



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:43 PM UTC

PDB ID : 1PWU / pdb_00001pwu
Title : Crystal Structure of Anthrax Lethal Factor complexed with (3-(N-hydroxycarbonylamido)-2-isobutylpropanoyl-Trp-methylamide), a known small molecule inhibitor of matrix metalloproteases.
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
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

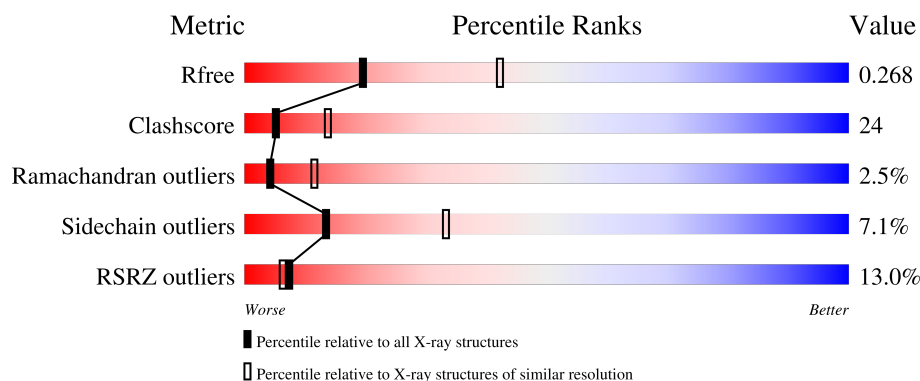
1 Overall quality at a glance

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	776	14% 52% 36% 7% • •
1	B	776	11% 55% 34% 6% 5%

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
3	GM6	A	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12238 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			6134	3897	1032	1197	8			
1	B	736	Total	C	N	O	S	0	0	0
			6046	3846	1014	1178	8			

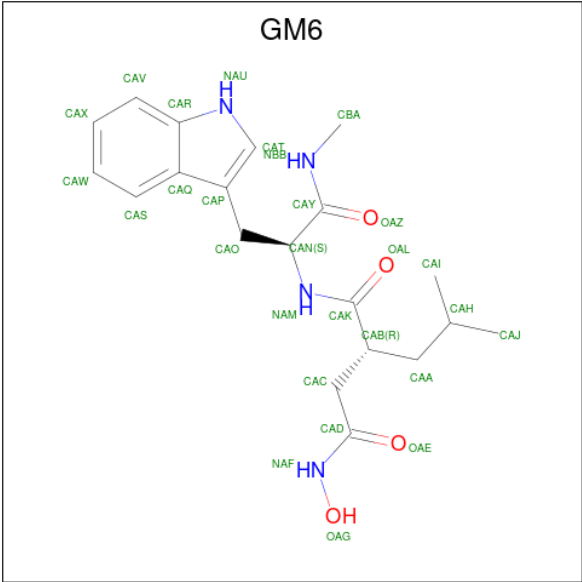
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	687	CYS	GLU	engineered mutation	UNP P15917
B	687	CYS	GLU	engineered mutation	UNP P15917

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3-(N-HYDROXYCARBOXAMIDO)-2-ISOBUTYLPROPANOYL-TRP-MET HYLAMIDE (CCD ID: GM6) (formula: C₂₀H₂₈N₄O₄).



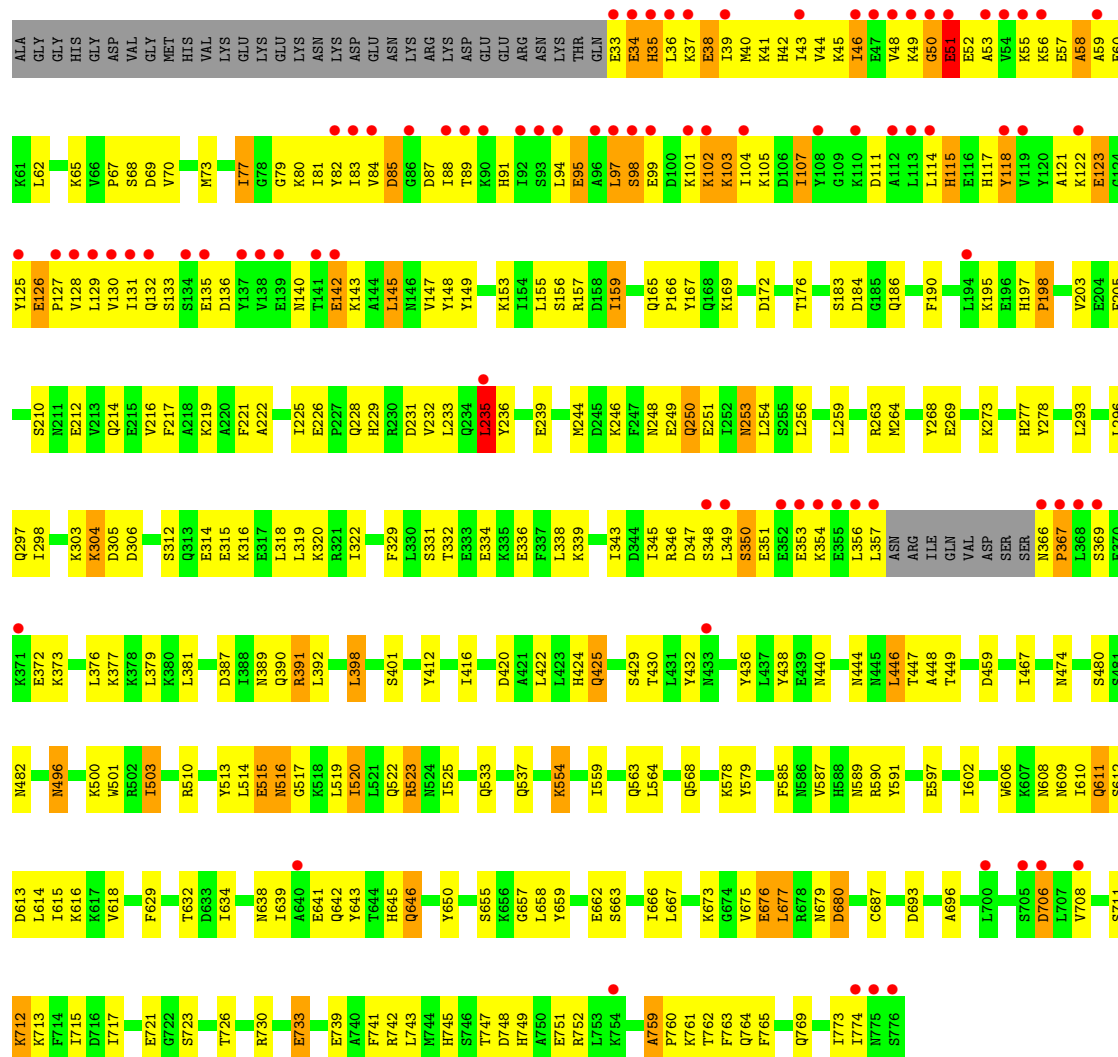
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	20	4	4		
3	B	1	Total	C	N	O	0	0
			28	20	4	4		

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.

Chain A: 14% 52% 36% 7% . .

● Molecule 1: Lethal factor

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	33.10 – 2.70 33.10 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.7 (33.10-2.70) 93.7 (33.10-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.270 0.234 , 0.268	Depositor DCC
R_{free} test set	3280 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12238	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: GM6, ZN

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	0.45	0/6243	0.98	25/8411 (0.3%)
1	B	0.50	0/6154	0.99	26/8290 (0.3%)
All	All	0.48	0/12397	0.99	51/16701 (0.3%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	GLN	OE1-CD-NE2	-10.54	112.06	122.60
1	A	323	GLN	OE1-CD-NE2	-10.43	112.17	122.60
1	A	362	VAL	N-CA-C	10.39	121.54	111.67
1	B	646	GLN	OE1-CD-NE2	-9.18	113.42	122.60
1	B	642	GLN	OE1-CD-NE2	-9.10	113.50	122.60
1	A	126	GLU	CA-C-N	8.88	128.95	119.90
1	A	126	GLU	C-N-CA	8.88	128.95	119.90
1	A	361	GLN	N-CA-C	8.49	120.23	110.97
1	A	589	ASN	N-CA-C	7.97	121.42	109.95
1	B	590	ARG	N-CA-C	7.63	122.03	112.87
1	B	759	ALA	CA-C-N	7.54	127.42	119.05
1	B	759	ALA	C-N-CA	7.54	127.42	119.05
1	B	589	ASN	N-CA-C	7.11	121.20	109.96
1	B	680	ASP	N-CA-C	-7.10	104.08	112.89
1	A	568	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	365	SER	N-CA-C	6.76	125.20	110.80
1	B	432	TYR	N-CA-C	6.71	118.40	108.60
1	B	642	GLN	CG-CD-NE2	6.70	126.45	116.40
1	A	323	GLN	CG-CD-NE2	6.64	126.36	116.40
1	A	590	ARG	N-CA-C	6.64	120.84	112.87
1	B	677	LEU	N-CA-C	-6.55	98.40	108.76
1	B	646	GLN	CG-CD-NE2	6.54	126.21	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	SER	N-CA-C	-6.14	100.50	110.20
1	A	348	SER	N-CA-C	6.14	119.71	109.95
1	B	97	LEU	CB-CA-C	-6.09	99.02	110.16
1	A	322	ILE	CA-C-N	-6.06	114.71	122.77
1	A	322	ILE	C-N-CA	-6.06	114.71	122.77
1	B	46	ILE	N-CA-C	5.96	112.59	106.21
1	A	587	VAL	N-CA-C	5.92	116.47	108.17
1	B	115	HIS	CA-C-N	-5.86	111.78	122.38
1	B	115	HIS	C-N-CA	-5.86	111.78	122.38
1	B	46	ILE	CB-CA-C	-5.72	106.82	113.22
1	A	301	GLU	CA-C-N	5.70	125.63	119.76
1	A	301	GLU	C-N-CA	5.70	125.63	119.76
1	B	235	LEU	N-CA-C	5.67	117.54	111.36
1	B	254	LEU	N-CA-C	-5.59	105.34	111.82
1	A	441	MET	N-CA-C	5.56	117.84	109.23
1	A	296	LEU	N-CA-C	-5.51	106.06	112.89
1	A	672	SER	N-CA-C	5.43	117.09	110.41
1	A	503	ILE	N-CA-C	5.39	115.71	108.17
1	B	629	PHE	N-CA-C	-5.36	98.50	107.99
1	A	263	ARG	N-CA-C	5.31	118.28	109.46
1	B	438	TYR	N-CA-C	5.23	118.09	109.72
1	B	515	GLU	N-CA-C	5.23	118.92	112.54
1	B	747	THR	N-CA-C	-5.23	105.75	111.82
1	B	430	THR	N-CA-C	-5.21	106.77	113.23
1	B	97	LEU	N-CA-C	5.19	116.96	108.76
1	A	647	ASP	N-CA-C	-5.11	105.62	111.14
1	B	263	ARG	N-CA-C	5.09	117.54	109.24
1	A	578	LYS	N-CA-C	5.07	117.47	111.33
1	A	677	LEU	N-CA-C	-5.07	99.03	107.80

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	6134	0	6123	302	0
1	B	6046	0	6033	299	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	28	11	0
3	B	28	0	28	5	0
All	All	12238	0	12212	598	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 24.

