	PRO	CB-CA-C	-11.47	92.48	110.49
1	B	100	ALA	CB-CA-C	-11.46	90.06	110.23
1	A	68	LYS	CB-CA-C	-11.00	93.61	110.88
1	B	73	THR	N-CA-C	-10.67	99.85	113.72
1	A	193	ASP	N-CA-CB	-10.46	94.64	110.33
1	B	272	GLN	CB-CA-C	9.96	126.12	109.38
1	B	1019	LYS	CB-CA-C	9.86	128.97	110.62
1	A	66	GLN	CB-CA-C	-9.44	93.54	109.50
1	A	38	LYS	N-CA-C	9.28	124.40	113.18
1	A	67	LYS	N-CA-CB	-9.14	98.43	110.59
1	A	147	PRO	N-CA-C	-9.12	93.69	112.47
1	A	1055	ASN	N-CA-C	8.81	123.32	112.58
1	A	146	ARG	N-CA-C	8.49	120.01	109.57
1	A	301	LEU	N-CA-C	8.42	122.66	112.38
1	A	298	ASN	N-CA-C	-8.11	101.72	112.75
1	A	181	ASP	N-CA-C	-7.97	98.21	109.69
1	B	272	GLN	N-CA-CB	-7.96	99.89	110.88
1	B	269	ILE	N-CA-C	7.90	117.95	110.53
1	A	147	PRO	CA-C-N	7.69	131.61	120.38
1	A	147	PRO	C-N-CA	7.69	131.61	120.38
1	A	69	LEU	N-CA-CB	7.57	124.04	110.95
1	A	168	THR	CA-C-N	7.53	126.35	120.33
1	A	168	THR	C-N-CA	7.53	126.35	120.33
1	B	113	HIS	CB-CG-CD2	-7.48	121.48	131.20
1	A	294	HIS	CB-CG-CD2	-7.43	121.55	131.20
1	B	1010	ASP	N-CA-C	7.42	122.72	112.04
1	B	294	HIS	CB-CG-CD2	-7.32	121.68	131.20
1	A	71	SER	N-CA-C	-7.26	98.72	110.20
1	A	154	LYS	N-CA-C	7.18	122.73	113.18
1	B	154	LYS	N-CA-CB	-7.08	98.02	110.34
1	B	1017	ILE	N-CA-CB	-6.95	99.76	111.23
1	A	146	ARG	N-CA-CB	-6.82	97.84	109.57
1	B	102	TRP	N-CA-CB	6.77	121.20	110.57
1	B	271	LYS	N-CA-C	6.61	118.22	107.32
1	B	154	LYS	N-CA-C	6.47	121.54	112.93
1	A	104	PHE	N-CA-C	6.43	118.29	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	PRO	CA-C-N	6.41	129.39	120.29
1	B	147	PRO	C-N-CA	6.41	129.39	120.29
1	A	1136	SER	CA-C-N	6.26	128.67	120.28
1	A	1136	SER	C-N-CA	6.26	128.67	120.28
1	B	208	LEU	N-CA-C	6.22	120.68	112.72
1	B	1142	THR	CB-CA-C	6.19	120.38	111.27
1	A	193	ASP	N-CA-C	-6.17	104.81	112.90
1	B	174	PHE	N-CA-C	6.11	120.47	112.89
1	A	201	PHE	N-CA-C	-6.05	105.93	113.55
1	A	67	LYS	CA-C-N	5.96	128.19	120.44
1	A	67	LYS	C-N-CA	5.96	128.19	120.44
1	A	228	HIS	N-CA-C	-5.96	106.55	113.88
1	B	104	PHE	N-CA-C	5.85	120.11	113.15
1	B	267	LEU	CB-CA-C	5.78	119.75	110.09
1	A	180	ALA	N-CA-C	5.64	117.90	111.02
1	A	40	PHE	CA-C-N	5.63	127.12	120.09
1	A	40	PHE	C-N-CA	5.63	127.12	120.09
1	B	238	LEU	N-CA-CB	-5.61	103.13	110.59
1	B	202	GLN	CA-C-N	5.57	127.74	120.28
1	B	202	GLN	C-N-CA	5.57	127.74	120.28
1	A	1137	ARG	CA-C-N	5.54	128.16	120.29
1	A	1137	ARG	C-N-CA	5.54	128.16	120.29
1	A	302	TYR	N-CA-CB	-5.53	101.75	110.49
1	B	88	VAL	N-CA-CB	5.53	118.06	110.54
1	B	237	ALA	CB-CA-C	-5.51	101.07	109.89
1	A	161	TRP	CA-C-N	5.50	124.73	120.33
1	A	161	TRP	C-N-CA	5.50	124.73	120.33
1	A	1053	ASN	CA-C-N	5.50	127.91	120.38
1	A	1053	ASN	C-N-CA	5.50	127.91	120.38
1	B	103	TYR	N-CA-C	-5.50	107.58	114.56
1	B	158	VAL	CB-CA-C	5.47	126.00	111.34
1	A	105	GLY	CA-C-N	5.46	127.86	120.65
1	A	105	GLY	C-N-CA	5.46	127.86	120.65
1	B	1016	LYS	CB-CA-C	-5.46	101.14	112.44
1	B	1017	ILE	N-CA-C	5.41	120.58	109.34
1	B	237	ALA	N-CA-C	5.40	118.06	109.96
1	B	301	LEU	N-CA-C	5.33	118.89	112.38
