



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 1PWQ / pdb_00001pwq
Title : Crystal structure of Anthrax Lethal Factor complexed with Thioacetyl-Tyr-Pro-Met-Amide, a metal-chelating peptidyl small molecule inhibitor
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 3.52 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

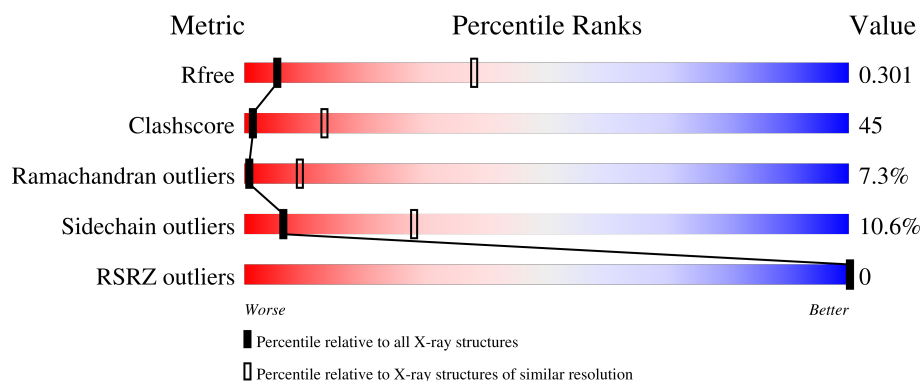
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	 29% 52% 12% • 6%
1	B	776	 28% 52% 14% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12120 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.

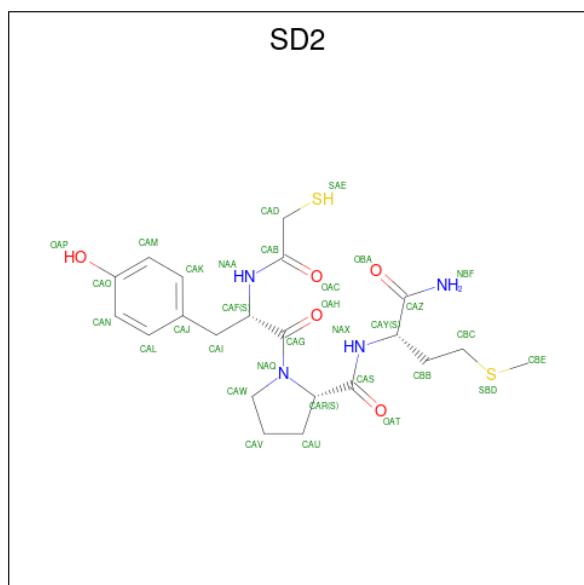
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6020	3827	1015	1171	7			
1	B	734	Total	C	N	O	S	0	0	0
			6034	3834	1017	1176	7			

- 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 N-(SULFANYLACETYL)TYROSYLPROLYLMETHIONINAMIDE (CCD ID: SD2) (formula: C₂₁H₃₀N₄O₅S₂).

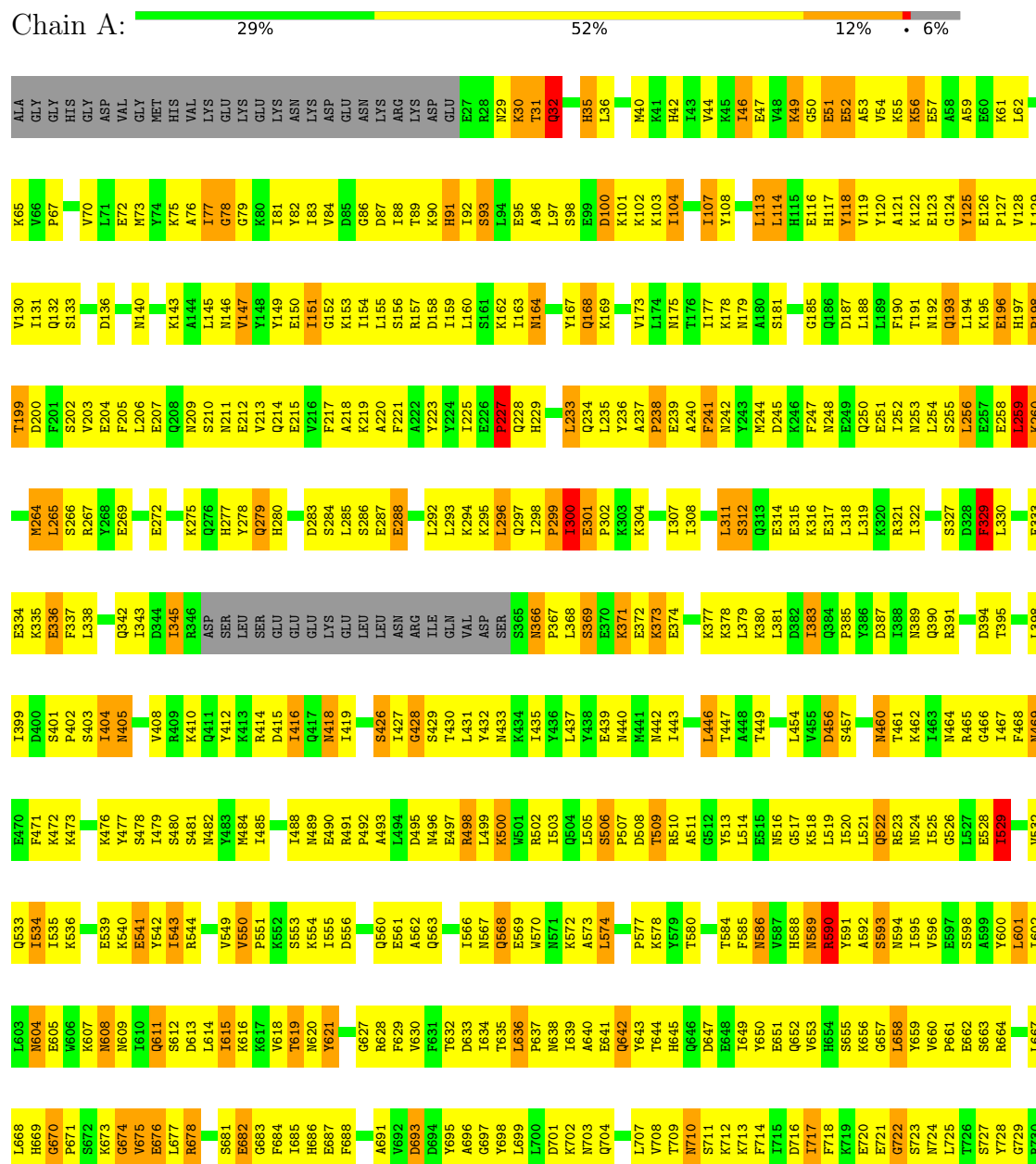


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	5	2		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	5	2		

3 Residue-property plots

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

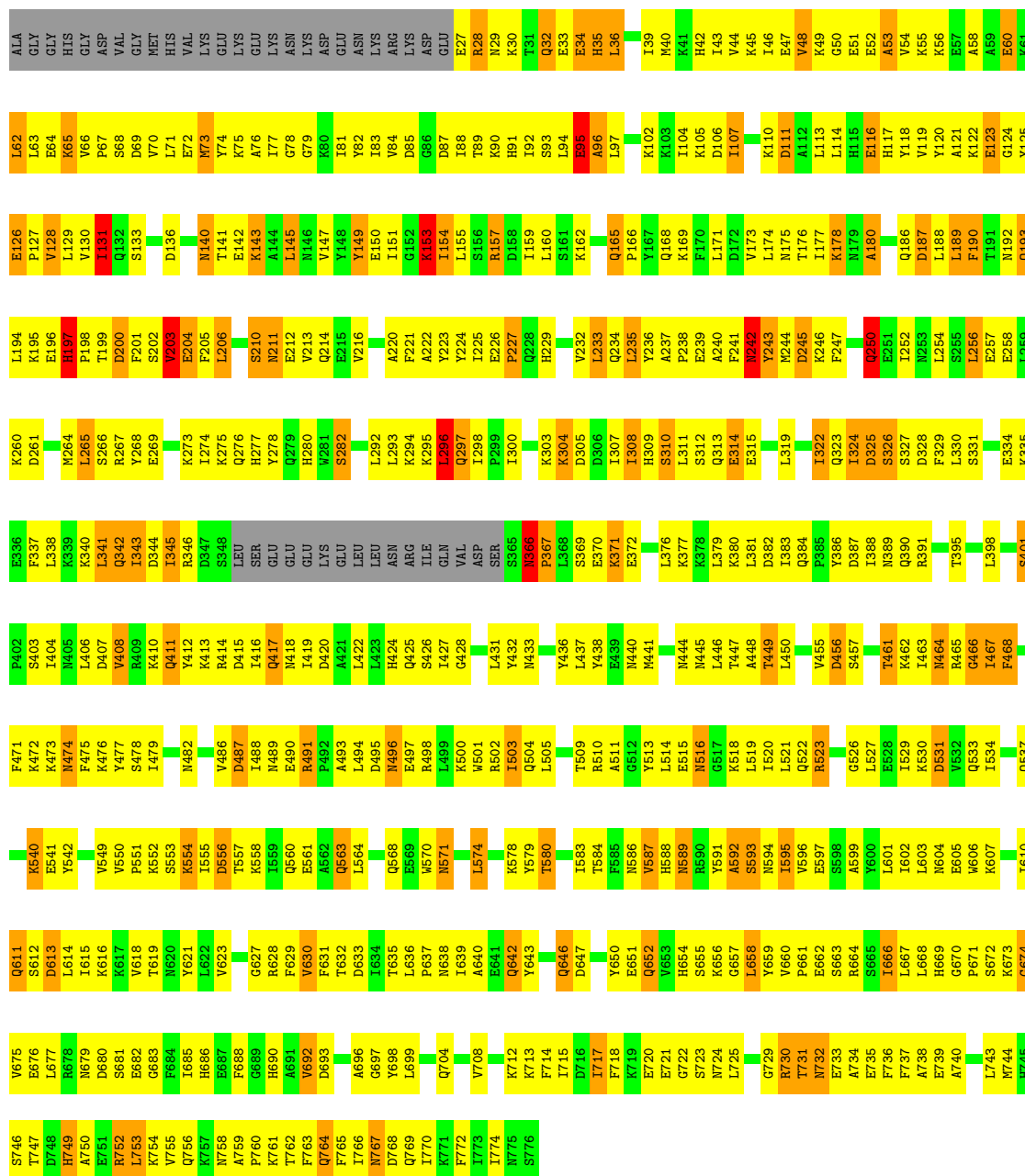
• Molecule 1: Lethal factor





• Molecule 1: Lethal factor

Chain B: 28% 52% 14% 5%



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)	24.86 – 3.52 24.86 – 3.52	Depositor EDS
% Data completeness (in resolution range)	86.7 (24.86-3.52) 82.4 (24.86-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.311 0.226 , 0.301	Depositor DCC
R_{free} test set	1331 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SD2

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	0.58	0/6128	1.08	43/8253 (0.5%)
1	B	0.62	3/6142 (0.0%)	1.12	62/8272 (0.7%)
All	All	0.60	3/12270 (0.0%)	1.10	105/16525 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	ASN	C-N	-5.63	1.25	1.33
1	B	95	GLU	C-N	5.53	1.41	1.33
1	B	243	TYR	N-CA	-5.08	1.39	1.46

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	B	411	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	704	GLN	OE1-CD-NE2	-10.04	112.56	122.60
1	A	642	GLN	OE1-CD-NE2	-10.02	112.58	122.60
1	A	342	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	A	32	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	A	568	GLN	OE1-CD-NE2	-9.60	113.00	122.60
1	B	704	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	B	642	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	B	342	GLN	OE1-CD-NE2	-9.42	113.18	122.60
1	B	34	GLU	N-CA-C	-8.36	100.00	112.04
1	A	288	GLU	N-CA-C	-8.25	103.35	113.41
1	B	457	SER	N-CA-C	7.99	122.28	112.54
1	B	126	GLU	N-CA-C	-7.84	97.62	109.30
1	B	28	ARG	N-CA-C	7.36	122.31	111.34
1	B	704	GLN	CG-CD-NE2	7.35	127.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	VAL	N-CA-C	-7.25	104.14	110.74
1	B	589	ASN	N-CA-C	7.06	120.14	109.63
1	B	126	GLU	CA-C-N	7.04	127.03	119.78
1	B	126	GLU	C-N-CA	7.04	127.03	119.78
1	B	730	ARG	N-CA-C	7.02	121.11	112.54
1	B	328	ASP	N-CA-C	-7.02	105.53	112.97
1	B	406	LEU	N-CA-C	6.97	118.67	111.14
1	B	411	GLN	CG-CD-NE2	6.92	126.78	116.40
1	A	642	GLN	CG-CD-NE2	6.86	126.69	116.40
1	B	642	GLN	CG-CD-NE2	6.84	126.66	116.40
1	B	165	GLN	N-CA-C	-6.78	99.72	110.10
1	A	168	GLN	CG-CD-NE2	6.77	126.56	116.40
1	B	597	GLU	N-CA-C	6.77	118.66	111.28
1	B	540	LYS	N-CA-C	-6.72	100.85	110.59
1	B	29	ASN	N-CA-C	6.70	123.00	113.02
1	B	153	LYS	N-CA-C	-6.67	104.06	112.93
1	A	151	ILE	N-CA-C	-6.63	103.39	110.36
1	A	32	GLN	CG-CD-NE2	6.60	126.31	116.40
1	B	629	PHE	N-CA-C	-6.56	98.52	108.96
1	B	612	SER	N-CA-C	6.54	119.25	111.33
1	A	93	SER	CA-C-N	-6.54	112.39	122.60
1	A	93	SER	C-N-CA	-6.54	112.39	122.60
1	A	568	GLN	CG-CD-NE2	6.53	126.19	116.40
1	B	119	VAL	N-CA-C	6.42	117.36	107.99
1	B	143	LYS	N-CA-C	-6.41	104.16	112.68
1	B	298	ILE	N-CA-C	6.37	114.99	107.73
1	B	342	GLN	CG-CD-NE2	6.36	125.94	116.40
1	B	554	LYS	N-CA-C	-6.35	106.12	114.31
1	B	307	ILE	N-CA-C	-6.34	106.55	112.83
1	A	342	GLN	CG-CD-NE2	6.32	125.88	116.40
1	B	605	GLU	N-CA-C	-6.29	104.47	111.71
1	A	704	GLN	CG-CD-NE2	6.21	125.72	116.40
1	B	308	ILE	N-CA-C	-6.18	106.89	111.90
1	B	371	LYS	N-CA-C	-6.17	105.65	113.43
1	A	287	GLU	N-CA-C	-6.15	105.87	113.19
1	A	589	ASN	N-CA-C	6.12	119.17	109.81
1	B	692	VAL	N-CA-C	-6.11	104.34	111.00
1	A	31	THR	CA-C-N	6.09	128.76	120.54
1	A	31	THR	C-N-CA	6.09	128.76	120.54
1	A	620	ASN	N-CA-C	-5.99	105.05	112.90
1	B	491	ARG	CA-C-N	5.85	126.18	119.92
1	B	491	ARG	C-N-CA	5.85	126.18	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	GLU	CA-C-N	5.84	132.70	121.54
1	B	95	GLU	C-N-CA	5.84	132.70	121.54
1	B	630	VAL	N-CA-C	5.80	116.21	107.80
1	A	540	LYS	N-CA-C	5.79	117.41	109.18
1	A	196	GLU	N-CA-C	5.77	117.57	111.28
1	A	628	ARG	N-CA-C	5.75	118.03	108.99
1	B	73	MET	N-CA-C	-5.69	105.16	111.36
1	A	506	SER	N-CA-C	-5.63	100.86	109.64
1	B	722	GLY	N-CA-C	5.62	119.02	112.50
1	A	371	LYS	N-CA-C	-5.62	105.93	112.89
1	B	621	TYR	N-CA-C	-5.61	104.56	111.40
1	B	752	ARG	N-CA-C	-5.61	105.70	112.54
1	B	699	LEU	N-CA-C	5.55	119.15	112.38
1	B	116	GLU	N-CA-C	-5.53	106.57	113.15
1	B	563	GLN	N-CA-C	-5.50	105.29	111.28
1	B	189	LEU	N-CA-C	5.46	119.92	111.56
1	A	301	GLU	CA-C-N	5.46	125.38	119.76
1	A	301	GLU	C-N-CA	5.46	125.38	119.76
1	B	749	HIS	N-CA-C	5.43	117.28	111.36
1	A	416	ILE	N-CA-C	5.43	115.88	110.23
1	B	401	SER	CA-C-N	5.42	126.61	119.84
1	B	401	SER	C-N-CA	5.42	126.61	119.84
1	A	621	TYR	N-CA-C	-5.38	105.31	111.07
1	B	190	PHE	N-CA-C	5.38	117.67	110.35
1	B	145	LEU	N-CA-C	-5.37	104.47	111.02
1	A	35	HIS	N-CA-C	-5.35	105.89	112.90
1	A	717	ILE	N-CA-C	-5.33	107.58	111.90
1	B	296	LEU	N-CA-C	-5.33	105.60	112.68
1	B	256	LEU	N-CA-C	-5.32	105.13	111.03
1	A	503	ILE	N-CA-C	5.30	116.93	108.87
1	A	32	GLN	N-CA-C	5.30	117.47	111.11
1	A	674	GLY	N-CA-C	-5.27	105.34	112.14
1	B	254	LEU	N-CA-C	-5.25	105.16	112.45
1	A	259	LEU	N-CA-C	-5.24	104.62	111.02
1	B	197	HIS	CA-C-N	5.23	126.38	119.84
1	B	197	HIS	C-N-CA	5.23	126.38	119.84
1	A	522	GLN	N-CA-C	-5.22	103.99	110.41
1	A	669	HIS	N-CA-C	-5.21	103.73	110.19
1	A	710	ASN	N-CA-C	-5.20	107.11	112.93
1	A	590	ARG	N-CA-C	5.12	121.70	110.80
1	B	131	ILE	N-CA-C	-5.10	102.51	109.55
1	A	534	ILE	CB-CA-C	-5.10	104.23	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	HIS	N-CA-C	5.09	117.37	108.76
1	B	149	TYR	N-CA-C	-5.09	106.92	113.23
1	A	136	ASP	N-CA-C	5.04	116.38	107.61
1	B	322	ILE	N-CA-C	5.04	115.59	109.30
1	B	658	LEU	N-CA-C	5.03	116.17	108.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6020	0	6008	534	0
1	B	6034	0	6017	546	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	28	9	0
3	B	32	0	29	9	0
All	All	12120	0	12082	1081	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 45.

