



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:42 PM UTC

PDB ID : 3KAK / pdb_00003kak
Title : Structure of homogluthathione synthetase from Glycine max in open conformation with gamma-glutamyl-cysteine bound.
Authors : Galant, A.; Arkus, K.A.J.; Zubieta, C.; Cahoon, R.E.; Jez, J.M.
Deposited on : 2009-10-19
Resolution : 2.11 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

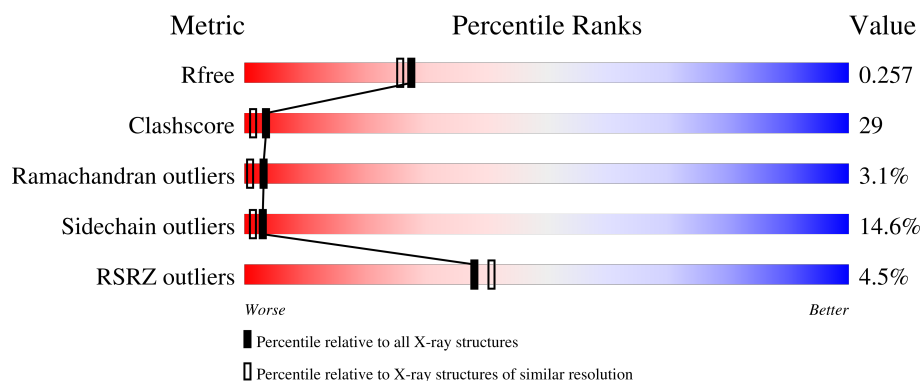
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	2% 47% 29% 9% • 11%
1	B	499	6% 43% 31% 11% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3GC	A	501	X	-	X	-
2	3GC	B	501	X	-	-	-
2	3GC	B	502	X	-	X	-

2 Entry composition [i](#)

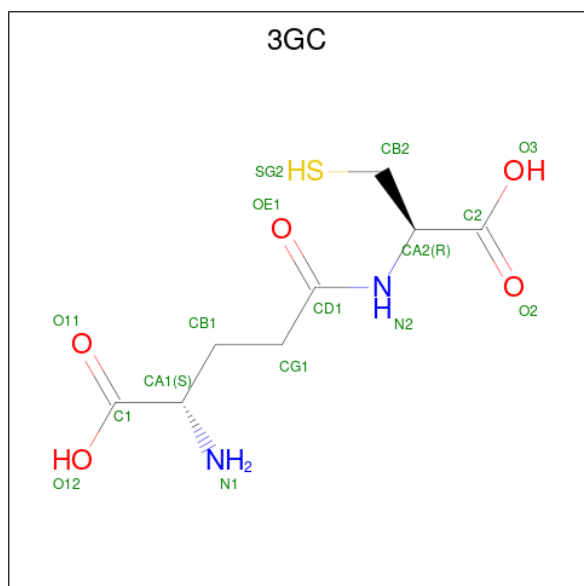
There are 3 unique types of molecules in this entry. The entry contains 7414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Homoglutathione synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	6	0
			3574	2275	619	665	15			
1	B	437	Total	C	N	O	S	0	6	0
			3511	2230	608	658	15			

- Molecule 2 is GAMMA-GLUTAMYLCYSTEINE (CCD ID: 3GC) (formula: $C_8H_{14}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			16	8	2	5	1		

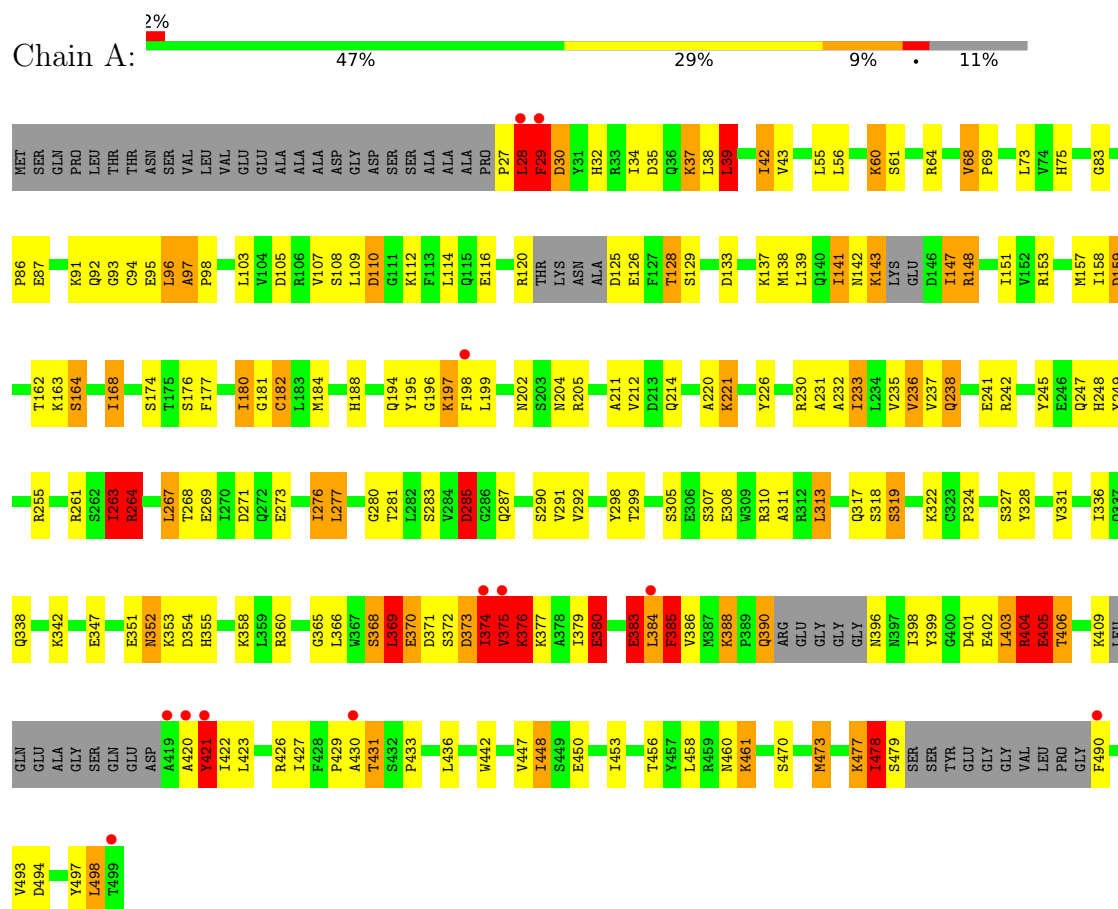
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	151	Total 151	O 151	0	0

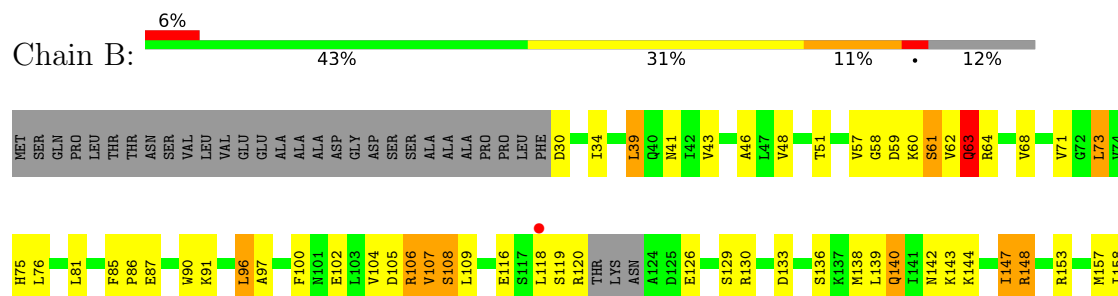
3 Residue-property plots

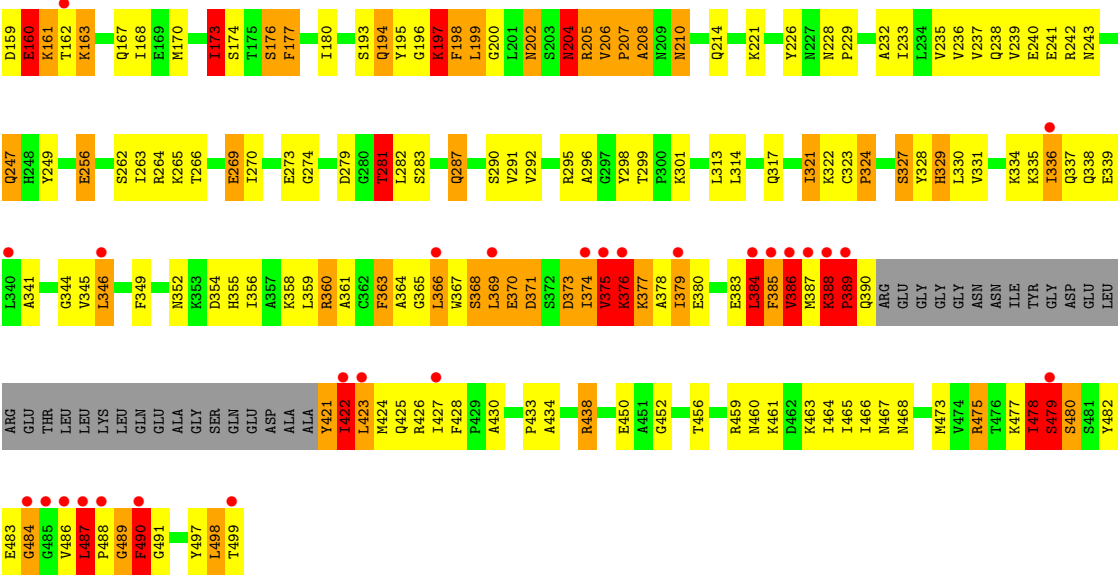
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Homogluthathione synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.88Å 80.95Å 89.12Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	19.80 – 2.11 19.80 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.80-2.11) 99.6 (19.80-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.288 (Not available) , 0.257	Depositor DCC
R_{free} test set	2635 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7414	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2346e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 3GC

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	1.56	29/3639 (0.8%)	1.56	47/4913 (1.0%)
1	B	1.64	37/3578 (1.0%)	1.65	72/4835 (1.5%)
All	All	1.60	66/7217 (0.9%)	1.61	119/9748 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	10
All	All	0	17