All (598) 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:104:ILE:CD1	1:B:114:LEU:HD23	1.48	1.39
1:B:104:ILE:HD11	1:B:114:LEU:CD2	1.54	1.36
1:A:48:VAL:CG2	1:A:52:GLU:HG2	1.63	1.29
1:A:99:GLU:HA	1:A:102:LYS:HD2	1.11	1.10
1:B:366:ASN:HB3	1:B:367:PRO:HD3	1.26	1.09
1:A:324:ILE:H	1:A:324:ILE:HD12	0.93	1.04
1:A:48:VAL:HG23	1:A:52:GLU:HG2	1.35	1.04
1:A:324:ILE:H	1:A:324:ILE:CD1	1.69	1.02
1:A:99:GLU:HA	1:A:102:LYS:CD	1.92	1.00
1:A:324:ILE:HD12	1:A:324:ILE:N	1.76	1.00
1:B:48:VAL:HG23	1:B:84:VAL:HA	1.47	0.95
1:B:48:VAL:CG2	1:B:84:VAL:HA	1.97	0.94
1:B:97:LEU:CD1	1:B:102:LYS:HG3	1.97	0.94
1:A:563:GLN:HE21	1:A:585:PHE:H	1.08	0.93
1:B:712:LYS:H	1:B:712:LYS:HD2	1.34	0.93
1:B:51:GLU:OE2	1:B:53:ALA:HB2	1.70	0.91
1:A:99:GLU:CA	1:A:102:LYS:HD2	2.00	0.90
1:A:435:ILE:HD12	1:A:435:ILE:H	1.33	0.89
1:A:30:LYS:HD3	1:A:33:GLU:HG3	1.52	0.88
1:B:510:ARG:H	1:B:522:GLN:HE21	0.91	0.88
1:A:354:LYS:HB3	1:A:358:ASN:HD21	1.38	0.87
1:B:98:SER:OG	1:B:101:LYS:HG2	1.73	0.87
1:A:704:GLN:HG2	1:A:705:SER:H	1.40	0.87
1:A:615:ILE:O	1:A:619:THR:HG23	1.75	0.86
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.56	0.86
1:A:48:VAL:CG2	1:A:52:GLU:CG	2.53	0.85
1:A:369:SER:O	1:A:373:LYS:HG2	1.76	0.85
1:A:712:LYS:HD2	1:A:713:LYS:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLU:O	1:A:359:ARG:HB2	1.77	0.84
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.41	0.84
1:B:97:LEU:HD13	1:B:102:LYS:HG3	1.55	0.84
1:B:366:ASN:HB3	1:B:367:PRO:CD	2.07	0.84
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.76	0.83
1:B:103:LYS:HE2	1:B:111:ASP:OD1	1.79	0.83
1:A:354:LYS:HB3	1:A:358:ASN:ND2	1.93	0.83
1:A:721:GLU:HA	1:A:724:ASN:HD22	1.41	0.83
1:A:715:ILE:HG22	1:A:719:LYS:HE2	1.61	0.82
1:B:510:ARG:H	1:B:522:GLN:NE2	1.76	0.82
1:B:366:ASN:CB	1:B:367:PRO:HD3	2.09	0.82
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.58	0.82
1:A:435:ILE:HD12	1:A:435:ILE:N	1.95	0.81
1:B:712:LYS:HD2	1:B:712:LYS:N	1.96	0.81
1:A:322:ILE:HD11	1:A:376:LEU:HD11	1.64	0.80
1:A:48:VAL:HG22	1:A:52:GLU:HG2	1.60	0.80
1:B:253:ASN:HD22	1:B:253:ASN:H	1.25	0.80
1:B:169:LYS:HD2	1:B:533:GLN:NE2	1.97	0.80
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.62	0.79
1:A:346:ARG:HD2	1:A:346:ARG:N	1.95	0.79
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.65	0.79
1:B:510:ARG:N	1:B:522:GLN:HE21	1.76	0.79
1:B:48:VAL:HG21	1:B:133:SER:HB3	1.63	0.79
1:A:46:ILE:HG22	1:A:83:ILE:HB	1.65	0.78
1:A:563:GLN:NE2	1:A:585:PHE:H	1.81	0.78
1:B:88:ILE:HD11	1:B:118:TYR:C	2.10	0.77
1:B:304:LYS:CE	1:B:304:LYS:H	1.98	0.77
1:B:677:LEU:HD11	3:B:2001:GM6:HAI2	1.67	0.77
1:B:712:LYS:H	1:B:712:LYS:CD	1.93	0.76
1:A:677:LEU:HD11	3:A:1001:GM6:HAI2	1.68	0.75
1:B:126:GLU:N	1:B:127:PRO:HD3	2.00	0.75
1:B:39:ILE:O	1:B:43:ILE:HG12	1.86	0.75
1:B:748:ASP:OD2	1:B:751:GLU:HG2	1.87	0.74
1:B:693:ASP:OD2	1:B:708:VAL:HG12	1.86	0.74
1:A:721:GLU:HA	1:A:724:ASN:ND2	2.03	0.74
1:A:704:GLN:HG2	1:A:705:SER:N	2.02	0.74
1:B:121:ALA:HB2	1:B:129:LEU:HD23	1.70	0.74
1:A:268:TYR:HB3	1:B:125:TYR:CE2	2.23	0.73
1:B:34:GLU:O	1:B:37:LYS:N	2.21	0.73
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.69	0.72
1:A:741:PHE:O	1:A:745:HIS:HD2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:HG22	1:B:105:LYS:H	1.54	0.72
1:A:439:GLU:HB2	1:A:486:VAL:HG12	1.72	0.72
1:B:320:LYS:HB3	1:B:356:LEU:HD21	1.71	0.71
1:A:268:TYR:HB3	1:B:125:TYR:CZ	2.24	0.71
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.56	0.71
1:A:322:ILE:CD1	1:A:376:LEU:HD11	2.21	0.71
1:A:317:GLU:HA	1:A:320:LYS:HE3	1.73	0.70
1:A:346:ARG:HD2	1:A:346:ARG:H	1.53	0.70
1:B:97:LEU:HD12	1:B:102:LYS:HG3	1.72	0.70
1:B:104:ILE:HG22	1:B:105:LYS:N	2.06	0.70
1:B:346:ARG:HH12	1:B:357:LEU:HD13	1.56	0.70
1:A:676:GLU:OE1	1:A:676:GLU:HA	1.92	0.70
1:B:169:LYS:HD2	1:B:533:GLN:HE22	1.57	0.69
1:A:55:LYS:HG2	1:A:133:SER:OG	1.93	0.69
1:A:496:ASN:C	1:A:496:ASN:HD22	1.99	0.69
1:A:275:LYS:NZ	1:A:279:GLN:HE22	1.90	0.69
1:A:103:LYS:HD2	1:A:111:ASP:HB3	1.73	0.69
1:A:753:LEU:O	1:A:756:GLN:HB3	1.93	0.69
1:A:675:VAL:HG22	3:A:1001:GM6:HAJ1	1.74	0.68
1:B:662:GLU:H	1:B:662:GLU:CD	2.02	0.68
1:B:312:SER:OG	1:B:315:GLU:HG3	1.94	0.68
1:B:611:GLN:NE2	1:B:613:ASP:HB2	2.08	0.67
1:A:48:VAL:HG23	1:A:52:GLU:CG	2.18	0.67
1:A:349:LEU:O	1:A:352:GLU:HG2	1.95	0.67
1:B:643:TYR:HA	1:B:646:GLN:HG3	1.76	0.67
1:A:611:GLN:NE2	1:A:770:ILE:HG21	2.11	0.66
1:A:123:GLU:HG2	1:A:124:GLY:H	1.61	0.66
1:B:107:ILE:HD13	1:B:107:ILE:O	1.96	0.66
1:B:98:SER:O	1:B:101:LYS:HG3	1.96	0.66
1:B:677:LEU:HD11	3:B:2001:GM6:CAI	2.26	0.66
1:B:563:GLN:NE2	1:B:585:PHE:H	1.94	0.66
1:A:316:LYS:O	1:A:320:LYS:HG3	1.97	0.65
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.31	0.65
1:B:48:VAL:HG13	1:B:85:ASP:OD2	1.97	0.65
1:A:57:GLU:O	1:A:61:LYS:HG2	1.96	0.65
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.32	0.65
1:B:40:MET:O	1:B:44:VAL:HB	1.97	0.65
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.79	0.65
1:B:608:ASN:C	1:B:609:ASN:HD22	2.05	0.65
1:B:496:ASN:N	1:B:496:ASN:HD22	1.94	0.64
1:B:706:ASP:OD1	1:B:706:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD12	1:A:505:LEU:HD11	1.78	0.64
1:A:83:ILE:HD12	1:A:83:ILE:N	2.12	0.64
1:A:182:ASP:OD2	1:A:184:ASP:HB2	1.98	0.64
1:B:331:SER:OG	1:B:334:GLU:HG3	1.98	0.64
1:A:728:TYR:CE2	3:A:1001:GM6:HAH	2.33	0.64
1:A:175:ASN:HA	1:A:178:LYS:HG2	1.80	0.64
1:A:312:SER:HB3	1:A:315:GLU:HG3	1.80	0.64
1:B:480:SER:HB3	1:B:525:ILE:HG22	1.78	0.64
1:A:98:SER:O	1:A:102:LYS:HG3	1.98	0.63
1:A:48:VAL:HG22	1:A:52:GLU:CG	2.25	0.63
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.27	0.63
1:A:264:MET:HE3	1:A:265:LEU:CD2	2.29	0.63
1:B:496:ASN:HD22	1:B:496:ASN:H	1.47	0.63
1:B:474:ASN:HB3	1:B:597:GLU:HG3	1.80	0.63
1:A:268:TYR:HB3	1:B:125:TYR:OH	1.99	0.62
1:A:314:GLU:O	1:A:317:GLU:HB2	1.99	0.62
1:A:564:LEU:O	1:A:568:GLN:HG3	1.99	0.62
1:A:474:ASN:HB3	1:A:597:GLU:HG3	1.81	0.62
1:B:401:SER:OG	1:B:638:ASN:ND2	2.28	0.62
1:A:655:SER:HB2	3:A:1001:GM6:OAL	2.00	0.62
1:B:48:VAL:HG22	1:B:84:VAL:HA	1.78	0.62
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.81	0.62
1:B:126:GLU:N	1:B:127:PRO:CD	2.63	0.62
1:A:48:VAL:HG22	1:A:52:GLU:OE2	2.00	0.62
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.15	0.61
1:B:140:ASN:C	1:B:140:ASN:HD22	2.08	0.61
1:B:89:THR:HG22	1:B:95:GLU:HG2	1.82	0.61
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.35	0.61
1:B:655:SER:HB2	3:B:2001:GM6:OAL	1.99	0.61
1:A:535:ILE:HD13	1:A:544:ARG:HB2	1.83	0.61
1:B:167:TYR:CZ	1:B:203:VAL:HG21	2.36	0.61
1:B:249:GLU:O	1:B:250:GLN:HG3	2.00	0.61
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.31	0.61
1:B:221:PHE:HA	1:B:244:MET:HE2	1.81	0.61
1:B:578:LYS:O	1:B:579:TYR:HB2	2.01	0.61
1:B:34:GLU:O	1:B:36:LEU:N	2.34	0.61
1:A:322:ILE:HD11	1:A:376:LEU:CD1	2.30	0.60
1:B:98:SER:O	1:B:101:LYS:CG	2.49	0.60
1:B:34:GLU:C	1:B:36:LEU:N	2.59	0.60
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.66	0.60
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG23	1:B:84:VAL:CA	2.28	0.60
1:B:373:LYS:HG2	1:B:377:LYS:HE3	1.84	0.60
1:B:662:GLU:OE2	1:B:662:GLU:N	2.24	0.60
1:B:34:GLU:O	1:B:35:HIS:C	2.44	0.60
1:A:49:LYS:HB2	1:A:49:LYS:NZ	2.17	0.60
1:A:263:ARG:HB2	1:A:266:SER:HB2	1.84	0.60
1:A:45:LYS:NZ	1:A:45:LYS:HB3	2.17	0.59
1:B:304:LYS:H	1:B:304:LYS:HE3	1.67	0.59
1:A:244:MET:HE3	1:A:244:MET:HA	1.83	0.59
1:A:99:GLU:OE2	1:A:102:LYS:HE3	2.02	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.18	0.59
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.02	0.59
1:B:741:PHE:O	1:B:745:HIS:HD2	1.85	0.59
1:B:97:LEU:HD12	1:B:102:LYS:CG	2.32	0.59
1:A:715:ILE:O	1:A:719:LYS:HG3	2.02	0.59
1:B:97:LEU:HD12	1:B:102:LYS:CE	2.33	0.59
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.68	0.58
1:A:424:HIS:O	1:A:510:ARG:HD2	2.03	0.58
1:B:449:THR:HA	1:B:673:LYS:HD3	1.85	0.58
1:B:102:LYS:HA	1:B:114:LEU:CD1	2.34	0.58
1:A:103:LYS:HE3	1:A:113:LEU:CD2	2.33	0.58
1:A:107:ILE:HG12	1:A:149:TYR:CG	2.38	0.58
1:A:737:PHE:CE1	1:A:766:ILE:HG12	2.39	0.58
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.85	0.58
1:B:97:LEU:HD12	1:B:102:LYS:HE3	1.85	0.58
1:B:264:MET:O	1:B:268:TYR:HD1	1.87	0.58
1:A:97:LEU:HD23	1:A:98:SER:N	2.18	0.58
1:A:657:GLY:O	3:A:1001:GM6:HAC2	2.03	0.58
1:A:677:LEU:HD11	3:A:1001:GM6:CAI	2.33	0.58
1:A:696:ALA:HB2	1:A:773:ILE:HD11	1.86	0.58
1:A:767:ASN:O	1:A:771:LYS:HG3	2.03	0.58
1:B:35:HIS:O	1:B:39:ILE:HG13	2.04	0.58
1:A:204:GLU:CD	1:A:204:GLU:H	2.11	0.58
1:A:691:ALA:O	1:A:694:ASP:HB3	2.04	0.57
1:A:119:VAL:HG12	1:A:131:ILE:HG12	1.84	0.57
1:B:104:ILE:CD1	1:B:114:LEU:CD2	2.40	0.57
1:A:35:HIS:HD2	1:A:68:SER:OG	1.87	0.57
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.37	0.57
1:A:577:PRO:O	1:A:580:THR:CG2	2.51	0.57
1:A:301:GLU:HG3	1:A:302:PRO:HD2	1.86	0.57
1:B:48:VAL:HG23	1:B:83:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.40	0.56
1:B:723:SER:CB	1:B:730:ARG:HD3	2.36	0.56
1:B:733:GLU:CD	1:B:733:GLU:H	2.11	0.56
1:B:765:PHE:O	1:B:769:GLN:HG2	2.05	0.56
1:A:104:ILE:HG13	1:A:120:TYR:HE1	1.71	0.56
1:B:496:ASN:H	1:B:496:ASN:ND2	2.04	0.56
1:A:107:ILE:HG12	1:A:149:TYR:CD1	2.41	0.56
1:B:319:LEU:HD23	1:B:345:ILE:HG13	1.86	0.56
