



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:03 PM UTC

PDB ID : 4GSF / pdb_00004gsf
Title : The structure analysis of cysteine free insulin degrading enzyme (ide) with (s)-2-{2-[carboxymethyl-(3-phenyl-propionyl)-amino]-acetylamino}-3-(3h-imidazol-4-yl)-propionic acid methyl ester
Authors : Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on : 2012-08-27
Resolution : 2.70 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

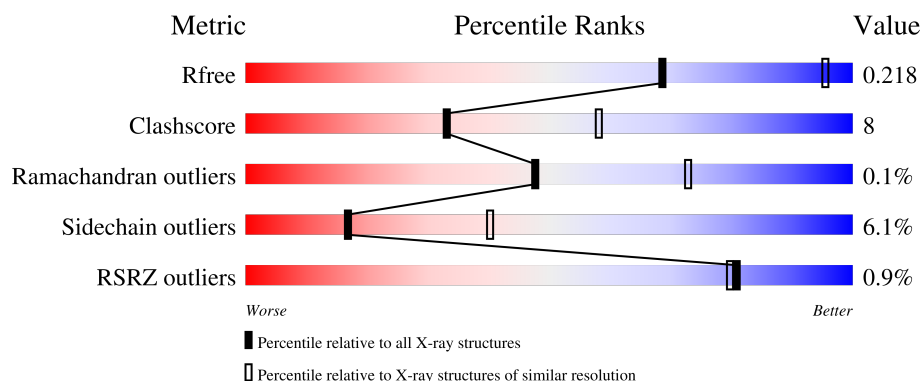
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	990	77% 18% ..
1	B	990	75% 19% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15908 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	956	Total	C	N	O	S	0	0	0
			7768	5008	1307	1431	22			
1	B	954	Total	C	N	O	S	0	0	0
			7758	5002	1305	1429	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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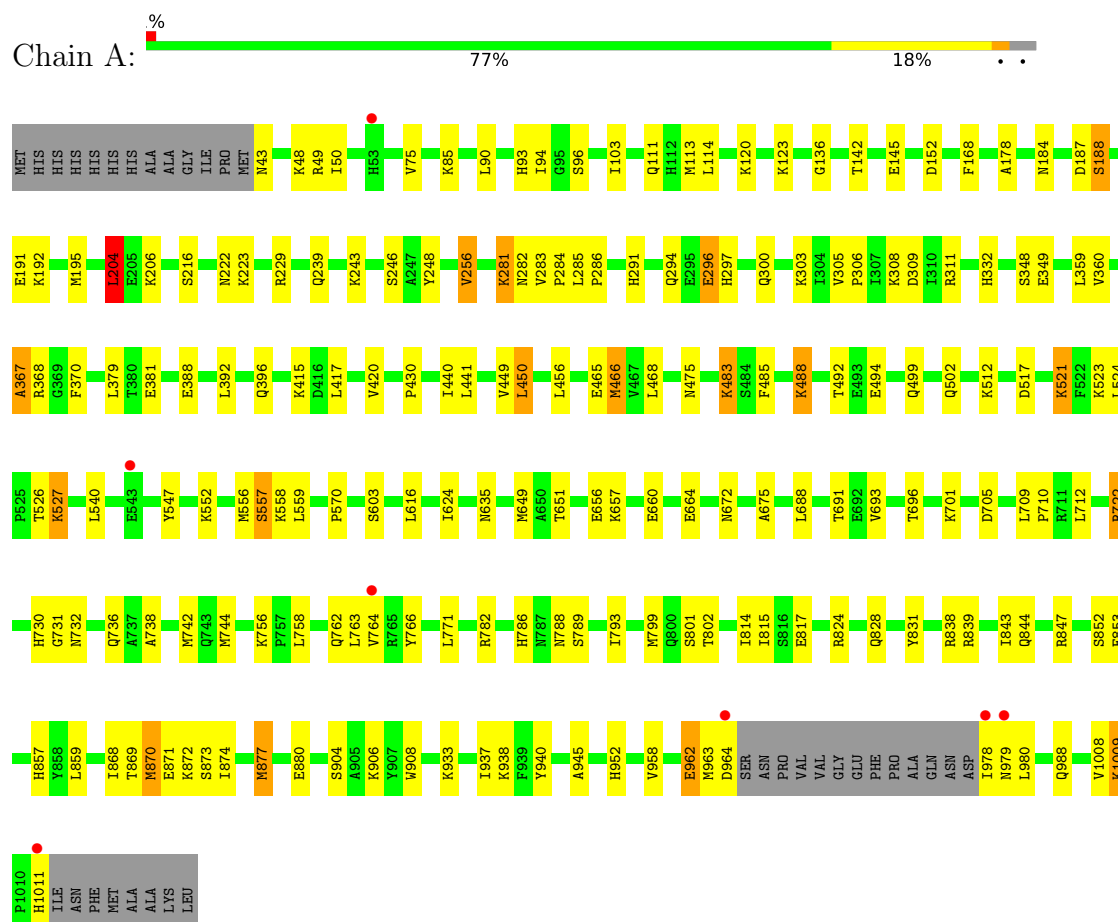
Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is methyl N-(carboxymethyl)-N-(3-phenylpropanoyl)glycyl-D-histidinate (CCD ID: MGH) (formula: C₂₀H₂₄N₄O₆).