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ARG	CA-C	11.27	1.67	1.52
1	A	404	ARG	N-CA	10.18	1.59	1.46
1	B	321	ILE	C-O	-8.77	1.15	1.24
1	A	368	SER	CA-C	8.55	1.64	1.52
1	B	427	ILE	CA-CB	8.53	1.64	1.54
1	A	385	PHE	N-CA	-8.17	1.35	1.46
1	A	236	VAL	CA-CB	8.14	1.63	1.54
1	A	375	VAL	CA-CB	8.07	1.65	1.54
1	B	68	VAL	CA-C	8.02	1.59	1.53
1	A	214	GLN	CA-C	-7.35	1.43	1.52
1	B	41	ASN	N-CA	7.23	1.54	1.46
1	A	404	ARG	C-O	7.22	1.33	1.24
1	B	206	VAL	CA-CB	7.02	1.61	1.53
1	A	374	ILE	CA-CB	6.88	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	VAL	CA-C	6.83	1.61	1.52
1	A	248	HIS	C-O	-6.79	1.15	1.24
1	B	43	VAL	CA-CB	6.65	1.62	1.54
1	B	170	MET	CA-C	-6.63	1.44	1.52
1	A	383	GLU	CB-CG	6.33	1.71	1.52
1	A	43	VAL	CA-CB	6.30	1.61	1.54
1	B	468	ASN	N-CA	-6.29	1.38	1.46
1	B	296	ALA	CA-C	-6.18	1.45	1.52
1	A	453	ILE	CA-CB	6.12	1.61	1.54
1	B	147	ILE	CA-CB	6.07	1.61	1.53
1	A	153	ARG	C-O	-6.03	1.17	1.23
1	A	116	GLU	N-CA	5.90	1.53	1.46
1	A	384	LEU	CG-CD2	5.88	1.72	1.52
1	A	478	ILE	CA-CB	5.88	1.60	1.54
1	B	314	LEU	C-O	-5.85	1.17	1.24
1	B	41	ASN	C-O	-5.84	1.17	1.24
1	B	104	VAL	C-O	-5.84	1.17	1.24
1	A	292	VAL	N-CA	5.80	1.53	1.46
1	B	281	THR	CA-CB	5.77	1.62	1.53
1	B	323	CYS	CA-C	5.76	1.59	1.52
1	A	369	LEU	N-CA	5.67	1.53	1.46
1	A	365	GLY	N-CA	5.66	1.51	1.45
1	A	212	VAL	CA-CB	5.59	1.61	1.54
1	A	430	ALA	CA-CB	5.59	1.59	1.52
1	B	62	VAL	CA-C	5.58	1.59	1.52
1	B	210	ASN	CB-CG	5.56	1.66	1.52
1	B	427	ILE	CG1-CD1	5.52	1.73	1.51
1	B	282	LEU	C-O	-5.48	1.17	1.23
1	A	232	ALA	CA-C	5.46	1.60	1.53
1	A	97	ALA	N-CA	5.41	1.51	1.46
1	B	359	LEU	N-CA	-5.41	1.39	1.46
1	B	456	THR	C-O	-5.39	1.17	1.24
1	B	207	PRO	CA-C	5.38	1.59	1.52
1	B	422	ILE	CA-C	5.36	1.59	1.52
1	B	361	ALA	CA-CB	-5.34	1.44	1.53
1	B	467	ASN	N-CA	5.31	1.52	1.46
1	A	233	ILE	CA-CB	5.27	1.60	1.54
1	B	176	SER	N-CA	5.22	1.52	1.46
1	B	208	ALA	CA-CB	5.22	1.61	1.53
1	B	107	VAL	C-O	5.18	1.30	1.24
1	B	263	ILE	C-O	5.16	1.29	1.23
1	B	173	ILE	CA-CB	5.15	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	ARG	CA-C	5.15	1.59	1.52
1	A	148	ARG	CA-C	-5.13	1.46	1.52
1	B	46	ALA	CA-CB	5.13	1.61	1.53
1	A	182	CYS	CA-C	5.10	1.59	1.52
1	B	232	ALA	CA-CB	5.09	1.61	1.53
1	B	464	ILE	CA-CB	5.09	1.60	1.54
1	A	238	GLN	CA-C	-5.07	1.45	1.53
1	B	269	GLU	N-CA	5.07	1.52	1.46
1	B	434	ALA	C-O	5.04	1.29	1.23
1	A	93	GLY	N-CA	5.03	1.52	1.45

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	PHE	CA-CB-CG	16.03	129.83	113.80
1	A	376	LYS	N-CA-C	12.94	128.53	112.23
1	B	373	ASP	N-CA-C	-9.30	100.51	114.64
1	A	380	GLU	O-C-N	-8.95	113.02	123.22
1	B	228	ASN	CA-C-N	8.81	129.69	119.47
1	B	228	ASN	C-N-CA	8.81	129.69	119.47
1	A	375	VAL	N-CA-C	-8.55	91.56	109.34
1	B	422	ILE	N-CA-C	8.44	126.89	109.34
1	A	372	SER	N-CA-C	8.41	120.52	111.36
1	B	205	ARG	CA-C-N	-8.32	116.60	122.59
1	B	205	ARG	C-N-CA	-8.32	116.60	122.59
1	A	68	VAL	N-CA-C	8.25	115.72	107.55
1	A	405	GLU	N-CA-C	-8.17	101.44	111.33
1	A	277	LEU	CA-C-N	-8.02	111.47	119.56
1	A	277	LEU	C-N-CA	-8.02	111.47	119.56
1	B	374	ILE	CB-CA-C	-7.97	102.53	111.45
1	B	176	SER	N-CA-C	7.81	120.40	110.24
1	B	489	GLY	CA-C-N	7.64	136.12	121.54
1	B	489	GLY	C-N-CA	7.64	136.12	121.54
1	A	29	PHE	CA-CB-CG	-7.55	106.25	113.80
1	B	81	LEU	CA-C-N	7.53	127.52	119.76
1	B	81	LEU	C-N-CA	7.53	127.52	119.76
1	A	421	TYR	N-CA-C	7.50	121.69	112.23
1	B	489	GLY	O-C-N	7.48	132.42	122.70
1	B	85	PHE	CA-C-N	-7.41	112.14	119.78
1	B	85	PHE	C-N-CA	-7.41	112.14	119.78
1	A	181	GLY	N-CA-C	-7.38	103.87	112.73
1	A	285	ASP	CA-CB-CG	7.23	119.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	LEU	N-CA-C	7.16	120.87	108.76
1	A	147	ILE	N-CA-C	-7.07	98.25	108.36
1	B	478	ILE	CA-C-N	7.04	134.99	121.54
1	B	478	ILE	C-N-CA	7.04	134.99	121.54
1	A	311	ALA	N-CA-C	-7.03	102.82	111.40
1	A	28	LEU	O-C-N	6.96	131.68	122.36
1	A	182	CYS	CB-CA-C	6.78	122.75	109.72
1	B	487	LEU	N-CA-C	-6.77	94.85	109.81
1	A	383	GLU	N-CA-C	6.71	125.09	110.80
1	B	367	TRP	N-CA-C	6.64	117.01	108.24
1	B	206	VAL	CB-CA-C	6.62	117.80	110.71
1	B	97	ALA	CA-C-N	-6.57	112.06	119.28
1	B	97	ALA	C-N-CA	-6.57	112.06	119.28
1	A	384	LEU	CB-CA-C	-6.54	97.39	110.42
1	A	404	ARG	N-CA-C	6.53	124.71	110.80
1	B	336	ILE	CB-CA-C	-6.51	103.49	112.02
1	A	299	THR	CA-C-N	-6.50	112.93	119.56
1	A	299	THR	C-N-CA	-6.50	112.93	119.56
1	B	104	VAL	N-CA-C	-6.34	104.15	110.62
1	A	405	GLU	CB-CA-C	-6.33	99.92	110.68
1	B	384	LEU	O-C-N	-6.30	115.58	122.38
1	B	63	GLN	N-CA-C	6.29	119.80	111.75
1	B	482	TYR	N-CA-C	6.14	118.10	108.96
1	A	281	THR	CB-CA-C	6.06	119.52	109.53
1	B	148	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	A	164	SER	N-CA-C	6.03	119.44	110.52
1	B	479	SER	N-CA-C	6.02	123.62	110.80
1	A	39	LEU	N-CA-CB	6.00	119.75	110.38
1	A	420	ALA	N-CA-C	5.97	117.35	107.20
1	A	375	VAL	CB-CA-C	5.90	120.97	111.29
1	B	295	ARG	N-CA-C	-5.90	104.74	112.41
1	B	68	VAL	CA-C-O	5.90	122.63	119.15
1	A	94	CYS	N-CA-C	5.88	118.16	111.11
1	B	199	LEU	N-CA-C	5.85	118.44	111.71
1	B	61	SER	N-CA-C	5.82	119.20	111.75
1	B	480	SER	N-CA-C	5.78	123.12	110.80
1	B	180	ILE	N-CA-C	5.76	116.50	110.62
1	A	255	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	B	292	VAL	CB-CA-C	-5.72	103.24	111.19
1	B	249	TYR	N-CA-C	-5.71	104.66	111.69
1	B	130	ARG	N-CA-C	-5.69	106.29	113.18
1	A	264	ARG	NE-CZ-NH1	-5.68	115.82	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ASN	CB-CA-C	-5.68	104.24	111.22
1	B	478	ILE	O-C-N	5.68	129.67	122.57
1	B	108	SER	N-CA-C	-5.63	105.14	111.28
1	A	498	LEU	O-C-N	5.60	129.76	122.87
1	B	102	GLU	N-CA-C	5.58	117.36	111.28
1	A	404	ARG	CB-CA-C	-5.51	99.45	110.42
1	B	489	GLY	N-CA-C	-5.51	100.13	113.18
1	A	37	LYS	N-CA-C	-5.50	105.36	112.68
1	B	498	LEU	CA-C-N	5.50	131.59	121.70
1	B	498	LEU	C-N-CA	5.50	131.59	121.70
1	A	249	TYR	N-CA-C	-5.46	104.98	111.69
1	B	377	LYS	N-CA-C	-5.44	105.86	113.37
1	B	355	HIS	N-CA-C	-5.43	105.39	112.23
1	B	204	ASN	CB-CA-C	-5.42	99.63	110.42
1	B	371	ASP	N-CA-C	5.42	118.14	110.50
1	B	68	VAL	CB-CA-C	5.41	116.49	110.71
1	A	283	SER	CA-C-N	-5.37	115.65	123.06
1	A	283	SER	C-N-CA	-5.37	115.65	123.06
1	A	388	LYS	CA-C-N	5.37	125.38	119.90
1	A	388	LYS	C-N-CA	5.37	125.38	119.90
1	A	403	LEU	N-CA-C	5.35	117.87	111.71
1	B	461	LYS	CB-CA-C	-5.31	110.01	117.23
1	B	422	ILE	CA-C-N	-5.25	114.66	122.74
1	B	422	ILE	C-N-CA	-5.25	114.66	122.74
1	B	367	TRP	CA-C-N	5.24	131.55	121.54
1	B	367	TRP	C-N-CA	5.24	131.55	121.54
1	A	29	PHE	N-CA-CB	5.24	119.34	110.49
1	B	376	LYS	N-CA-C	-5.22	99.67	110.80
1	A	385	PHE	CB-CA-C	5.21	120.79	110.42
1	B	239	VAL	CB-CA-C	-5.18	105.14	112.14
1	B	236	VAL	N-CA-C	-5.16	100.46	107.99
1	A	220	ALA	N-CA-C	-5.15	105.75	111.36
1	B	68	VAL	N-CA-C	5.15	112.96	107.76
1	B	130	ARG	CG-CD-NE	5.15	123.32	112.00
1	B	206	VAL	N-CA-CB	5.15	117.56	111.08
1	B	329	HIS	N-CA-C	-5.12	102.92	111.37
1	A	110	ASP	N-CA-C	5.11	117.49	107.57
1	A	383	GLU	CB-CG-CD	5.11	121.29	112.60
1	B	197	LYS	CD-CE-NZ	5.10	128.22	111.90
1	B	270	ILE	N-CA-C	-5.09	105.88	110.82
1	A	276	ILE	N-CA-CB	5.08	117.08	110.99
1	B	148	ARG	CG-CD-NE	-5.07	100.84	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	ILE	N-CA-C	-5.06	104.49	110.21
1	A	263	ILE	CA-C-N	-5.05	116.03	123.00
1	A	263	ILE	C-N-CA	-5.05	116.03	123.00
1	B	206	VAL	CA-C-N	5.05	125.28	119.83
1	B	206	VAL	C-N-CA	5.05	125.28	119.83
1	B	48	VAL	N-CA-C	5.03	115.64	110.36
1	B	427	ILE	N-CA-C	-5.00	100.69	107.99

