



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:34 PM UTC

PDB ID : 2X6J / pdb_00002x6j
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-93
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
Resolution : 3.50 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

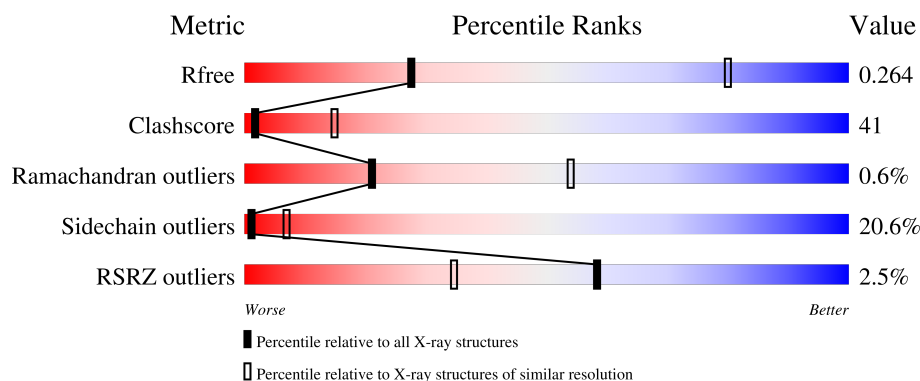
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	696	2% 28% 34% 13% • 22%
1	B	696	2% 33% 34% 11% • 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	093	A	1949	-	X	X	-
2	093	B	1950	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8967 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.

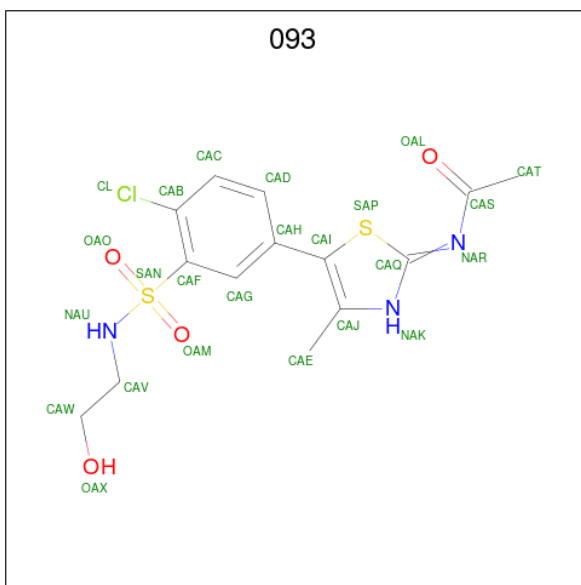
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4457	2882	757	791	27			
1	B	546	Total	C	N	O	S	0	0	0
			4462	2886	759	790	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression tag	UNP Q9W1M7
B	256	HIS	-	expression tag	UNP Q9W1M7
B	257	MET	-	expression tag	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIAZOLE-2-YL)-ACETAMIDE (CCD ID: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).

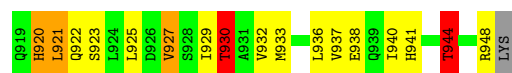


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0	0
2	B	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0	0

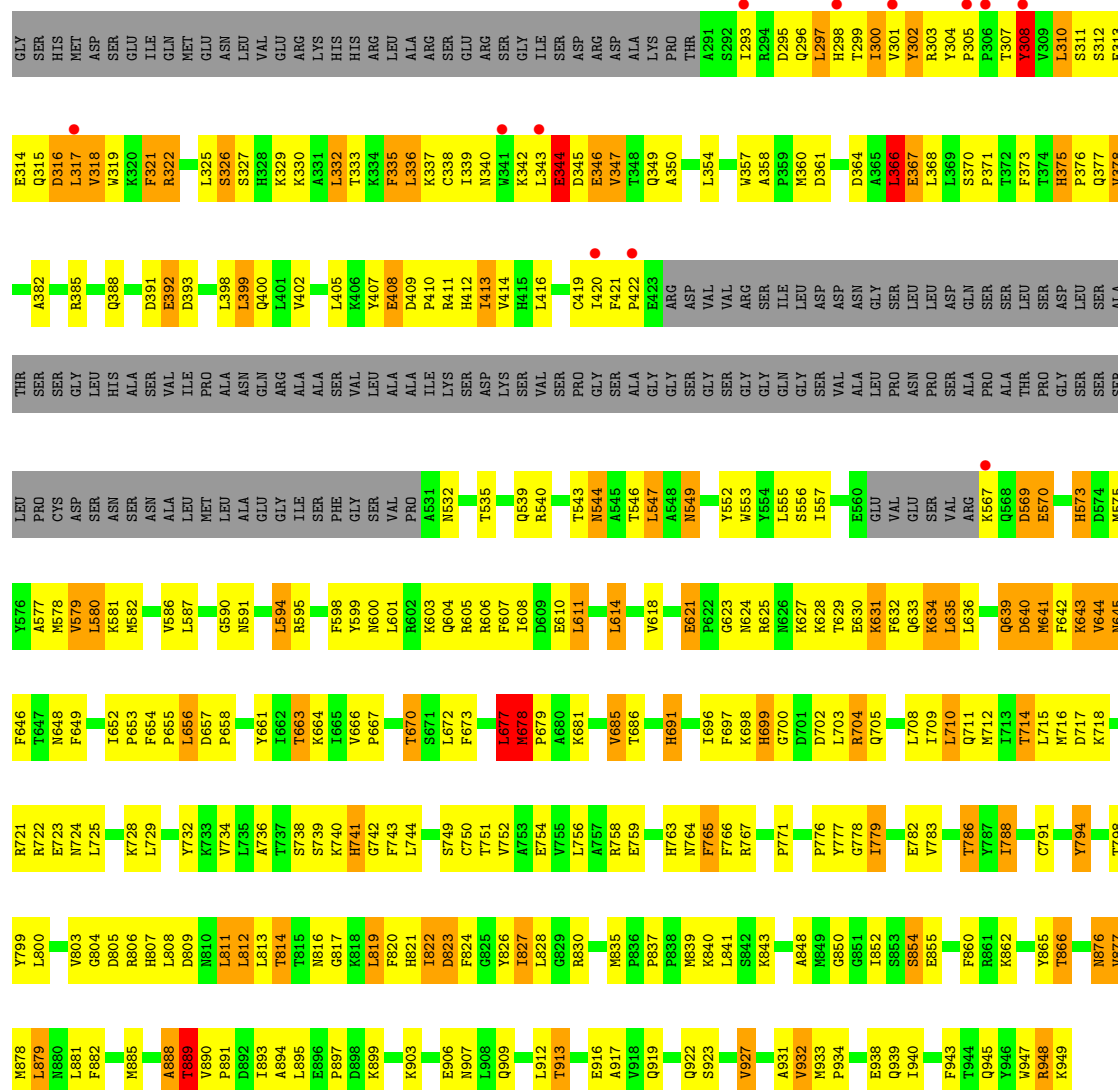
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

The visualization displays the amino acid sequence of Chain A, with the central bar indicating a score or probability. The sequence is represented by a series of amino acid codes (e.g., K380, Y381, A382, etc.) arranged in a grid. The color gradient of the bar suggests a range of values, with green indicating lower values and red indicating higher values. The vertical columns on the left and right provide additional context for the sequence, showing the distribution of amino acids across different positions.



• Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.95Å 156.33Å 242.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.62 – 3.50 61.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.62-3.50) 99.5 (61.62-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.272 0.225 , 0.264	Depositor DCC
R_{free} test set	1313 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 093

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	0.77	1/4566 (0.0%)	1.47	97/6183 (1.6%)
1	B	0.58	0/4571	1.06	17/6189 (0.3%)
All	All	0.68	1/9137 (0.0%)	1.28	114/12372 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	591	ASN	C-O	6.11	1.31	1.24

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	LYS	N-CA-C	-9.23	96.86	110.52
1	B	344	GLU	N-CA-C	8.93	121.09	111.36
1	A	340	ASN	N-CA-C	8.38	121.24	111.02
1	A	681	LYS	N-CA-C	-8.32	98.17	110.48
1	A	535	THR	N-CA-C	-7.74	102.93	111.36
1	A	757	ALA	N-CA-C	-7.70	102.89	111.82
1	A	375	HIS	CA-C-N	7.60	127.98	119.32
1	A	375	HIS	C-N-CA	7.60	127.98	119.32
1	A	551	PHE	N-CA-C	-7.38	103.31	111.36
1	A	364	ASP	N-CA-C	-7.27	103.39	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ALA	N-CA-C	-7.27	103.36	111.28
1	A	595	ARG	N-CA-C	-7.23	103.40	111.28
1	A	862	LYS	N-CA-C	-7.06	103.59	111.28
1	A	627	LYS	N-CA-C	-7.05	103.64	111.82
1	A	309	VAL	N-CA-C	-7.02	104.20	112.98
1	A	321	PHE	N-CA-C	-6.98	103.75	112.90
1	A	328	HIS	N-CA-C	6.91	119.26	108.96
1	A	868	TYR	N-CA-C	-6.87	103.88	111.36
1	B	666	VAL	CA-C-N	6.84	126.30	118.85
1	B	666	VAL	C-N-CA	6.84	126.30	118.85
1	B	678	MET	CA-C-N	6.76	126.67	119.85
1	B	678	MET	C-N-CA	6.76	126.67	119.85
1	A	297	LEU	N-CA-C	-6.74	104.00	111.82
1	A	389	ALA	CA-C-N	6.69	126.67	119.78
1	A	389	ALA	C-N-CA	6.69	126.67	119.78
1	A	790	SER	N-CA-C	-6.69	104.07	111.36
1	A	352	TRP	N-CA-C	-6.68	104.08	111.82
1	A	711	GLN	N-CA-C	-6.63	104.05	111.28
1	A	798	THR	N-CA-C	-6.53	104.24	111.36
1	A	767	ARG	N-CA-C	-6.52	104.26	111.82
1	A	915	GLU	N-CA-C	-6.48	104.06	112.23
1	A	865	TYR	N-CA-C	-6.48	104.30	111.36
1	A	944	THR	N-CA-C	-6.40	104.40	111.82
1	B	308	TYR	N-CA-C	6.39	118.88	108.26
1	A	693	TYR	CA-C-N	-6.35	112.83	122.81
1	A	693	TYR	C-N-CA	-6.35	112.83	122.81
1	A	592	PHE	N-CA-C	-6.35	104.74	113.18
1	A	369	LEU	N-CA-C	-6.31	105.55	113.18
1	A	602	ARG	N-CA-C	-6.29	104.42	111.28
1	A	403	GLN	N-CA-C	-6.23	104.57	111.36
1	A	409	ASP	CA-C-N	6.20	125.76	119.19
1	A	409	ASP	C-N-CA	6.20	125.76	119.19
1	A	722	ARG	N-CA-C	-6.20	104.63	111.82
1	A	416	LEU	N-CA-C	-6.14	104.67	111.36
1	A	901	VAL	N-CA-C	-6.12	104.54	110.72
1	A	930	THR	N-CA-C	-6.06	104.79	111.82
1	A	594	LEU	N-CA-C	-6.04	104.25	111.69
1	A	330	LYS	N-CA-C	-6.00	104.81	111.71
1	A	316	ASP	N-CA-C	-5.94	104.89	111.36
1	A	795	CYS	N-CA-C	-5.92	104.91	111.36
1	A	735	LEU	CA-C-N	-5.92	111.97	122.74
1	A	735	LEU	C-N-CA	-5.92	111.97	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	816	ASN	CA-C-N	-5.85	113.39	122.69
1	A	816	ASN	C-N-CA	-5.85	113.39	122.69
1	A	541	ALA	N-CA-C	-5.84	105.04	111.82
1	A	817	GLY	N-CA-C	5.83	122.80	114.64
1	B	678	MET	N-CA-C	5.83	121.07	109.01
1	A	673	PHE	N-CA-C	5.80	119.07	110.48
1	A	400	GLN	N-CA-C	-5.77	104.95	112.23
1	A	414	VAL	N-CA-C	-5.76	104.72	111.00
1	A	617	LEU	N-CA-C	-5.76	104.97	112.23
1	A	604	GLN	N-CA-C	-5.74	105.10	111.36
1	A	630	GLU	N-CA-C	-5.73	105.12	111.36
1	A	346	GLU	N-CA-C	-5.66	105.25	111.82
1	A	533	LEU	N-CA-C	5.65	117.44	111.28
1	A	578	MET	N-CA-C	-5.64	105.21	111.36
1	A	888	ALA	N-CA-C	5.64	120.00	113.18
1	A	557	ILE	N-CA-C	-5.63	104.05	111.09
1	A	906	GLU	N-CA-C	-5.61	104.80	111.69
1	B	375	HIS	CA-C-N	5.58	125.25	119.05
1	B	375	HIS	C-N-CA	5.58	125.25	119.05
1	B	823	ASP	N-CA-C	5.58	118.06	109.07
1	A	801	LEU	N-CA-C	-5.57	106.07	112.92