All (1081) 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:91:HIS:CD2	1:B:93:SER:HB3	1.69	1.27
1:A:635:THR:HG22	1:A:637:PRO:HD2	1.21	1.16
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.16	1.12
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.32	1.10
1:B:91:HIS:HD2	1:B:93:SER:HB3	0.92	1.09
1:B:91:HIS:CD2	1:B:93:SER:CB	2.38	1.07
1:A:49:LYS:HG3	1:A:50:GLY:H	1.24	1.02
1:B:340:LYS:O	1:B:344:ASP:OD1	1.81	0.99
1:B:366:ASN:CB	1:B:367:PRO:HD3	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASN:HD21	1:A:500:LYS:HE2	1.29	0.98
1:B:175:ASN:ND2	1:B:200:ASP:HB3	1.81	0.96
1:B:366:ASN:HB2	1:B:367:PRO:CD	1.89	0.96
1:B:175:ASN:HD21	1:B:200:ASP:HB3	1.28	0.95
1:A:304:LYS:H	1:A:304:LYS:HD2	1.31	0.95
1:B:165:GLN:HG3	1:B:166:PRO:HA	1.48	0.95
1:A:477:TYR:H	1:A:593:SER:HB2	1.30	0.94
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.48	0.94
1:A:426:SER:HA	1:A:510:ARG:HA	1.50	0.93
1:B:273:LYS:HD2	1:B:431:LEU:HD22	1.53	0.91
1:A:31:THR:O	1:A:35:HIS:HB3	1.70	0.91
1:A:643:TYR:HB3	1:A:652:GLN:OE1	1.72	0.90
3:B:9003:SD2:OAT	3:B:9003:SD2:HAL	1.74	0.88
1:A:500:LYS:HZ2	1:A:500:LYS:HB3	1.36	0.88
1:A:301:GLU:HG3	1:A:385:PRO:HG3	1.56	0.88
1:B:140:ASN:C	1:B:140:ASN:HD22	1.79	0.87
1:A:373:LYS:HG2	1:A:377:LYS:HE3	1.54	0.87
1:A:655:SER:HB2	3:A:9002:SD2:OAH	1.75	0.86
1:A:173:VAL:O	1:A:177:ILE:HG12	1.75	0.86
1:A:40:MET:O	1:A:44:VAL:HB	1.76	0.85
1:B:686:HIS:ND1	3:B:9003:SD2:HAK	1.92	0.85
1:A:412:TYR:O	1:A:416:ILE:HG13	1.77	0.85
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.42	0.85
1:B:516:ASN:H	1:B:516:ASN:HD22	1.23	0.84
1:B:366:ASN:HD22	1:B:367:PRO:CD	1.90	0.84
1:B:516:ASN:HD22	1:B:516:ASN:N	1.75	0.84
1:A:308:ILE:HD12	1:A:345:ILE:CD1	2.06	0.84
1:A:469:ASN:N	1:A:469:ASN:HD22	1.74	0.84
1:A:608:ASN:C	1:A:609:ASN:HD22	1.85	0.83
1:B:221:PHE:HA	1:B:244:MET:HE2	1.60	0.83
1:A:442:ASN:HB2	1:A:496:ASN:HD22	1.44	0.82
1:A:59:ALA:HB1	1:A:83:ILE:HD13	1.62	0.82
1:B:516:ASN:H	1:B:516:ASN:ND2	1.75	0.82
1:B:91:HIS:CD2	1:B:93:SER:H	1.98	0.81
1:B:468:PHE:CZ	1:B:534:ILE:HG13	2.16	0.81
1:B:36:LEU:HD13	1:B:64:GLU:OE1	1.80	0.81
1:A:440:ASN:ND2	1:A:500:LYS:HE2	1.96	0.81
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.16	0.80
1:A:308:ILE:CD1	1:A:345:ILE:HD11	2.11	0.80
1:A:102:LYS:HA	1:A:114:LEU:HD11	1.61	0.80
1:A:490:GLU:OE2	1:A:544:ARG:NH2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:SER:HA	3:A:9002:SD2:HBE3	1.62	0.79
1:B:81:ILE:HG23	1:B:129:LEU:HD22	1.65	0.79
1:B:113:LEU:O	1:B:116:GLU:HG2	1.83	0.79
1:B:557:THR:O	1:B:561:GLU:HG3	1.82	0.78
1:B:570:TRP:CE3	1:B:574:LEU:HD21	2.17	0.78
1:B:401:SER:CB	1:B:638:ASN:HD22	1.96	0.77
1:B:186:GLN:HE21	1:B:195:LYS:HB2	1.50	0.77
1:B:75:LYS:O	1:B:78:GLY:N	2.16	0.76
1:B:304:LYS:HD3	1:B:304:LYS:H	1.47	0.76
1:B:611:GLN:HE21	1:B:774:ILE:CD1	1.99	0.76
1:A:167:TYR:CE1	1:A:536:LYS:HB2	2.21	0.76
1:B:224:TYR:HD2	1:B:225:ILE:HD13	1.51	0.76
1:B:324:ILE:O	1:B:326:SER:N	2.18	0.76
1:A:233:LEU:O	1:A:237:ALA:HB3	1.85	0.76
1:A:518:LYS:O	1:A:519:LEU:HD23	1.86	0.75
1:A:676:GLU:O	1:A:677:LEU:HD23	1.85	0.75
1:B:463:ILE:HD12	1:B:534:ILE:HG23	1.68	0.75
1:A:61:LYS:HA	1:A:61:LYS:HE2	1.69	0.75
1:A:764:GLN:O	1:A:768:ASP:HB2	1.87	0.75
1:A:73:MET:HG2	1:A:256:LEU:HD23	1.69	0.75
1:A:87:ASP:HB3	1:A:90:LYS:HE3	1.69	0.74
1:B:343:ILE:HD13	1:B:343:ILE:N	2.02	0.74
1:A:87:ASP:O	1:A:90:LYS:HG2	1.87	0.74
1:A:49:LYS:HG3	1:A:50:GLY:N	1.97	0.74
1:A:567:ASN:C	1:A:569:GLU:H	1.96	0.74
1:B:635:THR:HB	1:B:637:PRO:HD2	1.69	0.74
1:A:709:THR:HG21	1:A:734:ALA:HA	1.67	0.74
1:B:366:ASN:HD22	1:B:367:PRO:HD3	1.50	0.74
1:A:500:LYS:HB3	1:A:500:LYS:NZ	2.02	0.74
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.88	0.74
1:B:401:SER:HB2	1:B:638:ASN:HD22	1.51	0.73
1:A:658:LEU:HD23	3:A:9002:SD2:SAE	2.28	0.73
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.03	0.73
1:B:610:ILE:HD12	1:B:610:ILE:H	1.53	0.72
1:A:611:GLN:HE21	1:A:774:ILE:HD11	1.54	0.72
1:A:258:GLU:HG3	1:A:502:ARG:HH12	1.54	0.72
1:B:211:ASN:HA	1:B:214:GLN:NE2	2.04	0.72
1:A:613:ASP:HB3	1:A:774:ILE:HG23	1.72	0.71
1:B:145:LEU:HD23	1:B:226:GLU:HG3	1.72	0.71
1:A:677:LEU:HD11	3:A:9002:SD2:CAO	2.20	0.71
1:B:343:ILE:O	1:B:346:ARG:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:PHE:O	1:B:692:VAL:HG23	1.90	0.70
1:A:298:ILE:O	1:A:298:ILE:HD12	1.91	0.70
1:B:88:ILE:HB	1:B:130:VAL:HG11	1.73	0.70
1:B:583:ILE:HG23	1:B:631:PHE:HE1	1.56	0.70
1:B:123:GLU:HG3	1:B:157:ARG:NH1	2.06	0.70
1:A:202:SER:O	1:A:205:PHE:N	2.25	0.70
1:A:107:ILE:HG23	1:A:108:TYR:H	1.57	0.70
1:B:570:TRP:HE3	1:B:574:LEU:HD21	1.55	0.70
1:B:646:GLN:NE2	1:B:652:GLN:HB3	2.07	0.70
1:A:95:GLU:HG3	1:A:95:GLU:O	1.91	0.70
1:B:630:VAL:HB	1:B:667:LEU:HD23	1.74	0.70
1:A:113:LEU:O	1:A:117:HIS:HB2	1.91	0.69
1:B:366:ASN:CB	1:B:367:PRO:CD	2.58	0.69
1:A:314:GLU:HA	1:A:317:GLU:CD	2.17	0.69
1:B:27:GLU:HG3	1:B:27:GLU:O	1.92	0.69
1:A:693:ASP:OD2	1:A:707:LEU:HB2	1.93	0.69
1:A:500:LYS:HZ2	1:A:544:ARG:HH21	1.40	0.69
1:B:111:ASP:N	1:B:111:ASP:OD2	2.26	0.69
1:B:461:THR:HG22	1:B:540:LYS:HA	1.74	0.69
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.57	0.69
1:A:513:TYR:HA	1:A:519:LEU:CD2	2.23	0.69
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.74	0.68
1:B:278:TYR:HE2	1:B:511:ALA:O	1.76	0.68
1:A:107:ILE:HG23	1:A:108:TYR:N	2.06	0.68
1:B:675:VAL:HG23	3:B:9003:SD2:CAZ	2.24	0.68
1:A:513:TYR:HA	1:A:519:LEU:HD22	1.74	0.68
1:B:114:LEU:HA	1:B:117:HIS:HB3	1.75	0.68
1:B:300:ILE:O	1:B:300:ILE:HG22	1.93	0.68
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.75	0.68
1:A:395:THR:HB	1:A:398:LEU:O	1.93	0.68
1:A:442:ASN:ND2	1:A:496:ASN:HB2	2.09	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.75	0.68
1:B:246:LYS:O	1:B:250:GLN:HB2	1.94	0.68
1:B:610:ILE:CG2	1:B:614:LEU:HD23	2.24	0.68
1:A:284:SER:O	1:A:285:LEU:HD23	1.95	0.67
1:A:498:ARG:HD3	1:A:542:TYR:CD2	2.30	0.67
1:A:585:PHE:CE1	1:A:596:VAL:HG13	2.30	0.67
1:B:129:LEU:HD21	1:B:131:ILE:HG12	1.75	0.67
1:B:603:LEU:O	1:B:606:TRP:HB3	1.93	0.67
1:A:103:LYS:HG3	1:A:113:LEU:HD21	1.77	0.67
1:A:577:PRO:O	1:A:580:THR:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HG23	1:A:193:GLN:H	1.60	0.67
1:A:369:SER:OG	1:A:372:GLU:HB2	1.93	0.67
1:B:366:ASN:ND2	1:B:367:PRO:HD3	2.09	0.67
1:B:733:GLU:CD	1:B:733:GLU:H	2.03	0.67
1:B:746:SER:O	1:B:752:ARG:HD2	1.94	0.67
1:A:107:ILE:C	1:A:107:ILE:HD13	2.19	0.66
1:B:126:GLU:N	1:B:127:PRO:HD3	2.10	0.66
1:B:140:ASN:HD22	1:B:141:THR:N	1.93	0.66
1:A:102:LYS:HA	1:A:114:LEU:CD1	2.25	0.66
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.30	0.66
1:B:475:PHE:CD1	1:B:529:ILE:HG12	2.30	0.66
1:A:296:LEU:C	1:A:296:LEU:HD23	2.20	0.66
1:B:107:ILE:HD13	1:B:107:ILE:O	1.96	0.66
1:B:386:TYR:OH	1:B:411:GLN:HG3	1.95	0.66
1:B:643:TYR:HA	1:B:646:GLN:HB2	1.77	0.66
1:B:755:VAL:HG12	1:B:763:PHE:HB2	1.78	0.66
1:A:335:LYS:C	1:A:337:PHE:H	2.02	0.65
1:A:296:LEU:HD12	1:A:419:ILE:HD13	1.78	0.65
1:B:221:PHE:CD1	1:B:244:MET:HE1	2.28	0.65
1:B:242:ASN:O	1:B:243:TYR:C	2.39	0.65
1:B:477:TYR:H	1:B:593:SER:HB2	1.62	0.65
1:A:427:ILE:HG23	1:A:428:GLY:N	2.09	0.65
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.11	0.65
1:B:125:TYR:C	1:B:127:PRO:HD3	2.21	0.65
1:B:438:TYR:CE2	1:B:502:ARG:HD3	2.32	0.65
1:B:212:GLU:O	1:B:216:VAL:HG23	1.96	0.65
1:A:500:LYS:HZ2	1:A:544:ARG:NH2	1.94	0.65
1:A:334:GLU:O	1:A:337:PHE:HB3	1.96	0.65
1:B:627:GLY:O	1:B:628:ARG:HG2	1.96	0.65
1:B:655:SER:HB2	3:B:9003:SD2:OAH	1.96	0.65
1:B:377:LYS:O	1:B:380:LYS:HB3	1.97	0.64
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.79	0.64
1:B:366:ASN:HD22	1:B:367:PRO:HD2	1.62	0.64
1:A:59:ALA:CB	1:A:83:ILE:HD13	2.27	0.64
1:B:49:LYS:HG3	1:B:85:ASP:HB3	1.80	0.64
1:B:670:GLY:H	1:B:671:PRO:HD3	1.63	0.64
1:B:36:LEU:O	1:B:40:MET:HG3	1.98	0.64
1:B:245:ASP:C	1:B:245:ASP:OD2	2.41	0.64
1:A:304:LYS:H	1:A:304:LYS:CD	2.08	0.64
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.78	0.64
1:A:151:ILE:O	1:A:154:ILE:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:O	1:A:634:ILE:HB	1.98	0.63
1:A:427:ILE:CG2	1:A:428:GLY:N	2.61	0.63
1:A:76:ALA:C	1:A:78:GLY:H	2.04	0.63
1:A:241:PHE:CD1	1:A:241:PHE:C	2.76	0.63
1:A:252:ILE:HG23	1:A:253:ASN:N	2.13	0.63
1:B:140:ASN:C	1:B:140:ASN:ND2	2.50	0.63
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.61	0.63
1:A:329:PHE:N	1:A:329:PHE:HD2	1.97	0.63
1:A:498:ARG:HD3	1:A:542:TYR:CE2	2.34	0.63
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.81	0.63
1:A:673:LYS:O	3:A:9002:SD2:HAY	1.99	0.63
1:B:686:HIS:CE1	3:B:9003:SD2:HAK	2.34	0.63
1:A:36:LEU:O	1:A:40:MET:HG2	1.99	0.63
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.33	0.63
1:B:650:TYR:CE1	1:B:651:GLU:HG3	2.33	0.63
1:A:73:MET:HB3	1:A:159:ILE:HD13	1.81	0.62
1:A:550:VAL:HG12	1:A:551:PRO:HD2	1.81	0.62
1:B:257:GLU:O	1:B:260:LYS:HB2	1.99	0.62
1:A:119:VAL:HG13	1:A:131:ILE:HG12	1.81	0.62
1:B:552:LYS:O	1:B:554:LYS:N	2.33	0.62
1:B:456:ASP:HB3	1:B:462:LYS:O	1.98	0.62
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.34	0.62
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.81	0.62
1:B:494:LEU:O	1:B:496:ASN:N	2.31	0.62
1:B:723:SER:HA	1:B:730:ARG:HD3	1.81	0.62
1:A:126:GLU:O	1:A:128:VAL:HG23	1.99	0.62
1:A:477:TYR:N	1:A:593:SER:HB2	2.10	0.62
1:B:232:VAL:O	1:B:235:LEU:HD12	2.00	0.62
1:B:43:ILE:HG13	1:B:44:VAL:HG23	1.81	0.62
1:B:366:ASN:ND2	1:B:367:PRO:CD	2.61	0.62
1:B:570:TRP:HH2	1:B:607:LYS:HB2	1.65	0.62
1:B:236:TYR:C	1:B:238:PRO:HD3	2.24	0.62
1:A:635:THR:HG22	1:A:637:PRO:CD	2.14	0.62
1:B:574:LEU:N	1:B:574:LEU:HD23	2.15	0.62
1:A:221:PHE:HA	1:A:244:MET:HE3	1.82	0.61
1:A:329:PHE:HD2	1:A:329:PHE:H	1.46	0.61
1:A:256:LEU:HD11	1:A:260:LYS:HE3	1.81	0.61
1:A:707:LEU:HD12	1:A:709:THR:CG2	2.30	0.61
1:B:105:LYS:HD2	1:B:105:LYS:N	2.15	0.61
1:A:221:PHE:O	1:A:225:ILE:HG12	2.00	0.61
1:B:240:ALA:O	1:B:244:MET:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HD13	1:B:503:ILE:N	2.15	0.61
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.82	0.61
1:B:650:TYR:CD1	1:B:651:GLU:HG3	2.36	0.61
1:B:686:HIS:HD2	1:B:738:ALA:HB1	1.66	0.61
1:B:725:LEU:HD12	1:B:736:PHE:CE1	2.36	0.61
1:A:67:PRO:O	1:A:70:VAL:HG22	2.01	0.61
1:B:73:MET:HG2	1:B:256:LEU:HD12	1.83	0.61
1:A:30:LYS:O	1:A:30:LYS:HG3	1.99	0.61
1:B:540:LYS:HD3	1:B:542:TYR:OH	2.00	0.61
1:A:102:LYS:O	1:A:114:LEU:HG	2.01	0.60
1:A:319:LEU:HA	1:A:322:ILE:HD12	1.81	0.60
1:B:131:ILE:HD11	1:B:147:VAL:CG1	2.30	0.60
1:B:292:LEU:HD11	1:B:418:ASN:HB3	1.82	0.60
1:B:673:LYS:O	1:B:673:LYS:HG3	2.01	0.60
1:B:708:VAL:HG21	1:B:769:GLN:HE22	1.67	0.60
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.01	0.60
1:A:635:THR:CG2	1:A:637:PRO:HD2	2.14	0.60
1:A:543:ILE:HG22	1:A:543:ILE:O	2.01	0.60
1:A:258:GLU:HG3	1:A:502:ARG:NH1	2.15	0.60
1:A:637:PRO:HG3	1:A:653:VAL:O	2.02	0.60
1:A:329:PHE:N	1:A:329:PHE:CD2	2.69	0.60
1:B:513:TYR:O	1:B:514:LEU:HD23	2.01	0.60
1:A:191:THR:HG22	1:A:194:LEU:HG	1.83	0.60
1:B:210:SER:O	1:B:212:GLU:N	2.35	0.60
1:A:681:SER:O	1:A:682:GLU:C	2.44	0.60
1:B:447:THR:HG21	1:B:450:LEU:HD12	1.84	0.60
1:A:766:ILE:O	1:A:770:ILE:HG12	2.02	0.59
1:B:766:ILE:C	1:B:768:ASP:H	2.10	0.59
1:A:737:PHE:C	1:A:737:PHE:CD2	2.80	0.59
1:B:440:ASN:ND2	1:B:500:LYS:HD3	2.17	0.59
1:A:476:LYS:H	1:A:593:SER:CB	2.13	0.59
1:A:737:PHE:C	1:A:737:PHE:HD2	2.09	0.59
1:B:280:HIS:C	1:B:282:SER:H	2.10	0.59
1:A:301:GLU:HG3	1:A:385:PRO:CG	2.30	0.59
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.82	0.59
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.85	0.59
1:A:338:LEU:HD21	1:A:383:ILE:HG21	1.84	0.59
1:B:83:ILE:HG23	1:B:131:ILE:HG22	1.83	0.59
1:A:608:ASN:N	1:A:608:ASN:HD22	1.99	0.59
1:A:636:LEU:C	1:A:638:ASN:H	2.11	0.59
1:B:210:SER:O	1:B:211:ASN:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:O	1:B:204:GLU:N	2.35	0.59
1:B:557:THR:O	1:B:560:GLN:HG2	2.02	0.59
1:A:330:LEU:HD21	1:A:380:LYS:HB2	1.83	0.59
1:A:454:LEU:HA	1:A:467:ILE:HG21	1.85	0.59
1:B:666:ILE:HG22	1:B:667:LEU:N	2.18	0.59
1:A:739:GLU:O	1:A:743:LEU:HD12	2.03	0.59
1:B:413:LYS:O	1:B:417:GLN:HG3	2.03	0.59
1:A:464:ASN:OD1	1:A:467:ILE:HD13	2.03	0.58
1:B:636:LEU:N	1:B:636:LEU:HD12	2.16	0.58
1:A:307:ILE:O	1:A:311:LEU:HD13	2.02	0.58
1:B:619:THR:O	1:B:623:VAL:HG23	2.03	0.58
1:B:656:LYS:HD3	1:B:672:SER:HB3	1.83	0.58
1:A:601:LEU:HD23	1:A:601:LEU:H	1.68	0.58
1:B:221:PHE:O	1:B:225:ILE:HG12	2.04	0.58
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.18	0.58
1:A:73:MET:CG	1:A:256:LEU:HD23	2.34	0.58
1:A:267:ARG:O	1:A:489:ASN:ND2	2.36	0.58
1:B:467:ILE:O	1:B:468:PHE:C	2.45	0.58
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.86	0.58
1:B:202:SER:OG	1:B:204:GLU:HG3	2.03	0.58
1:B:686:HIS:CD2	1:B:738:ALA:HB1	2.39	0.58
1:A:677:LEU:HD21	3:A:9002:SD2:OAP	2.02	0.58
1:A:461:THR:O	1:A:541:GLU:HB2	2.04	0.58
1:B:636:LEU:O	1:B:637:PRO:C	2.46	0.58
1:B:69:ASP:O	1:B:73:MET:HG3	2.04	0.57
1:B:155:LEU:O	1:B:159:ILE:HB	2.03	0.57
1:B:338:LEU:O	1:B:341:LEU:HB3	2.03	0.57
1:B:496:ASN:HD22	1:B:497:GLU:N	2.02	0.57
1:B:444:ASN:OD1	1:B:448:ALA:HA	2.04	0.57
1:A:338:LEU:HD22	1:A:379:LEU:HD13	1.85	0.57
1:A:368:LEU:O	1:A:369:SER:HB3	2.04	0.57
3:A:9002:SD2:HAL	3:A:9002:SD2:OAT	2.04	0.57
1:B:224:TYR:CD2	1:B:225:ILE:HD13	2.37	0.57
1:A:146:ASN:O	1:A:147:VAL:C	2.46	0.57
1:B:571:ASN:HD21	1:B:580:THR:HG22	1.68	0.57
1:B:280:HIS:C	1:B:282:SER:N	2.60	0.57
1:B:510:ARG:O	1:B:522:GLN:HB3	2.04	0.57
1:A:202:SER:O	1:A:205:PHE:HB3	2.04	0.57
1:A:221:PHE:CA	1:A:244:MET:HE3	2.35	0.57
1:B:84:VAL:O	1:B:133:SER:N	2.31	0.57
1:B:330:LEU:O	1:B:335:LYS:HE3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:C	1:A:280:HIS:H	2.13	0.57
1:B:91:HIS:CD2	1:B:93:SER:N	2.71	0.57
1:B:555:ILE:O	1:B:558:LYS:HB2	2.05	0.57
1:A:122:LYS:N	1:A:128:VAL:O	2.38	0.57
1:A:601:LEU:HD23	1:A:601:LEU:N	2.20	0.57
1:A:602:ILE:HG23	1:A:681:SER:HA	1.87	0.57
1:A:762:THR:HG22	1:A:766:ILE:HD13	1.87	0.57
1:B:468:PHE:CE1	1:B:534:ILE:CG1	2.87	0.57
1:B:673:LYS:O	1:B:674:GLY:C	2.46	0.57
1:A:286:SER:C	1:A:288:GLU:H	2.11	0.57
1:B:221:PHE:HD1	1:B:244:MET:CE	2.16	0.57
1:B:386:TYR:HH	1:B:411:GLN:HG3	1.69	0.57
1:A:196:GLU:O	1:A:197:HIS:C	2.48	0.56
1:B:257:GLU:O	1:B:260:LYS:N	2.38	0.56
1:B:438:TYR:HE2	1:B:502:ARG:HD3	1.70	0.56
1:A:335:LYS:C	1:A:337:PHE:N	2.63	0.56
1:A:253:ASN:C	1:A:255:SER:N	2.62	0.56
1:A:674:GLY:O	1:A:676:GLU:N	2.38	0.56
1:B:714:PHE:HE2	1:B:733:GLU:HB2	1.70	0.56
1:A:253:ASN:C	1:A:255:SER:H	2.12	0.56
1:B:611:GLN:HE21	1:B:774:ILE:HD11	1.70	0.56
1:A:391:ARG:NH2	1:A:399:ILE:O	2.38	0.56
1:A:469:ASN:N	1:A:469:ASN:ND2	2.45	0.56
1:A:643:TYR:CB	1:A:652:GLN:OE1	2.48	0.56
1:B:94:LEU:O	1:B:96:ALA:N	2.38	0.56
1:B:105:LYS:HE2	1:B:111:ASP:HB3	1.87	0.56
1:B:404:ILE:HD12	1:B:408:VAL:HB	1.87	0.56
1:A:167:TYR:CE1	1:A:536:LYS:CB	2.88	0.56
1:B:221:PHE:CE1	1:B:225:ILE:HD11	2.41	0.56
1:B:403:SER:OG	1:B:638:ASN:ND2	2.39	0.56
1:A:598:SER:O	1:A:602:ILE:HG13	2.05	0.56
1:B:438:TYR:O	1:B:486:VAL:HB	2.06	0.56
1:B:552:LYS:C	1:B:554:LYS:H	2.14	0.56
1:B:583:ILE:HG23	1:B:631:PHE:CE1	2.39	0.56
1:B:656:LYS:CD	1:B:672:SER:HB3	2.36	0.56
1:B:131:ILE:HD11	1:B:147:VAL:HG13	1.86	0.56
1:B:592:ALA:O	1:B:593:SER:C	2.49	0.56
1:B:68:SER:O	1:B:71:LEU:N	2.39	0.56
1:B:91:HIS:CD2	1:B:93:SER:HB2	2.37	0.56
1:A:634:ILE:O	1:A:635:THR:C	2.48	0.55
1:B:463:ILE:HD11	1:B:541:GLU:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:O	1:A:255:SER:N	2.40	0.55
1:A:506:SER:OG	1:A:508:ASP:HB2	2.06	0.55
1:A:658:LEU:HD22	1:A:659:TYR:N	2.21	0.55
1:B:117:HIS:CG	1:B:118:TYR:H	2.24	0.55
1:B:127:PRO:O	1:B:128:VAL:HG13	2.07	0.55
1:A:123:GLU:O	1:A:123:GLU:HG3	2.05	0.55
1:B:427:ILE:HG23	1:B:428:GLY:N	2.21	0.55
1:A:639:ILE:HG21	1:A:667:LEU:CD2	2.36	0.55
1:B:226:GLU:CD	1:B:229:HIS:HD1	2.14	0.55
1:B:602:ILE:HD13	1:B:668:LEU:HD21	1.87	0.55
1:A:107:ILE:CG2	1:A:108:TYR:H	2.18	0.55
1:A:525:ILE:HG22	1:A:526:GLY:N	2.21	0.55
1:B:35:HIS:O	1:B:39:ILE:HG12	2.06	0.55
1:B:192:ASN:C	1:B:194:LEU:H	2.14	0.55
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.72	0.55
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.89	0.55
1:A:304:LYS:HD2	1:A:304:LYS:N	2.12	0.55
1:A:477:TYR:CE1	1:A:593:SER:HA	2.40	0.55
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.07	0.55