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LEU	Peptide
1	A	373	ASP	Peptide
1	A	374	ILE	Peptide
1	A	375	VAL	Peptide
1	A	380	GLU	Mainchain
1	A	403	LEU	Peptide
1	A	404	ARG	Peptide
1	B	160	GLU	Peptide
1	B	368	SER	Peptide
1	B	384	LEU	Mainchain
1	B	388	LYS	Peptide
1	B	389	PRO	Peptide
1	B	422	ILE	Peptide
1	B	478	ILE	Mainchain
1	B	479	SER	Peptide
1	B	486	VAL	Peptide
1	B	487	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3574	0	3616	178	0
1	B	3511	0	3541	247	0
2	A	16	0	11	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	0	22	15	0
3	A	130	0	0	16	0
3	B	151	0	0	29	0
All	All	7414	0	7190	423	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 29.

All (423) 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:384:LEU:O	1:B:426:ARG:HB2	1.26	1.29
1:A:398:ILE:HG21	1:A:405:GLU:OE1	1.28	1.28
1:A:39:LEU:HD12	1:A:442:TRP:CZ3	1.69	1.25
1:B:374:ILE:O	1:B:376:LYS:N	1.72	1.19
1:B:479:SER:HB3	3:B:640:HOH:O	1.51	1.11
1:B:487:LEU:HB2	1:B:489:GLY:H	1.18	1.08
1:B:375:VAL:HG22	1:B:379:ILE:HG13	1.29	1.06
1:A:384:LEU:O	1:A:426:ARG:HB2	1.57	1.04
1:B:344:GLY:HA2	3:B:649:HOH:O	1.57	1.03
1:B:375:VAL:HG23	1:B:388:LYS:HG3	1.38	1.03
1:B:378:ALA:HB1	1:B:388:LYS:NZ	1.72	1.03
1:B:479:SER:CB	3:B:640:HOH:O	2.01	1.02
1:A:404:ARG:O	1:A:404:ARG:CG	2.06	1.02
1:A:373:ASP:HB2	1:A:374:ILE:HG22	1.39	1.01
1:A:374:ILE:HD12	1:A:374:ILE:O	1.61	1.01
1:B:207:PRO:HA	2:B:502:3GC:H22	1.25	0.99
1:A:383:GLU:OE1	1:A:384:LEU:HB2	1.60	0.99
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.26	0.98
1:B:160:GLU:C	1:B:163:LYS:HZ1	1.72	0.98
1:B:384:LEU:O	1:B:426:ARG:CB	2.12	0.97
1:A:60:LYS:HD3	1:A:242[A]:ARG:NH1	1.81	0.96
1:B:138:MET:CE	1:B:143:LYS:HD2	1.94	0.96
1:A:39:LEU:HD12	1:A:442:TRP:HZ3	1.17	0.96
1:B:384:LEU:C	1:B:426:ARG:HB2	1.91	0.95
1:B:160:GLU:C	1:B:163:LYS:NZ	2.25	0.95
1:A:277:LEU:HD11	3:A:605:HOH:O	1.67	0.94
1:B:337:GLN:HG3	3:B:613:HOH:O	1.65	0.94
1:A:404:ARG:O	1:A:404:ARG:HG2	1.11	0.93
1:B:238:GLN:NE2	2:B:501:3GC:H22	1.66	0.93
1:B:346:LEU:HA	3:B:623:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ALA:HB1	1:B:388:LYS:HZ3	1.33	0.90
1:A:384:LEU:HG	1:A:426:ARG:H	1.37	0.90
1:B:208:ALA:HB3	2:B:502:3GC:HA1	1.52	0.89
1:B:430:ALA:HA	3:B:617:HOH:O	1.72	0.89
1:B:349:PHE:HD1	3:B:623:HOH:O	1.56	0.88
1:B:423:LEU:HD12	1:B:424:MET:N	1.87	0.88
1:B:160:GLU:O	1:B:163:LYS:NZ	2.06	0.88
1:B:487:LEU:HB2	1:B:489:GLY:N	1.88	0.88
1:A:202:ASN:HD22	1:A:204:ASN:H	1.18	0.87
1:B:159:ASP:HB3	3:B:603:HOH:O	1.75	0.87
1:B:161:LYS:O	1:B:162:THR:HG22	1.76	0.86
1:A:384:LEU:O	1:A:385:PHE:O	1.93	0.86
1:B:118:LEU:HD21	1:B:336:ILE:HG12	1.56	0.86
1:B:374:ILE:C	1:B:376:LYS:H	1.84	0.85
1:A:373:ASP:HB2	1:A:374:ILE:CG2	2.07	0.85
1:A:379:ILE:HD11	1:A:406:THR:HG22	1.59	0.85
1:B:377:LYS:HE2	3:B:643:HOH:O	1.77	0.84
1:B:207:PRO:HA	2:B:502:3GC:N1	1.93	0.84
1:A:261:ARG:HH11	1:A:287:GLN:NE2	1.75	0.83
1:A:277:LEU:CD1	3:A:605:HOH:O	2.21	0.83
1:B:423:LEU:HB2	3:B:580:HOH:O	1.79	0.83
1:A:379:ILE:CG1	1:A:406:THR:HG22	2.07	0.82
1:A:39:LEU:CD1	1:A:442:TRP:CZ3	2.61	0.82
1:B:390:GLN:HG2	3:B:615:HOH:O	1.79	0.82
1:A:247:GLN:OE1	1:A:264:ARG:NH1	2.11	0.81
1:B:375:VAL:HG13	1:B:379:ILE:HB	1.62	0.81
1:B:375:VAL:HG23	1:B:388:LYS:CG	2.11	0.81
1:A:285:ASP:OD1	1:A:285:ASP:O	1.99	0.81
1:B:422:ILE:HG23	1:B:423:LEU:H	1.47	0.79
1:B:422:ILE:HG23	1:B:423:LEU:N	1.97	0.79
1:A:398:ILE:CG2	1:A:405:GLU:OE1	2.23	0.78
1:A:384:LEU:O	1:A:385:PHE:C	2.22	0.78
1:A:371:ASP:HA	1:A:375:VAL:HG23	1.64	0.78
1:A:125:ASP:OD2	1:A:128:THR:HB	1.85	0.77
1:A:39:LEU:CD1	1:A:442:TRP:HZ3	1.97	0.77
1:A:176:SER:OG	2:A:501:3GC:HG11	1.84	0.77
1:B:384:LEU:O	1:B:385:PHE:O	2.02	0.77
1:A:261:ARG:HH11	1:A:287:GLN:HE22	1.32	0.77
1:A:379:ILE:CD1	1:A:406:THR:HG22	2.15	0.76
1:B:138:MET:HE3	1:B:143:LYS:CG	2.15	0.76
1:B:161:LYS:HA	1:B:163:LYS:HZ1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:TYR:O	1:B:421:TYR:CD1	2.39	0.76
1:A:230:ARG:HD3	3:A:558:HOH:O	1.85	0.75
1:B:423:LEU:HD12	1:B:424:MET:H	1.50	0.75
1:B:344:GLY:CA	3:B:649:HOH:O	2.22	0.74
1:A:442:TRP:H	1:A:442:TRP:CD1	2.06	0.74
1:B:90:TRP:CD1	2:B:502:3GC:HA2	2.22	0.74
1:B:160:GLU:N	1:B:428:PHE:O	2.16	0.74
1:A:379:ILE:CG1	1:A:406:THR:CG2	2.65	0.74
1:B:484:GLY:HA3	3:B:525:HOH:O	1.86	0.74
1:B:390:GLN:CG	3:B:615:HOH:O	2.36	0.73
1:A:383:GLU:OE1	1:A:384:LEU:N	2.21	0.73
1:A:268:THR:HG22	3:A:554:HOH:O	1.87	0.73
1:B:376:LYS:C	1:B:378:ALA:H	1.95	0.73
1:B:378:ALA:HB1	1:B:388:LYS:HZ1	1.52	0.73
1:A:268:THR:HB	1:A:308:GLU:OE2	1.89	0.73
1:A:379:ILE:HG13	1:A:406:THR:HG21	1.68	0.73
1:B:364:ALA:HB3	1:B:424:MET:HE3	1.69	0.73
1:B:374:ILE:HG22	1:B:375:VAL:HB	1.71	0.72
1:B:207:PRO:CA	2:B:502:3GC:H22	2.02	0.72
1:A:370:GLU:O	1:A:374:ILE:HG13	1.88	0.72
1:B:142:ASN:O	1:B:142:ASN:ND2	2.23	0.72
1:A:374:ILE:O	1:A:374:ILE:CD1	2.36	0.72
1:B:138:MET:HE3	1:B:143:LYS:HD2	1.71	0.72
1:B:375:VAL:CG2	1:B:379:ILE:HG13	2.15	0.72
1:A:473:MET:HE1	3:A:545:HOH:O	1.89	0.71
1:B:379:ILE:CD1	3:B:532:HOH:O	2.38	0.71
1:A:368:SER:OG	1:A:369:LEU:N	2.23	0.70
1:B:386:VAL:O	1:B:423:LEU:HD13	1.90	0.70
1:B:208:ALA:CB	2:B:502:3GC:HA1	2.21	0.70
1:B:105:ASP:OD1	1:B:148:ARG:HD2	1.91	0.70
1:B:366:LEU:HA	1:B:423:LEU:O	1.92	0.70
1:A:379:ILE:HG13	1:A:406:THR:CG2	2.22	0.69
1:B:279:ASP:OD1	1:B:281:THR:CG2	2.40	0.69
1:B:194[A]:GLN:O	1:B:197:LYS:HD2	1.93	0.69
1:B:360:ARG:HG3	1:B:360:ARG:NH1	2.03	0.69
1:B:241:GLU:OE1	2:B:501:3GC:N1	2.26	0.69
1:A:384:LEU:C	1:A:426:ARG:HB2	2.18	0.69
1:B:374:ILE:HG22	1:B:375:VAL:N	2.07	0.68
1:A:409:LYS:C	3:A:546:HOH:O	2.36	0.68
1:B:238:GLN:HE21	2:B:501:3GC:H22	1.37	0.68
1:A:241:GLU:OE1	2:A:501:3GC:N1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:MET:CE	1:B:143:LYS:CD	2.71	0.67
1:B:161:LYS:HA	1:B:163:LYS:NZ	2.09	0.67
1:B:138:MET:HE2	1:B:143:LYS:HD2	1.76	0.67
1:B:120:ARG:HD2	1:B:335:LYS:CE	2.24	0.67
1:B:161:LYS:O	1:B:162:THR:CG2	2.43	0.67
1:B:120:ARG:HD2	1:B:335:LYS:HD3	1.77	0.67
1:A:384:LEU:HG	1:A:426:ARG:N	2.08	0.66
1:A:86:PRO:HD2	1:A:158:ILE:HD11	1.76	0.65
1:B:90:TRP:HD1	2:B:502:3GC:HA2	1.61	0.65
1:B:202:ASN:ND2	1:B:204:ASN:HB2	2.10	0.65
1:B:379:ILE:HD11	3:B:532:HOH:O	1.95	0.65
1:A:390:GLN:CG	1:A:422:ILE:HG23	2.26	0.65
1:B:63:GLN:CD	1:B:63:GLN:N	2.55	0.65
1:B:138:MET:HE3	1:B:143:LYS:CD	2.27	0.65
1:A:138:MET:SD	1:A:143:LYS:HD2	2.37	0.64
1:B:334:LYS:HZ3	1:B:421:TYR:HB2	1.61	0.64
1:B:269:GLU:O	1:B:273:GLU:HB2	1.97	0.64
1:B:374:ILE:CG2	1:B:375:VAL:N	2.60	0.64
1:A:388:LYS:NZ	3:A:596:HOH:O	2.29	0.64
1:A:34:ILE:HB	1:A:39:LEU:CD2	2.28	0.64
1:B:346:LEU:HD12	1:B:356:ILE:HG23	1.80	0.64
1:A:269:GLU:O	1:A:273:GLU:HB2	1.97	0.64
1:A:383:GLU:OE1	1:A:384:LEU:CB	2.40	0.64