1	A	417	HIS	N-CA-C	-5.53	105.33	111.36
1	A	577	ALA	N-CA-C	-5.53	105.33	111.36
1	A	641	MET	N-CA-C	-5.52	106.05	112.89
1	A	366	LEU	N-CA-C	-5.51	105.35	111.36
1	B	366	LEU	N-CA-C	-5.50	105.38	111.71
1	A	597	ILE	N-CA-C	-5.49	105.18	110.72
1	B	677	LEU	N-CA-C	-5.49	101.78	109.96
1	A	793	GLY	N-CA-C	-5.47	106.16	112.73
1	A	393	ASP	N-CA-C	-5.46	105.35	112.23
1	A	786	THR	N-CA-C	-5.45	105.49	111.82
1	A	581	LYS	N-CA-C	-5.43	105.52	111.82
1	A	883	SER	N-CA-C	-5.42	105.48	111.71
1	A	633	GLN	N-CA-C	-5.39	105.41	111.28
1	A	941	HIS	N-CA-C	-5.35	105.45	111.28
1	A	817	GLY	CA-C-N	-5.35	111.32	122.07
1	A	817	GLY	C-N-CA	-5.35	111.32	122.07
1	B	621	GLU	CA-C-N	5.34	124.85	119.19
1	B	621	GLU	C-N-CA	5.34	124.85	119.19
1	A	574	ASP	N-CA-C	-5.34	105.63	111.82
1	A	800	LEU	N-CA-C	-5.34	105.50	112.23
1	A	698	LYS	N-CA-C	5.33	117.21	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	682	LEU	CA-C-N	-5.33	113.54	122.92
1	A	682	LEU	C-N-CA	-5.33	113.54	122.92
1	B	888	ALA	N-CA-C	5.27	117.11	111.36
1	A	298	HIS	N-CA-C	-5.27	105.62	111.36
1	A	723	GLU	N-CA-C	-5.25	106.82	113.18
1	B	794	TYR	N-CA-C	5.23	117.06	111.36
1	A	847	GLU	N-CA-C	-5.19	105.80	111.82
1	A	921	LEU	N-CA-C	-5.19	105.70	111.36
1	A	576	TYR	N-CA-C	-5.18	105.81	111.82
1	A	768	LYS	N-CA-C	-5.18	105.72	111.36
1	A	368	LEU	N-CA-C	-5.16	105.83	111.82
1	A	614	LEU	N-CA-C	-5.16	105.73	111.36
1	A	905	GLU	N-CA-C	-5.16	105.83	111.82
1	A	788	ILE	N-CA-C	-5.16	105.51	110.72
1	A	680	ALA	CA-C-O	-5.16	115.73	121.81
1	A	938	GLU	N-CA-C	-5.14	105.75	112.23
1	A	677	LEU	N-CA-C	-5.13	102.61	110.30
1	A	715	LEU	N-CA-C	-5.09	105.81	111.36
1	B	375	HIS	N-CA-C	5.08	116.79	109.48
1	A	587	LEU	N-CA-C	-5.07	105.45	111.69

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide
1	A	737	THR	Mainchain
1	A	740	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4457	0	4490	361	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4462	0	4499	365	1
2	A	24	0	16	9	0
2	B	24	0	16	6	0
All	All	8967	0	9021	729	2

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 41.

All (729) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:CD2	1:A:377:GLN:H	1.54	1.24
1:B:311:SER:HB3	1:B:314:GLU:CB	1.76	1.15
1:B:299:THR:HB	1:B:303:ARG:HH11	1.10	1.14
1:A:705:GLN:HG2	1:A:890:VAL:HG13	1.22	1.13
1:A:629:THR:HB	1:A:672:LEU:HD12	1.18	1.10
1:A:421:PHE:HB3	1:A:422:PRO:HD2	1.33	1.10
1:A:322:ARG:HH12	1:A:353:MET:HG3	1.13	1.09
1:B:412:HIS:CE1	1:B:532:ASN:HB3	1.86	1.09
1:A:830:ARG:NH2	1:A:903:LYS:HZ1	1.50	1.09
1:A:638:GLU:HG2	1:A:641:MET:HG3	1.32	1.09
1:A:645:ASN:C	1:A:645:ASN:HD22	1.62	1.06
1:A:629:THR:HB	1:A:672:LEU:CD1	1.86	1.05
1:A:298:HIS:HB3	1:A:302:TYR:CE1	1.91	1.04
1:A:591:ASN:O	1:A:595:ARG:HD3	1.58	1.04
1:A:299:THR:HA	1:A:302:TYR:CE2	1.94	1.01
1:A:335:PHE:HD2	1:A:335:PHE:C	1.69	1.00
1:B:311:SER:HB3	1:B:314:GLU:HB3	1.44	1.00
1:A:532:ASN:OD1	1:A:535:THR:HG23	1.63	0.99
1:A:561:GLU:CD	1:A:561:GLU:H	1.71	0.98
1:B:570:GLU:CD	1:B:570:GLU:H	1.67	0.98
1:B:408:GLU:HB3	1:B:409:ASP:HA	1.41	0.98
1:A:737:THR:HG22	1:A:738:SER:H	1.26	0.97
1:A:814:THR:HG23	1:A:818:LYS:H	1.27	0.97
1:B:702:ASP:HB3	1:B:739:SER:HA	1.47	0.95
1:A:830:ARG:HH22	1:A:903:LYS:NZ	1.64	0.95
1:B:667:PRO:O	1:B:670:THR:HG22	1.65	0.95
1:A:319:TRP:CD1	1:A:323:PHE:HE2	1.84	0.95
1:A:375:HIS:HD2	1:A:377:GLN:N	1.63	0.95
1:B:329:LYS:NZ	1:B:361:ASP:H	1.64	0.94
1:A:734:VAL:HG22	1:A:744:LEU:HD23	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PHE:HD2	1:B:335:PHE:C	1.75	0.94
1:B:654:PHE:HD1	1:B:655:PRO:HD2	1.33	0.93
1:B:421:PHE:HB3	1:B:422:PRO:HD2	1.51	0.92
1:A:577:ALA:O	1:A:581:LYS:HD2	1.69	0.92
1:B:710:LEU:CD2	1:B:732:TYR:O	2.18	0.92
1:B:634:LYS:HA	1:B:634:LYS:HE2	1.50	0.91
1:A:335:PHE:C	1:A:335:PHE:CD2	2.44	0.90