1:B:117:HIS:ND1	1:B:118:TYR:CD1	2.74	0.56
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.71	0.56
1:B:639:ILE:HG22	1:B:641:GLU:H	1.71	0.56
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.05	0.56
1:A:435:ILE:N	1:A:435:ILE:CD1	2.62	0.55
1:A:101:LYS:C	1:A:103:LYS:H	2.14	0.55
1:A:312:SER:HB3	1:A:315:GLU:CG	2.35	0.55
1:A:577:PRO:O	1:A:580:THR:HG23	2.07	0.55
1:A:348:SER:O	1:A:349:LEU:HB2	2.06	0.55
1:A:371:LYS:H	1:A:371:LYS:HD3	1.71	0.55
1:A:712:LYS:CD	1:A:713:LYS:H	2.17	0.55
1:B:339:LYS:O	1:B:343:ILE:HG12	2.06	0.55
1:B:440:ASN:HD21	1:B:500:LYS:NZ	2.05	0.55
1:A:675:VAL:CG2	3:A:1001:GM6:HAJ1	2.36	0.55
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.89	0.55
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.69	0.55
1:B:516:ASN:ND2	1:B:516:ASN:H	2.04	0.55
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.42	0.55
1:B:516:ASN:N	1:B:516:ASN:HD22	2.05	0.55
1:A:84:VAL:HG11	1:A:91:HIS:CD2	2.42	0.54
1:A:420:ASP:OD1	1:A:523:ARG:HD3	2.07	0.54
1:B:186:GLN:HE21	1:B:195:LYS:HG2	1.72	0.54
1:B:332:THR:O	1:B:336:GLU:HG2	2.07	0.54
1:B:322:ILE:HD13	1:B:376:LEU:HD21	1.90	0.54
1:A:65:LYS:HE2	1:A:227:PRO:HG2	1.88	0.54
1:B:155:LEU:HA	1:B:159:ILE:HG13	1.89	0.54
1:A:618:VAL:O	1:A:622:LEU:HG	2.08	0.54
1:B:149:TYR:HA	1:B:222:ALA:HB2	1.89	0.54
1:B:440:ASN:ND2	1:B:500:LYS:HG2	2.23	0.54
1:A:352:GLU:HA	1:A:355:GLU:HG2	1.90	0.54
1:B:304:LYS:HE3	1:B:304:LYS:N	2.22	0.54
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.43	0.54
1:B:675:VAL:HG13	1:B:675:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.88	0.54
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.90	0.54
1:A:675:VAL:O	1:A:675:VAL:HG23	2.08	0.54
1:B:79:GLY:HA2	1:B:127:PRO:HB2	1.90	0.54
3:A:1001:GM6:HAJ2	3:A:1001:GM6:CAK	2.38	0.53
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.42	0.53
1:B:316:LYS:O	1:B:320:LYS:HG3	2.08	0.53
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.19	0.53
1:A:313:GLN:H	1:A:313:GLN:CD	2.17	0.53
1:A:379:LEU:O	1:A:383:ILE:HG12	2.08	0.53
1:A:48:VAL:HG11	1:A:55:LYS:HD3	1.90	0.53
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.91	0.53
1:A:662:GLU:OE2	1:A:662:GLU:N	2.29	0.53
1:B:37:LYS:O	1:B:41:LYS:N	2.42	0.53
1:B:46:ILE:HD11	1:B:56:LYS:HG3	1.90	0.53
1:A:40:MET:HE3	1:A:63:LEU:HD12	1.91	0.53
1:A:614:LEU:O	1:A:618:VAL:HG23	2.09	0.53
1:A:48:VAL:HG22	1:A:52:GLU:CD	2.34	0.52
1:A:244:MET:HE2	1:A:248:ASN:HD21	1.74	0.52
1:B:347:ASP:OD1	1:B:347:ASP:O	2.28	0.52
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.91	0.52
3:B:2001:GM6:HAJ2	3:B:2001:GM6:CAK	2.39	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.10	0.52
1:A:675:VAL:HG13	3:A:1001:GM6:OAZ	2.08	0.52
1:B:726:THR:OG1	1:B:739:GLU:HG2	2.09	0.52
1:A:97:LEU:HD23	1:A:98:SER:H	1.75	0.52
1:A:268:TYR:CB	1:B:125:TYR:CE2	2.93	0.52
1:A:768:ASP:HA	1:A:771:LYS:HE2	1.91	0.52
1:B:346:ARG:NH1	1:B:357:LEU:HD13	2.24	0.52
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.25	0.52
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.91	0.52
1:A:658:LEU:HD22	1:A:659:TYR:N	2.25	0.52
1:B:297:GLN:O	1:B:298:ILE:HD13	2.09	0.52
1:B:516:ASN:ND2	1:B:516:ASN:N	2.57	0.52
1:B:749:HIS:HA	1:B:752:ARG:HD2	1.91	0.52
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.39	0.52
1:B:153:LYS:O	1:B:157:ARG:HB3	2.10	0.52
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.92	0.52
1:B:723:SER:HA	1:B:730:ARG:CG	2.39	0.52
1:A:612:SER:O	1:A:616:LYS:HG3	2.09	0.52
1:A:712:LYS:HD2	1:A:713:LYS:N	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:CD1	1:B:56:LYS:HG3	2.40	0.52
1:B:156:SER:HB3	1:B:217:PHE:CD2	2.45	0.52
1:A:126:GLU:N	1:A:127:PRO:HD3	2.25	0.52
1:A:163:ILE:HG13	1:A:165:GLN:HG3	1.91	0.52
1:A:178:LYS:HG3	1:A:179:ASN:N	2.23	0.52
1:A:443:ILE:HD12	1:A:454:LEU:HD22	1.92	0.52
1:B:140:ASN:HD22	1:B:142:GLU:H	1.57	0.52
1:B:250:GLN:O	1:B:253:ASN:ND2	2.43	0.52
1:A:456:ASP:HB3	1:A:459:ASP:O	2.10	0.52
1:A:679:ASN:HD22	1:A:679:ASN:H	1.58	0.52
1:B:253:ASN:H	1:B:253:ASN:ND2	2.02	0.52
1:A:695:TYR:O	1:A:698:TYR:HB3	2.10	0.51
1:B:33:GLU:C	1:B:36:LEU:HB2	2.36	0.51
1:B:711:SER:O	1:B:715:ILE:HG13	2.10	0.51
1:B:726:THR:HG23	1:B:743:LEU:HD11	1.93	0.51
1:A:364:SER:O	1:A:365:SER:HB2	2.09	0.51
1:B:221:PHE:O	1:B:225:ILE:HG12	2.11	0.51
1:B:645:HIS:CD2	1:B:663:SER:HB3	2.45	0.51
1:A:45:LYS:HD2	1:A:82:TYR:CE2	2.46	0.51
1:A:412:TYR:O	1:A:416:ILE:HG13	2.11	0.51
1:B:564:LEU:O	1:B:568:GLN:HG3	2.10	0.51
1:B:104:ILE:CG2	1:B:105:LYS:N	2.74	0.51
1:B:726:THR:CG2	1:B:743:LEU:HD11	2.41	0.51
1:A:118:TYR:CD1	1:A:118:TYR:N	2.79	0.51
1:A:160:LEU:HB3	1:A:165:GLN:HB2	1.93	0.51
1:A:616:LYS:O	1:A:620:ASN:HB2	2.11	0.51
1:B:88:ILE:HD11	1:B:118:TYR:CA	2.40	0.51
1:B:104:ILE:CG2	1:B:105:LYS:H	2.22	0.51
1:B:304:LYS:H	1:B:304:LYS:HE2	1.74	0.51
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.92	0.50
1:B:632:THR:OG1	1:B:634:ILE:HG12	2.11	0.50
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.11	0.50
1:A:43:ILE:HD11	1:A:71:LEU:HG	1.93	0.50
1:A:119:VAL:HG11	1:A:147:VAL:HG22	1.92	0.50
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.11	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.45	0.50
1:A:95:GLU:C	1:A:97:LEU:H	2.20	0.50
1:B:88:ILE:HG23	1:B:130:VAL:CG1	2.42	0.50
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.94	0.50
1:A:98:SER:HB2	1:A:100:ASP:OD1	2.11	0.50
1:A:656:LYS:O	1:A:656:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:O	1:A:499:LEU:HB2	2.11	0.50
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.76	0.50
1:B:212:GLU:O	1:B:216:VAL:HG23	2.12	0.50
1:A:675:VAL:HG22	3:A:1001:GM6:CAJ	2.40	0.49
1:A:99:GLU:HA	1:A:102:LYS:CE	2.42	0.49
1:B:721:GLU:OE1	1:B:761:LYS:HG2	2.12	0.49
1:B:741:PHE:O	1:B:745:HIS:CD2	2.65	0.49
1:B:117:HIS:ND1	1:B:118:TYR:N	2.54	0.49
1:B:500:LYS:HE3	1:B:537:GLN:OE1	2.12	0.49
1:A:187:ASP:HA	1:A:195:LYS:NZ	2.28	0.49
1:B:36:LEU:HD21	1:B:68:SER:OG	2.12	0.49
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.95	0.49
1:B:609:ASN:C	1:B:610:ILE:HG13	2.38	0.49
1:A:333:GLU:OE2	1:A:333:GLU:HA	2.12	0.49
1:B:244:MET:CE	1:B:248:ASN:HD21	2.26	0.49
1:B:123:GLU:CD	1:B:157:ARG:HD2	2.38	0.49
1:B:723:SER:HB3	1:B:730:ARG:HD3	1.95	0.49
1:B:440:ASN:HD21	1:B:500:LYS:HZ2	1.60	0.49
1:A:677:LEU:O	1:A:678:ARG:C	2.56	0.48
1:B:55:LYS:O	1:B:58:ALA:HB3	2.12	0.48
1:B:129:LEU:HD11	1:B:131:ILE:HD11	1.95	0.48
1:A:171:LEU:HD21	1:A:201:PHE:HB2	1.95	0.48
1:B:33:GLU:HA	1:B:36:LEU:HB2	1.95	0.48
1:B:303:LYS:HB2	1:B:306:ASP:OD2	2.13	0.48
1:A:40:MET:O	1:A:44:VAL:HB	2.14	0.48
1:A:101:LYS:O	1:A:103:LYS:N	2.46	0.48
1:A:354:LYS:HD2	1:A:358:ASN:OD1	2.14	0.48
1:A:730:ARG:O	1:A:730:ARG:HG2	2.13	0.48
1:B:145:LEU:HD23	1:B:222:ALA:HB1	1.95	0.48
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.48	0.48
1:A:394:ASP:O	1:A:634:ILE:HB	2.13	0.48
1:B:723:SER:HA	1:B:730:ARG:HG2	1.95	0.48
1:B:609:ASN:HD22	1:B:609:ASN:N	2.11	0.48
1:A:67:PRO:HB2	1:A:70:VAL:HG13	1.95	0.48
1:A:323:GLN:HG2	1:A:325:ASP:H	1.78	0.48
1:B:36:LEU:O	1:B:40:MET:HG3	2.14	0.48
1:B:45:LYS:HB2	1:B:82:TYR:CE2	2.49	0.48
1:A:87:ASP:OD2	1:A:115:HIS:HA	2.15	0.47
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.48	0.47
1:A:307:ILE:HG21	1:A:341:LEU:CD1	2.45	0.47
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:HIS:NE2	1:B:663:SER:HB3	2.30	0.47
1:A:94:LEU:HD22	1:A:97:LEU:HD12	1.97	0.47
1:A:275:LYS:HZ3	1:A:279:GLN:HE22	1.59	0.47
1:A:437:LEU:HD12	1:A:505:LEU:CD1	2.44	0.47
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.15	0.47
1:A:771:LYS:C	1:A:773:ILE:H	2.23	0.47
1:B:381:LEU:HD11	1:B:650:TYR:HA	1.96	0.47
1:B:696:ALA:HB2	1:B:773:ILE:HD11	1.96	0.47
1:A:722:GLY:O	1:A:723:SER:OG	2.33	0.47
1:B:89:THR:C	1:B:91:HIS:H	2.23	0.47
1:B:759:ALA:N	1:B:760:PRO:HD3	2.30	0.47
1:A:536:LYS:HG3	1:A:537:GLN:N	2.29	0.47
1:A:303:LYS:O	1:A:307:ILE:HG12	2.15	0.46
1:A:437:LEU:CD1	1:A:505:LEU:HD11	2.45	0.46
1:B:769:GLN:HA	1:B:769:GLN:NE2	2.30	0.46
1:B:253:ASN:HD22	1:B:253:ASN:N	2.00	0.46
1:B:762:THR:O	1:B:763:PHE:C	2.59	0.46
1:A:369:SER:OG	1:A:372:GLU:HG2	2.14	0.46
1:B:34:GLU:C	1:B:36:LEU:H	2.24	0.46
1:B:50:GLY:O	1:B:55:LYS:NZ	2.48	0.46
1:A:45:LYS:HB3	1:A:45:LYS:HZ2	1.78	0.46
1:A:366:ASN:N	1:A:367:PRO:CD	2.79	0.46
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.96	0.46
1:B:210:SER:O	1:B:214:GLN:HG3	2.16	0.46
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.40	0.46
1:A:660:VAL:HG12	1:A:663:SER:H	1.81	0.46
1:B:149:TYR:HE1	1:B:219:LYS:HG3	1.81	0.46
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.49	0.46
1:A:243:TYR:CD1	1:A:243:TYR:C	2.93	0.46
1:B:87:ASP:OD2	1:B:115:HIS:HA	2.16	0.46
1:B:38:GLU:OE1	1:B:42:HIS:HB2	2.16	0.46
1:B:578:LYS:O	1:B:579:TYR:CB	2.64	0.46
1:A:301:GLU:HG3	1:A:302:PRO:CD	2.46	0.45
1:A:313:GLN:O	1:A:317:GLU:HG3	2.16	0.45
1:B:57:GLU:HA	1:B:60:GLU:HB3	1.97	0.45
1:A:360:ILE:O	1:A:364:SER:HB2	2.16	0.45
1:A:49:LYS:HB2	1:A:49:LYS:HZ2	1.79	0.45
1:B:559:ILE:HD13	1:B:587:VAL:HB	1.98	0.45
1:B:612:SER:O	1:B:616:LYS:HD3	2.16	0.45
1:A:94:LEU:O	1:A:97:LEU:HB2	2.16	0.45
1:A:103:LYS:HE3	1:A:113:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ASN:ND2	1:A:682:GLU:H	2.14	0.45
1:A:721:GLU:CA	1:A:724:ASN:HD22	2.19	0.45