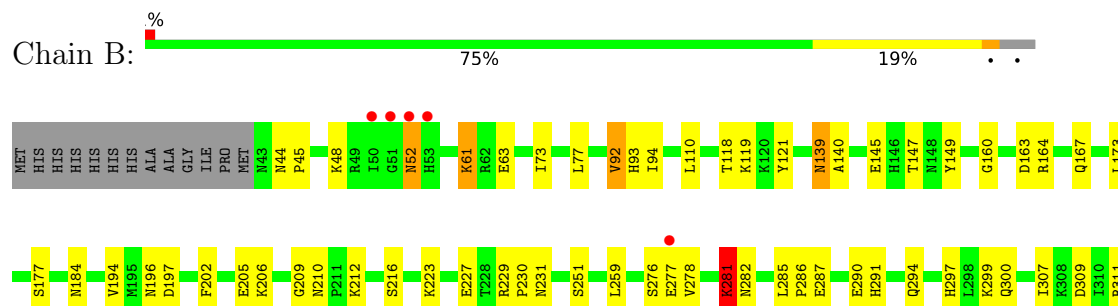
3 Residue-property plots

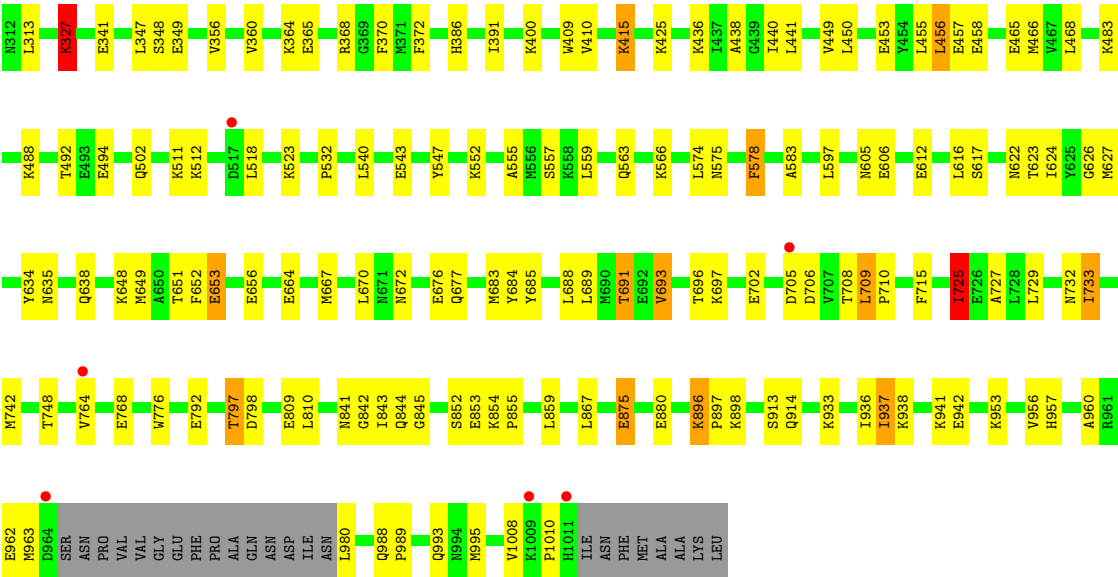
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Insulin-degrading enzyme



• Molecule 1: Insulin-degrading enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.18Å 263.18Å 90.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.70) 100.0 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.174 , 0.220 0.172 , 0.218	Depositor DCC
R_{free} test set	4913 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15908	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	16/7963 (0.2%)	1.24	26/10779 (0.2%)
1	B	1.27	16/7953 (0.2%)	1.23	31/10765 (0.3%)
All	All	1.28	32/15916 (0.2%)	1.24	57/21544 (0.3%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	LEU	CG-CD2	10.38	1.86	1.52
1	B	693	VAL	CA-CB	8.95	1.66	1.54
1	A	367	ALA	CA-CB	-8.46	1.42	1.53
1	B	543	GLU	CA-CB	7.28	1.61	1.53
1	A	517	ASP	CA-CB	6.82	1.62	1.53
1	A	523	LYS	CG-CD	6.67	1.72	1.52
1	B	764	VAL	CA-CB	6.08	1.61	1.54
1	B	438	ALA	CA-CB	-6.07	1.43	1.53
1	A	178	ALA	CA-CB	-5.90	1.44	1.53
1	A	763	LEU	CA-C	5.85	1.59	1.53
1	A	657	LYS	CA-CB	5.84	1.62	1.53
1	B	725	ILE	CA-C	-5.82	1.45	1.52
1	B	365	GLU	CA-CB	5.62	1.62	1.53
1	B	670	LEU	C-O	-5.43	1.17	1.24
1	B	492	THR	C-O	-5.42	1.17	1.23
1	A	523	LYS	CD-CE	5.41	1.68	1.52
1	A	675	ALA	CA-CB	-5.34	1.45	1.53
1	B	327	LYS	CD-CE	5.33	1.68	1.52
1	A	256	VAL	C-O	5.27	1.29	1.24
1	B	855	PRO	CA-C	5.26	1.55	1.52
1	A	764	VAL	CA-CB	5.25	1.60	1.53
1	A	693	VAL	CA-CB	5.24	1.60	1.54
1	A	908	TRP	N-CA	-5.20	1.40	1.46
1	A	738	ALA	CA-CB	-5.14	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLU	C-O	-5.14	1.18	1.24
1	B	705	ASP	CA-CB	5.13	1.62	1.53
1	B	205	GLU	CA-C	5.13	1.59	1.52
1	B	511	LYS	CA-CB	5.12	1.61	1.53
1	A	48	LYS	C-O	-5.12	1.18	1.24
1	B	202	PHE	N-CA	-5.08	1.40	1.46
1	B	494	GLU	CG-CD	5.07	1.64	1.52
1	B	465	GLU	CG-CD	5.04	1.64	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	ASP	N-CA-C	8.92	123.81	113.19
1	B	962	GLU	N-CA-C	7.21	122.19	112.88
1	A	817	GLU	CA-C-N	-7.13	112.29	119.56
1	A	817	GLU	C-N-CA	-7.13	112.29	119.56
1	B	456	LEU	N-CA-C	-7.11	98.21	109.23
1	B	617	SER	N-CA-C	7.08	119.69	109.14
1	A	1009	LYS	CA-C-N	6.80	127.73	120.11
1	A	1009	LYS	C-N-CA	6.80	127.73	120.11
1	B	511	LYS	N-CA-C	-6.50	104.27	111.36
1	B	938	LYS	N-CA-CB	6.45	119.37	110.01
1	A	870	MET	N-CA-C	6.41	118.27	111.28
1	B	988	GLN	CA-C-N	-6.40	114.03	120.31
1	B	988	GLN	C-N-CA	-6.40	114.03	120.31
1	A	420	VAL	N-CA-C	-6.37	104.29	110.72
1	B	555	ALA	N-CA-C	-6.34	105.03	112.89
1	A	547	TYR	CA-C-N	-6.31	113.28	119.78
1	A	547	TYR	C-N-CA	-6.31	113.28	119.78
1	B	197	ASP	N-CA-C	6.20	118.83	111.33
1	A	557	SER	N-CA-C	6.13	118.48	108.55
1	A	980	LEU	N-CA-C	6.12	119.14	109.96
1	A	282	ASN	N-CA-C	6.08	119.81	111.54
1	B	715	PHE	N-CA-C	6.04	117.86	111.28
1	B	92	VAL	CB-CA-C	-6.03	102.71	110.98
1	A	962	GLU	N-CA-C	5.97	120.15	107.67
1	B	281	LYS	N-CA-C	-5.87	105.88	113.16
1	B	229	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	75	VAL	CB-CA-C	-5.70	102.01	110.33
1	B	173	LEU	N-CA-C	5.61	118.12	111.33
1	B	605	ASN	N-CA-C	5.60	117.83	111.11
1	B	210	ASN	CA-C-N	-5.54	113.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASN	C-N-CA	-5.54	113.97	119.56
1	B	653	GLU	N-CA-C	5.51	117.88	108.90
1	B	52	ASN	CA-C-N	-5.46	114.41	123.37
1	B	52	ASN	C-N-CA	-5.46	114.41	123.37
1	B	853	GLU	N-CA-C	-5.45	106.48	113.23
1	B	651	THR	N-CA-C	-5.44	104.91	112.30
1	B	667	MET	N-CA-C	-5.43	105.26	111.07
1	A	651	THR	N-CA-C	-5.42	104.44	111.71
1	B	547	TYR	CA-C-N	-5.35	114.44	119.85
1	B	547	TYR	C-N-CA	-5.35	114.44	119.85
1	A	229	ARG	CA-C-N	-5.33	113.42	119.28
1	A	229	ARG	C-N-CA	-5.33	113.42	119.28
1	B	209	GLY	N-CA-C	-5.31	106.42	112.79
1	B	578	PHE	CB-CA-C	-5.25	102.22	110.79
1	A	766	TYR	N-CA-C	5.18	118.15	110.48
1	B	957	HIS	CA-C-N	-5.14	116.43	123.12
1	B	957	HIS	C-N-CA	-5.14	116.43	123.12
1	A	305	VAL	N-CA-C	5.12	112.93	107.76
1	A	499	GLN	N-CA-C	5.11	117.05	108.73
1	A	979	ASN	CA-C-N	5.08	128.07	120.95
1	A	979	ASN	C-N-CA	5.08	128.07	120.95
1	A	712	LEU	N-CA-C	5.08	116.82	111.28
1	A	731	GLY	N-CA-C	5.08	116.79	110.29
1	A	616	LEU	CA-C-N	-5.07	113.98	123.01
1	A	616	LEU	C-N-CA	-5.07	113.98	123.01
1	B	52	ASN	N-CA-C	5.07	121.24	113.28
1	A	282	ASN	CB-CA-C	-5.04	104.44	111.80