1:B:379:LEU:O	1:B:380:LYS:C	2.49	0.55
1:A:206:LEU:O	1:A:210:SER:HB3	2.07	0.54
1:A:769:GLN:O	1:A:772:PHE:HB3	2.07	0.54
1:B:32:GLN:O	1:B:34:GLU:N	2.39	0.54
1:B:431:LEU:O	1:B:432:TYR:HB3	2.08	0.54
1:B:714:PHE:HA	1:B:717:ILE:HG12	1.89	0.54
1:A:122:LYS:HB3	1:A:128:VAL:HB	1.89	0.54
1:A:762:THR:CG2	1:A:766:ILE:HD13	2.37	0.54
1:B:303:LYS:HD2	1:B:305:ASP:OD1	2.06	0.54
1:B:369:SER:OG	1:B:372:GLU:HG3	2.07	0.54
1:A:49:LYS:CG	1:A:50:GLY:N	2.69	0.54
1:A:250:GLN:HG3	1:A:251:GLU:HG2	1.90	0.54
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.90	0.54
1:A:76:ALA:C	1:A:78:GLY:N	2.66	0.54
1:A:247:PHE:CZ	1:A:252:ILE:HD12	2.42	0.54
1:B:83:ILE:HD12	1:B:131:ILE:HG21	1.88	0.54
1:B:94:LEU:HD11	1:B:130:VAL:HG21	1.90	0.54
1:B:729:GLY:O	1:B:736:PHE:HB2	2.07	0.54
1:A:749:HIS:O	1:A:752:ARG:N	2.41	0.54
1:B:275:LYS:HG3	1:B:513:TYR:CE2	2.42	0.54
1:A:156:SER:HA	1:A:160:LEU:HD12	1.89	0.54
1:A:563:GLN:HE21	1:A:584:THR:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:THR:CB	1:B:637:PRO:HD2	2.37	0.54
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.08	0.54
1:A:72:GLU:O	1:A:75:LYS:HB3	2.07	0.54
1:A:146:ASN:O	1:A:149:TYR:HB3	2.08	0.54
1:A:674:GLY:HA2	3:A:9002:SD2:OAT	2.07	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.36	0.54
1:A:152:GLY:O	1:A:153:LYS:C	2.50	0.54
1:A:314:GLU:C	1:A:317:GLU:HG2	2.33	0.54
1:A:440:ASN:ND2	1:A:493:ALA:HB2	2.23	0.54
1:A:563:GLN:O	1:A:566:ILE:HG22	2.08	0.54
1:B:221:PHE:CE2	1:B:225:ILE:HG13	2.42	0.54
1:A:150:GLU:OE2	1:A:153:LYS:HE2	2.07	0.53
1:A:508:ASP:O	1:A:509:THR:C	2.51	0.53
1:A:572:LYS:C	1:A:574:LEU:H	2.16	0.53
1:A:612:SER:O	1:A:616:LYS:HG3	2.08	0.53
1:A:614:LEU:O	1:A:618:VAL:HG23	2.08	0.53
1:B:410:LYS:O	1:B:414:ARG:HB2	2.09	0.53
1:A:472:LYS:HE3	1:A:532:VAL:O	2.07	0.53
1:B:77:ILE:HG22	1:B:127:PRO:HG2	1.90	0.53
1:A:585:PHE:CZ	1:A:596:VAL:HG13	2.44	0.53
1:A:608:ASN:N	1:A:608:ASN:ND2	2.56	0.53
1:A:314:GLU:HA	1:A:317:GLU:CG	2.38	0.53
1:A:670:GLY:H	1:A:671:PRO:CD	2.20	0.53
1:A:265:LEU:O	1:A:269:GLU:HB2	2.08	0.53
1:A:314:GLU:HA	1:A:317:GLU:HG2	1.89	0.53
1:A:442:ASN:CG	1:A:496:ASN:HB2	2.34	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG13	2.44	0.53
1:B:478:SER:O	1:B:527:LEU:HB2	2.08	0.53
1:A:167:TYR:HD2	1:A:168:GLN:H	1.57	0.53
1:A:204:GLU:O	1:A:207:GLU:HB3	2.09	0.53
1:B:40:MET:C	1:B:42:HIS:H	2.17	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG12	2.44	0.53
1:B:737:PHE:CE1	1:B:766:ILE:HG13	2.43	0.53
1:A:190:PHE:CD1	1:A:194:LEU:HB3	2.44	0.53
1:A:210:SER:O	1:A:214:GLN:HG3	2.08	0.53
1:A:677:LEU:HD11	3:A:9002:SD2:CAN	2.39	0.53
1:B:243:TYR:CD1	1:B:244:MET:N	2.77	0.53
1:B:312:SER:O	1:B:313:GLN:C	2.51	0.53
1:B:610:ILE:HD12	1:B:610:ILE:N	2.22	0.53
1:A:124:GLY:C	1:A:126:GLU:H	2.15	0.53
1:A:223:TYR:HB3	1:A:233:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:O	1:A:296:LEU:HB3	2.09	0.53
1:B:40:MET:HA	1:B:44:VAL:HG23	1.90	0.53
1:B:720:GLU:OE2	1:B:761:LYS:HE2	2.08	0.53
1:A:443:ILE:HD11	1:A:471:PHE:CD1	2.44	0.53
1:A:489:ASN:O	1:A:490:GLU:C	2.51	0.53
1:B:640:ALA:HA	1:B:643:TYR:CZ	2.44	0.53
1:B:675:VAL:HG23	3:B:9003:SD2:NBF	2.23	0.53
1:A:237:ALA:HB1	1:A:240:ALA:HB3	1.91	0.53
1:A:693:ASP:OD1	1:A:709:THR:HG22	2.09	0.53
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.39	0.53
1:B:91:HIS:NE2	1:B:93:SER:HB2	2.24	0.53
1:B:243:TYR:HD1	1:B:244:MET:N	2.07	0.53
1:B:369:SER:C	1:B:371:LYS:H	2.17	0.53
1:B:448:ALA:HB3	1:B:672:SER:O	2.09	0.53
1:A:233:LEU:HD23	1:A:237:ALA:CB	2.40	0.52
1:A:484:MET:HE3	1:A:590:ARG:NH2	2.24	0.52
1:A:733:GLU:H	1:A:733:GLU:CD	2.17	0.52
1:A:82:TYR:HB2	1:A:130:VAL:HG22	1.90	0.52
1:A:553:SER:O	1:A:554:LYS:C	2.51	0.52
1:A:681:SER:O	1:A:684:PHE:N	2.42	0.52
1:B:441:MET:SD	1:B:446:LEU:HD13	2.48	0.52
1:B:636:LEU:N	1:B:636:LEU:CD1	2.72	0.52
1:A:429:SER:HB3	1:A:432:TYR:CZ	2.44	0.52
1:A:460:ASN:O	1:A:498:ARG:NH2	2.40	0.52
1:A:732:ASN:OD1	1:A:732:ASN:C	2.52	0.52
1:B:243:TYR:C	1:B:243:TYR:CD1	2.86	0.52
1:B:463:ILE:HG13	1:B:541:GLU:HB3	1.92	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.09	0.52
1:A:256:LEU:HD13	1:A:256:LEU:C	2.34	0.52
1:A:294:LYS:O	1:A:295:LYS:C	2.52	0.52
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.92	0.52
1:B:614:LEU:HD13	1:B:770:ILE:HG23	1.90	0.52
1:A:155:LEU:O	1:A:160:LEU:HG	2.09	0.52
1:B:461:THR:O	1:B:541:GLU:HB2	2.10	0.52
1:A:103:LYS:HG3	1:A:113:LEU:CD2	2.40	0.52
1:A:286:SER:C	1:A:288:GLU:N	2.68	0.52
1:A:584:THR:HG21	1:A:630:VAL:HG22	1.92	0.52
1:B:46:ILE:HG22	1:B:48:VAL:HG13	1.91	0.52
1:B:749:HIS:O	1:B:750:ALA:C	2.52	0.52
1:A:314:GLU:O	1:A:318:LEU:HG	2.09	0.52
1:A:701:ASP:O	1:A:703:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:TRP:CZ3	1:B:574:LEU:HD21	2.44	0.52
1:A:212:GLU:O	1:A:215:GLU:HB3	2.10	0.52
1:A:335:LYS:O	1:A:337:PHE:N	2.43	0.52
1:A:505:LEU:N	1:A:505:LEU:HD22	2.25	0.52
1:B:202:SER:C	1:B:204:GLU:N	2.66	0.52
1:B:324:ILE:HG22	1:B:325:ASP:N	2.24	0.52
1:B:640:ALA:HB2	1:B:643:TYR:CZ	2.45	0.52
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.44	0.52
1:B:319:LEU:CD2	1:B:345:ILE:HD11	2.39	0.52
1:B:416:ILE:O	1:B:418:ASN:N	2.42	0.52
1:B:732:ASN:OD1	1:B:734:ALA:N	2.43	0.52
1:A:55:LYS:HD2	1:A:133:SER:OG	2.10	0.51
1:A:456:ASP:OD1	1:A:464:ASN:HB2	2.10	0.51
1:A:468:PHE:HD1	1:A:543:ILE:HD11	1.75	0.51
1:A:693:ASP:CG	1:A:708:VAL:HG12	2.36	0.51
1:B:276:GLN:NE2	1:B:431:LEU:HD11	2.25	0.51
1:B:129:LEU:HD23	1:B:129:LEU:C	2.35	0.51
1:B:174:LEU:HD22	1:B:216:VAL:HG11	1.92	0.51
1:B:178:LYS:O	1:B:178:LYS:HG3	2.09	0.51
1:B:493:ALA:O	1:B:494:LEU:HD23	2.10	0.51
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.45	0.51
1:A:73:MET:CB	1:A:159:ILE:HD13	2.41	0.51
1:A:118:TYR:HH	1:A:143:LYS:HA	1.75	0.51
1:A:264:MET:O	1:A:267:ARG:N	2.44	0.51
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.40	0.51
1:B:66:VAL:HG21	1:B:151:ILE:HD13	1.91	0.51
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.92	0.51
1:B:278:TYR:CE2	1:B:511:ALA:O	2.61	0.51
1:B:601:LEU:O	1:B:604:ASN:N	2.39	0.51
1:A:509:THR:OG1	1:A:549:VAL:HG11	2.11	0.51
1:A:696:ALA:O	1:A:697:GLY:C	2.53	0.51
1:A:32:GLN:O	1:A:36:LEU:HB2	2.10	0.51
1:A:87:ASP:C	1:A:87:ASP:OD2	2.52	0.51
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.91	0.51
1:B:276:GLN:O	1:B:277:HIS:C	2.54	0.51
1:B:32:GLN:C	1:B:34:GLU:H	2.18	0.51
1:B:293:LEU:O	1:B:297:GLN:HG3	2.11	0.51
1:B:762:THR:HG22	1:B:766:ILE:HD13	1.91	0.51
1:A:374:GLU:O	1:A:377:LYS:HB2	2.11	0.51
1:A:442:ASN:HB2	1:A:496:ASN:ND2	2.22	0.51
1:B:426:SER:HA	1:B:509:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ILE:HG22	1:B:489:ASN:CG	2.36	0.51
1:A:191:THR:C	1:A:193:GLN:H	2.19	0.51
1:A:264:MET:O	1:A:265:LEU:C	2.54	0.51
1:A:500:LYS:NZ	1:A:544:ARG:NH2	2.58	0.51
1:A:584:THR:HG22	1:A:629:PHE:O	2.11	0.51
1:A:636:LEU:C	1:A:638:ASN:N	2.67	0.51
1:B:62:LEU:HD13	1:B:63:LEU:HD23	1.93	0.51
1:B:366:ASN:CG	1:B:367:PRO:HD3	2.34	0.51
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.43	0.51
1:B:729:GLY:HA2	1:B:739:GLU:HG3	1.93	0.51
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.75	0.51
1:A:674:GLY:O	1:A:675:VAL:C	2.53	0.51
1:B:304:LYS:O	1:B:308:ILE:HG13	2.11	0.51
1:B:331:SER:HB3	1:B:334:GLU:CD	2.36	0.51
1:B:520:ILE:HG23	1:B:520:ILE:O	2.11	0.51
1:A:83:ILE:HA	1:A:131:ILE:O	2.11	0.51
1:A:296:LEU:HD23	1:A:296:LEU:O	2.11	0.51
1:A:505:LEU:N	1:A:505:LEU:CD2	2.74	0.51
1:B:304:LYS:HD3	1:B:304:LYS:N	2.23	0.50
1:A:294:LYS:O	1:A:297:GLN:N	2.44	0.50
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.26	0.50
1:A:567:ASN:C	1:A:569:GLU:N	2.62	0.50
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.94	0.50
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.10	0.50
1:B:735:GLU:O	1:B:736:PHE:C	2.52	0.50
1:A:88:ILE:HD13	1:A:118:TYR:C	2.36	0.50
1:B:632:THR:OG1	1:B:633:ASP:N	2.43	0.50
1:B:660:VAL:O	1:B:664:ARG:N	2.44	0.50
1:A:522:GLN:HG3	1:A:523:ARG:O	2.10	0.50
1:B:269:GLU:O	1:B:273:LYS:HG2	2.12	0.50
1:A:755:VAL:O	1:A:759:ALA:HB3	2.11	0.50
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.92	0.50
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.93	0.50
1:A:404:ILE:O	1:A:405:ASN:O	2.30	0.50
1:A:718:PHE:CD1	1:A:733:GLU:HB3	2.47	0.50
1:B:87:ASP:O	1:B:90:LYS:HG2	2.12	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.46	0.50
1:A:279:GLN:O	1:A:279:GLN:HG3	2.11	0.50
1:B:319:LEU:HD21	1:B:341:LEU:HD22	1.94	0.50
1:B:390:GLN:NE2	1:B:390:GLN:HA	2.27	0.50
1:B:713:LYS:O	1:B:717:ILE:HD11	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:GLY:CA	1:B:739:GLU:HG3	2.42	0.49
1:A:59:ALA:HB1	1:A:83:ILE:CD1	2.38	0.49
1:A:637:PRO:HB3	1:A:652:GLN:NE2	2.27	0.49
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.49
1:A:30:LYS:O	1:A:30:LYS:CG	2.61	0.49
1:A:440:ASN:HD21	1:A:500:LYS:CE	2.12	0.49
1:B:125:TYR:HE2	1:B:162:LYS:HE3	1.77	0.49
1:A:185:GLY:HA3	1:A:236:TYR:O	2.13	0.49
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.93	0.49
1:A:658:LEU:CD2	1:A:659:TYR:N	2.76	0.49
1:A:78:GLY:O	1:A:127:PRO:HD2	2.12	0.49
1:A:86:GLY:O	1:A:132:GLN:NE2	2.45	0.49
1:A:298:ILE:HD12	1:A:299:PRO:O	2.12	0.49
1:A:737:PHE:HD2	1:A:737:PHE:O	1.95	0.49
1:B:123:GLU:HG3	1:B:157:ARG:HH11	1.76	0.49
1:B:714:PHE:CE2	1:B:733:GLU:HB2	2.47	0.49
3:B:9003:SD2:OAT	3:B:9003:SD2:CAL	2.54	0.49
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.13	0.49
1:A:588:HIS:C	1:A:589:ASN:HD22	2.20	0.49
1:B:83:ILE:HD12	1:B:131:ILE:CG2	2.42	0.49
1:B:679:ASN:O	1:B:680:ASP:C	2.56	0.49
1:B:681:SER:O	1:B:685:ILE:HG13	2.12	0.49
1:A:153:LYS:O	1:A:157:ARG:HB3	2.13	0.49
1:A:252:ILE:CG2	1:A:253:ASN:N	2.76	0.49
1:A:255:SER:O	1:A:256:LEU:C	2.55	0.49
1:A:427:ILE:O	1:A:428:GLY:C	2.54	0.49
1:A:528:GLU:OE1	1:A:550:VAL:HG21	2.13	0.49
1:A:733:GLU:HG2	1:A:734:ALA:H	1.78	0.49
1:B:40:MET:O	1:B:44:VAL:HB	2.13	0.49
1:B:479:ILE:O	1:B:589:ASN:C	2.56	0.49
1:B:654:HIS:O	3:B:9003:SD2:HBE3	2.13	0.49
1:B:759:ALA:N	1:B:760:PRO:HD3	2.27	0.49
1:A:169:LYS:HE3	1:A:533:GLN:CB	2.43	0.49
1:A:177:ILE:HD12	1:A:238:PRO:HD2	1.95	0.49
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.95	0.49
1:A:163:ILE:O	1:A:164:ASN:HB2	2.13	0.49
1:A:241:PHE:C	1:A:241:PHE:HD1	2.20	0.49
1:A:278:TYR:O	1:A:280:HIS:N	2.46	0.49
1:B:84:VAL:C	1:B:133:SER:HB3	2.37	0.49
1:B:91:HIS:CG	1:B:93:SER:H	2.31	0.49
1:B:594:ASN:O	1:B:595:ILE:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ILE:HG13	1:A:499:LEU:HD21	1.95	0.48
1:B:194:LEU:O	1:B:194:LEU:HG	2.12	0.48
1:B:466:GLY:O	1:B:467:ILE:C	2.56	0.48
1:B:487:ASP:OD1	1:B:518:LYS:HE2	2.13	0.48
1:B:730:ARG:O	1:B:731:THR:O	2.31	0.48
1:B:758:ASN:C	1:B:760:PRO:HD3	2.37	0.48
1:A:477:TYR:H	1:A:593:SER:CB	2.12	0.48
1:A:696:ALA:O	1:A:699:LEU:N	2.46	0.48
1:B:40:MET:HA	1:B:43:ILE:HG12	1.95	0.48
1:B:222:ALA:O	1:B:223:TYR:C	2.56	0.48
1:A:209:ASN:O	1:A:212:GLU:HB2	2.14	0.48
1:A:506:SER:O	1:A:507:PRO:C	2.56	0.48
1:A:589:ASN:HB2	1:A:633:ASP:OD2	2.13	0.48
1:A:713:LYS:O	1:A:717:ILE:HG13	2.13	0.48
1:B:226:GLU:OE1	1:B:229:HIS:ND1	2.36	0.48
1:B:416:ILE:C	1:B:418:ASN:N	2.71	0.48
1:B:596:VAL:O	1:B:599:ALA:HB3	2.13	0.48
1:B:718:PHE:CG	1:B:733:GLU:HB3	2.49	0.48
1:B:366:ASN:ND2	1:B:367:PRO:HD2	2.26	0.48
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.12	0.48
1:A:107:ILE:CG2	1:A:108:TYR:N	2.72	0.48
1:A:440:ASN:CG	1:A:493:ALA:HB2	2.38	0.48
1:A:465:ARG:O	1:A:469:ASN:ND2	2.46	0.48
1:B:102:LYS:O	1:B:113:LEU:HD22	2.13	0.48
1:B:682:GLU:HA	1:B:685:ILE:HD12	1.95	0.48
1:B:762:THR:C	1:B:764:GLN:N	2.70	0.48
1:A:442:ASN:CB	1:A:496:ASN:HD22	2.21	0.48
1:B:229:HIS:O	1:B:232:VAL:HG23	2.13	0.48
1:B:447:THR:HG23	1:B:447:THR:O	2.13	0.48
1:B:640:ALA:C	1:B:642:GLN:H	2.20	0.48
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.95	0.48
1:A:267:ARG:HE	1:A:491:ARG:HH21	1.60	0.48
1:B:314:GLU:HG3	1:B:314:GLU:O	2.13	0.48
1:B:498:ARG:NH1	1:B:540:LYS:HE3	2.28	0.48
1:B:640:ALA:C	1:B:642:GLN:N	2.69	0.48
1:A:187:ASP:HA	1:A:195:LYS:HE2	1.95	0.48
1:A:314:GLU:O	1:A:317:GLU:HG2	2.14	0.48
1:A:636:LEU:O	1:A:638:ASN:N	2.47	0.48
1:B:322:ILE:HG13	1:B:372:GLU:OE2	2.14	0.48
1:B:635:THR:HG22	1:B:654:HIS:CE1	2.48	0.48
1:A:741:PHE:O	1:A:742:ARG:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LYS:O	1:B:529:ILE:HB	2.14	0.48
1:B:715:ILE:O	1:B:718:PHE:HB3	2.13	0.48
1:A:741:PHE:O	1:A:744:MET:N	2.47	0.48
1:B:65:LYS:HB3	1:B:225:ILE:HG22	1.95	0.48
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.13	0.48
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.44	0.48
1:B:529:ILE:N	1:B:529:ILE:HD12	2.29	0.48
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.49	0.48
1:A:107:ILE:HG22	1:A:146:ASN:OD1	2.14	0.47
1:A:688:PHE:O	1:A:691:ALA:HB3	2.13	0.47
1:B:239:GLU:O	1:B:240:ALA:C	2.56	0.47
1:B:749:HIS:O	1:B:752:ARG:N	2.44	0.47
1:A:51:GLU:O	1:A:53:ALA:N	2.47	0.47
1:A:87:ASP:OD2	1:A:89:THR:N	2.47	0.47
1:A:217:PHE:CE1	1:A:244:MET:HE1	2.48	0.47
1:A:770:ILE:O	1:A:774:ILE:HG13	2.14	0.47
1:B:43:ILE:HG13	1:B:44:VAL:N	2.28	0.47
1:B:636:LEU:CD1	1:B:636:LEU:H	2.27	0.47
1:B:679:ASN:O	1:B:682:GLU:N	2.46	0.47
1:B:275:LYS:HG3	1:B:513:TYR:HE2	1.79	0.47
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.14	0.47
1:B:498:ARG:HH12	1:B:540:LYS:HG2	1.79	0.47
1:A:107:ILE:C	1:A:107:ILE:CD1	2.87	0.47
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.44	0.47
1:A:657:GLY:HA2	1:A:667:LEU:O	2.14	0.47
1:A:29:ASN:C	1:A:31:THR:H	2.21	0.47
1:A:118:TYR:OH	1:A:143:LYS:HA	2.14	0.47
1:B:587:VAL:O	1:B:588:HIS:CG	2.67	0.47
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.49	0.47
1:A:391:ARG:NH1	1:A:404:ILE:CD1	2.78	0.47
1:B:91:HIS:NE2	1:B:93:SER:CB	2.76	0.47
1:B:257:GLU:O	1:B:258:GLU:C	2.54	0.47
1:B:496:ASN:HD22	1:B:496:ASN:C	2.21	0.47
1:B:674:GLY:O	1:B:677:LEU:HB2	2.14	0.47
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.50	0.47
1:A:258:GLU:CG	1:A:502:ARG:HH12	2.25	0.47
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.49	0.47
1:A:401:SER:O	1:A:403:SER:N	2.37	0.47
1:A:656:LYS:O	1:A:668:LEU:HD12	2.14	0.47
1:A:718:PHE:O	1:A:722:GLY:HA3	2.15	0.47
1:B:107:ILE:HG12	1:B:149:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HD21	1:B:379:LEU:HB3	1.96	0.47
1:A:191:THR:HG23	1:A:194:LEU:H	1.80	0.47
1:A:550:VAL:HG12	1:A:551:PRO:CD	2.43	0.47
1:B:123:GLU:CG	1:B:124:GLY:H	2.28	0.47
1:B:530:LYS:O	1:B:531:ASP:HB2	2.14	0.47
1:A:476:LYS:N	1:A:593:SER:OG	2.34	0.47
1:A:686:HIS:CD2	1:A:686:HIS:C	2.93	0.47
1:A:693:ASP:OD2	1:A:693:ASP:O	2.33	0.47
1:A:718:PHE:HA	1:A:722:GLY:HA3	1.97	0.47
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.50	0.47
1:B:84:VAL:HG22	1:B:85:ASP:N	2.30	0.47
1:B:264:MET:C	1:B:266:SER:N	2.73	0.47
1:B:511:ALA:CB	1:B:521:LEU:HA	2.45	0.47
1:B:564:LEU:O	1:B:568:GLN:HB2	2.15	0.47
1:A:118:TYR:CD1	1:A:118:TYR:N	2.83	0.47
1:A:338:LEU:CD2	1:A:383:ILE:HG21	2.45	0.47
1:A:479:ILE:HG22	1:A:480:SER:N	2.30	0.47
1:B:660:VAL:HG13	1:B:662:GLU:OE2	2.14	0.47
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.98	0.46
1:A:191:THR:HG21	1:A:212:GLU:OE2	2.15	0.46
1:B:280:HIS:O	1:B:282:SER:N	2.48	0.46
1:B:614:LEU:O	1:B:618:VAL:HG23	2.14	0.46
1:A:220:ALA:HB3	1:A:244:MET:HE2	1.97	0.46
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.15	0.46
1:B:189:LEU:HD22	1:B:220:ALA:HB2	1.97	0.46
1:A:498:ARG:CD	1:A:542:TYR:CD2	2.97	0.46
1:A:639:ILE:HG21	1:A:667:LEU:HD21	1.96	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.15	0.46
1:B:472:LYS:HG3	1:B:473:LYS:N	2.29	0.46
1:B:526:GLY:HA3	1:B:550:VAL:O	2.16	0.46
1:A:96:ALA:O	1:A:97:LEU:C	2.59	0.46
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.46	0.46
1:A:560:GLN:O	1:A:561:GLU:C	2.59	0.46
1:A:586:ASN:HB3	1:A:632:THR:OG1	2.14	0.46
1:A:718:PHE:CE1	1:A:733:GLU:N	2.84	0.46
1:B:261:ASP:OD1	1:B:490:GLU:HB3	2.15	0.46
1:B:313:GLN:C	1:B:315:GLU:H	2.22	0.46
1:B:324:ILE:O	1:B:325:ASP:C	2.59	0.46
1:B:455:VAL:HG22	1:B:498:ARG:HE	1.79	0.46
1:A:199:THR:OG1	1:A:200:ASP:N	2.47	0.46
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.46
1:B:77:ILE:HG22	1:B:77:ILE:O	2.16	0.46
1:B:331:SER:HB3	1:B:334:GLU:HB2	1.97	0.46
1:A:316:LYS:O	1:A:319:LEU:HB3	2.15	0.46
1:A:410:LYS:NZ	1:A:414:ARG:HH21	2.14	0.46
1:A:439:GLU:OE1	1:A:590:ARG:NH2	2.49	0.46
1:A:498:ARG:HG2	1:A:498:ARG:HH11	1.81	0.46
1:B:769:GLN:O	1:B:772:PHE:HB3	2.16	0.46