1:B:118:TYR:HA	1:B:132:GLN:HG3	1.98	0.45
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.45
1:A:681:SER:O	1:A:682:GLU:C	2.59	0.45
1:B:639:ILE:CG2	1:B:641:GLU:H	2.30	0.45
1:B:666:ILE:HD12	1:B:687:CYS:HB3	1.98	0.45
1:B:48:VAL:HG23	1:B:83:ILE:C	2.42	0.45
1:B:104:ILE:HD11	1:B:114:LEU:CG	2.39	0.45
1:B:122:LYS:HB3	1:B:128:VAL:HG22	1.98	0.45
1:B:614:LEU:O	1:B:618:VAL:HG23	2.17	0.45
1:A:354:LYS:NZ	1:A:357:LEU:HD23	2.32	0.45
1:A:480:SER:OG	1:A:484:MET:HG3	2.17	0.45
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.46	0.45
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.98	0.45
1:B:84:VAL:HG22	1:B:85:ASP:N	2.32	0.45
1:B:350:SER:O	1:B:353:GLU:N	2.50	0.45
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.46	0.45
1:A:577:PRO:HB2	1:A:580:THR:HG22	1.98	0.45
1:B:117:HIS:CE1	1:B:118:TYR:CE1	3.04	0.45
1:B:149:TYR:CZ	1:B:153:LYS:HE3	2.52	0.45
1:B:231:ASP:O	1:B:235:LEU:HB2	2.17	0.45
1:B:659:TYR:HD1	1:B:666:ILE:HD13	1.82	0.45
1:A:40:MET:HE3	1:A:63:LEU:HB2	1.98	0.45
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.47	0.45
1:A:640:ALA:C	1:A:642:GLN:N	2.75	0.45
1:B:122:LYS:HE2	1:B:128:VAL:HG22	1.99	0.45
1:A:90:LYS:O	1:A:90:LYS:HG2	2.17	0.45
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.47	0.45
1:A:329:PHE:CD1	1:A:330:LEU:HG	2.52	0.44
1:A:741:PHE:O	1:A:745:HIS:CD2	2.62	0.44
1:A:204:GLU:O	1:A:208:GLN:HG2	2.18	0.44
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.17	0.44
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.98	0.44
1:A:40:MET:CE	1:A:63:LEU:HD12	2.47	0.44
1:A:118:TYR:CE2	1:A:143:LYS:HA	2.53	0.44
1:A:167:TYR:OH	1:A:536:LYS:HE2	2.18	0.44
1:B:48:VAL:CG2	1:B:84:VAL:CA	2.83	0.44
1:B:183:SER:O	1:B:184:ASP:C	2.60	0.44
1:A:598:SER:O	1:A:602:ILE:HG13	2.17	0.44
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HD12	1:B:102:LYS:CD	2.47	0.44
1:B:143:LYS:O	1:B:147:VAL:HG23	2.17	0.44
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.51	0.44
1:A:215:GLU:HG3	1:A:219:LYS:HE3	1.98	0.44
1:A:149:TYR:HA	1:A:222:ALA:HB2	1.98	0.44
1:A:323:GLN:NE2	1:A:325:ASP:HB2	2.31	0.44
1:A:371:LYS:H	1:A:371:LYS:CD	2.31	0.44
1:B:38:GLU:OE1	1:B:38:GLU:O	2.35	0.44
1:B:51:GLU:OE2	1:B:53:ALA:CB	2.54	0.44
1:B:81:ILE:HG23	1:B:129:LEU:HD12	1.99	0.44
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.83	0.44
1:A:566:ILE:HD13	1:A:583:ILE:HG21	2.00	0.44
1:B:97:LEU:CD1	1:B:114:LEU:HD12	2.48	0.44
1:A:225:ILE:O	1:A:227:PRO:HD3	2.18	0.44
1:A:637:PRO:HD3	1:A:654:HIS:HB2	2.00	0.44
1:B:33:GLU:CA	1:B:36:LEU:HB2	2.48	0.44
1:B:123:GLU:HG3	1:B:157:ARG:NE	2.33	0.44
1:A:725:LEU:O	1:A:726:THR:C	2.61	0.44
1:B:136:ASP:HB2	1:B:143:LYS:HD2	1.99	0.44
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.99	0.44
1:A:643:TYR:HA	1:A:646:GLN:HG3	2.00	0.43
1:B:350:SER:O	1:B:351:GLU:C	2.61	0.43
1:B:37:LYS:O	1:B:41:LYS:CB	2.66	0.43
1:B:104:ILE:CG1	1:B:114:LEU:CD2	2.96	0.43
1:A:437:LEU:HD11	1:A:519:LEU:HD12	2.00	0.43
1:A:739:GLU:CD	1:A:742:ARG:HH21	2.24	0.43
1:B:43:ILE:HA	1:B:80:LYS:HD3	1.99	0.43
1:A:46:ILE:HD12	1:A:46:ILE:O	2.18	0.43
1:A:94:LEU:HD21	1:A:122:LYS:HB2	1.99	0.43
1:A:433:ASN:O	1:A:435:ILE:HG13	2.17	0.43
1:A:693:ASP:HB2	1:A:737:PHE:CD2	2.54	0.43
1:B:244:MET:HE3	1:B:248:ASN:ND2	2.34	0.43
1:B:343:ILE:O	1:B:347:ASP:HB2	2.19	0.43
1:A:125:TYR:C	1:A:127:PRO:HD3	2.43	0.43
1:A:315:GLU:O	1:A:318:LEU:N	2.51	0.43
1:A:692:VAL:C	1:A:694:ASP:N	2.76	0.43
1:B:48:VAL:CG2	1:B:133:SER:HB3	2.41	0.43
1:B:104:ILE:HD11	1:B:114:LEU:HD23	0.60	0.43
1:B:126:GLU:O	1:B:128:VAL:HG13	2.19	0.43
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.53	0.43
1:A:354:LYS:HD2	1:A:358:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:O	1:A:367:PRO:O	2.36	0.43
1:A:693:ASP:CG	1:A:709:THR:HB	2.44	0.43
1:B:33:GLU:HA	1:B:36:LEU:HD12	2.01	0.43
1:A:107:ILE:HG22	1:A:108:TYR:CD1	2.52	0.43
1:A:637:PRO:CD	1:A:654:HIS:HB2	2.48	0.43
1:A:686:HIS:ND1	1:A:739:GLU:OE1	2.47	0.43
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.99	0.43
1:A:192:ASN:HA	1:A:195:LYS:HB2	2.00	0.43
1:A:701:ASP:C	1:A:703:ASN:N	2.76	0.43
1:B:205:PHE:CD1	1:B:205:PHE:C	2.96	0.43
1:A:293:LEU:HD22	1:A:520:ILE:HD12	2.01	0.43
1:B:184:ASP:HB3	1:B:236:TYR:HD1	1.84	0.43
1:B:197:HIS:HA	1:B:198:PRO:HD3	1.87	0.43
1:B:226:GLU:OE1	1:B:228:GLN:HB2	2.18	0.43
1:A:121:ALA:HB2	1:A:150:GLU:HG3	2.01	0.42
1:A:145:LEU:HD13	1:A:145:LEU:O	2.19	0.42
1:A:176:THR:O	1:A:180:ALA:HB2	2.19	0.42
1:B:391:ARG:HG3	1:B:412:TYR:CE1	2.54	0.42
1:B:739:GLU:OE2	1:B:739:GLU:HA	2.19	0.42
1:A:563:GLN:HE21	1:A:585:PHE:N	1.93	0.42
1:B:69:ASP:O	1:B:73:MET:HG3	2.19	0.42
1:A:372:GLU:O	1:A:375:PHE:HB3	2.20	0.42
1:A:655:SER:HB2	3:A:1001:GM6:CAK	2.50	0.42
1:B:84:VAL:O	1:B:132:GLN:HA	2.19	0.42
1:B:293:LEU:HD21	1:B:422:LEU:HD23	2.00	0.42
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.49	0.42
1:A:298:ILE:O	1:A:298:ILE:HG13	2.19	0.42
1:A:399:ILE:HD12	1:A:413:LYS:HG3	2.01	0.42
1:A:656:LYS:HD3	1:A:656:LYS:C	2.45	0.42
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.19	0.42
1:B:398:LEU:O	1:B:401:SER:HB3	2.19	0.42
1:B:677:LEU:CD2	1:B:742:ARG:CZ	2.97	0.42
1:A:292:LEU:HD22	1:A:419:ILE:HD11	2.02	0.42
1:A:307:ILE:HG21	1:A:341:LEU:HD11	2.02	0.42
1:A:675:VAL:O	1:A:676:GLU:C	2.62	0.42
1:B:655:SER:HB2	3:B:2001:GM6:CAK	2.50	0.42
1:A:352:GLU:O	1:A:355:GLU:HG2	2.19	0.42
1:B:104:ILE:O	1:B:111:ASP:HA	2.19	0.42
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.54	0.42
1:A:83:ILE:N	1:A:83:ILE:CD1	2.82	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASN:O	1:A:434:LYS:C	2.63	0.42
1:A:679:ASN:HD22	1:A:679:ASN:N	2.17	0.42
1:A:744:MET:HE3	1:A:763:PHE:CE1	2.55	0.42
1:A:241:PHE:CD1	1:A:241:PHE:C	2.98	0.42
1:B:278:TYR:HE2	1:B:425:GLN:HB3	1.85	0.42
1:B:609:ASN:C	1:B:610:ILE:CG1	2.93	0.42
1:A:119:VAL:CG1	1:A:147:VAL:HG22	2.49	0.41
1:B:89:THR:C	1:B:91:HIS:N	2.78	0.41
1:B:165:GLN:HA	1:B:166:PRO:C	2.44	0.41
1:B:229:HIS:O	1:B:232:VAL:HB	2.20	0.41
1:B:94:LEU:O	1:B:95:GLU:C	2.62	0.41
1:B:186:GLN:O	1:B:190:PHE:HB2	2.20	0.41
1:B:269:GLU:HG3	1:B:273:LYS:HE3	2.02	0.41
1:B:296:LEU:HD23	1:B:520:ILE:HD12	2.01	0.41
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.34	0.41
1:B:314:GLU:O	1:B:318:LEU:HD13	2.20	0.41
1:B:657:GLY:O	1:B:658:LEU:HB2	2.19	0.41
1:A:187:ASP:HA	1:A:195:LYS:CE	2.50	0.41
1:A:30:LYS:CD	1:A:33:GLU:HG3	2.36	0.41
1:A:135:GLU:O	1:A:135:GLU:HG2	2.20	0.41
1:B:57:GLU:O	1:B:57:GLU:HG2	2.21	0.41
1:B:140:ASN:C	1:B:140:ASN:ND2	2.76	0.41
1:B:140:ASN:OD1	1:B:143:LYS:HG3	2.19	0.41
1:A:173:VAL:O	1:A:177:ILE:HG12	2.20	0.41
1:B:50:GLY:O	1:B:55:LYS:CE	2.68	0.41
1:B:59:ALA:O	1:B:62:LEU:HB3	2.20	0.41
1:B:713:LYS:HE3	1:B:713:LYS:HB2	1.90	0.41
1:A:323:GLN:HA	1:A:324:ILE:HD12	2.01	0.41
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.34	0.41
1:A:573:ALA:C	1:A:574:LEU:HD12	2.46	0.41
1:A:50:GLY:O	1:A:51:GLU:C	2.64	0.41
1:A:187:ASP:HA	1:A:195:LYS:HE2	2.03	0.41
1:A:193:GLN:HA	1:A:193:GLN:NE2	2.35	0.41
1:A:627:GLY:HA3	1:A:664:ARG:O	2.21	0.41
1:B:145:LEU:CD2	1:B:222:ALA:HB1	2.50	0.41
1:A:321:ARG:HD2	1:A:321:ARG:HA	1.85	0.41
1:A:324:ILE:CD1	1:A:324:ILE:N	2.50	0.41
1:A:701:ASP:HB3	1:A:703:ASN:OD1	2.21	0.41
1:A:749:HIS:O	1:A:752:ARG:HB2	2.21	0.41
1:A:753:LEU:O	1:A:756:GLN:N	2.53	0.41
1:B:88:ILE:HG23	1:B:130:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:H	1:A:92:ILE:HG13	1.55	0.41
1:A:322:ILE:CD1	1:A:376:LEU:CD1	2.95	0.41
1:A:701:ASP:C	1:A:703:ASN:H	2.28	0.41
1:B:169:LYS:O	1:B:172:ASP:HB2	2.21	0.41
1:B:320:LYS:HG2	1:B:345:ILE:CG2	2.51	0.41
1:B:554:LYS:HD2	1:B:554:LYS:HA	1.79	0.41
1:B:713:LYS:O	1:B:717:ILE:HG12	2.20	0.41
1:A:204:GLU:CD	1:A:204:GLU:N	2.78	0.41
1:A:404:ILE:N	1:A:404:ILE:HD13	2.35	0.41
1:B:609:ASN:N	1:B:609:ASN:ND2	2.68	0.41
1:B:666:ILE:C	1:B:667:LEU:HD23	2.46	0.41
1:B:135:GLU:O	1:B:135:GLU:HG3	2.21	0.40
1:B:436:TYR:HA	1:B:503:ILE:O	2.21	0.40
1:B:515:GLU:C	1:B:517:GLY:H	2.29	0.40
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.02	0.40
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.21	0.40
1:B:107:ILE:HD13	1:B:107:ILE:C	2.46	0.40
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.78	0.40
1:A:743:LEU:C	1:A:745:HIS:H	2.29	0.40
1:B:88:ILE:HG22	1:B:94:LEU:CD2	2.51	0.40
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.20	0.40
1:B:118:TYR:CD1	1:B:118:TYR:N	2.89	0.40
1:B:249:GLU:C	1:B:250:GLN:HG3	2.46	0.40
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.90	0.40
1:A:94:LEU:HD12	1:A:130:VAL:HG21	2.03	0.40
1:A:97:LEU:HD22	1:A:98:SER:O	2.21	0.40
1:A:371:LYS:HD3	1:A:371:LYS:N	2.35	0.40
1:B:67:PRO:O	1:B:68:SER:C	2.65	0.40
1:B:329:PHE:HE2	1:B:373:LYS:HG3	1.86	0.40
1:B:459:ASP:C	1:B:459:ASP:OD2	2.63	0.40
1:B:602:ILE:HD11	1:B:680:ASP:HB2	2.02	0.40
1:A:155:LEU:HD12	1:A:159:ILE:HD12	2.02	0.40
1:A:392:LEU:HD21	1:A:416:ILE:HD13	2.04	0.40
1:A:744:MET:HE3	1:A:763:PHE:CD1	2.57	0.40
1:A:755:VAL:HG13	1:A:759:ALA:HB3	2.02	0.40
1:B:369:SER:OG	1:B:372:GLU:HG3	2.22	0.40
1:B:739:GLU:CD	1:B:742:ARG:HH21	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	745/776 (96%)	655 (88%)	66 (9%)	24 (3%)	3	7
1	B	732/776 (94%)	659 (90%)	60 (8%)	13 (2%)	6	18
All	All	1477/1552 (95%)	1314 (89%)	126 (8%)	37 (2%)	4	11