1:A:553:TRP:O	1:A:557:ILE:HG13	1.72	0.90
1:B:678:MET:C	1:B:699:HIS:HE2	1.79	0.90
1:A:322:ARG:NH1	1:A:353:MET:HG3	1.86	0.90
1:B:329:LYS:HZ3	1:B:361:ASP:CG	1.79	0.90
1:A:591:ASN:OD1	1:A:592:PHE:N	2.05	0.90
1:B:710:LEU:HD23	1:B:732:TYR:O	1.72	0.90
1:B:739:SER:O	1:B:740:LYS:HG2	1.71	0.89
1:B:412:HIS:CE1	1:B:532:ASN:CB	2.54	0.89
1:A:814:THR:CG2	1:A:818:LYS:H	1.84	0.89
1:B:827:ILE:HG23	1:B:828:LEU:HG	1.55	0.89
1:A:698:LYS:NZ	2:A:1949:093:CL	2.42	0.89
1:A:375:HIS:CD2	1:A:377:GLN:N	2.40	0.88
1:B:375:HIS:CD2	1:B:377:GLN:H	1.91	0.88
1:A:298:HIS:HB3	1:A:302:TYR:HE1	1.36	0.88
1:B:367:GLU:O	1:B:370:SER:OG	1.90	0.88
1:B:311:SER:HB3	1:B:314:GLU:HB2	1.52	0.88
1:A:319:TRP:CD1	1:A:323:PHE:CE2	2.60	0.88
1:B:549:ASN:C	1:B:549:ASN:HD22	1.80	0.87
1:A:319:TRP:NE1	1:A:322:ARG:HH21	1.73	0.87
1:A:654:PHE:HD1	1:A:655:PRO:HD2	1.40	0.87
1:B:332:LEU:CD1	1:B:336:LEU:HD11	2.03	0.87
1:B:335:PHE:C	1:B:335:PHE:CD2	2.52	0.87
1:A:363:GLU:HA	1:A:366:LEU:HD12	1.55	0.86
1:B:782:GLU:O	1:B:786:THR:HG23	1.74	0.86
1:B:299:THR:HB	1:B:303:ARG:NH1	1.88	0.86
1:A:678:MET:O	1:A:699:HIS:CD2	2.30	0.84
1:A:647:THR:O	1:A:664:LYS:HB3	1.77	0.84
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.42	0.84
1:A:842:SER:OG	1:A:844:GLU:OE1	1.94	0.83
1:A:319:TRP:CD1	1:A:322:ARG:HE	1.95	0.83
1:A:322:ARG:HD2	1:A:335:PHE:CD1	2.12	0.83
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.13	0.83
1:A:319:TRP:HE1	1:A:322:ARG:HH21	1.24	0.83
1:A:751:THR:HG22	1:A:754:GLU:HG3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:CD1	1:A:357:TRP:CZ3	2.67	0.82
1:B:412:HIS:HE1	1:B:532:ASN:CB	1.92	0.82
1:B:876:ASN:H	1:B:876:ASN:HD22	1.27	0.81
1:B:296:GLN:O	1:B:300:ILE:HG22	1.81	0.81
1:B:654:PHE:HD1	1:B:655:PRO:CD	1.94	0.81
1:B:663:THR:OG1	1:B:664:LYS:HG2	1.81	0.81
1:A:705:GLN:CG	1:A:890:VAL:HG13	2.09	0.81
1:B:326:SER:HA	1:B:357:TRP:CZ2	2.16	0.80
1:B:734:VAL:HG22	1:B:744:LEU:HD22	1.61	0.80
1:B:627:LYS:O	1:B:630:GLU:HG2	1.82	0.80
1:B:749:SER:HB2	1:B:812:LEU:CD1	2.11	0.80
1:B:329:LYS:NZ	1:B:361:ASP:CG	2.40	0.79
1:A:673:PHE:HB2	1:A:679:PRO:HD2	1.65	0.79
1:A:638:GLU:HG2	1:A:641:MET:CG	2.10	0.79
1:A:629:THR:CB	1:A:672:LEU:HD12	2.08	0.79
1:B:712:MET:HE1	1:B:878:MET:HG2	1.65	0.79
1:B:913:THR:HG23	1:B:916:GLU:HG3	1.65	0.79
1:B:329:LYS:HZ2	1:B:361:ASP:H	1.29	0.78
1:B:332:LEU:HD12	1:B:336:LEU:HD11	1.65	0.78
1:A:534:CYS:O	1:A:538:ILE:HG13	1.83	0.78
1:A:591:ASN:O	1:A:595:ARG:CD	2.31	0.78
1:B:400:GLN:HE22	1:B:711:GLN:HE22	1.31	0.78
1:B:728:LYS:HD3	1:B:786:THR:HB	1.64	0.78
1:B:310:LEU:HD13	1:B:311:SER:OG	1.82	0.78
1:A:568:GLN:HA	1:A:568:GLN:OE1	1.83	0.78
2:A:1949:093:HAD	2:A:1949:093:HAE1	1.66	0.78
1:A:294:ARG:HA	1:A:297:LEU:HD21	1.66	0.77
1:B:421:PHE:HB3	1:B:422:PRO:CD	2.14	0.77
1:A:645:ASN:C	1:A:645:ASN:ND2	2.35	0.76
1:A:298:HIS:HE1	1:A:318:VAL:HA	1.49	0.76
1:A:722:ARG:HH11	1:A:722:ARG:CG	1.98	0.76
1:A:737:THR:HG22	1:A:738:SER:N	1.99	0.76
1:A:322:ARG:NH1	1:A:335:PHE:HE1	1.83	0.76
1:A:678:MET:O	1:A:699:HIS:NE2	2.19	0.76
1:A:667:PRO:O	1:A:670:THR:HG23	1.85	0.75
1:A:322:ARG:HH11	1:A:335:PHE:HE1	1.33	0.75
1:B:315:GLN:HG3	1:B:338:CYS:HB2	1.67	0.75
1:B:791:CYS:SG	1:B:819:LEU:HD23	2.25	0.75
1:B:631:LYS:O	1:B:635:LEU:HD23	1.85	0.75
1:A:747:VAL:HG23	2:A:1949:093:HAK	1.52	0.74
1:A:807:HIS:H	1:A:810:ASN:HB2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PRO:O	1:A:414:VAL:HG23	1.88	0.74
1:A:677:LEU:HD11	1:A:700:GLY:H	1.50	0.74
1:A:706:ASP:O	1:A:710:LEU:HD12	1.87	0.74
1:A:626:ASN:HA	1:A:629:THR:CG2	2.18	0.74
1:B:332:LEU:HD22	1:B:357:TRP:HB3	1.69	0.74
1:B:302:TYR:HE2	1:B:303:ARG:HE	1.34	0.74
1:B:629:THR:O	1:B:633:GLN:HG3	1.87	0.73
1:A:843:LYS:O	1:A:847:GLU:HG3	1.88	0.73
1:A:335:PHE:HD1	1:A:357:TRP:CH2	2.06	0.73