1	B	1029	ILE	CB-CA-C	5.32	118.45	111.53
1	A	39	ILE	N-CA-C	-5.31	108.10	113.47
1	B	161	TRP	N-CA-C	5.28	116.89	111.03
1	A	140	HIS	N-CA-C	5.25	118.51	112.57
1	A	187	ASP	CA-CB-CG	5.24	117.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1057	VAL	N-CA-CB	5.22	118.92	111.82
1	A	281	HIS	CA-C-N	5.11	127.08	120.44
1	A	281	HIS	C-N-CA	5.11	127.08	120.44
1	A	67	LYS	N-CA-C	5.05	120.09	113.88
1	B	1003	ILE	CA-C-N	5.03	127.29	120.65
1	B	1003	ILE	C-N-CA	5.03	127.29	120.65
1	B	126	ILE	N-CA-C	-5.02	105.65	110.72
1	B	64	GLY	N-CA-C	-5.01	108.45	114.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	228	HIS	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	3383	0	3450	32	0
1	B	3343	0	3412	77	0
2	A	27	0	34	2	0
2	B	27	0	34	3	0
All	All	6780	0	6930	108	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 8.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:ARG:HH12	1:B:1026:THR:CG2	1.37	1.35
1:B:1014:ARG:NH1	1:B:1026:THR:CG2	2.04	1.21
1:B:1018:TYR:CE1	1:B:1019:LYS:O	1.96	1.19
1:B:271:LYS:N	1:B:271:LYS:HD3	1.59	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:ARG:HH12	1:B:1026:THR:HG22	1.21	1.04
1:B:1014:ARG:HH12	1:B:1026:THR:HG21	1.18	1.04
1:A:191:PRO:HB2	1:A:192:ASN:OD1	1.64	0.96
1:B:1014:ARG:NH1	1:B:1026:THR:HG21	1.78	0.92
1:B:271:LYS:HD3	1:B:271:LYS:H	1.20	0.91
1:B:1018:TYR:CD1	1:B:1019:LYS:N	2.46	0.83
1:B:101:ASN:OD1	1:B:102:TRP:N	2.15	0.80
1:B:1020:ASP:HB2	1:B:1024:TYR:HB2	1.64	0.79
1:A:37:ASN:O	1:A:41:LEU:HB2	1.87	0.73
1:B:99:VAL:HG23	1:B:100:ALA:N	2.03	0.73
1:B:1018:TYR:CG	1:B:1019:LYS:N	2.57	0.72
1:B:99:VAL:HG23	1:B:100:ALA:H	1.57	0.69
1:A:145:GLN:O	1:A:147:PRO:HD3	1.94	0.66
1:B:95:ALA:O	1:B:99:VAL:HG22	1.94	0.66
1:A:192:ASN:OD1	1:A:192:ASN:N	2.29	0.66
1:A:191:PRO:CB	1:A:192:ASN:OD1	2.42	0.65
1:B:101:ASN:HB3	1:B:103:TYR:CZ	2.31	0.65
1:B:1017:ILE:CG2	1:B:1018:TYR:N	2.60	0.65
1:A:151:LEU:HA	1:A:155:VAL:HB	1.79	0.65
1:B:63:MET:HG2	1:B:78:LEU:HD13	1.79	0.64
1:B:1014:ARG:NH1	1:B:1026:THR:HG22	1.91	0.64
1:B:271:LYS:HE2	1:B:271:LYS:O	1.99	0.63
1:B:126:ILE:HG13	1:B:160:VAL:HG11	1.82	0.61
1:A:192:ASN:OD1	1:A:195:TRP:HD1	1.84	0.61
1:B:1017:ILE:HG22	1:B:1018:TYR:N	2.14	0.61
1:A:1092:ASP:O	1:A:1096:ARG:HG3	2.01	0.60
1:B:1014:ARG:CZ	1:B:1026:THR:CG2	2.78	0.60
1:B:228:HIS:O	1:B:1004:PHE:HB3	2.01	0.59
1:A:192:ASN:CG	1:A:195:TRP:HD1	2.09	0.59
1:B:153:GLU:O	1:B:157:TYR:HE1	1.85	0.59
1:B:1018:TYR:O	1:B:1019:LYS:HB3	2.05	0.57
1:A:145:GLN:HE22	1:B:1060:LYS:NZ	2.03	0.56
1:A:1014:ARG:HD2	1:A:1018:TYR:HB2	1.86	0.56
1:B:298:ASN:HB3	1:B:299:PRO:HD3	1.87	0.56
1:A:192:ASN:OD1	1:A:195:TRP:CD1	2.59	0.56
1:B:1018:TYR:OH	1:B:1020:ASP:OD2	2.21	0.55
1:B:1014:ARG:HH22	1:B:1026:THR:HG22	1.71	0.55
1:B:96:VAL:O	1:B:99:VAL:CG2	2.55	0.55
1:B:153:GLU:O	1:B:157:TYR:CE1	2.59	0.55
1:B:1018:TYR:CZ	1:B:1019:LYS:O	2.59	0.55
1:B:1018:TYR:CD1	1:B:1019:LYS:O	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:O	1:B:99:VAL:HG22	2.09	0.52