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	367	PRO
1	A	370	GLU
1	A	473	LYS
1	B	34	GLU
1	B	51	GLU
1	B	123	GLU
1	B	350	SER
1	A	198	PRO
1	A	251	GLU
1	A	311	LEU
1	A	349	LEU
1	A	365	SER
1	A	676	GLU
1	A	723	SER
1	B	35	HIS
1	B	198	PRO
1	B	251	GLU
1	A	123	GLU
1	A	371	LYS
1	A	678	ARG
1	A	733	GLU
1	B	50	GLY
1	B	58	ALA
1	B	367	PRO

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	96	ALA
1	A	346	ARG
1	A	369	SER
1	B	349	LEU
1	A	700	LEU
1	A	307	ILE
1	A	726	THR
1	A	772	PHE
1	B	250	GLN
1	B	126	GLU
1	A	675	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	686/710 (97%)	631 (92%)	55 (8%)	11	28
1	B	675/710 (95%)	633 (94%)	42 (6%)	16	39
All	All	1361/1420 (96%)	1264 (93%)	97 (7%)	13	33

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	46	ILE
1	A	49	LYS
1	A	60	GLU
1	A	70	VAL
1	A	107	ILE
1	A	118	TYR
1	A	119	VAL
1	A	171	LEU
1	A	208	GLN
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	239	GLU
1	A	244	MET
1	A	256	LEU
1	A	259	LEU
1	A	266	SER
1	A	296	LEU
1	A	301	GLU
1	A	319	LEU
1	A	322	ILE
1	A	324	ILE
1	A	326	SER
1	A	348	SER
1	A	359	ARG
1	A	371	LYS
1	A	404	ILE
1	A	411	GLN
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	467	ILE
1	A	491	ARG
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU
1	A	505	LEU
1	A	555	ILE
1	A	564	LEU
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	619	THR
1	A	620	ASN
1	A	626	ASN
1	A	636	LEU
1	A	639	ILE
1	A	656	LYS
1	A	658	LEU
1	A	676	GLU
1	A	679	ASN
1	A	712	LYS
1	A	757	LYS