1:B:299:THR:CB	1:B:303:ARG:HH11	1.96	0.73
1:B:667:PRO:O	1:B:670:THR:CG2	2.35	0.73
1:B:703:LEU:HD13	1:B:744:LEU:HD21	1.71	0.73
1:A:319:TRP:NE1	1:A:323:PHE:CE2	2.57	0.73
1:B:311:SER:CB	1:B:314:GLU:HB3	2.18	0.73
1:A:913:THR:HG23	1:A:916:GLU:CD	2.13	0.73
1:A:405:LEU:HD23	1:A:533:LEU:HD21	1.68	0.73
1:B:549:ASN:C	1:B:549:ASN:ND2	2.43	0.73
1:B:948:ARG:O	1:B:949:LYS:HB2	1.87	0.73
1:A:639:GLN:NE2	1:A:645:ASN:OD1	2.22	0.73
1:A:375:HIS:HD2	1:A:377:GLN:H	0.87	0.72
1:A:638:GLU:CG	1:A:641:MET:HG3	2.16	0.72
1:A:322:ARG:HH12	1:A:353:MET:CG	1.96	0.72
1:B:765:PHE:C	1:B:765:PHE:CD2	2.67	0.72
1:A:421:PHE:HB3	1:A:422:PRO:CD	2.15	0.72
1:B:819:LEU:HD12	1:B:820:PHE:N	2.05	0.71
1:B:582:MET:O	1:B:586:VAL:HG23	1.90	0.71
1:B:738:SER:HB3	1:B:741:HIS:CE1	2.25	0.71
1:A:319:TRP:O	1:A:322:ARG:HB3	1.89	0.71
1:A:300:ILE:O	1:A:304:TYR:HB2	1.90	0.71
1:A:351:LEU:HD13	1:A:377:GLN:HG2	1.70	0.71
1:B:335:PHE:HD1	1:B:357:TRP:CZ3	2.08	0.71
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.19	0.71
1:A:722:ARG:HH11	1:A:722:ARG:HG3	1.55	0.70
1:A:296:GLN:O	1:A:299:THR:HG22	1.92	0.70
1:B:319:TRP:HA	1:B:322:ARG:NE	2.06	0.70
1:B:346:GLU:HA	1:B:349:GLN:CD	2.17	0.70
1:B:749:SER:HB2	1:B:812:LEU:HD12	1.72	0.70
1:A:319:TRP:NE1	1:A:323:PHE:HE2	1.87	0.70
1:A:332:LEU:HD12	1:A:336:LEU:CD2	2.21	0.70
1:A:654:PHE:CD1	1:A:655:PRO:HD2	2.26	0.70
1:A:322:ARG:NH1	1:A:335:PHE:CE1	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:HH11	1:A:722:ARG:CB	2.05	0.69
1:B:678:MET:O	1:B:699:HIS:NE2	2.21	0.69
1:B:798:THR:HG23	1:B:803:VAL:HB	1.75	0.69
1:B:749:SER:CB	1:B:812:LEU:HD12	2.23	0.69
1:A:798:THR:HG23	1:A:803:VAL:HB	1.73	0.69
1:B:319:TRP:CD1	1:B:319:TRP:C	2.71	0.69
1:B:375:HIS:CD2	1:B:377:GLN:N	2.61	0.69
1:A:793:GLY:O	1:A:797:ILE:HG13	1.93	0.69
1:A:718:LYS:O	1:A:722:ARG:HG2	1.92	0.68
1:A:751:THR:HG22	1:A:754:GLU:CG	2.22	0.68
1:A:304:TYR:CB	1:A:305:PRO:HD3	2.24	0.68
1:B:329:LYS:HZ3	1:B:361:ASP:H	1.39	0.68
1:B:549:ASN:OD1	1:B:658:PRO:HG3	1.93	0.68
1:A:329:LYS:HB3	1:A:360:MET:HA	1.75	0.68
1:B:314:GLU:O	1:B:318:VAL:HG12	1.93	0.68
1:A:322:ARG:HD2	1:A:335:PHE:CE1	2.27	0.68
1:A:811:LEU:C	1:A:812:LEU:HD23	2.18	0.68
1:B:297:LEU:HA	1:B:300:ILE:CG2	2.23	0.68
1:A:909:GLN:HG3	1:A:912:LEU:HG	1.75	0.68
1:B:610:GLU:CD	1:B:643:LYS:HG2	2.19	0.68
1:A:332:LEU:HD12	1:A:336:LEU:HD23	1.74	0.68
1:B:335:PHE:HE2	1:B:339:ILE:HD13	1.58	0.68
1:B:751:THR:HA	1:B:812:LEU:HB3	1.75	0.67
1:A:629:THR:HA	1:A:672:LEU:HD11	1.76	0.67
1:A:769:HIS:CD2	1:A:815:THR:HG22	2.29	0.67
1:B:763:HIS:CD2	1:B:848:ALA:HA	2.29	0.67
1:B:876:ASN:HD22	1:B:876:ASN:N	1.92	0.67
1:A:654:PHE:HD1	1:A:655:PRO:CD	2.08	0.67
1:A:657:ASP:OD2	1:A:657:ASP:C	2.37	0.67
1:B:578:MET:O	1:B:582:MET:HG3	1.95	0.67
1:B:877:VAL:O	1:B:881:LEU:HG	1.95	0.67
1:B:315:GLN:HB2	1:B:338:CYS:HB3	1.77	0.67
1:B:549:ASN:ND2	1:B:553:TRP:CD1	2.63	0.67
1:A:625:ARG:O	1:A:629:THR:HG22	1.95	0.66
1:B:913:THR:HG23	1:B:916:GLU:CG	2.25	0.66
1:B:705:GLN:OE1	1:B:890:VAL:HG13	1.96	0.66
1:A:335:PHE:HD1	1:A:357:TRP:CZ3	2.13	0.66
1:A:343:LEU:HD13	1:A:345:ASP:H	1.61	0.66
1:B:297:LEU:HD23	1:B:297:LEU:H	1.60	0.66
1:A:326:SER:HB2	1:A:357:TRP:CE2	2.31	0.66
1:A:332:LEU:O	1:A:336:LEU:HD23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:THR:CB	1:A:672:LEU:CD1	2.71	0.66
1:B:549:ASN:ND2	1:B:553:TRP:HD1	1.93	0.66
1:B:699:HIS:CD2	1:B:699:HIS:H	2.11	0.66
1:A:294:ARG:HA	1:A:297:LEU:CD2	2.27	0.65
1:B:329:LYS:NZ	1:B:361:ASP:CB	2.59	0.65
1:B:618:VAL:HG21	1:B:632:PHE:CD2	2.31	0.65
1:B:913:THR:HG23	1:B:916:GLU:CD	2.21	0.65
1:B:743:PHE:O	1:B:744:LEU:HD23	1.97	0.65
1:B:751:THR:HG23	1:B:754:GLU:H	1.59	0.65
1:B:749:SER:HB2	1:B:812:LEU:HD13	1.77	0.65
1:A:362:VAL:O	1:A:365:ALA:HB3	1.97	0.65
1:A:549:ASN:C	1:A:549:ASN:ND2	2.54	0.65