1:B:120:ARG:NE	1:B:335:LYS:HD3	2.12	0.63
1:A:261:ARG:NH1	1:A:287:GLN:NE2	2.47	0.63
1:B:194[A]:GLN:HE21	1:B:194[A]:GLN:HA	1.63	0.63
1:B:475:ARG:NH2	1:B:490:PHE:O	2.32	0.63
1:B:334:LYS:NZ	1:B:421:TYR:HB2	2.13	0.63
1:B:384:LEU:O	1:B:426:ARG:HD2	1.99	0.63
1:A:69:PRO:HA	1:A:245:TYR:OH	1.98	0.63
1:B:358:LYS:HE2	3:B:576:HOH:O	1.99	0.62
1:B:159:ASP:OD1	1:B:428:PHE:N	2.25	0.62
1:A:396:ASN:N	3:A:611:HOH:O	2.31	0.62
1:B:338:GLN:OE1	1:B:422:ILE:HG22	1.99	0.62
1:B:479:SER:HB2	3:B:640:HOH:O	1.78	0.62
1:B:118:LEU:HD21	1:B:336:ILE:CG1	2.30	0.61
1:B:475:ARG:CZ	1:B:490:PHE:O	2.48	0.61
1:B:87:GLU:OE2	1:B:91:LYS:NZ	2.33	0.61
1:B:108:SER:HB2	1:B:327:SER:HB2	1.81	0.61
1:B:138:MET:HE1	1:B:317:GLN:HA	1.83	0.61
1:A:174:SER:O	2:A:501:3GC:HB22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HB2	3:B:504:HOH:O	2.00	0.60
1:B:388:LYS:O	1:B:390:GLN:HB3	2.01	0.60
1:B:279:ASP:OD1	1:B:281:THR:HG23	2.00	0.60
1:A:86:PRO:HD2	1:A:158:ILE:CD1	2.31	0.60
1:A:108:SER:HB2	1:A:327:SER:HB2	1.82	0.60
1:B:138:MET:HE3	1:B:143:LYS:HG3	1.83	0.60
1:B:364:ALA:HB3	1:B:424:MET:CE	2.31	0.60
1:B:375:VAL:HG13	1:B:379:ILE:CB	2.30	0.60
1:B:120:ARG:CD	1:B:335:LYS:HD3	2.32	0.60
1:B:160:GLU:C	1:B:163:LYS:HZ3	2.05	0.60
1:A:442:TRP:CD1	1:A:442:TRP:N	2.68	0.60
1:B:334:LYS:HG2	1:B:338:GLN:HE21	1.65	0.60
1:B:129:SER:O	1:B:133[A]:ASP:OD1	2.20	0.60
1:A:405:GLU:CA	1:A:405:GLU:OE2	2.49	0.59
1:A:352:ASN:HD22	1:A:352:ASN:C	2.10	0.59
1:B:375:VAL:O	1:B:379:ILE:HB	2.03	0.59
1:B:118:LEU:HD22	1:B:335:LYS:HB3	1.85	0.59
1:B:168:ILE:HG21	1:B:450:GLU:OE2	2.02	0.59
1:A:34:ILE:HB	1:A:39:LEU:HD21	1.85	0.59
1:A:157:MET:HG3	1:A:168[B]:ILE:HD13	1.84	0.58
1:B:198:PHE:HD2	1:B:199:LEU:HG	1.68	0.58
1:B:174:SER:O	1:B:174:SER:OG	2.14	0.58
1:A:379:ILE:HD11	1:A:406:THR:CG2	2.33	0.58
1:B:279:ASP:OD1	1:B:281:THR:HG22	2.03	0.58
1:B:365:GLY:O	1:B:424:MET:HA	2.04	0.58
1:B:423:LEU:HD12	1:B:423:LEU:C	2.28	0.58
1:B:120:ARG:HD2	1:B:335:LYS:CD	2.33	0.58
1:B:360:ARG:NH1	1:B:360:ARG:CG	2.65	0.58
1:A:133:ASP:O	1:A:137:LYS:HG3	2.04	0.57
1:A:202:ASN:ND2	1:A:204:ASN:CG	2.62	0.57
1:B:430:ALA:CA	3:B:617:HOH:O	2.43	0.57
1:A:450:GLU:OE2	1:A:477:LYS:HE2	2.03	0.57
1:B:389:PRO:HB2	3:B:557:HOH:O	2.04	0.57
1:B:478:ILE:HG22	1:B:479:SER:N	2.19	0.57
1:A:233:ILE:HG12	1:A:291:VAL:HB	1.85	0.57
1:A:379:ILE:HG12	1:A:406:THR:HG22	1.84	0.57
1:B:369:LEU:O	1:B:370:GLU:HG3	2.04	0.57
1:B:383:GLU:O	1:B:428:PHE:HZ	1.88	0.57
1:B:376:LYS:C	1:B:378:ALA:N	2.58	0.56
1:B:488:PRO:HG2	1:B:490:PHE:HA	1.87	0.56
1:B:160:GLU:O	1:B:161:LYS:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LYS:O	1:B:385:PHE:CE1	2.58	0.56
1:B:147:ILE:HB	1:B:321:ILE:CD1	2.35	0.56
1:B:210:ASN:OD1	1:B:214:GLN:HG3	2.06	0.56
1:B:322:LYS:HD3	1:B:322:LYS:N	2.21	0.56
1:B:202:ASN:HD22	1:B:204:ASN:H	1.52	0.56
1:A:129:SER:O	1:A:133:ASP:OD1	2.24	0.55
1:B:208:ALA:H	2:B:502:3GC:CA1	2.19	0.55
1:A:236:VAL:HG11	1:A:267:LEU:HD13	1.89	0.55
1:B:313:LEU:O	1:B:317:GLN:HG3	2.07	0.55
1:A:353:LYS:HE3	3:A:555:HOH:O	2.07	0.55
1:B:376:LYS:O	1:B:378:ALA:N	2.38	0.55
1:A:176:SER:HG	2:A:501:3GC:HG11	1.68	0.55
1:A:197:LYS:HE3	1:A:198:PHE:H	1.71	0.55
1:A:409:LYS:HE3	3:A:586:HOH:O	2.06	0.55
1:B:161:LYS:CA	1:B:163:LYS:HZ1	2.18	0.55
1:B:298:TYR:CE1	2:B:501:3GC:HG12	2.42	0.55
1:B:59:ASP:OD1	1:B:61:SER:HB3	2.08	0.54
1:B:120:ARG:HD2	1:B:335:LYS:NZ	2.23	0.54
1:B:328:TYR:O	1:B:329:HIS:C	2.50	0.54
1:A:376:LYS:HZ3	1:A:380:GLU:CG	2.21	0.54
1:B:147:ILE:HB	1:B:321:ILE:HD11	1.90	0.54
1:B:153:ARG:HD2	1:B:452:GLY:HA3	1.89	0.54
1:B:375:VAL:C	1:B:379:ILE:H	2.16	0.54
1:B:422:ILE:CG2	1:B:423:LEU:N	2.70	0.54
1:A:386:VAL:HG22	1:A:399:TYR:CD2	2.42	0.54
1:A:298:TYR:CZ	2:A:501:3GC:OE1	2.61	0.54
1:B:378:ALA:CB	1:B:388:LYS:NZ	2.59	0.54
1:A:157:MET:CE	1:A:429:PRO:HB3	2.38	0.53
1:B:324:PRO:HB2	1:B:328:TYR:HB2	1.90	0.53
1:A:377:LYS:O	1:A:380:GLU:O	2.26	0.53
1:A:276:ILE:CG2	1:A:280:GLY:HA2	2.39	0.53
1:A:352:ASN:ND2	1:A:354:ASP:H	2.06	0.53
1:A:56:LEU:HD23	1:A:75:HIS:HA	1.90	0.53
1:A:109:LEU:HD11	1:A:148:ARG:NH1	2.23	0.53
1:B:489:GLY:C	1:B:491:GLY:H	2.16	0.53
1:A:352:ASN:ND2	1:A:354:ASP:N	2.57	0.53
1:A:370:GLU:HB2	1:A:374:ILE:HG23	1.91	0.53
1:B:379:ILE:HD13	3:B:532:HOH:O	2.07	0.53
1:B:63:GLN:CD	1:B:63:GLN:H	2.17	0.53
1:B:138:MET:CE	1:B:143:LYS:HG3	2.39	0.53
1:B:163:LYS:HE3	1:B:163:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:THR:OG1	1:B:269:GLU:HG3	2.09	0.52
1:B:378:ALA:CB	1:B:388:LYS:HZ1	2.20	0.52
1:A:322:LYS:HD3	1:A:322:LYS:N	2.24	0.52
1:B:34:ILE:CG2	1:B:39:LEU:HD13	2.40	0.52
1:B:120:ARG:HE	1:B:335:LYS:HD3	1.73	0.52
1:A:384:LEU:CG	1:A:426:ARG:H	2.17	0.52
1:B:375:VAL:HA	1:B:379:ILE:N	2.24	0.52
1:A:401:ASP:O	1:A:404:ARG:HB3	2.10	0.52
1:B:63:GLN:OE1	1:B:64:ARG:N	2.38	0.52
1:B:138:MET:CE	1:B:143:LYS:CG	2.87	0.52
1:B:339:GLU:O	1:B:345:VAL:HG21	2.10	0.51
1:B:118:LEU:HD12	1:B:330:LEU:HD22	1.91	0.51
1:B:375:VAL:HA	1:B:379:ILE:H	1.76	0.51
1:B:30:ASP:HA	1:B:433:PRO:HG2	1.93	0.50
1:A:374:ILE:O	1:A:374:ILE:CG1	2.59	0.50
1:B:194[A]:GLN:HE21	1:B:194[A]:GLN:CA	2.24	0.50
1:B:460:ASN:O	1:B:463:LYS:HE3	2.12	0.50
1:A:352:ASN:HD21	1:A:354:ASP:HB3	1.76	0.50
1:A:55:LEU:HD21	1:A:184:MET:SD	2.52	0.50
1:A:267:LEU:HD22	3:A:513:HOH:O	2.12	0.50
1:B:388:LYS:HG2	1:B:389:PRO:HD2	1.94	0.50
1:B:204:ASN:HB3	1:B:205:ARG:HG2	1.93	0.50
1:B:173:ILE:HD12	1:B:324:PRO:HD2	1.92	0.50
1:B:198:PHE:HZ	3:B:524:HOH:O	1.95	0.50
1:B:221:LYS:HD2	1:B:466:ILE:HD11	1.94	0.50
1:B:210:ASN:HB3	3:B:631:HOH:O	2.12	0.50
1:A:460:ASN:O	1:A:461:LYS:C	2.55	0.49
1:A:338:GLN:HG2	1:A:366:LEU:HD11	1.94	0.49
1:B:138:MET:HE3	1:B:143:LYS:CB	2.42	0.49
1:B:196:GLY:O	1:B:200:GLY:N	2.45	0.49
1:A:390:GLN:HG2	1:A:422:ILE:HG23	1.93	0.49
1:B:324:PRO:HB2	1:B:328:TYR:CB	2.43	0.49
1:A:159:ASP:HB2	1:A:427:ILE:HG23	1.94	0.48
1:B:63:GLN:H	1:B:63:GLN:NE2	2.10	0.48
1:B:368:SER:HB3	1:B:422:ILE:HG12	1.95	0.48
1:B:426:ARG:HD3	1:B:428:PHE:CZ	2.49	0.48
1:A:376:LYS:NZ	1:A:380:GLU:HB2	2.29	0.48
1:A:245:TYR:CE2	1:B:51:THR:HG21	2.48	0.48
1:B:426:ARG:NH1	1:B:428:PHE:CE2	2.82	0.48
1:A:32:HIS:CD2	1:A:433:PRO:HB3	2.48	0.48
1:A:174:SER:OG	2:A:501:3GC:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:SER:O	1:B:197:LYS:HE3	2.12	0.48
1:B:341:ALA:HB1	1:B:366:LEU:HD13	1.96	0.47
1:A:231:ALA:CB	1:A:290:SER:HB3	2.45	0.47
1:B:488:PRO:HD2	1:B:490:PHE:HA	1.95	0.47
1:B:360:ARG:HA	1:B:363:PHE:HB2	1.96	0.47
1:B:438:ARG:HD3	3:B:552:HOH:O	2.13	0.47
1:A:226:TYR:CG	1:A:290:SER:HB2	2.50	0.47
1:A:271:ASP:HB2	1:A:307:SER:O	2.14	0.47
1:A:313:LEU:HD22	1:A:317:GLN:HG3	1.95	0.47
1:A:73:LEU:HB2	1:B:73:LEU:HB2	1.96	0.47
1:A:370:GLU:O	1:A:374:ILE:CG1	2.59	0.47