1:B:48:ILE:HG23	1:B:91:LEU:HD13	1.92	0.52
1:B:99:VAL:CG2	1:B:100:ALA:N	2.72	0.52
1:B:132:LEU:HD23	1:B:151:LEU:HD21	1.92	0.52
1:B:1014:ARG:NH1	1:B:1026:THR:HG23	2.14	0.52
1:B:88:VAL:HA	1:B:91:LEU:HD12	1.93	0.51
1:A:195:TRP:NE1	1:B:267:LEU:O	2.39	0.51
1:B:228:HIS:O	1:B:1004:PHE:CB	2.59	0.50
1:B:138:ILE:HG21	1:B:222:ILE:HG23	1.93	0.50
1:A:1079:LEU:O	1:A:1085:LYS:HD3	2.11	0.50
1:B:1014:ARG:CZ	1:B:1026:THR:HG22	2.41	0.50
1:B:271:LYS:N	1:B:271:LYS:CD	2.49	0.50
1:B:125:TRP:NE1	1:B:206:VAL:O	2.41	0.49
1:B:1014:ARG:NH2	1:B:1026:THR:HG22	2.27	0.49
1:B:85:LEU:HA	1:B:88:VAL:HG22	1.95	0.48
1:B:1091:LEU:HD22	1:B:1095:ARG:HB3	1.95	0.48
1:A:145:GLN:HE22	1:B:1060:LYS:HZ2	1.61	0.48
1:B:101:ASN:OD1	1:B:102:TRP:O	2.31	0.48
1:A:1055:ASN:O	1:A:1055:ASN:OD1	2.32	0.47
1:A:80:LEU:HB2	1:A:126:ILE:HG21	1.96	0.47
1:B:274:CYS:HA	1:B:277:GLU:HB2	1.96	0.47
1:B:247:ALA:HB1	1:B:297:LEU:HD22	1.96	0.47
1:A:175:ALA:HA	1:A:188:ARG:HA	1.96	0.46
1:A:1106:MET:HB3	1:A:1110:GLY:HA3	1.96	0.46
1:B:139:VAL:HA	1:B:225:LYS:HG2	1.97	0.46
1:B:187:ASP:HB3	2:B:1500:ITD:S2	2.56	0.46
1:A:208:LEU:O	1:A:208:LEU:HD23	2.16	0.45
1:B:113:HIS:CE1	1:B:187:ASP:HA	2.50	0.45
1:A:37:ASN:O	1:A:41:LEU:CB	2.61	0.45
1:A:191:PRO:C	1:A:192:ASN:OD1	2.60	0.45
1:B:1120:MET:H	1:B:1120:MET:HG2	1.48	0.45
1:B:99:VAL:CG2	1:B:100:ALA:H	2.26	0.44
1:B:1019:LYS:HA	1:B:1024:TYR:O	2.16	0.44
1:A:247:ALA:HB3	1:A:297:LEU:HD21	1.99	0.44
1:B:134:ARG:HG3	1:B:241:THR:HG21	2.00	0.44
1:A:1006:MET:HE1	1:A:1098:ALA:HA	1.99	0.44
1:B:1017:ILE:CG2	1:B:1018:TYR:H	2.31	0.43
1:A:113:HIS:CE1	2:A:1500:ITD:H19	2.54	0.43
1:B:1017:ILE:CG2	1:B:1025:TYR:HD2	2.32	0.43
1:A:183:ARG:NH1	2:A:1500:ITD:H13	2.33	0.43
1:B:139:VAL:O	1:B:139:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:TYR:HE1	1:B:1019:LYS:O	1.87	0.43
1:B:1017:ILE:HD13	1:B:1039:LEU:HD11	2.00	0.43
1:B:1118:LEU:HA	1:B:1121:LEU:HD12	2.00	0.43
1:B:125:TRP:HZ2	1:B:210:LEU:HB3	1.84	0.42
1:A:193:ASP:O	1:A:196:VAL:N	2.43	0.42
1:B:73:THR:O	1:B:77:ARG:HG3	2.19	0.42
1:B:296:CYS:O	1:B:299:PRO:HD2	2.20	0.42
1:B:1105:GLN:HE22	1:B:1142:THR:HG21	1.84	0.42
1:B:71:SER:O	1:B:72:MET:HB3	2.20	0.41
1:B:96:VAL:O	1:B:99:VAL:HG23	2.20	0.41
1:B:1133:LEU:HB3	1:B:1150:ILE:HD11	2.00	0.41
1:A:1143:PRO:O	1:A:1147:LYS:HB2	2.20	0.41
2:B:1500:ITD:H3	2:B:1500:ITD:H18	2.02	0.40
1:A:41:LEU:N	1:A:42:PRO:HD2	2.35	0.40
1:A:41:LEU:HD13	1:A:286:ILE:HG22	2.03	0.40
1:B:262:ASP:HB2	1:B:284:ILE:HD11	2.03	0.40
2:B:1500:ITD:S2	2:B:1500:ITD:H17	2.61	0.40
1:A:111:ALA:HA	1:A:114:VAL:HG22	2.03	0.40
1:B:48:ILE:HD11	1:B:295:CYS:HB2	2.03	0.40
1:B:73:THR:O	1:B:73:THR:CG2	2.68	0.40
1:A:1130:ALA:HB1	1:A:1150:ILE:HG23	2.02	0.40
1:B:261:ILE:O	1:B:265:ILE:HG13	2.22	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	410/499 (82%)	388 (95%)	21 (5%)	1 (0%)	43	73
1	B	407/499 (82%)	385 (95%)	22 (5%)	0	100	100
All	All	817/998 (82%)	773 (95%)	43 (5%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO

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	362/430 (84%)	303 (84%)	59 (16%)	2	11
1	B	360/430 (84%)	296 (82%)	64 (18%)	2	9
All	All	722/860 (84%)	599 (83%)	123 (17%)	2	10

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	50	LEU
1	A	53	ILE
1	A	60	ILE
1	A	65	TYR
1	A	66	GLN
1	A	90	THR
1	A	117	THR
1	A	126	ILE
1	A	130	ILE
1	A	132	LEU
1	A	145	GLN
1	A	146	ARG
1	A	150	LEU
1	A	158	VAL
1	A	165	LEU
1	A	168	THR
1	A	172	PHE
1	A	173	ILE
1	A	192	ASN
1	A	193	ASP
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	208	LEU
1	A	216	LEU
1	A	220	CYS
1	A	223	ILE
1	A	225	LYS
1	A	1007	LEU
1	A	1011	GLU
1	A	1013	LEU
1	A	1029	ILE
1	A	1032	LEU
1	A	1035	LYS
1	A	1048	LYS
1	A	1050	ILE
1	A	1052	ARG
1	A	1054	THR
1	A	1060	LYS
1	A	1062	GLU
1	A	1066	LEU
1	A	1090	SER
1	A	1099	LEU
1	A	1117	SER
1	A	1128	GLU
1	A	1137	ARG
1	A	1150	ILE
1	A	1151	THR
1	A	239	LYS
1	A	241	THR
1	A	246	LEU
1	A	249	PHE
1	A	266	LEU
1	A	270	ILE
1	A	275	GLU
1	A	279	THR
1	A	280	VAL
1	A	282	LYS
1	A	284	ILE
1	A	293	PHE
1	B	48	ILE
1	B	53	ILE
1	B	63	MET
1	B	65	TYR
1	B	72	MET