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.84	0.65
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.25	0.65
1:B:830:ARG:HH22	1:B:903:LYS:NZ	1.95	0.64
1:A:335:PHE:HD2	1:A:335:PHE:O	1.80	0.64
1:A:751:THR:CG2	1:A:754:GLU:H	2.10	0.64
1:A:363:GLU:HA	1:A:366:LEU:CD1	2.27	0.64
1:B:573:HIS:C	1:B:573:HIS:CD2	2.75	0.64
1:A:785:ASP:OD1	1:A:789:LYS:HE3	1.98	0.64
1:B:912:LEU:HD12	1:B:917:ALA:HA	1.78	0.64
1:A:920:HIS:C	1:A:920:HIS:CD2	2.75	0.64
1:B:645:ASN:OD1	1:B:645:ASN:C	2.40	0.64
1:A:405:LEU:CD2	1:A:533:LEU:HD21	2.28	0.64
1:A:830:ARG:NH2	1:A:903:LYS:NZ	2.34	0.64
1:A:751:THR:CG2	1:A:754:GLU:HG3	2.27	0.64
1:A:806:ARG:HA	1:A:810:ASN:HD22	1.62	0.64
1:A:827:ILE:CG2	1:A:828:LEU:HG	2.28	0.64
1:A:830:ARG:HH22	1:A:903:LYS:HZ1	0.76	0.64
1:A:862:LYS:O	1:A:866:THR:HG23	1.97	0.64
1:A:806:ARG:CZ	1:A:810:ASN:ND2	2.61	0.63
1:B:698:LYS:O	1:B:741:HIS:HA	1.98	0.63
1:B:332:LEU:HD12	1:B:336:LEU:CD1	2.29	0.63
1:A:533:LEU:HD23	1:A:534:CYS:N	2.14	0.63
1:B:549:ASN:HD21	1:B:553:TRP:CD1	2.15	0.63
1:B:712:MET:CE	1:B:878:MET:HG2	2.28	0.63
1:B:812:LEU:HD21	1:B:822:ILE:HG21	1.81	0.63
1:A:866:THR:O	1:A:870:HIS:HD2	1.82	0.63
1:B:614:LEU:HD12	1:B:614:LEU:C	2.24	0.63
1:A:549:ASN:HD22	1:A:550:TYR:N	1.97	0.62
1:B:314:GLU:O	1:B:317:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:NZ	1:B:361:ASP:N	2.43	0.62
1:A:363:GLU:CD	1:A:363:GLU:N	2.57	0.62
1:A:813:LEU:HD12	1:A:818:LYS:O	1.98	0.62
1:B:621:GLU:HG2	1:B:623:GLY:H	1.63	0.62
1:A:319:TRP:HD1	1:A:323:PHE:CE2	2.17	0.62
1:B:806:ARG:NH1	1:B:823:ASP:O	2.29	0.62
1:A:677:LEU:HD21	1:A:699:HIS:HB2	1.80	0.62
1:B:544:ASN:OD1	1:B:544:ASN:C	2.42	0.62
1:A:363:GLU:CA	1:A:366:LEU:HD12	2.29	0.62
1:B:319:TRP:O	1:B:319:TRP:HD1	1.82	0.62
1:B:751:THR:HG22	1:B:754:GLU:HB2	1.82	0.62
1:B:749:SER:CB	1:B:812:LEU:CD1	2.76	0.62
1:A:664:LYS:H	1:A:685:VAL:CG2	2.12	0.62
1:A:578:MET:O	1:A:582:MET:HG3	2.00	0.61
1:B:411:ARG:HA	1:B:414:VAL:HG22	1.81	0.61
1:B:549:ASN:HD21	1:B:553:TRP:HD1	1.46	0.61
1:B:751:THR:HG22	1:B:754:GLU:CG	2.31	0.61
1:B:826:TYR:HB3	1:B:830:ARG:O	2.00	0.61
1:A:813:LEU:CD1	1:A:818:LYS:O	2.49	0.61
1:A:723:GLU:O	1:A:724:ASN:HB3	1.99	0.61
1:A:335:PHE:CD1	1:A:357:TRP:HZ3	2.17	0.60
1:A:580:LEU:HD22	1:A:581:LYS:HE2	1.82	0.60
1:A:689:ALA:HB3	1:A:691:HIS:CE1	2.34	0.60
1:A:803:VAL:HG12	1:A:806:ARG:HD3	1.83	0.60
1:A:415:HIS:C	1:A:415:HIS:ND1	2.59	0.60
1:A:417:HIS:ND1	1:A:417:HIS:C	2.58	0.60
1:A:580:LEU:HD22	1:A:581:LYS:CE	2.32	0.60
1:A:716:MET:SD	1:A:797:ILE:HG23	2.42	0.60
1:B:703:LEU:CD1	1:B:744:LEU:HD21	2.31	0.60
1:A:812:LEU:HD11	1:A:822:ILE:CD1	2.31	0.60
1:A:315:GLN:HG3	1:A:316:ASP:OD2	2.01	0.60
1:A:405:LEU:HB3	1:A:575:MET:HE1	1.83	0.60
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.84	0.60
1:B:618:VAL:HG21	1:B:632:PHE:HD2	1.66	0.60
1:A:751:THR:HG22	1:A:754:GLU:CB	2.31	0.60
1:B:315:GLN:HG2	1:B:316:ASP:N	2.17	0.60
1:B:722:ARG:HH11	1:B:722:ARG:HB3	1.66	0.60
1:B:749:SER:OG	2:B:1950:093:NAR	2.35	0.60
1:A:722:ARG:HG3	1:A:722:ARG:NH1	2.17	0.60
1:B:412:HIS:HE1	1:B:532:ASN:HB2	1.64	0.60
1:B:570:GLU:CD	1:B:570:GLU:N	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.66	0.60
1:B:807:HIS:CD2	1:B:809:ASP:HB2	2.36	0.60
1:B:339:ILE:O	1:B:342:LYS:HB3	2.01	0.60
1:B:629:THR:HG22	1:B:672:LEU:HB3	1.84	0.60
1:B:716:MET:HG2	1:B:878:MET:HE2	1.82	0.60
1:A:806:ARG:CZ	1:A:810:ASN:HD22	2.14	0.59
1:A:297:LEU:O	1:A:301:VAL:HG23	2.03	0.59
1:B:329:LYS:HZ3	1:B:361:ASP:N	2.00	0.59
1:B:614:LEU:HD21	1:B:636:LEU:HD23	1.84	0.59
1:A:391:ASP:CG	1:A:540:ARG:HH12	2.10	0.59
1:A:709:ILE:HD12	1:A:801:LEU:HD13	1.83	0.59
1:B:335:PHE:CD1	1:B:357:TRP:HZ3	2.21	0.59
1:A:645:ASN:HD22	1:A:646:PHE:N	2.01	0.58
1:B:412:HIS:NE2	1:B:532:ASN:HB3	2.18	0.58
1:B:814:THR:OG1	1:B:816:ASN:HB3	2.03	0.58