1:A:450:GLU:CD	1:A:477:LYS:HE2	2.40	0.47
1:B:375:VAL:H	1:B:388:LYS:HE2	1.80	0.47
1:A:352:ASN:C	1:A:352:ASN:ND2	2.72	0.47
1:A:405:GLU:OE2	1:A:405:GLU:HA	2.13	0.47
1:A:92:GLN:NE2	3:A:634:HOH:O	2.48	0.47
1:A:404:ARG:C	1:A:406:THR:N	2.70	0.47
1:A:238:GLN:NE2	2:A:501:3GC:H22	2.13	0.47
1:A:180:ILE:HG21	1:A:493:VAL:HG11	1.96	0.46
1:A:87:GLU:OE2	1:A:91:LYS:NZ	2.46	0.46
1:A:151:ILE:HG12	1:A:456:THR:HG22	1.98	0.46
1:B:34:ILE:HG22	1:B:39:LEU:HD13	1.98	0.46
1:B:161:LYS:N	1:B:163:LYS:HZ1	2.12	0.46
1:B:176:SER:O	1:B:177:PHE:HB2	2.15	0.46
1:A:157:MET:HE2	1:A:429:PRO:HB3	1.97	0.46
1:B:364:ALA:O	1:B:365:GLY:C	2.58	0.46
1:B:479:SER:HA	3:B:525:HOH:O	2.15	0.46
1:A:318[B]:SER:O	1:A:322:LYS:NZ	2.48	0.46
1:A:347:GLU:OE1	1:A:360:ARG:NH1	2.49	0.46
1:B:205:ARG:HB2	1:B:497:TYR:CE2	2.51	0.46
1:A:237:VAL:HG11	1:A:264:ARG:NH1	2.31	0.46
1:A:404:ARG:NH2	3:A:609:HOH:O	2.47	0.46
1:B:75:HIS:ND1	1:B:76:LEU:O	2.42	0.46
1:B:388:LYS:CG	1:B:389:PRO:HD2	2.45	0.46
1:A:83:GLY:O	1:A:497:TYR:N	2.47	0.46
1:A:120:ARG:HD2	1:A:120:ARG:HA	1.80	0.46
1:B:341:ALA:CB	1:B:366:LEU:HD13	2.45	0.46
1:A:221:LYS:HB3	1:A:458:LEU:CD2	2.46	0.45
1:A:383:GLU:OE1	1:A:384:LEU:CA	2.64	0.45
1:A:431:THR:HG23	3:A:529:HOH:O	2.16	0.45
1:A:38:LEU:O	1:A:42:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:HD22	1:A:354:ASP:N	2.15	0.45
1:B:167:GLN:O	1:B:424:MET:HE1	2.17	0.45
1:A:376:LYS:HZ2	1:A:380:GLU:HB2	1.81	0.45
1:B:375:VAL:HG13	1:B:379:ILE:CG1	2.46	0.45
1:B:118:LEU:HD21	1:B:336:ILE:CD1	2.46	0.45
1:B:488:PRO:CG	1:B:490:PHE:HA	2.46	0.45
1:A:197:LYS:NZ	1:A:198:PHE:HB2	2.31	0.45
1:A:105:ASP:OD1	1:A:148:ARG:HD2	2.16	0.45
1:A:271:ASP:OD1	1:A:310:ARG:HD2	2.17	0.45
1:B:426:ARG:NH1	1:B:428:PHE:HE2	2.15	0.45
1:A:226:TYR:HE2	1:A:319[B]:SER:O	2.00	0.45
1:A:177:PHE:CD1	1:A:180:ILE:HG12	2.52	0.45
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.61	0.45
1:B:202:ASN:CG	1:B:204:ASN:HB2	2.41	0.45
1:B:487:LEU:N	1:B:487:LEU:HD22	2.32	0.45
1:A:95:GLU:OE2	1:A:358:LYS:HE2	2.17	0.44
1:A:402:GLU:O	1:A:405:GLU:CD	2.61	0.44
1:A:369:LEU:HA	1:A:374:ILE:HD11	1.99	0.44
1:A:376:LYS:O	1:A:376:LYS:CD	2.65	0.44
1:A:108:SER:HB2	1:A:327:SER:CB	2.48	0.44
1:B:488:PRO:HB2	1:B:491:GLY:N	2.32	0.44
1:A:64:ARG:HB3	1:A:68:VAL:HG23	1.99	0.44
1:A:188:HIS:HE1	1:A:494:ASP:OD1	2.01	0.44
1:A:376:LYS:HD3	1:A:379:ILE:HB	1.98	0.44
1:B:379:ILE:HG12	3:B:615:HOH:O	2.18	0.44
1:B:421:TYR:CD1	1:B:421:TYR:C	2.96	0.44
1:B:374:ILE:C	1:B:376:LYS:N	2.50	0.44
1:A:352:ASN:HD22	1:A:355:HIS:H	1.66	0.44
1:A:386:VAL:CG2	1:A:399:TYR:CE2	3.01	0.44
1:B:384:LEU:O	1:B:426:ARG:CG	2.66	0.44
1:A:105:ASP:OD2	1:A:148:ARG:NH1	2.51	0.43
1:B:136:SER:O	1:B:140:GLN:HB2	2.18	0.43
1:B:194[B]:GLN:O	1:B:197:LYS:HD2	2.18	0.43
1:A:379:ILE:CD1	1:A:406:THR:CG2	2.91	0.43
1:A:96:LEU:HA	1:A:96:LEU:HD12	1.66	0.43
1:A:195:TYR:O	1:A:199:LEU:HD12	2.17	0.43
1:A:376:LYS:NZ	1:A:380:GLU:CG	2.81	0.43
1:A:386:VAL:HG22	1:A:399:TYR:CE2	2.54	0.43
1:B:86:PRO:HA	1:B:499:THR:HA	2.00	0.43
1:B:274:GLY:HA2	1:B:283:SER:O	2.19	0.43
1:A:376:LYS:O	1:A:377:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.85	0.43
1:B:247:GLN:OE1	1:B:264:ARG:NH2	2.51	0.43
1:A:383:GLU:CG	1:A:384:LEU:N	2.81	0.43
1:B:118:LEU:CD1	1:B:330:LEU:HD22	2.48	0.43
1:B:197:LYS:O	1:B:198:PHE:C	2.61	0.42
1:B:233:ILE:O	1:B:262:SER:HA	2.19	0.42
1:A:331:VAL:HA	1:A:336:ILE:HG21	2.01	0.42
1:A:342:LYS:O	1:A:360:ARG:NH2	2.52	0.42
1:B:256:GLU:HB3	3:B:635:HOH:O	2.19	0.42
1:A:27:PRO:CB	1:A:30:ASP:HB3	2.49	0.42
1:B:105:ASP:O	1:B:108:SER:OG	2.32	0.42
1:B:87:GLU:HB2	1:B:498:LEU:HB3	2.00	0.42
1:B:157:MET:HB2	1:B:168:ILE:HD11	2.01	0.42
1:A:110:ASP:O	1:A:114:LEU:HG	2.20	0.42
1:A:448:ILE:HD12	1:A:448:ILE:HG21	1.73	0.42
1:A:97:ALA:HB3	1:A:98:PRO:HD3	2.02	0.42
1:A:107:VAL:H	1:A:107:VAL:HG23	1.63	0.42
1:A:236:VAL:CG1	1:A:267:LEU:HD13	2.50	0.42
1:B:58:GLY:HA3	1:B:242[B]:ARG:HG2	2.02	0.42
1:B:120:ARG:HD2	1:B:335:LYS:HZ3	1.85	0.42
1:B:422:ILE:CG2	1:B:423:LEU:H	2.23	0.42
1:B:265:LYS:HA	1:B:269:GLU:OE1	2.20	0.41
1:A:263:ILE:HG21	1:A:263:ILE:HD12	1.83	0.41
1:A:384:LEU:HA	1:A:426:ARG:HB3	2.01	0.41
1:B:287:GLN:HE21	1:B:287:GLN:HB2	1.70	0.41
1:A:162:THR:OG1	1:A:164:SER:HB2	2.20	0.41
1:B:208:ALA:N	2:B:502:3GC:HA1	2.35	0.41
1:A:157:MET:HE1	1:A:429:PRO:HB3	2.01	0.41
1:A:352:ASN:ND2	1:A:355:HIS:H	2.18	0.41
1:B:147:ILE:HA	1:B:459:ARG:O	2.20	0.41
1:B:238:GLN:NE2	2:B:501:3GC:N1	2.49	0.41
1:B:247:GLN:H	1:B:247:GLN:HG3	1.63	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.46	0.41
1:A:103:LEU:O	1:A:107:VAL:HG23	2.20	0.41
1:B:118:LEU:CD2	1:B:335:LYS:HG2	2.50	0.41
1:B:140:GLN:C	1:B:142:ASN:H	2.29	0.41
1:B:142:ASN:O	1:B:142:ASN:CG	2.63	0.41
1:B:331:VAL:HA	1:B:336:ILE:HG21	2.03	0.41
1:A:436:LEU:HD21	1:A:447:VAL:HG11	2.02	0.41
1:B:247:GLN:OE1	1:B:264:ARG:NH1	2.52	0.41
1:B:299:THR:OG1	1:B:301:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HG	1:B:426:ARG:H	1.85	0.41
1:A:261:ARG:NH1	1:A:287:GLN:HE21	2.17	0.41
1:A:211:ALA:HA	1:A:470:SER:O	2.20	0.41
1:B:96:LEU:HG	1:B:100:PHE:CE2	2.56	0.41
1:B:147:ILE:HB	1:B:321:ILE:HD12	2.02	0.41
1:B:208:ALA:N	2:B:502:3GC:N1	2.63	0.41
1:B:226:TYR:CD1	1:B:290:SER:HB2	2.56	0.41
1:B:331:VAL:O	1:B:337:GLN:OE1	2.38	0.41
1:B:388:LYS:O	1:B:389:PRO:C	2.63	0.41
1:A:143:LYS:HE2	1:A:143:LYS:HB2	1.22	0.41
1:A:421:TYR:HD2	1:A:421:TYR:HA	1.46	0.41
1:A:478:ILE:O	1:A:479:SER:HB2	2.21	0.41
1:B:385:PHE:HB3	1:B:423:LEU:HD11	2.01	0.40
1:B:106:ARG:O	1:B:107:VAL:C	2.61	0.40
1:B:148:ARG:NH2	3:B:629:HOH:O	2.51	0.40
1:B:374:ILE:HG22	1:B:375:VAL:CB	2.47	0.40
1:B:118:LEU:HG	1:B:336:ILE:HD11	2.04	0.40
1:B:195:TYR:C	1:B:197:LYS:HG2	2.46	0.40
1:A:197:LYS:N	3:A:628:HOH:O	2.39	0.40
1:A:324:PRO:HB2	1:A:328:TYR:HB2	2.03	0.40
1:A:409:LYS:HE2	3:A:563:HOH:O	2.21	0.40
1:B:197:LYS:CG	1:B:198:PHE:H	2.34	0.40
1:B:385:PHE:CD1	1:B:385:PHE:N	2.78	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	437/499 (88%)	406 (93%)	23 (5%)	8 (2%)	6	3
1	B	437/499 (88%)	387 (89%)	31 (7%)	19 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	874/998 (88%)	793 (91%)	54 (6%)	27 (3%)	3 1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ARG
1	A	461	LYS
1	B	197	LYS
1	B	370	GLU
1	B	375	VAL
1	B	385	PHE
1	B	387	MET
1	B	389	PRO
1	B	483	GLU
1	B	487	LEU
1	B	490	PHE
1	A	383	GLU
1	A	385	PHE
1	B	204	ASN
1	B	478	ILE
1	B	479	SER
1	B	480	SER
1	A	29	PHE
1	B	422	ILE
1	A	196	GLY
1	B	198	PHE
1	B	376	LYS
1	B	386	VAL
1	A	141	ILE
1	B	177	PHE
1	A	375	VAL
1	B	484	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	397/431 (92%)	340 (86%)	57 (14%)	3	1
1	B	390/431 (90%)	331 (85%)	59 (15%)	3	1
All	All	787/862 (91%)	671 (85%)	116 (15%)	3	1