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.46
1:A:57:GLU:O	1:A:61:LYS:N	2.36	0.46
1:A:311:LEU:O	1:A:312:SER:HB3	2.15	0.46
1:B:171:LEU:O	1:B:175:ASN:HB2	2.15	0.46
1:B:238:PRO:O	1:B:241:PHE:HB3	2.15	0.46
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.51	0.46
1:B:420:ASP:CG	1:B:523:ARG:HH11	2.24	0.46
1:B:468:PHE:CG	1:B:534:ILE:HD11	2.51	0.46
1:A:114:LEU:C	1:A:116:GLU:H	2.24	0.46
1:A:439:GLU:OE1	1:A:484:MET:HE3	2.16	0.46
1:A:529:ILE:HD13	1:A:529:ILE:N	2.31	0.46
1:B:294:LYS:HG3	1:B:295:LYS:N	2.31	0.46
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.97	0.46
1:A:592:ALA:HA	1:A:595:ILE:HG12	1.97	0.46
1:A:167:TYR:OH	1:A:536:LYS:HB2	2.15	0.46
1:A:264:MET:HE3	1:A:265:LEU:HD22	1.98	0.46
1:A:319:LEU:C	1:A:319:LEU:HD13	2.41	0.46
1:B:376:LEU:HD23	1:B:379:LEU:HD12	1.98	0.46
1:B:636:LEU:N	1:B:637:PRO:CD	2.79	0.46
1:B:743:LEU:O	1:B:744:MET:C	2.59	0.46
1:A:46:ILE:O	1:A:47:GLU:HG3	2.16	0.45
1:A:76:ALA:O	1:A:78:GLY:N	2.49	0.45
1:A:151:ILE:O	1:A:152:GLY:C	2.57	0.45
1:A:205:PHE:CE2	1:A:209:ASN:ND2	2.82	0.45
1:A:753:LEU:O	1:A:756:GLN:N	2.48	0.45
1:B:294:LYS:C	1:B:296:LEU:H	2.22	0.45
1:B:557:THR:HA	1:B:560:GLN:HG2	1.97	0.45
1:A:481:SER:HA	1:A:524:ASN:HD22	1.80	0.45
1:A:615:ILE:HG22	1:A:616:LYS:N	2.31	0.45
1:A:693:ASP:OD2	1:A:693:ASP:C	2.58	0.45
1:B:643:TYR:HB3	1:B:646:GLN:OE1	2.16	0.45
1:B:670:GLY:H	1:B:671:PRO:CD	2.28	0.45
1:A:314:GLU:CA	1:A:317:GLU:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:CG2	1:A:428:GLY:H	2.30	0.45
1:A:615:ILE:O	1:A:619:THR:HG23	2.15	0.45
1:A:695:TYR:O	1:A:698:TYR:HB3	2.17	0.45
1:A:191:THR:OG1	1:A:192:ASN:N	2.50	0.45
1:A:299:PRO:O	1:A:300:ILE:HG23	2.16	0.45
1:A:301:GLU:H	1:A:301:GLU:CD	2.24	0.45
1:B:49:LYS:HB2	1:B:50:GLY:H	1.58	0.45
1:B:113:LEU:H	1:B:116:GLU:CD	2.25	0.45
1:B:239:GLU:O	1:B:242:ASN:N	2.49	0.45
1:B:369:SER:O	1:B:371:LYS:N	2.49	0.45
1:B:661:PRO:C	1:B:663:SER:N	2.75	0.45
1:A:122:LYS:CB	1:A:128:VAL:HB	2.47	0.45
1:A:264:MET:O	1:A:266:SER:N	2.49	0.45
1:A:584:THR:HG23	1:A:630:VAL:HA	1.98	0.45
1:A:682:GLU:O	1:A:685:ILE:N	2.44	0.45
1:B:467:ILE:HD12	1:B:467:ILE:N	2.32	0.45
1:B:487:ASP:OD2	1:B:487:ASP:N	2.49	0.45
1:B:731:THR:HG22	1:B:732:ASN:H	1.81	0.45
1:B:733:GLU:CD	1:B:733:GLU:N	2.73	0.45
1:A:296:LEU:C	1:A:296:LEU:CD2	2.89	0.45
1:A:429:SER:HB3	1:A:432:TYR:CE1	2.52	0.45
1:A:495:ASP:C	1:A:497:GLU:N	2.68	0.45
1:A:749:HIS:O	1:A:750:ALA:C	2.60	0.45
1:B:51:GLU:O	1:B:53:ALA:N	2.50	0.45
1:B:74:TYR:CZ	1:B:79:GLY:HA3	2.52	0.45
1:B:563:GLN:NE2	1:B:584:THR:HA	2.32	0.45
1:B:717:ILE:N	1:B:717:ILE:HD13	2.31	0.45
1:A:126:GLU:O	1:A:126:GLU:HG3	2.16	0.45
1:A:191:THR:HG22	1:A:194:LEU:CG	2.47	0.45
1:A:264:MET:HG2	1:A:265:LEU:N	2.31	0.45
1:B:89:THR:HG21	1:B:97:LEU:HD12	1.98	0.45
1:B:256:LEU:O	1:B:257:GLU:C	2.59	0.45
1:B:303:LYS:HD3	1:B:304:LYS:NZ	2.32	0.45
1:B:679:ASN:C	1:B:681:SER:N	2.72	0.45
1:A:278:TYR:C	1:A:280:HIS:N	2.75	0.45
1:B:202:SER:O	1:B:203:VAL:C	2.60	0.45
1:B:202:SER:C	1:B:204:GLU:H	2.25	0.45
1:B:211:ASN:O	1:B:214:GLN:N	2.49	0.45
1:B:264:MET:O	1:B:267:ARG:N	2.48	0.45
1:B:427:ILE:HG23	1:B:428:GLY:H	1.80	0.45
1:B:477:TYR:N	1:B:593:SER:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HD11	1:B:521:LEU:HD21	1.98	0.45
1:A:73:MET:O	1:A:76:ALA:HB3	2.17	0.45
1:A:150:GLU:O	1:A:151:ILE:C	2.60	0.45
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.52	0.45
1:A:739:GLU:O	1:A:743:LEU:CD1	2.65	0.45
1:B:60:GLU:C	1:B:62:LEU:N	2.72	0.45
1:B:303:LYS:NZ	1:B:304:LYS:HZ1	2.15	0.45
1:B:467:ILE:HD12	1:B:467:ILE:H	1.82	0.45
1:B:681:SER:O	1:B:682:GLU:C	2.59	0.45
1:A:61:LYS:HA	1:A:61:LYS:CE	2.45	0.45
1:A:426:SER:HB3	1:A:508:ASP:O	2.17	0.45
1:A:611:GLN:NE2	1:A:774:ILE:HD11	2.29	0.45
1:A:707:LEU:HD23	1:A:707:LEU:H	1.81	0.45
1:A:728:TYR:O	1:A:729:GLY:C	2.59	0.45
1:B:587:VAL:HG11	1:B:592:ALA:HA	1.99	0.45
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.85	0.44
1:A:366:ASN:HB2	1:A:367:PRO:HD3	1.99	0.44
1:A:744:MET:SD	1:A:766:ILE:HG21	2.57	0.44
1:A:766:ILE:HD12	1:A:766:ILE:N	2.32	0.44
1:B:766:ILE:C	1:B:768:ASP:N	2.71	0.44
1:A:169:LYS:HE3	1:A:533:GLN:HB2	2.00	0.44
1:A:187:ASP:HA	1:A:195:LYS:CE	2.47	0.44
1:A:188:LEU:HD12	1:A:188:LEU:O	2.18	0.44
1:A:462:LYS:HA	1:A:541:GLU:OE2	2.17	0.44
1:B:48:VAL:HB	1:B:49:LYS:H	1.51	0.44
1:B:62:LEU:C	1:B:62:LEU:HD22	2.43	0.44
1:B:67:PRO:O	1:B:68:SER:C	2.59	0.44
1:B:192:ASN:C	1:B:194:LEU:N	2.76	0.44
1:A:311:LEU:O	1:A:315:GLU:HB2	2.17	0.44
1:B:131:ILE:HD11	1:B:147:VAL:HG11	1.99	0.44
1:B:766:ILE:HG22	1:B:767:ASN:N	2.31	0.44
1:A:185:GLY:CA	1:A:236:TYR:O	2.66	0.44
1:A:677:LEU:O	1:A:678:ARG:C	2.59	0.44
1:B:155:LEU:HD12	1:B:159:ILE:CG2	2.47	0.44
1:B:176:THR:O	1:B:180:ALA:N	2.46	0.44
1:B:591:TYR:O	1:B:595:ILE:HG12	2.17	0.44
1:B:658:LEU:HD23	1:B:659:TYR:N	2.32	0.44
1:B:721:GLU:OE2	1:B:760:PRO:N	2.51	0.44
1:A:244:MET:O	1:A:245:ASP:C	2.59	0.44
1:A:639:ILE:HG21	1:A:667:LEU:HD22	2.00	0.44
1:A:711:SER:OG	1:A:714:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.99	0.44
1:B:640:ALA:CA	1:B:643:TYR:CZ	3.01	0.44
1:A:371:LYS:HD2	1:A:371:LYS:HA	1.81	0.44
1:A:391:ARG:NH1	1:A:404:ILE:HD13	2.33	0.44
1:A:566:ILE:HG12	1:A:566:ILE:O	2.18	0.44
1:A:661:PRO:O	1:A:664:ARG:HG3	2.17	0.44
1:B:122:LYS:HB3	1:B:128:VAL:HG23	1.99	0.44
1:B:640:ALA:HB2	1:B:643:TYR:OH	2.17	0.44
1:B:693:ASP:HB2	1:B:737:PHE:CE2	2.52	0.44
1:A:31:THR:HG22	1:A:32:GLN:N	2.32	0.44
1:A:523:ARG:O	1:A:524:ASN:HB2	2.17	0.44
1:A:765:PHE:O	1:A:768:ASP:HB3	2.17	0.44
1:B:56:LYS:C	1:B:58:ALA:N	2.73	0.44
1:B:196:GLU:O	1:B:197:HIS:C	2.61	0.44
1:A:741:PHE:C	1:A:741:PHE:CD2	2.96	0.44
1:B:113:LEU:HB2	1:B:116:GLU:OE1	2.18	0.44
1:B:511:ALA:HB2	1:B:521:LEU:HA	2.00	0.44
1:A:378:LYS:HG2	1:A:650:TYR:CD2	2.53	0.44
1:A:488:ILE:HG13	1:A:517:GLY:O	2.18	0.44
1:A:600:TYR:O	1:A:604:ASN:HB2	2.17	0.44
1:A:649:ILE:C	1:A:651:GLU:H	2.24	0.44
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.99	0.44
1:B:670:GLY:N	1:B:671:PRO:CD	2.81	0.44
1:B:765:PHE:O	1:B:768:ASP:HB3	2.18	0.44
1:A:522:GLN:HG2	1:A:525:ILE:HD11	1.99	0.43
1:A:660:VAL:HA	1:A:661:PRO:HD3	1.91	0.43
1:B:503:ILE:N	1:B:503:ILE:CD1	2.78	0.43
1:A:335:LYS:CG	1:A:336:GLU:N	2.81	0.43
1:B:193:GLN:HE21	1:B:193:GLN:HB3	1.61	0.43
1:B:490:GLU:HG3	1:B:491:ARG:N	2.33	0.43
1:A:84:VAL:O	1:A:133:SER:N	2.51	0.43
1:A:500:LYS:HB3	1:A:544:ARG:HH21	1.83	0.43
1:A:614:LEU:HD22	1:A:770:ILE:HD12	2.00	0.43
1:B:412:TYR:O	1:B:416:ILE:HG12	2.18	0.43
1:A:154:ILE:HA	1:A:158:ASP:OD1	2.19	0.43
1:A:345:ILE:O	1:A:345:ILE:HG22	2.18	0.43
1:B:60:GLU:C	1:B:62:LEU:H	2.26	0.43
1:B:468:PHE:O	1:B:471:PHE:HB3	2.18	0.43
1:A:145:LEU:HD22	1:A:229:HIS:NE2	2.33	0.43
1:A:608:ASN:C	1:A:609:ASN:ND2	2.64	0.43
1:A:662:GLU:H	1:A:662:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TYR:CD2	1:B:224:TYR:C	2.96	0.43
1:A:528:GLU:O	1:A:529:ILE:C	2.61	0.43
1:B:415:ASP:O	1:B:419:ILE:HG13	2.19	0.43
1:A:218:ALA:O	1:A:219:LYS:C	2.61	0.43
1:A:435:ILE:HG22	1:A:437:LEU:HG	2.01	0.43
1:A:479:ILE:CG2	1:A:480:SER:N	2.82	0.43
1:A:634:ILE:HG13	1:A:635:THR:O	2.18	0.43
1:A:640:ALA:HA	1:A:643:TYR:CZ	2.53	0.43
1:A:714:PHE:O	1:A:717:ILE:N	2.39	0.43
1:B:83:ILE:HG23	1:B:131:ILE:CG2	2.47	0.43
1:B:89:THR:O	1:B:89:THR:HG22	2.18	0.43
1:B:155:LEU:HD12	1:B:159:ILE:HB	2.01	0.43
1:B:297:GLN:OE1	1:B:514:LEU:HD13	2.19	0.43
1:B:309:HIS:O	1:B:310:SER:HB3	2.18	0.43
1:A:56:LYS:O	1:A:56:LYS:HG3	2.18	0.43
1:A:79:GLY:HA3	1:A:127:PRO:HB2	1.99	0.43
1:A:534:ILE:HG22	1:A:535:ILE:N	2.33	0.43
1:B:79:GLY:HA2	1:B:127:PRO:HB2	2.00	0.43
1:B:104:ILE:C	1:B:105:LYS:HD2	2.44	0.43
1:B:369:SER:C	1:B:371:LYS:N	2.77	0.43
1:B:379:LEU:O	1:B:382:ASP:N	2.51	0.43
1:B:388:ILE:HG23	1:B:416:ILE:HD11	2.00	0.43
1:B:476:LYS:N	1:B:593:SER:OG	2.42	0.43
1:B:610:ILE:HG21	1:B:614:LEU:HD23	1.98	0.43
1:B:690:HIS:CE1	1:B:735:GLU:OE1	2.72	0.43
1:A:140:ASN:HD21	1:A:143:LYS:NZ	2.16	0.43
1:A:155:LEU:HG	1:A:160:LEU:HD11	2.00	0.43
1:A:234:GLN:HG3	1:A:241:PHE:CD2	2.53	0.43
1:A:525:ILE:CG2	1:A:526:GLY:N	2.82	0.43
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.53	0.43
1:A:214:GLN:O	1:A:215:GLU:C	2.62	0.43
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.54	0.43
1:B:639:ILE:O	1:B:642:GLN:N	2.44	0.43
1:B:766:ILE:O	1:B:768:ASP:N	2.52	0.43
1:A:98:SER:C	1:A:100:ASP:H	2.25	0.42
1:A:145:LEU:O	1:A:146:ASN:C	2.62	0.42
1:A:621:TYR:CE1	1:A:664:ARG:CZ	3.02	0.42
1:B:202:SER:O	1:B:205:PHE:N	2.51	0.42
1:A:404:ILE:C	1:A:405:ASN:O	2.62	0.42
1:A:480:SER:HB3	1:A:525:ILE:HB	2.00	0.42
1:B:65:LYS:HD2	1:B:65:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:CG	1:B:118:TYR:N	2.87	0.42
1:A:32:GLN:O	1:A:36:LEU:CB	2.68	0.42
1:A:429:SER:OG	1:A:430:THR:N	2.52	0.42
1:A:506:SER:C	1:A:508:ASP:N	2.76	0.42
1:A:611:GLN:HE22	1:A:770:ILE:CG2	2.32	0.42
1:B:264:MET:HE2	1:B:265:LEU:HD22	2.01	0.42
1:B:718:PHE:HZ	1:B:731:THR:O	2.02	0.42
1:A:206:LEU:CD1	1:A:213:VAL:HG11	2.49	0.42
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.54	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.19	0.42
1:A:555:ILE:N	1:A:555:ILE:HD12	2.34	0.42
1:B:91:HIS:HE2	1:B:93:SER:HB2	1.83	0.42
1:B:160:LEU:C	1:B:162:LYS:N	2.77	0.42
1:B:238:PRO:O	1:B:239:GLU:C	2.62	0.42
1:B:472:LYS:O	1:B:473:LYS:C	2.62	0.42
1:B:610:ILE:H	1:B:610:ILE:CD1	2.27	0.42
1:B:615:ILE:O	1:B:616:LYS:C	2.63	0.42
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.53	0.42
1:B:737:PHE:O	1:B:740:ALA:HB3	2.19	0.42
1:A:467:ILE:H	1:A:467:ILE:CD1	2.33	0.42
1:A:562:ALA:O	1:A:563:GLN:C	2.63	0.42
1:B:388:ILE:O	1:B:391:ARG:N	2.47	0.42
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.54	0.42
1:A:77:ILE:CG2	1:A:162:LYS:HD2	2.50	0.42
1:A:190:PHE:HD1	1:A:194:LEU:HB3	1.84	0.42
1:A:570:TRP:HH2	1:A:607:LYS:HB2	1.85	0.42
1:A:592:ALA:O	1:A:593:SER:C	2.63	0.42
1:A:707:LEU:HD23	1:A:707:LEU:N	2.34	0.42
1:A:744:MET:HE1	1:A:766:ILE:HG22	2.01	0.42
1:B:60:GLU:O	1:B:62:LEU:N	2.52	0.42
1:B:153:LYS:O	1:B:154:ILE:C	2.62	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.49	0.42
1:B:551:PRO:O	1:B:552:LYS:C	2.63	0.42
1:A:645:HIS:NE2	1:A:663:SER:HB3	2.34	0.42
1:B:70:VAL:HG22	1:B:252:ILE:HD11	2.02	0.42
1:B:437:LEU:HD11	1:B:519:LEU:HD12	2.02	0.42
1:B:654:HIS:O	3:B:9003:SD2:CBE	2.68	0.42
1:A:159:ILE:HG23	1:A:259:LEU:HD11	2.01	0.42
1:A:191:THR:HG21	1:A:212:GLU:CD	2.44	0.42
1:A:366:ASN:H	1:A:367:PRO:CD	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASN:ND2	1:A:469:ASN:H	2.15	0.42
1:A:725:LEU:HB2	1:A:736:PHE:HE1	1.83	0.42
1:B:30:LYS:HG3	1:B:30:LYS:O	2.20	0.42
1:B:416:ILE:HG22	1:B:420:ASP:OD1	2.20	0.42
1:A:70:VAL:HG12	1:A:252:ILE:HD11	2.01	0.42
1:A:311:LEU:O	1:A:312:SER:CB	2.67	0.42
1:A:403:SER:HB2	1:A:638:ASN:OD1	2.20	0.42
1:A:607:LYS:C	1:A:609:ASN:H	2.28	0.42
1:B:427:ILE:O	1:B:432:TYR:OH	2.35	0.42
1:B:456:ASP:OD1	1:B:456:ASP:C	2.63	0.42
1:B:657:GLY:HA2	1:B:667:LEU:O	2.20	0.42
1:B:698:TYR:CD1	1:B:698:TYR:C	2.98	0.42
1:A:118:TYR:C	1:A:119:VAL:CG2	2.93	0.42
1:A:563:GLN:HE21	1:A:585:PHE:H	1.68	0.42
1:B:190:PHE:CB	1:B:194:LEU:HD23	2.50	0.42
1:B:578:LYS:O	1:B:579:TYR:HB2	2.20	0.42
1:B:601:LEU:O	1:B:602:ILE:C	2.63	0.42
1:B:659:TYR:CE2	1:B:661:PRO:HG3	2.55	0.42
1:A:416:ILE:C	1:A:418:ASN:N	2.77	0.41
1:B:77:ILE:CG2	1:B:77:ILE:O	2.68	0.41
1:B:498:ARG:HA	1:B:498:ARG:HD2	1.92	0.41
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.41
1:A:29:ASN:C	1:A:31:THR:N	2.77	0.41
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.86	0.41
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.41
1:B:264:MET:O	1:B:266:SER:N	2.53	0.41
1:B:303:LYS:O	1:B:304:LYS:C	2.63	0.41
1:A:567:ASN:O	1:A:569:GLU:N	2.49	0.41
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.80	0.41
1:B:75:LYS:C	1:B:78:GLY:H	2.19	0.41
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.03	0.41
1:B:327:SER:C	1:B:329:PHE:H	2.28	0.41
1:B:529:ILE:N	1:B:529:ILE:CD1	2.83	0.41
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.19	0.41
1:A:369:SER:OG	1:A:372:GLU:CB	2.67	0.41
1:A:394:ASP:HB3	1:A:635:THR:OG1	2.20	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.50	0.41
1:B:619:THR:O	1:B:619:THR:HG22	2.19	0.41
1:A:118:TYR:CE2	1:A:143:LYS:HB3	2.56	0.41
1:A:178:LYS:HG3	1:A:179:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLU:HG2	1:A:734:ALA:N	2.35	0.41
1:B:555:ILE:O	1:B:556:ASP:C	2.64	0.41
1:B:635:THR:C	1:B:637:PRO:HD2	2.45	0.41
1:A:175:ASN:O	1:A:178:LYS:HG2	2.21	0.41
1:A:213:VAL:O	1:A:214:GLN:C	2.61	0.41
1:A:272:GLU:HA	1:A:275:LYS:HB3	2.01	0.41
1:A:465:ARG:O	1:A:466:GLY:C	2.63	0.41
1:A:649:ILE:C	1:A:651:GLU:N	2.77	0.41
1:B:114:LEU:HD22	1:B:120:TYR:HB2	2.01	0.41
1:B:160:LEU:C	1:B:162:LYS:H	2.29	0.41
1:B:174:LEU:CD2	1:B:216:VAL:HG11	2.51	0.41
1:B:313:GLN:C	1:B:315:GLU:N	2.77	0.41
1:B:342:GLN:C	1:B:343:ILE:HD13	2.46	0.41
1:B:467:ILE:H	1:B:467:ILE:CD1	2.33	0.41
1:B:610:ILE:HG23	1:B:614:LEU:HD23	1.99	0.41
1:B:658:LEU:HD23	1:B:658:LEU:C	2.46	0.41
1:B:696:ALA:O	1:B:697:GLY:C	2.63	0.41
1:A:247:PHE:O	1:A:247:PHE:CG	2.73	0.41
1:B:74:TYR:CE1	1:B:79:GLY:HA3	2.55	0.41
1:B:187:ASP:O	1:B:188:LEU:C	2.64	0.41
1:B:401:SER:CB	1:B:638:ASN:ND2	2.75	0.41
1:B:468:PHE:CD2	1:B:534:ILE:HD11	2.56	0.41
1:A:121:ALA:HA	1:A:129:LEU:HA	2.02	0.41
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.56	0.41
1:A:301:GLU:HA	1:A:302:PRO:HD3	1.84	0.41
1:A:311:LEU:O	1:A:315:GLU:OE1	2.39	0.41
1:A:563:GLN:NE2	1:A:585:PHE:H	2.17	0.41
1:A:721:GLU:OE1	1:A:759:ALA:HA	2.20	0.41
1:B:54:VAL:O	1:B:55:LYS:C	2.61	0.41
1:B:75:LYS:O	1:B:76:ALA:C	2.64	0.41
1:B:257:GLU:HA	1:B:260:LYS:HD3	2.03	0.41
1:B:473:LYS:O	1:B:474:ASN:HB2	2.20	0.41
1:B:540:LYS:HD3	1:B:542:TYR:CZ	2.55	0.41
1:B:661:PRO:C	1:B:663:SER:H	2.28	0.41
1:B:755:VAL:HG12	1:B:756:GLN:N	2.34	0.41
1:A:118:TYR:HE2	1:A:143:LYS:HB3	1.86	0.41
1:A:169:LYS:HE3	1:A:533:GLN:HB3	2.03	0.41
1:A:202:SER:O	1:A:203:VAL:C	2.62	0.41
1:A:241:PHE:HD1	1:A:242:ASN:N	2.18	0.41
1:A:391:ARG:CZ	1:A:395:THR:HG21	2.51	0.41
1:A:427:ILE:HD12	1:A:427:ILE:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:O	1:A:431:LEU:HD23	2.21	0.41
1:B:27:GLU:O	1:B:27:GLU:CG	2.63	0.41
1:B:64:GLU:CD	1:B:64:GLU:O	2.64	0.41
1:B:143:LYS:O	1:B:147:VAL:HG23	2.21	0.41
1:B:186:GLN:NE2	1:B:195:LYS:HB2	2.25	0.41
1:B:416:ILE:C	1:B:418:ASN:H	2.29	0.41
1:B:465:ARG:O	1:B:466:GLY:C	2.62	0.41
1:B:490:GLU:HG2	1:B:537:GLN:HE22	1.86	0.41
1:B:502:ARG:C	1:B:503:ILE:HD13	2.46	0.41
1:A:154:ILE:HG22	1:A:155:LEU:N	2.35	0.41
1:A:522:GLN:HG3	1:A:523:ARG:N	2.36	0.41
1:A:721:GLU:C	1:A:723:SER:H	2.29	0.41
1:B:235:LEU:HD13	1:B:236:TYR:CD1	2.56	0.41
1:B:267:ARG:HG2	1:B:489:ASN:CG	2.45	0.41
1:B:341:LEU:O	1:B:341:LEU:HD23	2.21	0.41
1:B:416:ILE:O	1:B:417:GLN:C	2.62	0.41
1:B:673:LYS:O	1:B:673:LYS:CG	2.68	0.41
1:B:753:LEU:O	1:B:754:LYS:C	2.64	0.41
1:A:223:TYR:HB3	1:A:233:LEU:CD1	2.50	0.40
1:A:740:ALA:O	1:A:741:PHE:C	2.62	0.40
1:B:408:VAL:O	1:B:411:GLN:HB3	2.21	0.40
1:A:73:MET:SD	1:A:159:ILE:HG21	2.61	0.40
1:A:511:ALA:HB2	1:A:521:LEU:HD23	2.03	0.40
1:A:634:ILE:HD11	1:A:639:ILE:HD12	2.02	0.40
1:A:681:SER:O	1:A:684:PHE:HB3	2.21	0.40
1:A:733:GLU:O	1:A:734:ALA:C	2.63	0.40
1:B:106:ASP:OD2	1:B:110:LYS:HB2	2.21	0.40
1:B:343:ILE:HG23	1:B:346:ARG:HD2	2.01	0.40
1:A:467:ILE:N	1:A:467:ILE:HD12	2.36	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.20	0.40
1:B:89:THR:HG21	1:B:97:LEU:CD1	2.52	0.40
1:B:234:GLN:HB2	1:B:241:PHE:CE2	2.57	0.40
1:B:762:THR:O	1:B:763:PHE:C	2.64	0.40
1:A:36:LEU:C	1:A:40:MET:HG2	2.47	0.40
1:A:640:ALA:O	1:A:644:THR:HG23	2.22	0.40
1:B:177:ILE:CG2	1:B:186:GLN:HA	2.51	0.40
1:B:226:GLU:HA	1:B:227:PRO:HD3	1.94	0.40
1:B:681:SER:C	1:B:683:GLY:N	2.78	0.40
1:A:266:SER:O	1:A:269:GLU:HB3	2.22	0.40
1:A:605:GLU:C	1:A:607:LYS:N	2.77	0.40
1:A:721:GLU:HA	1:A:724:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:O	1:B:342:GLN:NE2	2.53	0.40
1:B:335:LYS:C	1:B:337:PHE:N	2.79	0.40
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.81	0.40
1:B:448:ALA:O	1:B:449:THR:C	2.65	0.40
1:B:510:ARG:HB2	1:B:522:GLN:OE1	2.22	0.40
1:B:511:ALA:CB	1:B:521:LEU:HD23	2.51	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	728/776 (94%)	529 (73%)	144 (20%)	55 (8%)	1	8
1	B	730/776 (94%)	536 (73%)	143 (20%)	51 (7%)	1	10
All	All	1458/1552 (94%)	1065 (73%)	287 (20%)	106 (7%)	1	9