There are no chirality outliers.

There are no planarity outliers.

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	7768	0	7676	120	0
1	B	7758	0	7672	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	23	7	0
2	B	30	0	23	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	183	0	0	21	0
4	B	137	0	0	8	0
All	All	15908	0	15394	242	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 (242) 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:204:LEU:CD2	1:A:204:LEU:CG	1.86	1.51
1:A:705:ASP:CB	4:A:1270:HOH:O	1.84	1.22
1:A:557:SER:HB2	1:A:742:MET:HE3	1.49	0.94
1:B:309:ASP:H	1:B:672:ASN:HD21	1.15	0.94
1:B:386:HIS:HE1	4:B:1215:HOH:O	1.49	0.94
1:A:978:ILE:N	4:A:1339:HOH:O	2.00	0.92
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.20	0.89
1:B:797:THR:CG2	1:B:798:ASP:H	1.88	0.87
1:A:309:ASP:H	1:A:672:ASN:HD21	1.24	0.84
1:A:332:HIS:HD2	2:A:1101:MGH:H101	1.44	0.82
1:B:797:THR:HG23	1:B:798:ASP:N	1.95	0.82
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.62	0.81
1:A:204:LEU:HD12	4:A:1279:HOH:O	1.82	0.80
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.80	0.79
1:B:309:ASP:H	1:B:672:ASN:ND2	1.79	0.79
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.00	0.79
1:B:797:THR:HG23	1:B:798:ASP:H	1.46	0.79
1:B:436:LYS:NZ	4:B:1217:HOH:O	2.15	0.78
1:A:204:LEU:CD2	1:A:204:LEU:HG	2.10	0.77
1:A:300:GLN:NE2	1:A:502:GLN:HE21	1.81	0.77
1:A:296:GLU:HG2	4:A:1210:HOH:O	1.85	0.76
1:A:332:HIS:HD2	2:A:1101:MGH:C01	1.97	0.76
1:B:368:ARG:HD2	4:B:1242:HOH:O	1.87	0.75
1:B:635:ASN:ND2	1:B:732:ASN:HD22	1.85	0.75
2:B:1101:MGH:H223	2:B:1101:MGH:O20	1.86	0.74
1:B:61:LYS:HE2	1:B:61:LYS:HA	1.68	0.74
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:THR:CG2	1:B:798:ASP:N	2.50	0.74
1:B:294:GLN:H	1:B:297:HIS:HD2	1.34	0.73
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.70	0.72
1:A:300:GLN:HE21	1:A:502:GLN:HE21	1.37	0.72
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.73	0.70
1:A:204:LEU:CB	4:A:1279:HOH:O	2.39	0.70
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.37	0.70
1:B:453:GLU:OE2	4:B:1250:HOH:O	2.09	0.69
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.40	0.69
1:B:300:GLN:NE2	1:B:502:GLN:HE21	1.90	0.69
1:A:360:VAL:HA	2:A:1101:MGH:H08	1.75	0.69
1:A:184:ASN:HD21	1:A:223:LYS:HE3	1.56	0.68
1:A:309:ASP:H	1:A:672:ASN:ND2	1.91	0.68
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.41	0.68
1:A:296:GLU:HB3	4:A:1210:HOH:O	1.94	0.68
1:A:964:ASP:N	4:A:1312:HOH:O	2.27	0.67
1:A:294:GLN:H	1:A:297:HIS:HD2	1.42	0.67
1:B:616:LEU:HD11	1:B:638:GLN:HG2	1.77	0.67
1:B:309:ASP:N	1:B:672:ASN:HD21	1.90	0.66
1:B:623:THR:HB	1:B:626:GLY:O	1.95	0.66
1:A:204:LEU:CG	4:A:1279:HOH:O	2.43	0.66
1:A:756:LYS:HB2	1:A:756:LYS:HZ3	1.62	0.64
1:A:557:SER:HB2	1:A:742:MET:CE	2.24	0.64
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.80	0.64
1:A:332:HIS:CD2	2:A:1101:MGH:C01	2.81	0.63
1:B:93:HIS:HD2	1:B:145:GLU:O	1.81	0.63
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.81	0.62
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.82	0.61
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.82	0.61
1:A:296:GLU:CB	4:A:1210:HOH:O	2.49	0.61
1:B:360:VAL:CG1	2:B:1101:MGH:H215	2.31	0.61
1:A:656:GLU:HB2	1:A:709:LEU:HD22	1.82	0.60
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.82	0.60
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.02	0.60
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.84	0.59
1:B:61:LYS:HA	1:B:61:LYS:CE	2.32	0.59
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.10	0.59
1:A:557:SER:CB	1:A:742:MET:HE3	2.28	0.58
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.98	0.58
1:A:782:ARG:HH12	1:A:963:MET:H	1.52	0.58
1:A:789:SER:HB2	1:A:958:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLU:HG3	1:B:709:LEU:CD2	2.35	0.57
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.87	0.56
1:A:736:GLN:HB3	4:A:1379:HOH:O	2.06	0.56
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.41	0.56
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.33	0.55
1:B:797:THR:HG22	1:B:798:ASP:H	1.70	0.55
1:A:306:PRO:O	1:A:483:LYS:HE3	2.07	0.55
1:A:204:LEU:CD1	4:A:1279:HOH:O	2.46	0.55
1:A:246:SER:O	1:A:281:LYS:HE3	2.07	0.55