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	29	PHE
1	A	30	ASP
1	A	35	ASP
1	A	37	LYS
1	A	39	LEU
1	A	42	ILE
1	A	60	LYS
1	A	61	SER
1	A	96	LEU
1	A	112	LYS
1	A	126	GLU
1	A	128	THR
1	A	139	LEU
1	A	141	ILE
1	A	142	ASN
1	A	143	LYS
1	A	147	ILE
1	A	159	ASP
1	A	163	LYS
1	A	168[A]	ILE
1	A	168[B]	ILE
1	A	180	ILE
1	A	182	CYS
1	A	194	GLN
1	A	197	LYS
1	A	205	ARG
1	A	221	LYS
1	A	235	VAL
1	A	263	ILE
1	A	264	ARG
1	A	267	LEU
1	A	285	ASP
1	A	305	SER
1	A	313	LEU

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Mol	Chain	Res	Type
1	A	319[A]	SER
1	A	319[B]	SER
1	A	351	GLU
1	A	352	ASN
1	A	369	LEU
1	A	370	GLU
1	A	374	ILE
1	A	376	LYS
1	A	383	GLU
1	A	390	GLN
1	A	404	ARG
1	A	405	GLU
1	A	406	THR
1	A	421	TYR
1	A	423	LEU
1	A	431	THR
1	A	448	ILE
1	A	473	MET
1	A	477	LYS
1	A	478	ILE
1	A	490	PHE
1	A	498	LEU
1	B	39	LEU
1	B	57	VAL
1	B	60	LYS
1	B	63	GLN
1	B	71	VAL
1	B	73	LEU
1	B	96	LEU
1	B	106	ARG
1	B	116	GLU
1	B	119	SER
1	B	126	GLU
1	B	139	LEU
1	B	140	GLN
1	B	144	LYS
1	B	158	ILE
1	B	160	GLU
1	B	161	LYS
1	B	163	LYS
1	B	173	ILE
1	B	194[A]	GLN