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Mol	Chain	Res	Type
1	A	769	GLN
1	A	774	ILE
1	B	38	GLU
1	B	49	LYS
1	B	51	GLU
1	B	52	GLU
1	B	77	ILE
1	B	85	ASP
1	B	95	GLU
1	B	102	LYS
1	B	103	LYS
1	B	107	ILE
1	B	118	TYR
1	B	142	GLU
1	B	145	LEU
1	B	159	ILE
1	B	233	LEU
1	B	235	LEU
1	B	246	LYS
1	B	253	ASN
1	B	256	LEU
1	B	304	LYS
1	B	305	ASP
1	B	348	SER
1	B	354	LYS
1	B	391	ARG
1	B	398	LEU
1	B	425	GLN
1	B	446	LEU
1	B	447	THR
1	B	467	ILE
1	B	496	ASN
1	B	503	ILE
1	B	516	ASN
1	B	520	ILE
1	B	523	ARG
1	B	554	LYS
1	B	611	GLN
1	B	676	GLU
1	B	679	ASN
1	B	706	ASP
1	B	712	LYS

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Mol	Chain	Res	Type
1	B	733	GLU
1	B	764	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	42	HIS
1	A	164	ASN
1	A	192	ASN
1	A	193	GLN
1	A	197	HIS
1	A	209	ASN
1	A	211	ASN
1	A	214	GLN
1	A	242	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN
1	A	313	GLN
1	A	323	GLN
1	A	366	ASN
1	A	390	GLN
1	A	425	GLN
1	A	474	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	537	GLN
1	A	563	GLN
1	A	565	ASN
1	A	571	ASN
1	A	588	HIS
1	A	589	ASN
1	A	594	ASN
1	A	608	ASN
1	A	645	HIS
1	A	646	GLN
1	A	679	ASN
1	A	710	ASN
1	A	724	ASN
1	A	745	HIS

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Mol	Chain	Res	Type
1	A	756	GLN
1	A	769	GLN
1	B	115	HIS
1	B	132	GLN
1	B	164	ASN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	211	ASN
1	B	214	GLN
1	B	242	ASN
1	B	250	GLN
1	B	253	ASN
1	B	262	GLN
1	B	277	HIS
1	B	279	GLN
1	B	297	GLN
1	B	313	GLN
1	B	390	GLN
1	B	393	GLN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	464	ASN
1	B	474	ASN
1	B	489	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	563	GLN
1	B	568	GLN
1	B	571	ASN
1	B	586	ASN
1	B	589	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN

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Mol	Chain	Res	Type
1	B	645	HIS
1	B	679	ASN
1	B	745	HIS
1	B	756	GLN
1	B	769	GLN
1	B	775	ASN

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](#)

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	$\# Z > 2$
3	GM6	B	2001	2	29,29,29	1.19	4 (13%)	37,39,39	1.14	4 (10%)
3	GM6	A	1001	2	29,29,29	1.18	4 (13%)	37,39,39	1.18	4 (10%)

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
3	GM6	B	2001	2	-	2/28/28/28	0/2/2/2
3	GM6	A	1001	2	-	2/28/28/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	GM6	CAQ-CAP	-3.23	1.38	1.44
3	A	1001	GM6	CAQ-CAP	-3.18	1.38	1.44
3	B	2001	GM6	CAR-NAU	-2.64	1.33	1.37
3	A	1001	GM6	CAR-NAU	-2.49	1.33	1.37
3	B	2001	GM6	CAT-CAP	-2.37	1.33	1.36
3	A	1001	GM6	CAT-NAU	-2.16	1.33	1.37
3	B	2001	GM6	CAO-CAP	2.06	1.54	1.50
3	A	1001	GM6	CAT-CAP	-2.05	1.33	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GM6	CAQ-CAR-NAU	-3.50	104.61	107.52
3	B	2001	GM6	CAQ-CAR-NAU	-3.47	104.63	107.52
3	B	2001	GM6	CBA-NBB-CAY	-2.71	117.49	122.21
3	A	1001	GM6	CBA-NBB-CAY	-2.69	117.53	122.21
3	A	1001	GM6	CAR-CAQ-CAP	2.53	109.73	107.17
3	B	2001	GM6	CAR-CAQ-CAP	2.18	109.36	107.17
3	B	2001	GM6	CAV-CAR-NAU	2.06	134.04	130.74
3	A	1001	GM6	CAV-CAR-NAU	2.01	133.96	130.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GM6	CAN-CAY-NBB-CBA
3	A	1001	GM6	OAZ-CAY-NBB-CBA
3	B	2001	GM6	CAN-CAY-NBB-CBA
3	B	2001	GM6	OAZ-CAY-NBB-CBA

There are no ring outliers.