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.42	0.55
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.89	0.55
1:B:294:GLN:H	1:B:297:HIS:CD2	2.20	0.55
2:A:1101:MGH:H215	2:A:1101:MGH:O19	2.06	0.54
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.90	0.54
1:B:121:TYR:OH	1:B:163:ASP:OD2	2.14	0.54
1:A:730:HIS:HD2	1:A:904:SER:OG	1.90	0.54
1:A:465:GLU:HB2	4:A:1244:HOH:O	2.08	0.54
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.90	0.54
1:B:688:LEU:HD13	1:B:696:THR:HG22	1.89	0.53
1:A:801:SER:O	1:A:802:THR:C	2.52	0.53
1:A:297:HIS:HE1	4:A:1212:HOH:O	1.91	0.53
1:B:455:LEU:HD22	4:B:1202:HOH:O	2.08	0.53
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.91	0.52
1:A:635:ASN:ND2	1:A:732:ASN:HD22	2.07	0.52
1:A:204:LEU:HB2	4:A:1279:HOH:O	2.07	0.52
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.54	0.51
1:B:300:GLN:HE21	1:B:502:GLN:HE21	1.56	0.51
1:A:392:LEU:O	1:A:396:GLN:HG3	2.10	0.51
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.43	0.51
1:A:49:ARG:HD2	4:A:1201:HOH:O	2.10	0.51
1:B:441:LEU:HD23	1:B:449:VAL:CG1	2.36	0.51
1:B:566:LYS:HE3	1:B:896:LYS:NZ	2.25	0.51
1:B:597:LEU:HD11	1:B:627:MET:HG2	1.92	0.51
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.93	0.50
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.93	0.50
1:B:623:THR:CB	1:B:626:GLY:O	2.60	0.50
1:B:623:THR:N	1:B:626:GLY:O	2.43	0.50
1:A:526:THR:O	1:A:527:LYS:C	2.54	0.50
1:B:797:THR:HB	1:B:845:GLY:HA2	1.93	0.50
1:A:297:HIS:CE1	4:A:1212:HOH:O	2.63	0.50
1:B:139:ASN:ND2	1:B:140:ALA:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.94	0.50
1:A:360:VAL:HA	2:A:1101:MGH:C08	2.42	0.50
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.47	0.50
1:A:857:HIS:HD2	4:A:1247:HOH:O	1.95	0.50
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.41	0.50
1:A:877:MET:O	1:A:933:LYS:NZ	2.44	0.49
1:A:136:GLY:HA3	1:A:152:ASP:O	2.12	0.49
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.20	0.49
1:A:556:MET:HG3	1:A:556:MET:O	2.12	0.49
1:A:782:ARG:NH1	1:A:963:MET:H	2.10	0.49
1:B:139:ASN:HD22	1:B:140:ALA:H	1.60	0.49
1:B:566:LYS:HE3	1:B:896:LYS:HZ1	1.78	0.48
1:B:648:LYS:O	1:B:652:PHE:HB2	2.13	0.48
1:B:676:GLU:HA	1:B:676:GLU:OE1	2.13	0.48
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.94	0.48
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.94	0.48
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.14	0.48
1:A:466:MET:HE2	1:A:466:MET:C	2.39	0.48
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.96	0.48
1:B:852:SER:HB3	1:B:859:LEU:HD11	1.95	0.48
2:A:1101:MGH:H117	2:A:1101:MGH:H123	1.59	0.48
1:B:875:GLU:O	1:B:933:LYS:NZ	2.45	0.48
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.48
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.27	0.47
1:B:348:SER:OG	1:B:606:GLU:OE2	2.27	0.47
1:A:415:LYS:HD2	1:A:456:LEU:O	2.14	0.47
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.37	0.47
1:B:349:GLU:HA	1:B:349:GLU:OE1	2.14	0.47
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.45	0.47
1:A:359:LEU:HD23	1:A:360:VAL:N	2.29	0.47
1:A:843:ILE:HG22	1:A:844:GLN:H	1.79	0.47
1:B:563:GLN:HG3	1:B:733:ILE:O	2.13	0.47
1:A:722:ARG:HA	1:A:756:LYS:O	2.15	0.47
1:A:349:GLU:OE1	1:A:521:LYS:HD3	2.15	0.47
1:B:281:LYS:HE3	1:B:281:LYS:HB3	1.72	0.47
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.50	0.47
1:A:359:LEU:HD23	1:A:359:LEU:C	2.40	0.47
1:A:756:LYS:HZ3	1:A:756:LYS:CB	2.25	0.46
1:A:793:ILE:O	1:A:847:ARG:HA	2.15	0.46
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.45	0.46
1:B:691:THR:HG23	4:B:1206:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:H	1:A:297:HIS:CD2	2.29	0.46
1:A:868:ILE:O	1:A:869:THR:C	2.59	0.46
1:A:852:SER:HB3	1:A:859:LEU:HD11	1.98	0.46
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.45	0.46
1:A:184:ASN:ND2	1:A:223:LYS:HE3	2.25	0.46
1:B:797:THR:CG2	1:B:844:GLN:HG3	2.47	0.45
1:B:937:ILE:O	1:B:941:LYS:HG3	2.15	0.45
1:A:388:GLU:HB3	4:A:1253:HOH:O	2.15	0.45
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.98	0.45
1:B:797:THR:HG21	1:B:844:GLN:HG3	1.99	0.45
1:A:308:LYS:HE3	1:A:672:ASN:HB3	1.97	0.45
1:B:110:LEU:HD23	1:B:110:LEU:C	2.41	0.45
1:B:327:LYS:HZ3	1:B:327:LYS:HB2	1.82	0.45
1:B:683:MET:HA	1:B:792:GLU:OE1	2.16	0.45