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Mol	Chain	Res	Type
1	B	73	THR
1	B	75	LYS
1	B	85	LEU
1	B	86	LEU
1	B	89	ILE
1	B	97	ASP
1	B	106	ASN
1	B	108	LEU
1	B	130	ILE
1	B	138	ILE
1	B	143	ASN
1	B	151	LEU
1	B	158	VAL
1	B	165	LEU
1	B	168	THR
1	B	172	PHE
1	B	179	GLU
1	B	187	ASP
1	B	193	ASP
1	B	194	LEU
1	B	200	GLN
1	B	206	VAL
1	B	213	ILE
1	B	216	LEU
1	B	220	CYS
1	B	223	ILE
1	B	1002	ASN
1	B	1015	LEU
1	B	1016	LYS
1	B	1018	TYR
1	B	1019	LYS
1	B	1020	ASP
1	B	1026	THR
1	B	1027	ILE
1	B	1029	ILE
1	B	1032	LEU
1	B	1035	LYS
1	B	1050	ILE
1	B	1059	THR
1	B	1065	LYS
1	B	1066	LEU
1	B	1099	LEU

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Mol	Chain	Res	Type
1	B	1120	MET
1	B	1124	LYS
1	B	1141	GLN
1	B	1150	ILE
1	B	245	ILE
1	B	251	CYS
1	B	259	ILE
1	B	265	ILE
1	B	270	ILE
1	B	271	LYS
1	B	275	GLU
1	B	277	GLU
1	B	283	TRP
1	B	286	ILE
1	B	290	LEU
1	B	297	LEU
1	B	301	LEU

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

Mol	Chain	Res	Type
1	A	37	ASN
1	A	56	ASN
1	A	106	ASN
1	A	145	GLN
1	A	228	HIS
1	A	1055	ASN
1	A	1123	GLN
1	B	56	ASN
1	B	1002	ASN
1	B	1069	GLN
1	B	1105	GLN
1	B	1122	GLN
1	B	1123	GLN
1	B	1141	GLN

5.3.3 RNA ⓘ

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](#)

2 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	2.66	6 (21%)	30,42,42	2.48	12 (40%)
2	ITD	B	1500	-	28,30,30	2.64	5 (17%)	30,42,42	2.66	16 (53%)

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	B	1500	-	-	4/12/39/39	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C9-S2	-7.50	1.65	1.75
2	B	1500	ITD	C5-C7	7.45	1.43	1.34
2	B	1500	ITD	C9-S2	-7.42	1.65	1.75
2	A	1500	ITD	C4-N1	6.99	1.34	1.28
2	A	1500	ITD	C5-C7	6.92	1.42	1.34
2	B	1500	ITD	C4-N1	6.47	1.33	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C4-N2	-4.08	1.30	1.38
2	B	1500	ITD	C2-N1	-4.04	1.45	1.49
2	B	1500	ITD	C4-N2	-3.93	1.30	1.38
2	A	1500	ITD	C2-N1	-2.93	1.46	1.49
2	A	1500	ITD	C8-S2	-2.23	1.77	1.80

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ITD	C17-C16-N4	6.34	119.15	109.34
2	B	1500	ITD	C17-C16-N4	6.10	118.79	109.34
2	B	1500	ITD	N2-C4-N1	-4.72	110.30	116.95
2	A	1500	ITD	C6-C2-N1	4.61	106.59	102.83
2	A	1500	ITD	N2-C4-N1	-4.60	110.48	116.95
2	B	1500	ITD	C10-N3-C9	4.43	132.25	124.48
2	B	1500	ITD	S1-C4-N2	4.28	115.65	109.31
2	A	1500	ITD	C3-C2-C6	-4.07	106.49	112.09
2	A	1500	ITD	S1-C4-N2	3.90	115.08	109.31
2	B	1500	ITD	C19-C18-C17	3.80	119.24	111.42
2	A	1500	ITD	C10-N3-C9	3.76	131.07	124.48
2	B	1500	ITD	C11-C10-N3	3.57	117.70	110.57
2	B	1500	ITD	C8-S2-C9	3.50	108.72	100.98
2	B	1500	ITD	C12-C11-C10	-3.25	105.27	111.09
2	A	1500	ITD	C7-C5-S1	-3.25	108.56	113.11
2	B	1500	ITD	C15-C10-N3	3.13	116.83	110.57
2	B	1500	ITD	C18-C17-C16	3.04	116.48	111.40
2	A	1500	ITD	C8-S2-C9	2.94	107.48	100.98
2	B	1500	ITD	C21-C16-C17	2.86	115.28	110.33
2	B	1500	ITD	C7-C5-S1	-2.72	109.30	113.11
2	A	1500	ITD	C21-C16-C17	2.71	115.02	110.33
2	B	1500	ITD	C3-C2-C6	-2.60	108.51	112.09
2	A	1500	ITD	C18-C17-C16	2.32	115.29	111.40
2	A	1500	ITD	C21-C16-N4	2.32	112.93	109.34
2	A	1500	ITD	C19-C18-C17	2.20	115.93	111.42
2	B	1500	ITD	C21-C16-N4	2.19	112.72	109.34
2	B	1500	ITD	C14-C15-C10	-2.19	107.17	111.09
2	B	1500	ITD	C6-C2-N1	2.14	104.58	102.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