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Mol	Chain	Res	Type
1	B	194[B]	GLN
1	B	197	LYS
1	B	202	ASN
1	B	206	VAL
1	B	229	PRO
1	B	235	VAL
1	B	237	VAL
1	B	240	GLU
1	B	247	GLN
1	B	256	GLU
1	B	281	THR
1	B	287	GLN
1	B	324	PRO
1	B	327	SER
1	B	346	LEU
1	B	352	ASN
1	B	354	ASP
1	B	360	ARG
1	B	363	PHE
1	B	366	LEU
1	B	369	LEU
1	B	371	ASP
1	B	373	ASP
1	B	375	VAL
1	B	379	ILE
1	B	380	GLU
1	B	386	VAL
1	B	388	LYS
1	B	421	TYR
1	B	422	ILE
1	B	425	GLN
1	B	438	ARG
1	B	465	ILE
1	B	473	MET
1	B	475	ARG
1	B	477	LYS
1	B	479	SER
1	B	487	LEU
1	B	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	92	GLN
1	A	202	ASN
1	A	214	GLN
1	A	238	GLN
1	A	272	GLN
1	A	287	GLN
1	A	337	GLN
1	A	352	ASN
1	A	381	ASN
1	A	468	ASN
1	B	40	GLN
1	B	142	ASN
1	B	202	ASN
1	B	238	GLN
1	B	272	GLN
1	B	287	GLN
1	B	337	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	3GC	B	502	-	14,15,15	2.55	2 (14%)	16,19,19	4.59	11 (68%)
2	3GC	A	501	-	14,15,15	1.86	2 (14%)	16,19,19	4.45	7 (43%)
2	3GC	B	501	-	14,15,15	1.79	2 (14%)	16,19,19	2.69	9 (56%)

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	3GC	B	502	-	1/1/5/6	8/19/19/19	-
2	3GC	A	501	-	1/1/5/6	11/19/19/19	-
2	3GC	B	501	-	1/1/5/6	4/19/19/19	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	3GC	OE1-CD1	7.87	1.38	1.23
2	A	501	3GC	OE1-CD1	5.07	1.33	1.23
2	B	501	3GC	OE1-CD1	4.93	1.33	1.23
2	B	502	3GC	CD1-N2	-4.07	1.25	1.34
2	A	501	3GC	CD1-N2	-3.54	1.26	1.34
2	B	501	3GC	CD1-N2	-3.36	1.26	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3GC	CB2-CA2-C2	-13.53	97.58	109.79
2	A	501	3GC	CB2-CA2-N2	-9.63	97.55	111.28
2	B	502	3GC	CA2-CB2-SG2	-8.39	104.69	114.16
2	B	502	3GC	CG1-CD1-N2	-8.26	101.31	115.86
2	B	502	3GC	CB2-CA2-C2	7.68	116.72	109.79
2	B	501	3GC	CB2-CA2-C2	6.21	115.39	109.79
2	B	502	3GC	CB1-CG1-CD1	-6.12	99.41	113.06
2	B	502	3GC	CB2-CA2-N2	-4.99	104.17	111.28
2	B	502	3GC	CA2-N2-CD1	4.26	132.37	121.68
2	B	502	3GC	OE1-CD1-CG1	4.26	129.74	122.02
2	B	501	3GC	CG1-CD1-N2	4.07	123.03	115.86
2	B	502	3GC	OE1-CD1-N2	3.54	128.94	122.95
2	B	501	3GC	CB1-CG1-CD1	-3.48	105.31	113.06
2	B	501	3GC	CA2-N2-CD1	-3.19	113.68	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3GC	CB1-CA1-C1	2.92	118.18	110.45
2	B	502	3GC	C2-CA2-N2	-2.86	103.93	110.57
2	A	501	3GC	O3-C2-CA2	2.85	123.15	113.51
2	B	501	3GC	CG1-CB1-CA1	-2.80	107.43	113.86
2	A	501	3GC	O2-C2-CA2	-2.65	113.69	122.26
2	A	501	3GC	C2-CA2-N2	2.39	116.11	110.57
2	B	501	3GC	OE1-CD1-CG1	-2.33	117.80	122.02
2	B	502	3GC	CG1-CB1-CA1	2.31	119.15	113.86
2	B	501	3GC	OE1-CD1-N2	-2.24	119.17	122.95
2	B	502	3GC	O3-C2-CA2	2.20	120.95	113.51
2	A	501	3GC	CA2-N2-CD1	2.08	126.91	121.68
2	B	501	3GC	CA2-CB2-SG2	2.04	116.46	114.16
2	B	501	3GC	CB2-CA2-N2	-2.02	108.40	111.28

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	3GC	CA1
2	B	501	3GC	CA1
2	B	502	3GC	CA1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3GC	C1-CA1-CB1-CG1
2	A	501	3GC	N2-CA2-CB2-SG2
2	A	501	3GC	C2-CA2-CB2-SG2
2	B	501	3GC	N2-CA2-CB2-SG2
2	B	501	3GC	C2-CA2-CB2-SG2
2	B	502	3GC	CB2-CA2-N2-CD1
2	A	501	3GC	CA1-CB1-CG1-CD1
2	B	501	3GC	O12-C1-CA1-N1
2	B	502	3GC	N2-CD1-CG1-CB1
2	B	502	3GC	OE1-CD1-CG1-CB1
2	A	501	3GC	O2-C2-CA2-N2
2	A	501	3GC	O3-C2-CA2-N2
2	B	502	3GC	N2-CA2-CB2-SG2
2	A	501	3GC	O11-C1-CA1-N1
2	A	501	3GC	O2-C2-CA2-CB2
2	B	502	3GC	C1-CA1-CB1-CG1
2	B	502	3GC	CA1-CB1-CG1-CD1
2	A	501	3GC	N1-CA1-CB1-CG1

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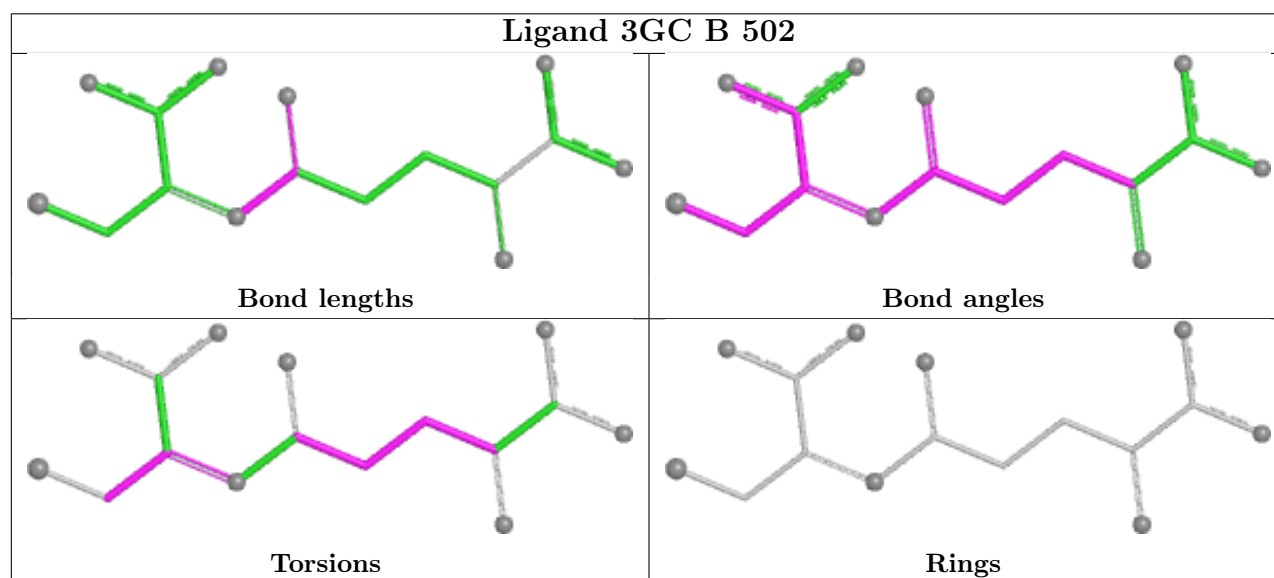
Mol	Chain	Res	Type	Atoms
2	A	501	3GC	O3-C2-CA2-CB2
2	A	501	3GC	O12-C1-CA1-N1
2	B	502	3GC	C2-CA2-CB2-SG2
2	B	502	3GC	N1-CA1-CB1-CG1
2	B	501	3GC	O11-C1-CA1-N1