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.98	0.45
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.98	0.45
1:B:557:SER:HB2	1:B:742:MET:HE3	1.99	0.45
1:A:660:GLU:HG3	4:A:1272:HOH:O	2.15	0.45
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.51	0.45
1:B:386:HIS:CE1	4:B:1215:HOH:O	2.38	0.45
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.99	0.45
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.50	0.44
1:B:627:MET:HE3	1:B:627:MET:HB2	1.77	0.44
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.99	0.44
1:B:285:LEU:HD12	1:B:286:PRO:CD	2.44	0.44
1:B:623:THR:HG22	1:B:624:ILE:N	2.32	0.44
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.98	0.44
1:A:145:GLU:CD	1:A:367:ALA:HB1	2.43	0.44
1:A:788:ASN:ND2	4:A:1357:HOH:O	2.50	0.44
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.66	0.44
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.84	0.44
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.64	0.44
1:B:867:LEU:HD23	1:B:867:LEU:HA	1.88	0.44
1:A:283:VAL:HG12	1:A:284:PRO:O	2.18	0.44
1:A:488:LYS:HD2	1:A:488:LYS:N	2.32	0.44
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.76	0.44
2:B:1101:MGH:O20	2:B:1101:MGH:C23	2.62	0.44
1:B:842:GLY:HA3	1:B:1008:VAL:HG23	1.99	0.43
1:A:93:HIS:HD2	1:A:145:GLU:O	2.00	0.43
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.53	0.43
1:A:824:ARG:O	1:A:828:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:LEU:HB2	1:B:742:MET:HE2	2.01	0.43
1:B:616:LEU:HD11	1:B:638:GLN:CG	2.47	0.43
1:A:838:ARG:C	1:A:839:ARG:HD2	2.43	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.63	0.43
1:A:814:ILE:HD13	1:A:814:ILE:HG21	1.76	0.43
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.00	0.43
1:B:552:LYS:HB3	1:B:559:LEU:HB3	2.00	0.43
1:B:196:ASN:OD1	1:B:196:ASN:C	2.61	0.43
1:A:843:ILE:HG22	1:A:844:GLN:N	2.33	0.43
1:B:160:GLY:O	1:B:164:ARG:HG3	2.19	0.43
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.54	0.43
1:B:227:GLU:C	1:B:230:PRO:HD2	2.44	0.42
1:B:559:LEU:C	1:B:559:LEU:HD12	2.44	0.42
1:B:597:LEU:HD12	1:B:622:ASN:N	2.34	0.42
1:B:896:LYS:HA	1:B:897:PRO:HD2	1.91	0.42
1:B:913:SER:O	1:B:914:GLN:HB2	2.18	0.42
1:B:231:ASN:HD22	1:B:231:ASN:HA	1.65	0.42
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.73	0.42
1:B:574:LEU:HD22	1:B:729:LEU:HD22	2.01	0.42
1:B:776:TRP:CD2	1:B:989:PRO:HB3	2.54	0.42
1:A:483:LYS:HB2	4:A:1214:HOH:O	2.18	0.42
1:B:708:THR:HB	1:B:710:PRO:HD2	2.00	0.42
1:B:685:TYR:HB2	1:B:956:VAL:HG11	2.02	0.42
1:A:206:LYS:HB3	1:A:216:SER:HA	2.02	0.42
1:B:313:LEU:HD11	1:B:391:ILE:HD11	2.01	0.42
1:B:341:GLU:OE2	2:B:1101:MGH:H10	2.20	0.42
1:B:578:PHE:CE2	1:B:725:ILE:HD13	2.55	0.42
1:A:782:ARG:HH12	1:A:963:MET:N	2.17	0.41
1:B:400:LYS:HA	1:B:518:LEU:HD21	2.01	0.41
1:B:415:LYS:HE3	4:B:1222:HOH:O	2.21	0.41
1:B:483:LYS:HA	1:B:483:LYS:HD3	1.69	0.41
1:B:372:PHE:CD1	1:B:372:PHE:N	2.88	0.41
1:B:575:ASN:O	1:B:727:ALA:HA	2.21	0.41
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.02	0.41
1:A:381:GLU:H	1:A:381:GLU:HG3	1.74	0.41
1:B:259:LEU:HD23	1:B:259:LEU:C	2.45	0.41
1:A:649:MET:HB2	1:A:649:MET:HE3	1.83	0.41
1:B:44:ASN:OD1	1:B:45:PRO:HD2	2.21	0.41
1:B:409:TRP:CE2	1:B:410:VAL:HG23	2.56	0.41
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.84	0.40
1:A:744:MET:O	1:A:744:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:HB3	1:B:216:SER:HA	2.03	0.40
1:B:689:LEU:HD23	1:B:995:MET:HG2	2.04	0.40
1:A:113:MET:HB3	1:A:113:MET:HE3	1.85	0.40
1:A:300:GLN:HE21	1:A:502:GLN:NE2	2.12	0.40
1:A:570:PRO:C	1:A:635:ASN:HD22	2.30	0.40
1:A:722:ARG:HB2	1:A:758:LEU:HD23	2.02	0.40
1:A:111:GLN:NE2	1:A:142:THR:OG1	2.43	0.40
1:A:799:MET:HE3	1:A:799:MET:HB3	1.83	0.40
1:B:118:THR:HG21	1:B:167:GLN:CB	2.52	0.40
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.56	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	952/990 (96%)	915 (96%)	36 (4%)	1 (0%)	48	73
1	B	950/990 (96%)	911 (96%)	38 (4%)	1 (0%)	48	73
All	All	1902/1980 (96%)	1826 (96%)	74 (4%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	PRO
1	A	103	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	837/879 (95%)	792 (95%)	45 (5%)	20	45
1	B	837/879 (95%)	780 (93%)	57 (7%)	14	35
All	All	1674/1758 (95%)	1572 (94%)	102 (6%)	17	40