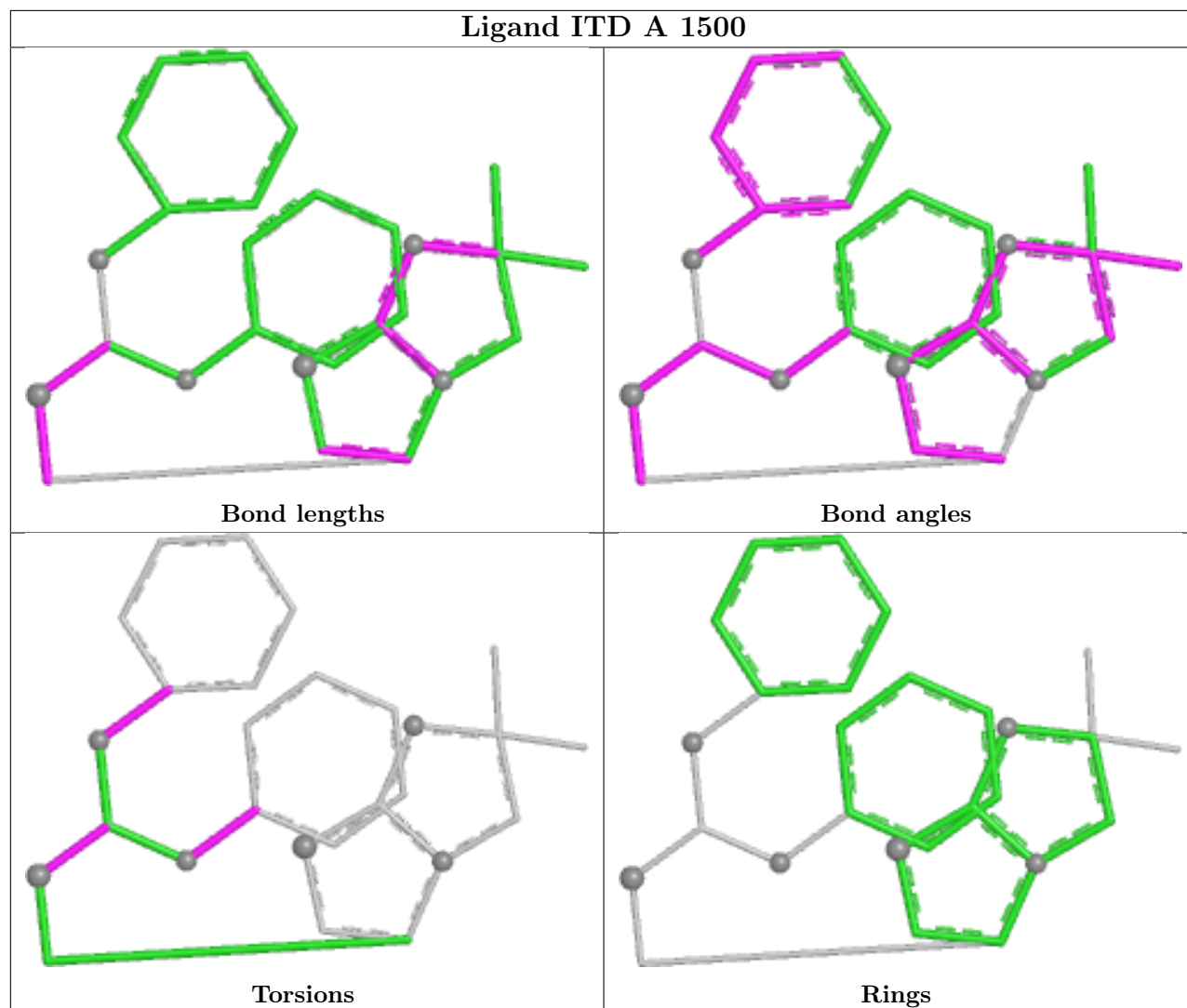
Mol	Chain	Res	Type	Atoms
2	A	1500	ITD	N3-C9-S2-C8
2	A	1500	ITD	C17-C16-N4-C9
2	B	1500	ITD	C17-C16-N4-C9
2	B	1500	ITD	C15-C10-N3-C9
2	B	1500	ITD	N3-C9-S2-C8
2	A	1500	ITD	C11-C10-N3-C9
2	B	1500	ITD	S2-C9-N4-C16