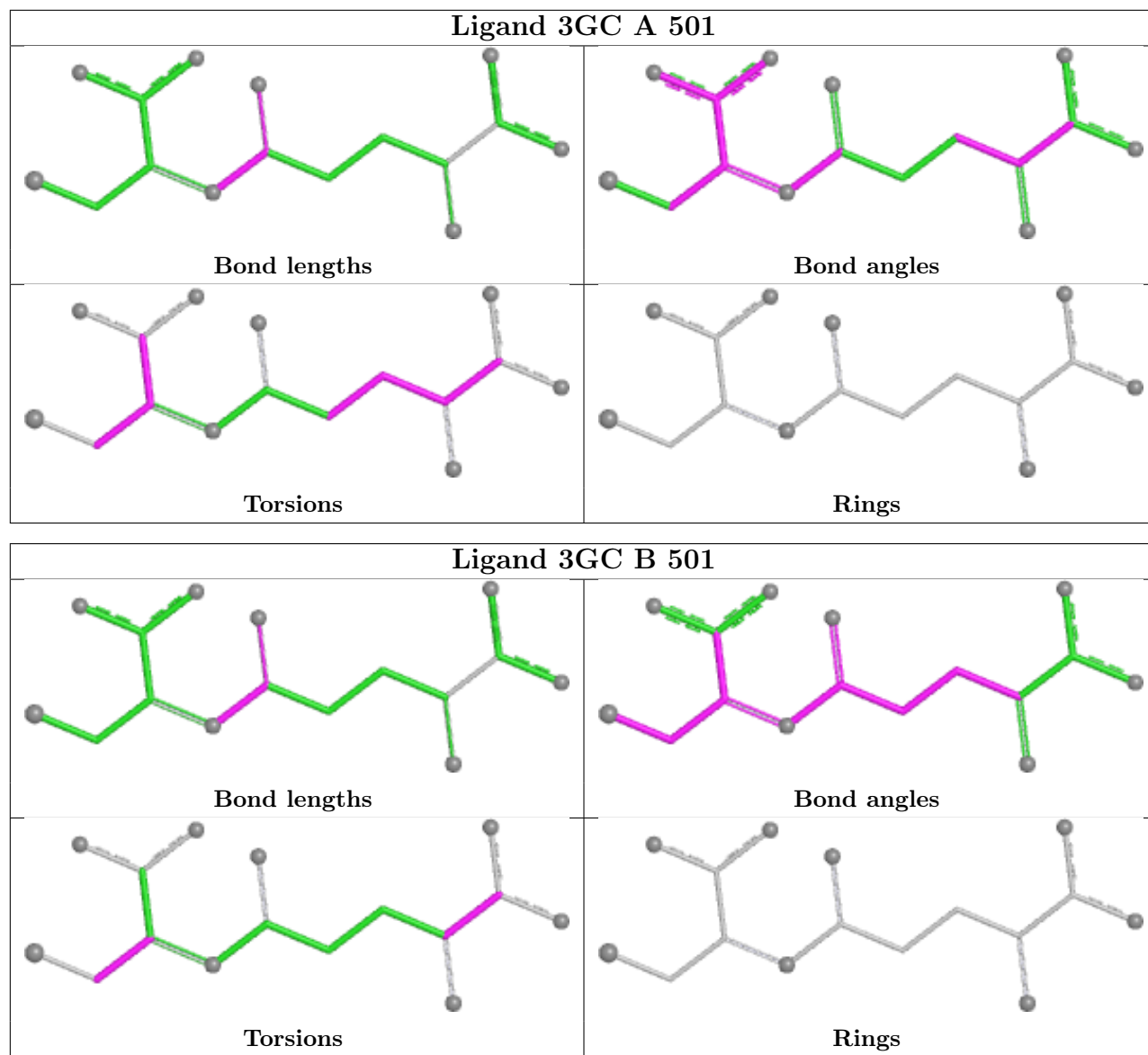
There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	3GC	10	0
2	A	501	3GC	7	0
2	B	501	3GC	5	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	443/499 (88%)	-0.09	12 (2%) 56 59	9, 27, 46, 71	6 (1%)
1	B	437/499 (87%)	-0.02	28 (6%) 25 28	7, 24, 59, 78	6 (1%)
All	All	880/998 (88%)	-0.06	40 (4%) 38 41	7, 26, 52, 78	12 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	375	VAL	6.3
1	A	375	VAL	5.6
1	A	374	ILE	5.3
1	B	484	GLY	4.2
1	B	369	LEU	4.2
1	A	28	LEU	4.2
1	A	384	LEU	3.9
1	B	486	VAL	3.7
1	A	421	TYR	3.6
1	A	419	ALA	3.5
1	B	389	PRO	3.4
1	B	374	ILE	3.4
1	B	488	PRO	3.2
1	B	384	LEU	3.2
1	B	479	SER	3.2
1	B	388	LYS	3.2
1	B	499	THR	3.1
1	A	430	ALA	3.0
1	B	346	LEU	3.0
1	B	485	GLY	2.9
1	B	427	ILE	2.9
1	A	198	PHE	2.8
1	B	490	PHE	2.8
1	B	379	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	2.7
1	B	386	VAL	2.7
1	B	422	ILE	2.6
1	A	420	ALA	2.6
1	A	490	PHE	2.5
1	B	487	LEU	2.4
1	A	29	PHE	2.4
1	B	385	PHE	2.4
1	B	366	LEU	2.4
1	B	387	MET	2.4
1	B	336	ILE	2.3
1	B	340	LEU	2.3
1	B	162	THR	2.3
1	A	499	THR	2.2
1	B	376	LYS	2.1
1	B	118	LEU	2.1

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](#)

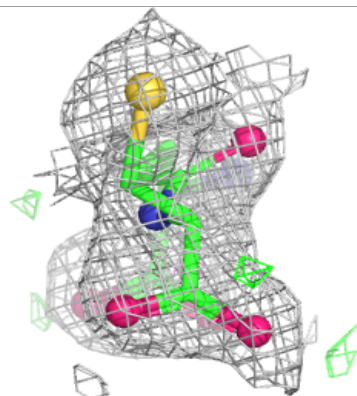
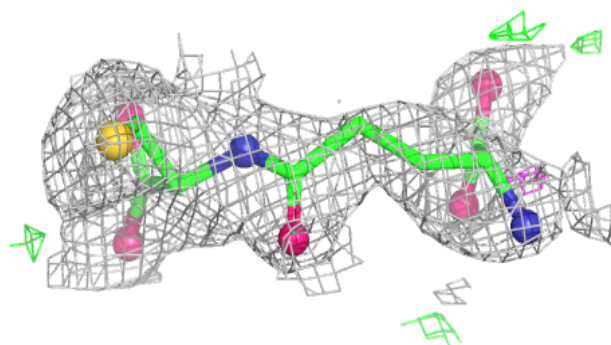
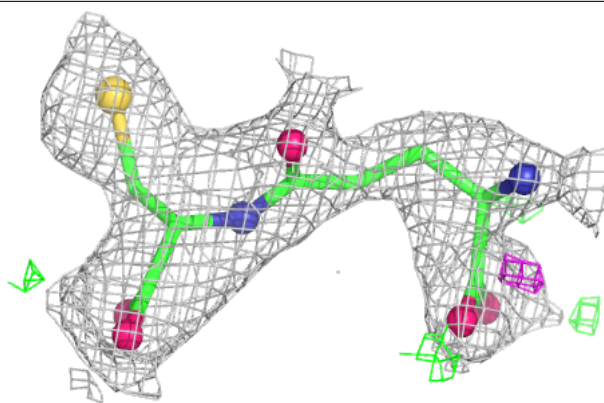
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3GC	A	501	16/16	0.83	0.11	46,51,57,61	0
2	3GC	B	501	16/16	0.84	0.10	35,43,47,50	0
2	3GC	B	502	16/16	0.87	0.14	13,20,24,24	16

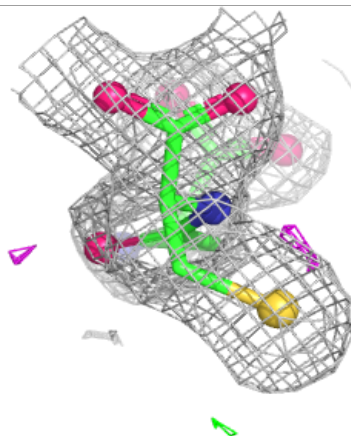
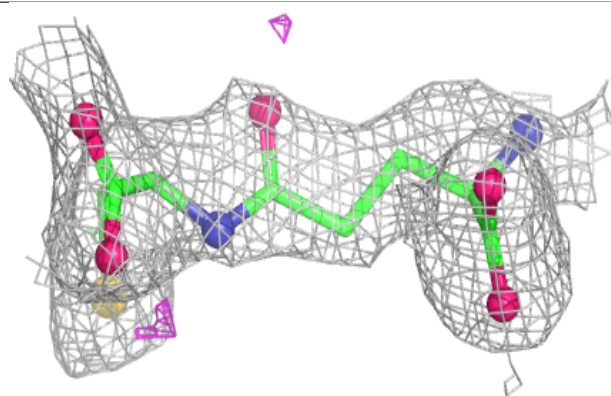
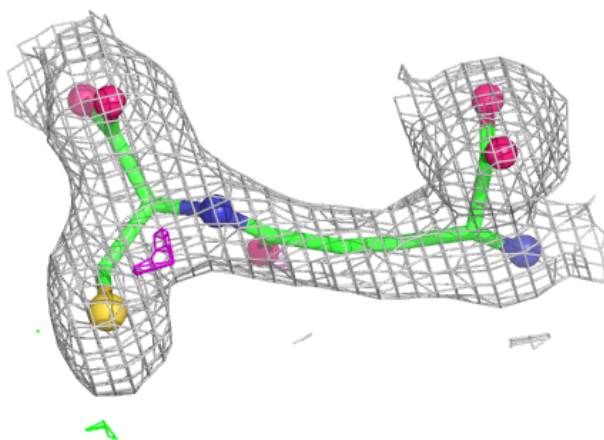
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3GC A 501:

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

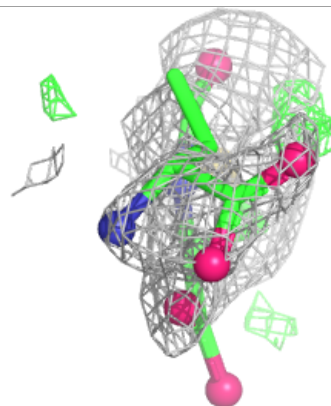
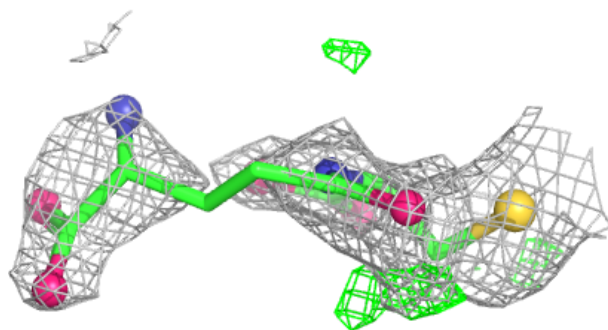
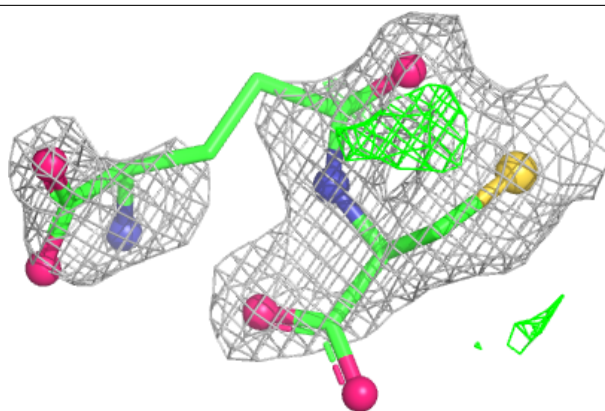
**Electron density around 3GC B 501:**

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



Electron density around 3GC B 502:

$2mF_o-DF_c$ (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.