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	92	ILE
1	A	227	PRO
1	A	238	PRO
1	A	405	ASN
1	A	457	SER
1	A	473	LYS
1	A	539	GLU
1	A	675	VAL
1	A	678	ARG
1	A	702	LYS
1	A	720	GLU

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Mol	Chain	Res	Type
1	B	33	GLU
1	B	95	GLU
1	B	211	ASN
1	B	310	SER
1	B	325	ASP
1	B	366	ASN
1	B	495	ASP
1	B	553	SER
1	B	731	THR
1	A	181	SER
1	A	279	GLN
1	A	336	GLU
1	A	369	SER
1	A	428	GLY
1	A	573	ALA
1	A	590	ARG
1	A	615	ILE
1	A	647	ASP
1	A	676	GLU
1	B	35	HIS
1	B	96	ALA
1	B	157	ARG
1	B	168	GLN
1	B	203	VAL
1	B	210	SER
1	B	242	ASN
1	B	250	GLN
1	B	324	ILE
1	B	326	SER
1	B	367	PRO
1	B	370	GLU
1	B	417	GLN
1	B	515	GLU
1	B	592	ALA
1	B	593	SER
1	A	30	LYS
1	A	125	TYR
1	A	254	LEU
1	A	265	LEU
1	A	312	SER
1	A	460	ASN
1	A	509	THR