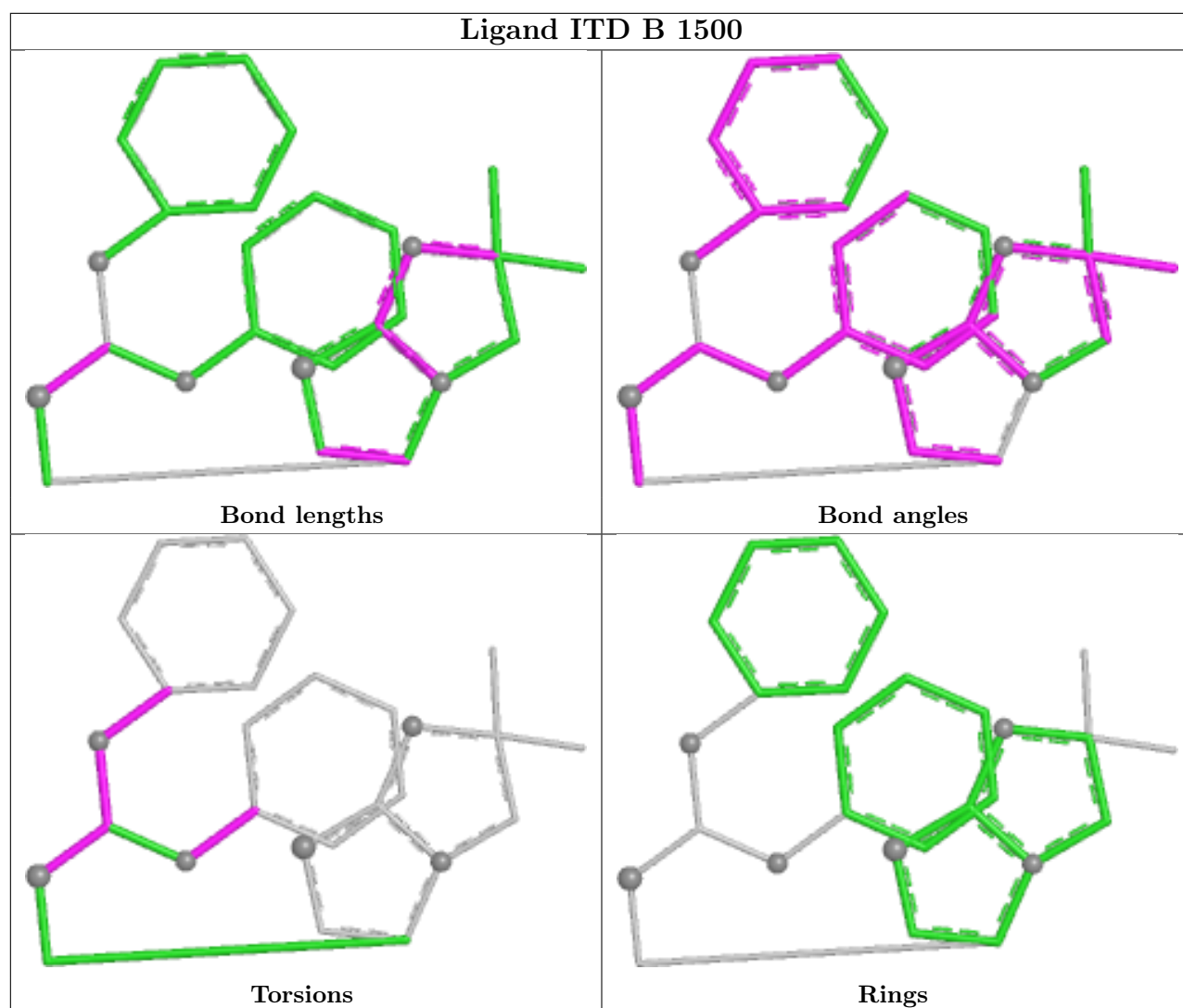
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ITD	2	0
2	B	1500	ITD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	420/499 (84%)	0.13	3 (0%)	84 68	70, 107, 152, 185	0
1	B	415/499 (83%)	0.04	3 (0%)	84 68	58, 94, 137, 161	0
All	All	835/998 (83%)	0.09	6 (0%)	84 68	58, 102, 146, 185	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1140	ASN	2.3
1	B	1017	ILE	2.1
1	A	121	TYR	2.1
1	B	101	ASN	2.1
1	A	123	SER	2.0
1	B	267	LEU	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](#)