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	50	ILE
1	A	85	LYS
1	A	96	SER
1	A	123	LYS
1	A	188	SER
1	A	192	LYS
1	A	204	LEU
1	A	239	GLN
1	A	243	LYS
1	A	281	LYS
1	A	296	GLU
1	A	348	SER
1	A	430	PRO
1	A	440	ILE
1	A	450	LEU
1	A	466	MET
1	A	468	LEU
1	A	475	ASN
1	A	483	LYS
1	A	488	LYS
1	A	492	THR
1	A	494	GLU
1	A	512	LYS
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS
1	A	558	LYS
1	A	603	SER
1	A	624	ILE
1	A	691	THR
1	A	701	LYS
1	A	722	ARG

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Mol	Chain	Res	Type
1	A	762	GLN
1	A	853	GLU
1	A	871	GLU
1	A	872	LYS
1	A	873	SER
1	A	877	MET
1	A	906	LYS
1	A	938	LYS
1	A	962	GLU
1	A	988	GLN
1	A	1009	LYS
1	A	1011	HIS
1	B	48	LYS
1	B	52	ASN
1	B	61	LYS
1	B	63	GLU
1	B	77	LEU
1	B	92	VAL
1	B	94	ILE
1	B	119	LYS
1	B	139	ASN
1	B	177	SER
1	B	194	VAL
1	B	212	LYS
1	B	276	SER
1	B	277	GLU
1	B	281	LYS
1	B	282	ASN
1	B	287	GLU
1	B	290	GLU
1	B	299	LYS
1	B	307	ILE
1	B	327	LYS
1	B	347	LEU
1	B	356	VAL
1	B	364	LYS
1	B	415	LYS
1	B	425	LYS
1	B	440	ILE
1	B	450	LEU
1	B	458	GLU
1	B	466	MET

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Mol	Chain	Res	Type
1	B	468	LEU
1	B	488	LYS
1	B	512	LYS
1	B	523	LYS
1	B	612	GLU
1	B	649	MET
1	B	653	GLU
1	B	677	GLN
1	B	691	THR
1	B	693	VAL
1	B	702	GLU
1	B	709	LEU
1	B	725	ILE
1	B	733	ILE
1	B	748	THR
1	B	797	THR
1	B	809	GLU
1	B	841	ASN
1	B	854	LYS
1	B	875	GLU
1	B	880	GLU
1	B	896	LYS
1	B	898	LYS
1	B	937	ILE
1	B	942	GLU
1	B	980	LEU
1	B	993	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	111	GLN
1	A	184	ASN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	332	HIS
1	A	336	HIS
1	A	376	ASN
1	A	399	GLN

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Mol	Chain	Res	Type
1	A	573	ASN
1	A	635	ASN
1	A	672	ASN
1	A	730	HIS
1	A	821	ASN
1	A	857	HIS
1	A	922	ASN
1	B	93	HIS
1	B	111	GLN
1	B	129	GLN
1	B	139	ASN
1	B	184	ASN
1	B	231	ASN
1	B	232	GLN
1	B	245	HIS
1	B	297	HIS
1	B	300	GLN
1	B	332	HIS
1	B	363	GLN
1	B	376	ASN
1	B	386	HIS
1	B	407	GLN
1	B	499	GLN
1	B	635	ASN
1	B	672	ASN
1	B	677	GLN
1	B	724	HIS
1	B	730	HIS
1	B	821	ASN
1	B	993	GLN

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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	MGH	A	1101	-	31,31,31	2.03	6 (19%)	40,40,40	2.82	13 (32%)
2	MGH	B	1101	-	31,31,31	2.14	10 (32%)	40,40,40	2.40	10 (25%)

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	MGH	A	1101	-	-	11/31/31/31	0/2/2/2
2	MGH	B	1101	-	-	14/31/31/31	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGH	C21-N16	6.44	1.47	1.35
2	A	1101	MGH	C21-N16	6.08	1.46	1.35
2	A	1101	MGH	O02-C03	5.93	1.47	1.33
2	B	1101	MGH	O02-C03	5.51	1.46	1.33
2	B	1101	MGH	C08-C07	3.38	1.43	1.36
2	A	1101	MGH	C17-N16	3.21	1.50	1.45
2	A	1101	MGH	C15-N16	2.96	1.49	1.45
2	B	1101	MGH	C17-N16	2.83	1.49	1.45
2	B	1101	MGH	C23-C21	2.47	1.56	1.51
2	A	1101	MGH	C10-N11	2.33	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGH	C29-C30	2.25	1.42	1.38
2	B	1101	MGH	C30-C25	2.25	1.43	1.38
2	B	1101	MGH	C26-C25	2.17	1.43	1.38
2	B	1101	MGH	O19-C18	-2.16	1.23	1.30
2	A	1101	MGH	C23-C21	2.09	1.55	1.51
2	B	1101	MGH	C27-C26	2.08	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGH	O02-C03-C05	8.25	132.48	111.49
2	A	1101	MGH	C17-N16-C15	-7.75	104.29	117.49
2	B	1101	MGH	C23-C21-N16	7.49	129.43	118.09
2	A	1101	MGH	O02-C03-O04	-6.33	111.53	123.85
2	B	1101	MGH	C24-C23-C21	6.10	119.27	112.33
2	B	1101	MGH	O22-C21-N16	-4.80	113.58	122.12
2	A	1101	MGH	C13-C15-N16	4.40	124.47	113.22
2	A	1101	MGH	C03-C05-N12	4.39	120.77	110.65
2	B	1101	MGH	C17-N16-C15	-4.37	110.06	117.49
2	B	1101	MGH	O02-C03-O04	-4.14	115.79	123.85
2	A	1101	MGH	C17-N16-C21	-4.08	108.86	120.81
2	B	1101	MGH	O02-C03-C05	3.97	121.60	111.49
2	B	1101	MGH	C05-C06-C07	3.88	122.86	113.75
2	A	1101	MGH	C05-N12-C13	3.88	131.41	121.68
2	A	1101	MGH	C23-C21-N16	3.55	123.47	118.09
2	A	1101	MGH	O14-C13-N12	3.51	128.89	122.95
2	A	1101	MGH	C24-C23-C21	2.98	115.72	112.33
2	B	1101	MGH	C06-C05-N12	-2.72	105.44	110.64
2	A	1101	MGH	O22-C21-N16	-2.70	117.32	122.12
2	A	1101	MGH	O04-C03-C05	-2.68	115.99	123.94
2	B	1101	MGH	C03-C05-N12	-2.48	104.93	110.65
2	B	1101	MGH	C13-C15-N16	2.15	118.72	113.22
2	A	1101	MGH	C07-C08-N09	2.03	109.65	106.54

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MGH	C03-C05-C06-C07
2	A	1101	MGH	N12-C05-C06-C07
2	A	1101	MGH	C13-C15-N16-C17
2	A	1101	MGH	C18-C17-N16-C21