2 monomers are involved in 16 short contacts:

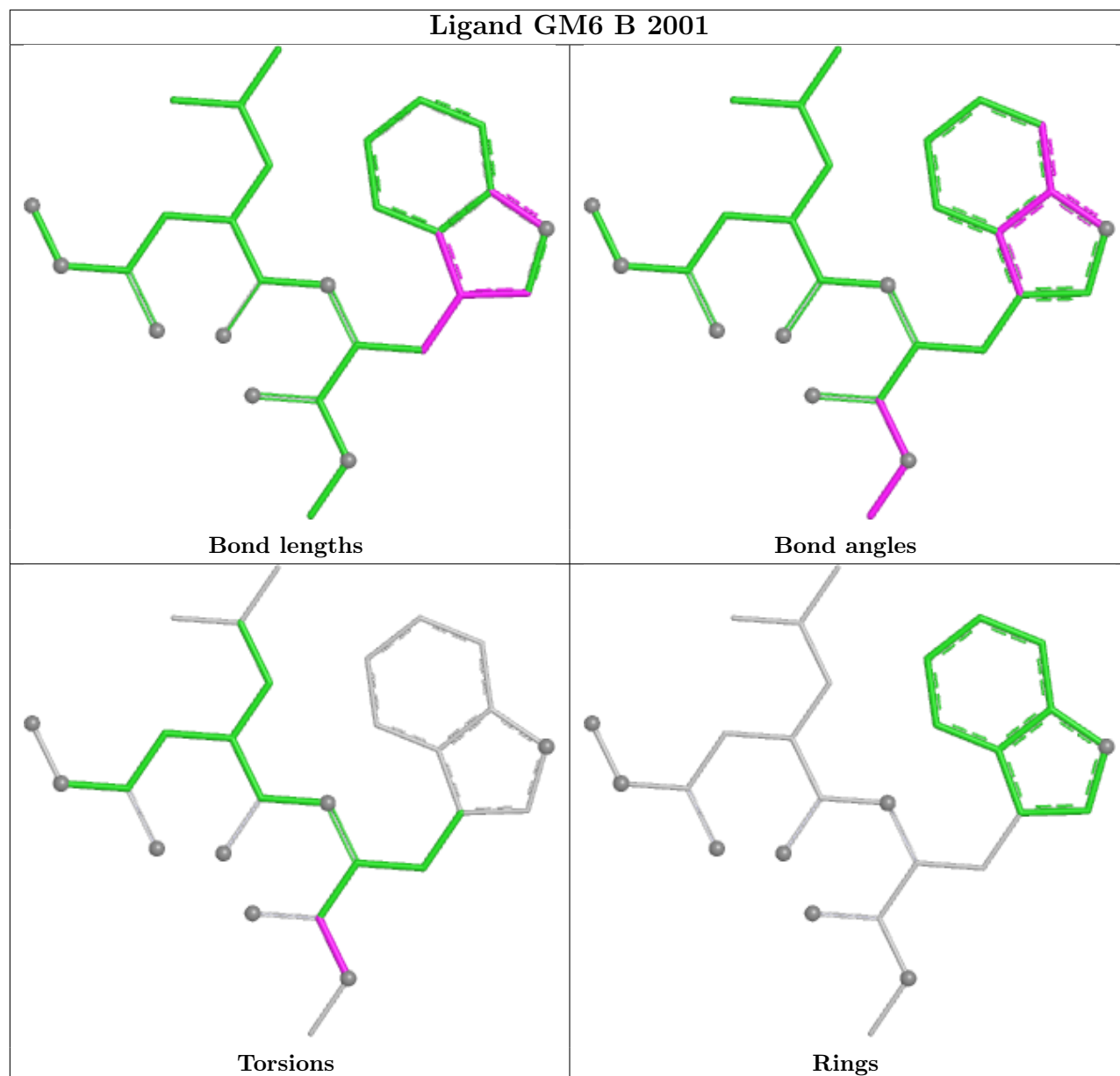
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	GM6	5	0

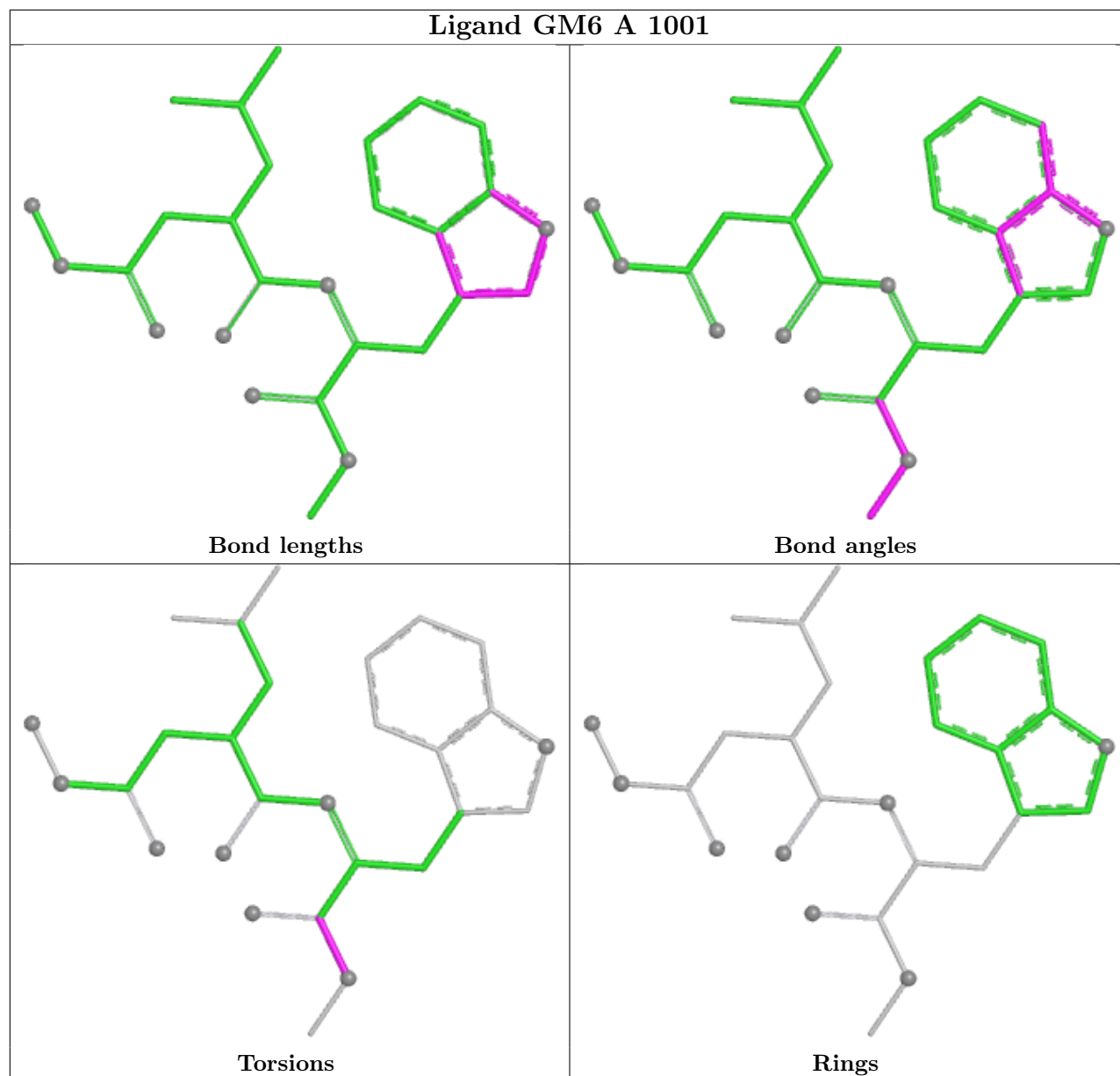
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GM6	11	0