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Mol	Chain	Res	Type
1	A	568	GLN
1	A	593	SER
1	A	741	PHE
1	A	760	PRO
1	B	48	VAL
1	B	52	GLU
1	B	123	GLU
1	B	187	ASP
1	B	531	ASP
1	B	767	ASN
1	A	114	LEU
1	A	198	PRO
1	A	264	MET
1	A	299	PRO
1	A	300	ILE
1	A	329	PHE
1	A	492	PRO
1	A	682	GLU
1	B	53	ALA
1	B	180	ALA
1	B	200	ASP
1	B	468	PHE
1	B	474	ASN
1	B	666	ILE
1	B	732	ASN
1	A	77	ILE
1	A	164	ASN
1	A	402	PRO
1	A	731	THR
1	A	742	ARG
1	B	142	GLU
1	B	169	LYS
1	B	265	LEU
1	B	314	GLU
1	B	464	ASN
1	B	647	ASP
1	A	78	GLY
1	A	433	ASN
1	A	670	GLY
1	B	674	GLY
1	A	529	ILE
1	A	627	GLY

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Mol	Chain	Res	Type
1	A	722	GLY
1	B	198	PRO
1	B	227	PRO
1	A	147	VAL
1	A	366	ASN
1	A	383	ILE
1	B	466	GLY
1	B	467	ILE
1	B	595	ILE
1	B	383	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/710 (94%)	599 (89%)	72 (11%)	6	28
1	B	673/710 (95%)	602 (90%)	71 (10%)	6	28
All	All	1344/1420 (95%)	1201 (89%)	143 (11%)	6	28