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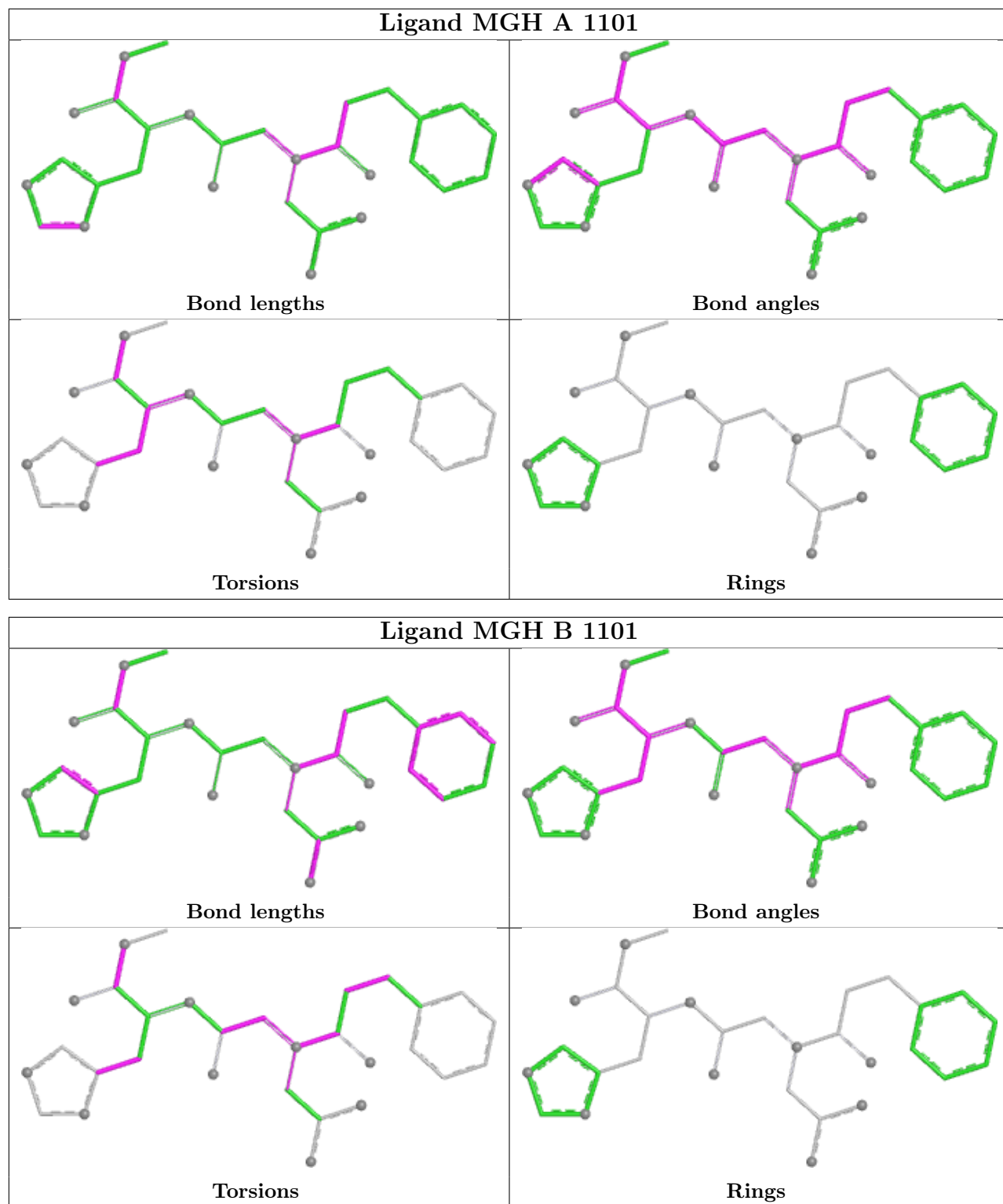
Mol	Chain	Res	Type	Atoms
2	B	1101	MGH	C13-C15-N16-C17
2	B	1101	MGH	C23-C21-N16-C15
2	B	1101	MGH	O22-C21-N16-C17
2	B	1101	MGH	C21-C23-C24-C25
2	A	1101	MGH	O22-C21-N16-C15
2	B	1101	MGH	O22-C21-N16-C15
2	A	1101	MGH	C05-C03-O02-C01
2	B	1101	MGH	C05-C03-O02-C01
2	B	1101	MGH	C05-C06-C07-C08
2	A	1101	MGH	C05-C06-C07-N11
2	B	1101	MGH	C05-C06-C07-N11
2	A	1101	MGH	C23-C21-N16-C15
2	B	1101	MGH	C23-C21-N16-C17
2	B	1101	MGH	C13-C15-N16-C21
2	A	1101	MGH	O04-C03-O02-C01
2	A	1101	MGH	C05-C06-C07-C08
2	B	1101	MGH	N12-C13-C15-N16
2	B	1101	MGH	O14-C13-C15-N16
2	B	1101	MGH	O04-C03-O02-C01
2	A	1101	MGH	C06-C05-N12-C13
2	B	1101	MGH	C18-C17-N16-C21

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MGH	7	0
2	B	1101	MGH	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	956/990 (96%)	-0.67	7 (0%) 84 83	19, 35, 51, 75	0
1	B	954/990 (96%)	-0.52	11 (1%) 76 75	25, 39, 55, 82	0
All	All	1910/1980 (96%)	-0.59	18 (0%) 81 80	19, 37, 53, 82	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	964	ASP	7.0
1	B	964	ASP	6.8
1	A	979	ASN	4.3
1	A	978	ILE	4.3
1	B	1011	HIS	4.2
1	A	1011	HIS	3.5
1	A	764	VAL	3.3
1	B	51	GLY	3.3
1	B	50	ILE	3.0
1	B	705	ASP	2.7
1	B	53	HIS	2.5
1	B	52	ASN	2.5
1	B	764	VAL	2.4
1	B	1009	LYS	2.4
1	A	53	HIS	2.2
1	B	517	ASP	2.2
1	B	277	GLU	2.1
1	A	543	GLU	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](#)