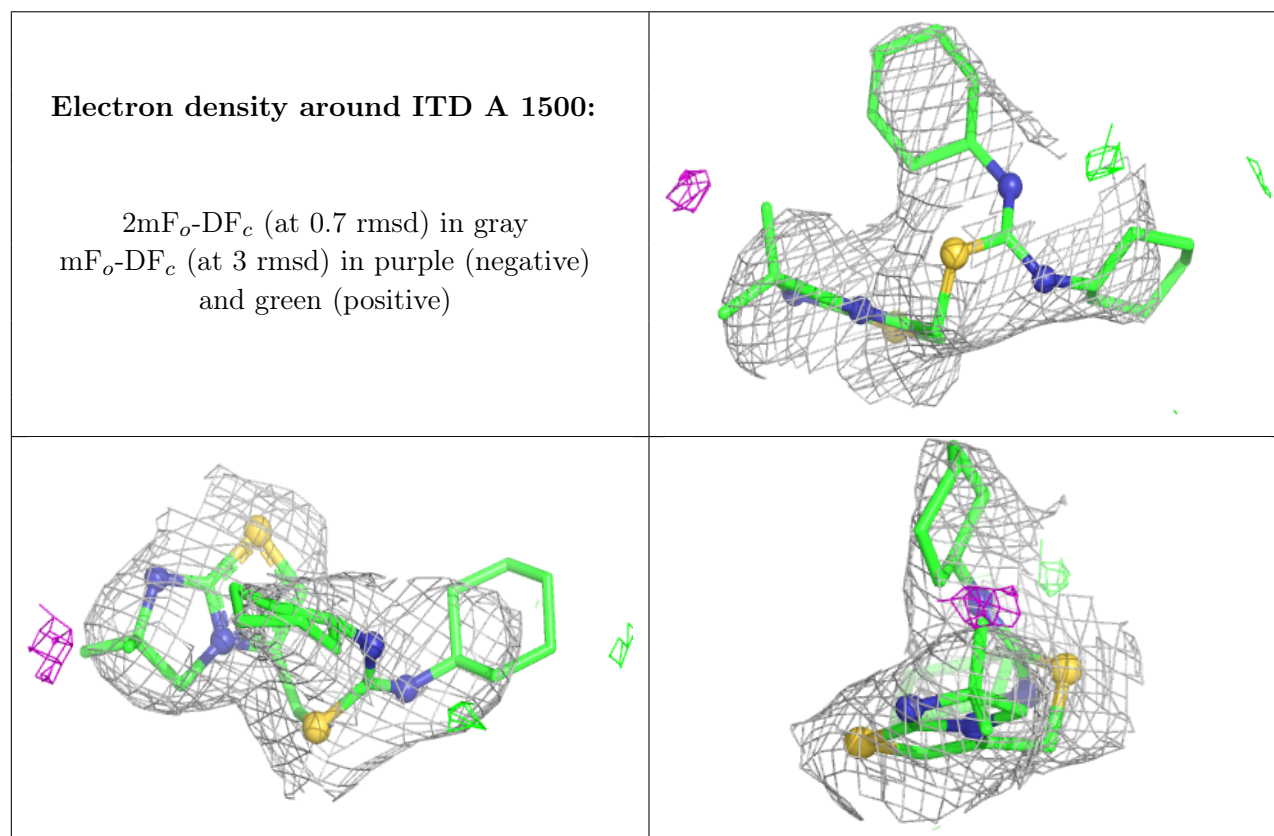
There are no oligosaccharides in this entry.

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.

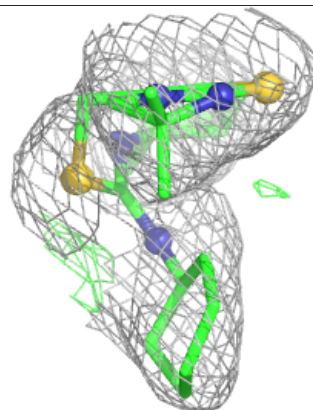
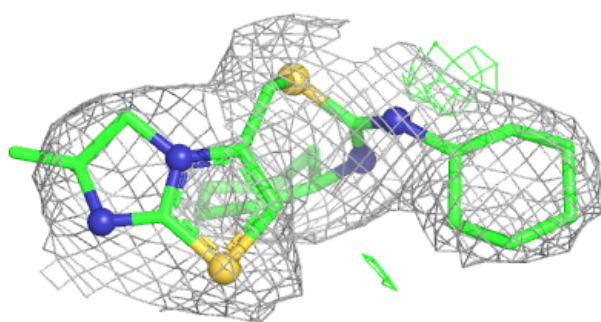
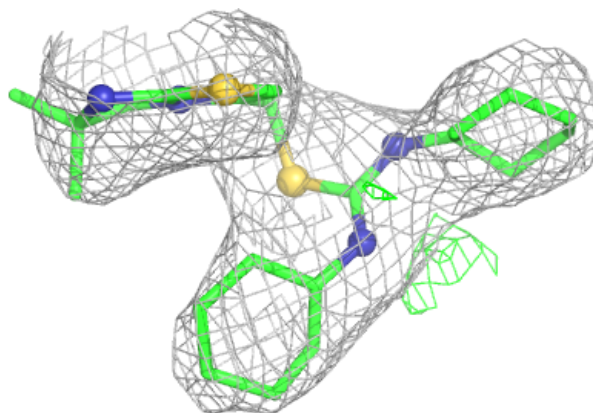
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ITD	A	1500	27/27	0.89	0.14	118,124,129,129	0
2	ITD	B	1500	27/27	0.92	0.12	75,80,93,93	0

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 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 ⓘ

There are no such residues in this entry.