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	42	HIS
1	A	46	ILE
1	A	49	LYS
1	A	51	GLU
1	A	52	GLU
1	A	56	LYS
1	A	91	HIS
1	A	93	SER
1	A	100	ASP
1	A	101	LYS
1	A	104	ILE
1	A	107	ILE

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	118	TYR
1	A	193	GLN
1	A	199	THR
1	A	211	ASN
1	A	227	PRO
1	A	233	LEU
1	A	239	GLU
1	A	241	PHE
1	A	256	LEU
1	A	259	LEU
1	A	260	LYS
1	A	283	ASP
1	A	292	LEU
1	A	296	LEU
1	A	300	ILE
1	A	311	LEU
1	A	321	ARG
1	A	329	PHE
1	A	333	GLU
1	A	343	ILE
1	A	345	ILE
1	A	373	LYS
1	A	381	LEU
1	A	404	ILE
1	A	408	VAL
1	A	418	ASN
1	A	426	SER
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	456	ASP
1	A	469	ASN
1	A	498	ARG
1	A	500	LYS
1	A	514	LEU
1	A	529	ILE
1	A	541	GLU
1	A	543	ILE
1	A	550	VAL
1	A	556	ASP
1	A	574	LEU

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Mol	Chain	Res	Type
1	A	578	LYS
1	A	586	ASN
1	A	594	ASN
1	A	601	LEU
1	A	604	ASN
1	A	608	ASN
1	A	611	GLN
1	A	619	THR
1	A	636	LEU
1	A	658	LEU
1	A	693	ASP
1	A	710	ASN
1	A	712	LYS
1	A	716	ASP
1	A	727	SER
1	A	737	PHE
1	A	764	GLN
1	B	28	ARG
1	B	32	GLN
1	B	36	LEU
1	B	47	GLU
1	B	60	GLU
1	B	62	LEU
1	B	65	LYS
1	B	92	ILE
1	B	95	GLU
1	B	107	ILE
1	B	111	ASP
1	B	128	VAL
1	B	131	ILE
1	B	136	ASP
1	B	140	ASN
1	B	153	LYS
1	B	154	ILE
1	B	178	LYS
1	B	193	GLN
1	B	197	HIS
1	B	199	THR
1	B	203	VAL
1	B	204	GLU
1	B	206	LEU
1	B	233	LEU