1:A:335:PHE:CD1	1:A:357:TRP:CH2	2.88	0.58
1:A:812:LEU:HD11	1:A:822:ILE:HD12	1.84	0.58
1:A:406:LYS:NZ	1:A:887:ASP:O	2.36	0.58
1:B:640:ASP:OD1	1:B:640:ASP:C	2.46	0.58
1:B:319:TRP:HA	1:B:322:ARG:HE	1.66	0.58
1:B:599:TYR:HD2	1:B:599:TYR:O	1.87	0.58
1:B:862:LYS:O	1:B:866:THR:HG22	2.03	0.58
1:B:799:TYR:O	1:B:907:ASN:ND2	2.37	0.58
1:B:375:HIS:CD2	1:B:375:HIS:C	2.82	0.58
1:A:305:PRO:O	1:A:334:LYS:NZ	2.37	0.58
1:B:710:LEU:HD22	1:B:732:TYR:O	2.03	0.58
1:A:373:PHE:N	1:A:373:PHE:CD2	2.71	0.57
1:B:812:LEU:HD12	1:B:820:PHE:CZ	2.39	0.57
1:A:657:ASP:OD2	1:A:659:GLU:N	2.37	0.57
1:B:634:LYS:HA	1:B:634:LYS:CE	2.21	0.57
1:A:538:ILE:HG23	1:A:583:PHE:HD1	1.69	0.57
1:A:621:GLU:O	1:A:628:LYS:HE2	2.04	0.57
1:B:329:LYS:HZ3	1:B:361:ASP:CB	2.16	0.57
1:B:830:ARG:NH2	1:B:903:LYS:NZ	2.52	0.57
1:B:392:GLU:HG2	1:B:393:ASP:N	2.19	0.57
1:A:373:PHE:N	1:A:373:PHE:HD2	2.02	0.57
1:A:807:HIS:HD2	1:A:809:ASP:HB2	1.70	0.57
1:B:375:HIS:NE2	1:B:377:GLN:HB2	2.19	0.57
1:B:841:LEU:O	1:B:932:VAL:HG21	2.05	0.57
1:A:335:PHE:CD2	1:A:335:PHE:O	2.57	0.57
1:A:575:MET:SD	1:A:575:MET:C	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:TYR:HD1	1:A:921:LEU:HD23	1.69	0.57
1:A:319:TRP:HE1	1:A:322:ARG:NH2	2.00	0.56
1:B:590:GLY:O	1:B:595:ARG:HD3	2.05	0.56
1:A:421:PHE:CB	1:A:422:PRO:HD2	2.22	0.56
1:A:677:LEU:HD11	1:A:700:GLY:N	2.20	0.56
1:A:898:ASP:N	1:A:898:ASP:OD1	2.37	0.56
1:B:344:GLU:O	1:B:347:VAL:HB	2.04	0.56
1:B:702:ASP:HB3	1:B:739:SER:CA	2.30	0.56
1:B:878:MET:O	1:B:882:PHE:HD2	1.88	0.56
1:A:326:SER:HB2	1:A:357:TRP:NE1	2.20	0.56
1:A:375:HIS:HB3	1:A:378:VAL:HG22	1.88	0.56
1:B:332:LEU:O	1:B:336:LEU:HD22	2.06	0.56
1:B:416:LEU:O	1:B:420:ILE:HG12	2.06	0.56
1:B:723:GLU:O	1:B:724:ASN:OD1	2.24	0.56
1:B:318:VAL:HG23	1:B:322:ARG:HB2	1.88	0.56
1:A:335:PHE:CE1	1:A:357:TRP:HZ3	2.24	0.56
1:B:335:PHE:HD1	1:B:357:TRP:HZ3	1.50	0.56
1:B:400:GLN:HE22	1:B:711:GLN:NE2	2.02	0.56
1:B:934:PRO:O	1:B:938:GLU:HG3	2.06	0.56
1:B:763:HIS:NE2	1:B:848:ALA:HA	2.21	0.55
1:B:657:ASP:OD2	1:B:657:ASP:C	2.49	0.55
1:B:649:PHE:CE2	1:B:664:LYS:HA	2.41	0.55
1:B:876:ASN:N	1:B:876:ASN:ND2	2.54	0.55
1:A:409:ASP:OD1	1:A:411:ARG:N	2.39	0.55
1:A:827:ILE:HG23	1:A:828:LEU:HG	1.87	0.55
1:B:402:VAL:O	1:B:405:LEU:HB2	2.05	0.55
1:A:869:LEU:HD11	1:A:918:VAL:CG2	2.36	0.55
1:B:343:LEU:O	1:B:346:GLU:HG2	2.07	0.55
1:A:872:ARG:HH12	1:A:909:GLN:C	2.14	0.55
1:B:325:LEU:O	1:B:327:SER:N	2.40	0.55
1:A:405:LEU:CD2	1:A:533:LEU:CD2	2.85	0.55
1:B:319:TRP:C	1:B:319:TRP:HD1	2.12	0.55
1:B:343:LEU:HG	1:B:344:GLU:H	1.71	0.55
1:B:806:ARG:N	1:B:806:ARG:HD2	2.22	0.55
1:A:772:CYS:O	1:A:778:GLY:HA2	2.07	0.54
1:B:333:THR:HA	1:B:336:LEU:CD2	2.38	0.54
1:A:409:ASP:HB3	1:A:412:HIS:CD2	2.42	0.54
1:B:569:ASP:OD1	1:B:569:ASP:C	2.51	0.54
1:A:751:THR:HG22	1:A:754:GLU:H	1.72	0.54
1:B:299:THR:O	1:B:302:TYR:HD2	1.90	0.54
1:B:315:GLN:CG	1:B:338:CYS:HB2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:THR:HA	1:A:936:LEU:HD12	1.90	0.54
1:A:409:ASP:OD1	1:A:409:ASP:C	2.50	0.54
1:A:629:THR:CA	1:A:672:LEU:HD11	2.37	0.54
1:A:645:ASN:ND2	1:A:647:THR:H	2.06	0.54
1:B:712:MET:O	1:B:716:MET:HG3	2.07	0.54
1:A:645:ASN:ND2	1:A:647:THR:N	2.56	0.53
1:A:610:GLU:HG3	1:A:644:VAL:HG12	1.90	0.53
1:B:366:LEU:HD12	1:B:881:LEU:HD21	1.91	0.53
1:A:677:LEU:O	1:A:679:PRO:HD3	2.08	0.53
1:B:767:ARG:O	1:B:771:PRO:HG3	2.09	0.53
1:A:304:TYR:HB2	1:A:305:PRO:HD3	1.89	0.53
1:A:811:LEU:O	1:A:812:LEU:HD23	2.09	0.53
1:A:402:VAL:O	1:A:576:TYR:OH	2.22	0.53
1:A:806:ARG:HA	1:A:810:ASN:ND2	2.23	0.53
1:A:807:HIS:HA	1:B:947:TRP:CZ3	2.44	0.53
1:A:544:ASN:C	1:A:544:ASN:OD1	2.52	0.53
1:B:765:PHE:HD2	1:B:766:PHE:N	2.06	0.53
1:A:705:GLN:HG3	1:A:891:PRO:HD2	1.91	0.53
1:B:408:GLU:HB3	1:B:409:ASP:CA	2.29	0.52