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	747/776 (96%)	0.69	111 (14%)	5 4	21, 58, 126, 154	0
1	B	736/776 (94%)	0.45	82 (11%)	10 8	21, 51, 120, 152	0
All	All	1483/1552 (95%)	0.57	193 (13%)	7 6	21, 54, 123, 154	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	6.3
1	A	324	ILE	5.6
1	B	349	LEU	5.4
1	A	360	ILE	5.3
1	B	98	SER	5.3
1	B	48	VAL	5.1
1	B	84	VAL	5.1
1	B	92	ILE	4.9
1	A	362	VAL	4.9
1	B	357	LEU	4.9
1	A	137	TYR	4.8
1	A	349	LEU	4.6
1	B	36	LEU	4.5
1	B	50	GLY	4.5
1	A	357	LEU	4.4
1	A	104	ILE	4.4
1	A	367	PRO	4.3
1	A	92	ILE	4.3
1	B	113	LEU	4.2
1	A	356	LEU	4.2
1	B	137	TYR	4.2
1	A	320	LYS	4.0
1	B	59	ALA	4.0
1	A	319	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	3.9
1	B	49	LYS	3.8
1	A	343	ILE	3.8
1	A	368	LEU	3.8
1	B	114	LEU	3.8
1	B	55	LYS	3.6
1	A	322	ILE	3.6
1	A	180	ALA	3.6
1	A	138	VAL	3.6
1	B	54	VAL	3.6
1	B	367	PRO	3.5
1	A	713	LYS	3.5
1	A	316	LYS	3.5
1	A	321	ARG	3.5
1	B	37	LYS	3.4
1	B	705	SER	3.4
1	A	354	LYS	3.4
1	B	101	LYS	3.4
1	B	356	LEU	3.4
1	B	94	LEU	3.4
1	A	50	GLY	3.3
1	A	112	ALA	3.3
1	B	433	ASN	3.3
1	A	36	LEU	3.3
1	A	327	SER	3.3
1	B	56	LYS	3.3
1	A	358	ASN	3.2
1	A	330	LEU	3.2
1	B	353	GLU	3.2
1	B	708	VAL	3.2
1	A	101	LYS	3.1
1	A	712	LYS	3.1
1	B	88	ILE	3.1
1	B	35	HIS	3.0
1	B	125	TYR	3.0
1	B	97	LEU	3.0
1	B	368	LEU	3.0
1	A	366	ASN	3.0
1	B	775	ASN	3.0
1	A	345	ILE	3.0
1	A	97	LEU	3.0
1	A	700	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	776	SER	3.0
1	B	131	ILE	3.0
1	A	54	VAL	3.0
1	A	56	LYS	2.9
1	A	702	LYS	2.9
1	A	181	SER	2.9
1	A	88	ILE	2.9
1	B	102	LYS	2.9
1	B	235	LEU	2.9
1	A	31	THR	2.9
1	A	708	VAL	2.9
1	B	129	LEU	2.9
1	B	352	GLU	2.8
1	A	323	GLN	2.8
1	A	119	VAL	2.8
1	A	326	SER	2.8
1	A	49	LYS	2.8
1	A	352	GLU	2.8
1	B	47	GLU	2.8
1	A	198	PRO	2.8
1	B	134	SER	2.8
1	A	776	SER	2.8
1	A	753	LEU	2.8
1	A	40	MET	2.7
1	A	369	SER	2.7
1	A	125	TYR	2.7
1	B	118	TYR	2.7
1	A	346	ARG	2.7
1	A	135	GLU	2.7
1	B	34	GLU	2.7
1	A	709	THR	2.7
1	A	39	ILE	2.6
1	B	194	LEU	2.6
1	A	30	LYS	2.6
1	A	711	SER	2.6
1	B	130	VAL	2.6
1	B	142	GLU	2.6
1	A	90	LYS	2.6
1	B	122	LYS	2.6
1	A	675	VAL	2.6
1	A	93	SER	2.5
1	B	93	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	2.5
1	A	677	LEU	2.5
1	B	354	LYS	2.5
1	B	99	GLU	2.5
1	A	268	TYR	2.5
1	A	772	PHE	2.5
1	A	332	THR	2.5
1	A	288	GLU	2.5
1	A	337	PHE	2.5
1	A	714	PHE	2.5
1	B	46	ILE	2.4
1	A	134	SER	2.4
1	A	363	ASP	2.4
1	A	765	PHE	2.4
1	A	114	LEU	2.4
1	A	719	LYS	2.4
1	B	53	ALA	2.4
1	B	366	ASN	2.4
1	A	705	SER	2.4
1	A	353	GLU	2.4
1	B	33	GLU	2.4
1	B	355	GLU	2.4
1	A	371	LYS	2.4
1	A	754	LYS	2.4
1	B	86	GLY	2.4
1	B	119	VAL	2.4
1	B	43	ILE	2.4
1	A	339	LYS	2.4
1	A	86	GLY	2.4
1	A	94	LEU	2.3
1	A	715	ILE	2.3
1	B	51	GLU	2.3
1	A	769	GLN	2.3
1	A	763	PHE	2.3
1	A	83	ILE	2.3
1	B	369	SER	2.3
1	A	46	ILE	2.3
1	B	39	ILE	2.3
1	B	141	THR	2.3
1	A	44	VAL	2.3
1	A	304	LYS	2.3
1	B	90	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLU	2.3
1	A	37	LYS	2.2
1	B	89	THR	2.2
1	A	136	ASP	2.2
1	B	706	ASP	2.2
1	A	53	ALA	2.2
1	B	104	ILE	2.2
1	B	112	ALA	2.2
1	B	371	LYS	2.2
1	B	135	GLU	2.2
1	A	699	LEU	2.2
1	A	131	ILE	2.2
1	A	307	ILE	2.2
1	B	774	ILE	2.2
1	A	338	LEU	2.2
1	A	725	LEU	2.2
1	B	700	LEU	2.2
1	A	678	ARG	2.2
1	B	127	PRO	2.2
1	B	83	ILE	2.2
1	B	640	ALA	2.1
1	A	141	THR	2.1
1	A	35	HIS	2.1
1	A	100	ASP	2.1
1	B	138	VAL	2.1
1	A	724	ASN	2.1
1	B	132	GLN	2.1
1	B	108	TYR	2.1
1	B	82	TYR	2.1
1	A	203	VAL	2.1
1	A	329	PHE	2.1
1	A	340	LYS	2.1
1	B	110	LYS	2.1
1	A	342	GLN	2.1
1	A	707	LEU	2.1
1	A	48	VAL	2.1
1	A	130	VAL	2.1
1	A	701	ASP	2.0
1	B	139	GLU	2.0
1	B	348	SER	2.0
1	A	41	LYS	2.0
1	B	128	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	754	LYS	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](#)

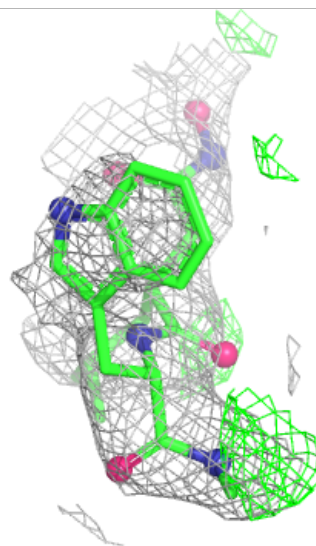
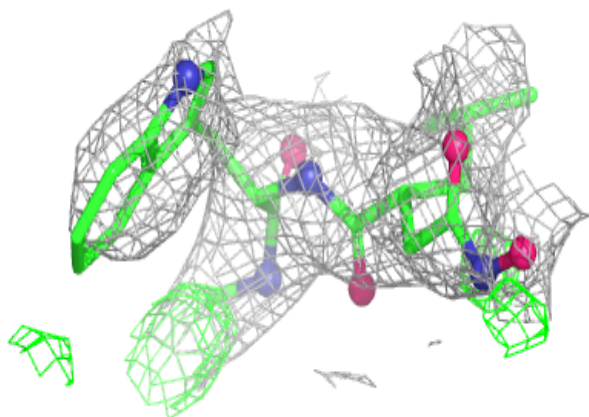
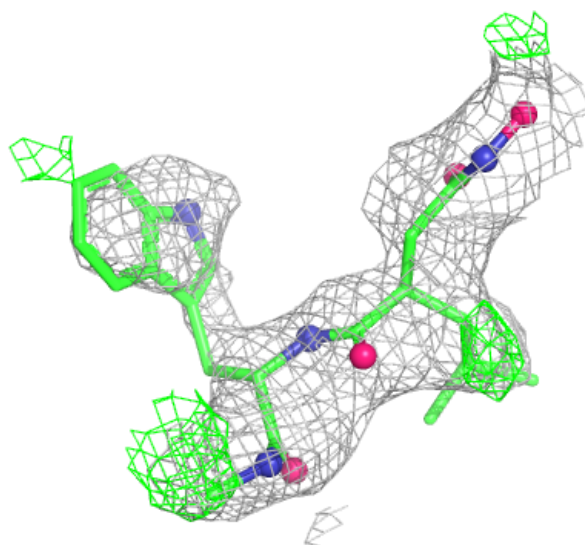
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GM6	A	1001	28/28	0.79	0.23	96,98,103,103	0
3	GM6	B	2001	28/28	0.84	0.22	95,98,102,103	0
2	ZN	A	9001	1/1	0.98	0.05	84,84,84,84	0
2	ZN	B	9002	1/1	0.99	0.03	75,75,75,75	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.

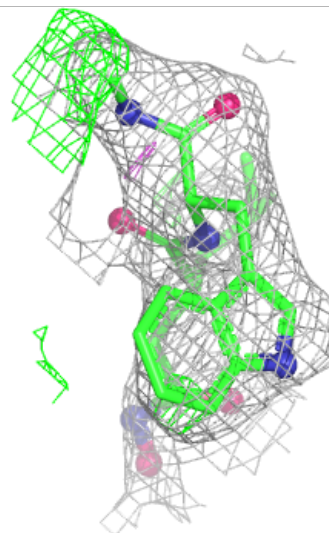
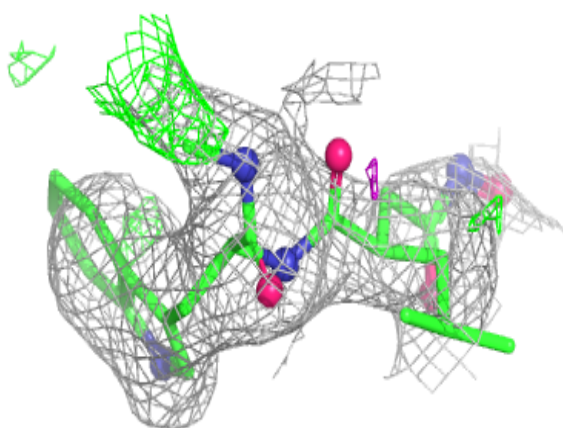
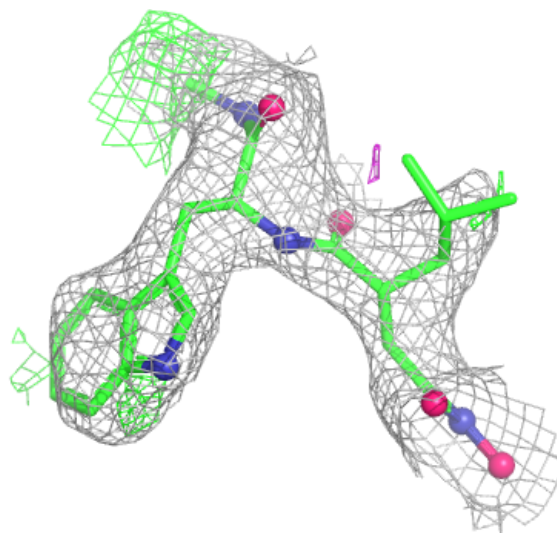
Electron density around GM6 A 1001:

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



Electron density around GM6 B 2001:

$2mF_o-DF_c$ (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.