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Mol	Chain	Res	Type
1	B	235	LEU
1	B	245	ASP
1	B	250	GLN
1	B	274	ILE
1	B	282	SER
1	B	296	LEU
1	B	297	GLN
1	B	304	LYS
1	B	323	GLN
1	B	341	LEU
1	B	343	ILE
1	B	345	ILE
1	B	366	ASN
1	B	381	LEU
1	B	384	GLN
1	B	398	LEU
1	B	407	ASP
1	B	408	VAL
1	B	425	GLN
1	B	433	ASN
1	B	445	ASN
1	B	449	THR
1	B	456	ASP
1	B	461	THR
1	B	464	ASN
1	B	487	ASP
1	B	496	ASN
1	B	503	ILE
1	B	516	ASN
1	B	523	ARG
1	B	533	GLN
1	B	556	ASP
1	B	571	ASN
1	B	574	LEU
1	B	580	THR
1	B	586	ASN
1	B	587	VAL
1	B	611	GLN
1	B	613	ASP
1	B	646	GLN
1	B	652	GLN
1	B	712	LYS

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Mol	Chain	Res	Type
1	B	717	ILE
1	B	747	THR
1	B	753	LEU
1	B	764	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	132	GLN
1	A	140	ASN
1	A	164	ASN
1	A	165	GLN
1	A	179	ASN
1	A	186	GLN
1	A	193	GLN
1	A	197	HIS
1	A	214	GLN
1	A	262	GLN
1	A	276	GLN
1	A	297	GLN
1	A	309	HIS
1	A	323	GLN
1	A	440	ASN
1	A	444	ASN
1	A	460	ASN
1	A	469	ASN
1	A	474	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	609	ASN
1	A	611	GLN
1	A	620	ASN
1	A	703	ASN
1	A	710	ASN

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Mol	Chain	Res	Type
1	A	745	HIS
1	A	756	GLN
1	B	91	HIS
1	B	140	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	276	GLN
1	B	277	HIS
1	B	342	GLN
1	B	366	ASN
1	B	390	GLN
1	B	440	ASN
1	B	445	ASN
1	B	464	ASN
1	B	496	ASN
1	B	516	ASN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	565	ASN
1	B	568	GLN
1	B	571	ASN
1	B	589	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN
1	B	645	HIS
1	B	690	HIS
1	B	710	ASN
1	B	749	HIS
1	B	756	GLN
1	B	769	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	SD2	B	9003	2	33,33,33	1.13	3 (9%)	43,44,44	2.24	6 (13%)
3	SD2	A	9002	2	33,33,33	0.96	1 (3%)	43,44,44	1.87	5 (11%)

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	SD2	B	9003	2	-	7/32/44/44	0/2/2/2
3	SD2	A	9002	2	-	5/32/44/44	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	SD2	CBB-CBC	-3.50	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9003	SD2	CBB-CBC	-3.30	1.38	1.51
3	B	9003	SD2	CAR-NAQ	2.32	1.51	1.47
3	B	9003	SD2	CBB-CAY	-2.05	1.48	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9003	SD2	CAY-NAX-CAS	10.39	143.97	121.65
3	A	9002	SD2	CAY-NAX-CAS	7.46	137.67	121.65
3	A	9002	SD2	CBB-CAY-NAX	-5.57	99.87	110.91
3	B	9003	SD2	CAR-CAS-NAX	5.50	128.60	116.52
3	B	9003	SD2	CBB-CAY-NAX	4.79	120.38	110.91
3	A	9002	SD2	CAR-CAS-NAX	-4.60	106.44	116.52
3	B	9003	SD2	OAT-CAS-NAX	-4.23	115.39	122.96
3	A	9002	SD2	OAT-CAS-NAX	4.20	130.48	122.96
3	B	9003	SD2	CAS-CAR-NAQ	-2.59	105.42	112.50
3	B	9003	SD2	CBB-CAY-CAZ	2.28	115.67	110.14
3	A	9002	SD2	CBC-CBB-CAY	2.26	119.87	112.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	9003	SD2	OAT-CAS-NAX-CAY
3	B	9003	SD2	CAR-CAS-NAX-CAY
3	B	9003	SD2	CBB-CAY-NAX-CAS
3	B	9003	SD2	CBB-CBC-SBD-CBE
3	B	9003	SD2	CAZ-CAY-CBB-CBC
3	A	9002	SD2	NAQ-CAR-CAS-NAX
3	B	9003	SD2	NAQ-CAR-CAS-NAX
3	A	9002	SD2	NAQ-CAR-CAS-OAT
3	A	9002	SD2	CAU-CAR-CAS-OAT
3	B	9003	SD2	NAQ-CAR-CAS-OAT
3	A	9002	SD2	CAU-CAR-CAS-NAX
3	A	9002	SD2	NAX-CAY-CBB-CBC

There are no ring outliers.

2 monomers are involved in 18 short contacts:

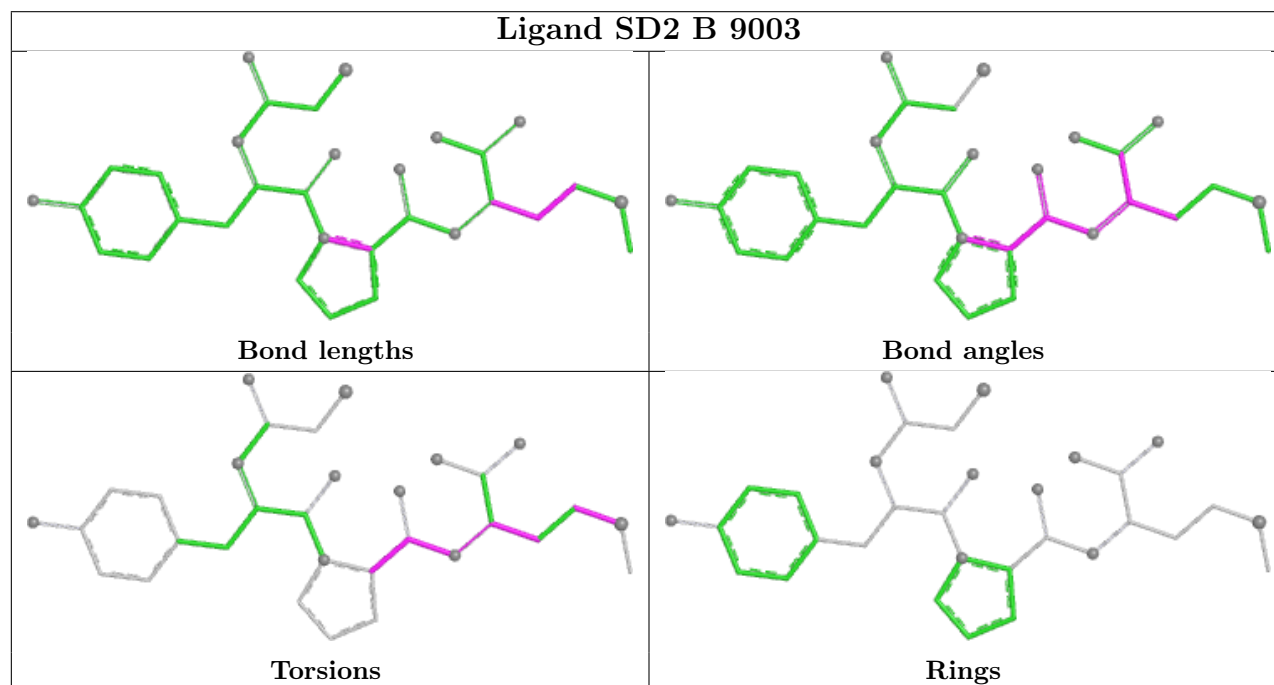
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9003	SD2	9	0

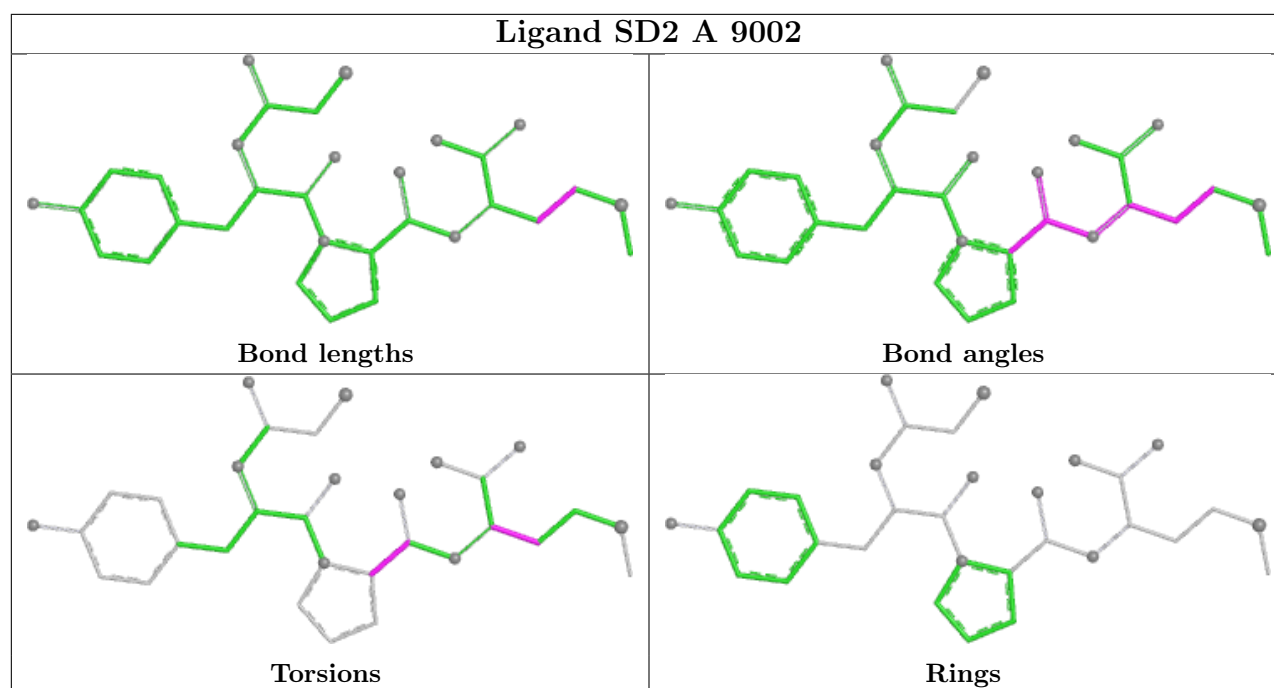
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	SD2	9	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	732/776 (94%)	-1.59	0 100 100	13, 39, 88, 93	0
1	B	734/776 (94%)	-1.60	0 100 100	11, 38, 84, 96	0
All	All	1466/1552 (94%)	-1.60	0 100 100	11, 38, 86, 96	0

There are no RSRZ outliers to report.

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.

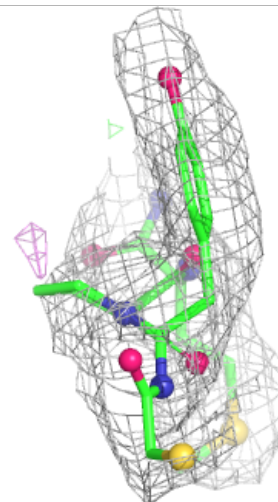
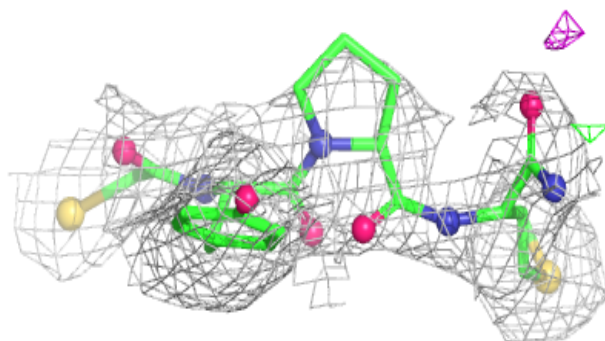
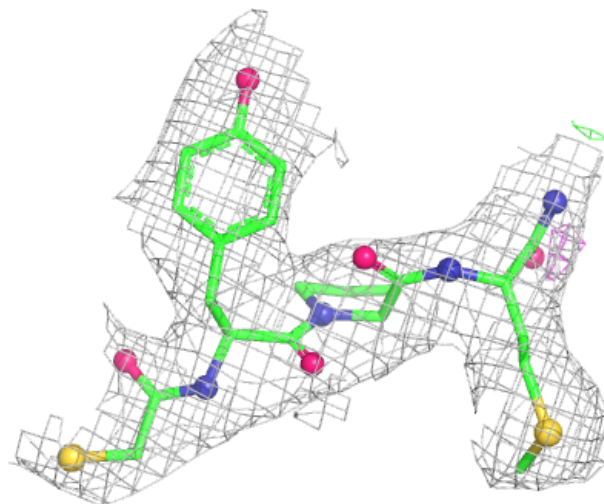
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SD2	B	9003	32/32	0.99	0.03	16,23,32,37	0
2	ZN	B	9002	1/1	1.00	0.00	17,17,17,17	0
3	SD2	A	9002	32/32	1.00	0.03	21,23,30,41	0
2	ZN	A	9001	1/1	1.00	0.01	21,21,21,21	0

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.

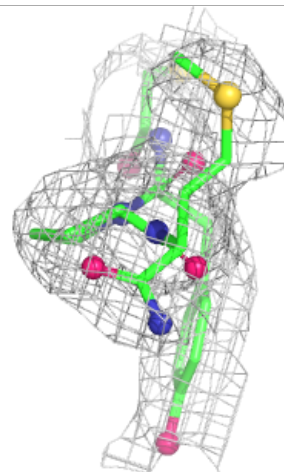
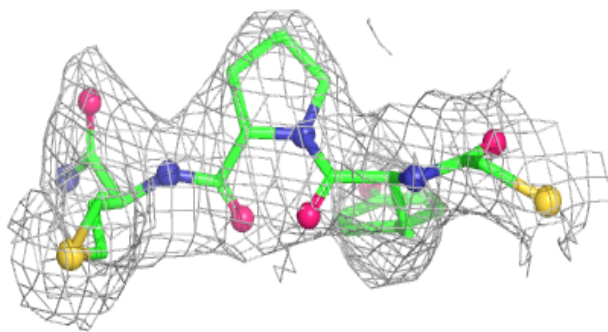
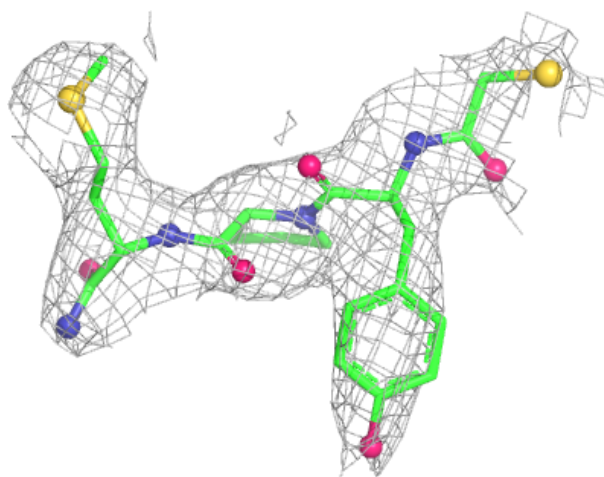
Electron density around SD2 B 9003:

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



Electron density around SD2 A 9002:

$2mF_o-DF_c$ (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.