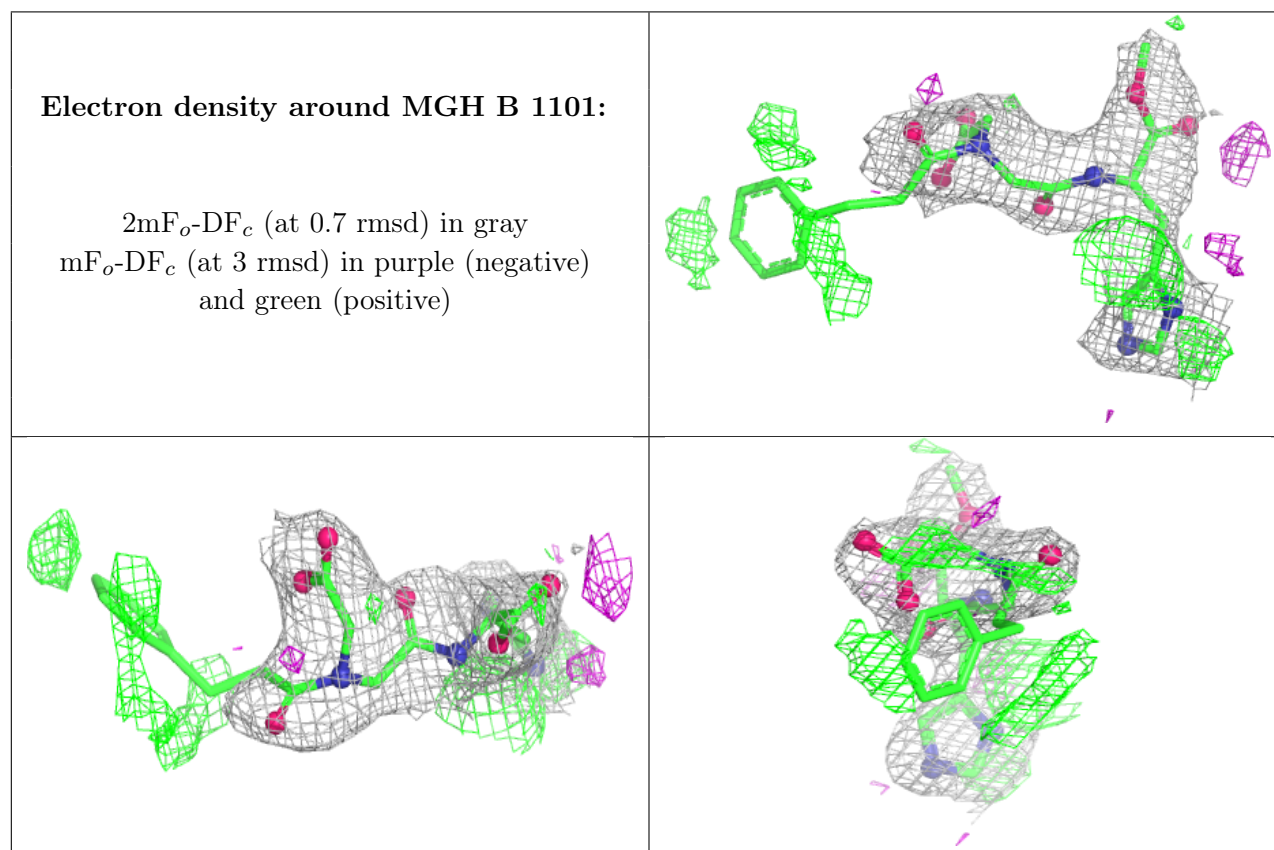
There are no oligosaccharides in this entry.

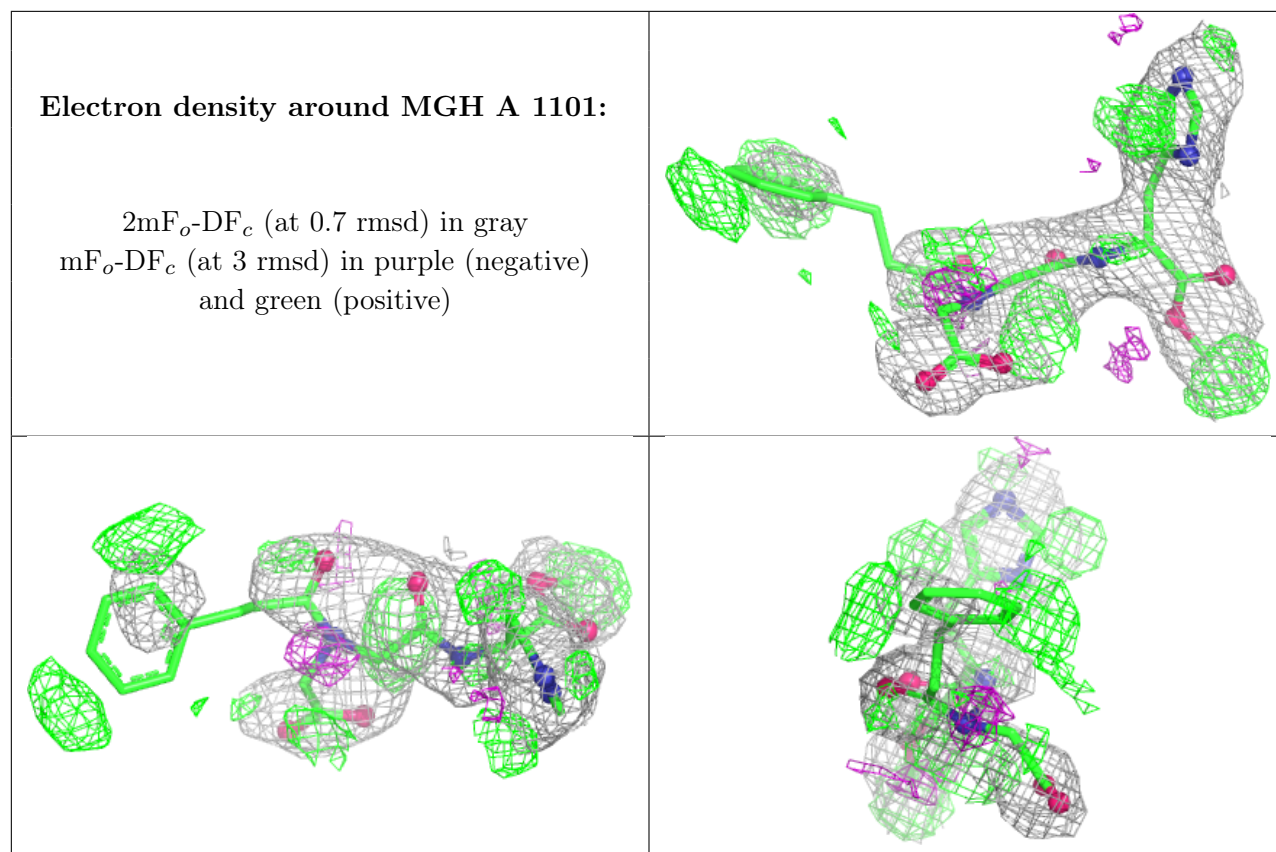
6.4 Ligands [i](#)

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	MGH	B	1101	30/30	0.82	0.23	59,69,105,105	0
2	MGH	A	1101	30/30	0.84	0.23	49,78,97,97	0
3	ZN	B	1102	1/1	0.98	0.04	49,49,49,49	0
3	ZN	A	1102	1/1	0.99	0.03	44,44,44,44	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.