1:B:567:LYS:C	1:B:570:GLU:OE1	2.53	0.52
1:B:766:PHE:CE1	1:B:817:GLY:HA2	2.44	0.52
1:A:375:HIS:O	1:A:378:VAL:HG23	2.09	0.52
1:B:656:LEU:C	1:B:656:LEU:HD23	2.34	0.52
1:B:744:LEU:HD13	2:B:1950:093:CAC	2.39	0.52
1:B:765:PHE:C	1:B:765:PHE:HD2	2.17	0.52
1:A:319:TRP:O	1:A:319:TRP:HD1	1.92	0.52
1:A:723:GLU:O	1:A:724:ASN:CB	2.58	0.52
1:B:598:PHE:C	1:B:598:PHE:CD2	2.87	0.52
1:A:567:LYS:HG3	1:A:568:GLN:H	1.75	0.52
1:A:847:GLU:HG2	1:A:933:MET:HE1	1.91	0.52
1:B:412:HIS:CE1	1:B:532:ASN:HB2	2.39	0.52
1:B:621:GLU:O	1:B:628:LYS:HE2	2.09	0.52
1:A:561:GLU:CD	1:A:561:GLU:N	2.53	0.51
1:B:552:TYR:CG	1:B:601:LEU:HD13	2.45	0.51
1:A:645:ASN:ND2	1:A:648:ASN:H	2.08	0.51
1:A:649:PHE:CE1	1:A:663:THR:O	2.64	0.51
1:A:363:GLU:CD	1:A:363:GLU:H	2.18	0.51
1:A:626:ASN:HA	1:A:629:THR:HG22	1.89	0.51
1:A:763:HIS:NE2	1:A:848:ALA:O	2.35	0.51
1:B:371:PRO:HB3	1:B:407:TYR:CE2	2.45	0.51
1:B:416:LEU:HG	1:B:582:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ALA:O	1:A:690:HIS:HB2	2.10	0.51
1:B:315:GLN:HA	1:B:318:VAL:HG13	1.93	0.51
1:B:751:THR:HG22	1:B:754:GLU:CB	2.41	0.51
1:A:944:THR:OG1	1:B:931:ALA:O	2.26	0.51
2:A:1949:093:OAL	2:A:1949:093:SAP	2.69	0.51
1:B:354:LEU:C	1:B:354:LEU:HD23	2.35	0.51
1:B:552:TYR:OH	1:B:605:ARG:NE	2.36	0.51
1:A:367:GLU:O	1:A:370:SER:HB3	2.10	0.51
1:A:375:HIS:HB3	1:A:378:VAL:CG2	2.41	0.51
1:A:764:ASN:OD1	1:A:767:ARG:NH1	2.44	0.51
1:B:843:LYS:HA	1:B:932:VAL:HG13	1.92	0.51
1:B:909:GLN:HB3	1:B:912:LEU:HG	1.93	0.51
2:B:1950:093:SAP	2:B:1950:093:CAT	2.99	0.51
1:B:830:ARG:HH22	1:B:903:LYS:CE	2.24	0.51
1:A:609:ASP:O	1:A:613:LYS:HG3	2.11	0.50
1:B:312:SER:HA	1:B:315:GLN:OE1	2.10	0.50
1:B:409:ASP:OD1	1:B:410:PRO:HD2	2.12	0.50
1:A:391:ASP:CG	1:A:540:ARG:NH1	2.68	0.50
1:A:722:ARG:CG	1:A:722:ARG:NH1	2.66	0.50
1:B:828:LEU:O	1:B:830:ARG:NH1	2.44	0.50
1:A:305:PRO:HB2	1:A:308:TYR:CD2	2.46	0.50
1:A:375:HIS:CD2	1:A:375:HIS:C	2.88	0.50
1:B:807:HIS:NE2	1:B:809:ASP:HB2	2.27	0.50
1:A:661:TYR:HB2	1:A:687:SER:HB3	1.92	0.50
1:A:807:HIS:HA	1:B:947:TRP:HZ3	1.77	0.50
1:B:345:ASP:O	1:B:349:GLN:HG3	2.11	0.50
1:B:375:HIS:HD2	1:B:377:GLN:N	2.10	0.50
1:B:634:LYS:HE2	1:B:634:LYS:CA	2.33	0.50
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.93	0.50
1:B:807:HIS:HD2	1:B:809:ASP:H	1.59	0.50
1:A:696:ILE:HG22	1:A:697:PHE:N	2.25	0.50
1:A:807:HIS:CD2	1:A:809:ASP:HB2	2.46	0.50
1:B:318:VAL:O	1:B:322:ARG:N	2.39	0.50
1:A:722:ARG:HH11	1:A:722:ARG:HB2	1.75	0.50
1:B:629:THR:HG22	1:B:672:LEU:CB	2.41	0.50
1:B:806:ARG:HB3	1:B:811:LEU:HD21	1.94	0.50
1:B:673:PHE:HB2	1:B:679:PRO:HD2	1.93	0.50
1:A:544:ASN:OD1	1:A:546:THR:N	2.45	0.49
1:A:827:ILE:HG22	1:A:828:LEU:HG	1.94	0.49
1:B:399:LEU:H	1:B:399:LEU:HD22	1.76	0.49
1:A:360:MET:HG2	1:A:364:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:THR:HG23	1:A:754:GLU:H	1.75	0.49
1:B:321:PHE:O	1:B:325:LEU:HD23	2.12	0.49
2:B:1950:093:NAU	2:B:1950:093:CL	2.81	0.49
1:A:549:ASN:C	1:A:549:ASN:HD22	2.18	0.49
2:A:1949:093:HAD	2:A:1949:093:CAE	2.40	0.49
1:B:297:LEU:HA	1:B:300:ILE:HG22	1.94	0.49
1:B:329:LYS:O	1:B:332:LEU:HB3	2.12	0.49
1:B:894:ALA:O	1:B:897:PRO:HD3	2.13	0.49
1:A:839:MET:HE1	1:A:921:LEU:HD11	1.94	0.49
1:B:339:ILE:HD12	1:B:350:ALA:CB	2.42	0.49
1:A:872:ARG:NH1	1:A:909:GLN:O	2.44	0.49
1:B:590:GLY:HA3	1:B:594:LEU:HB2	1.94	0.49
1:B:599:TYR:O	1:B:603:LYS:HG3	2.13	0.49
1:A:397:TYR:O	1:A:398:LEU:C	2.56	0.49
1:B:577:ALA:O	1:B:581:LYS:HD3	2.13	0.49
1:B:678:MET:C	1:B:699:HIS:NE2	2.60	0.49
1:A:399:LEU:HB3	1:A:400:GLN:NE2	2.28	0.48
1:A:806:ARG:HD2	1:A:806:ARG:N	2.28	0.48
1:B:300:ILE:O	1:B:304:TYR:HD2	1.95	0.48
1:B:335:PHE:HD2	1:B:335:PHE:O	1.94	0.48
1:B:346:GLU:HA	1:B:349:GLN:OE1	2.13	0.48
1:B:299:THR:O	1:B:302:TYR:CD2	2.66	0.48
1:B:413:ILE:HD13	1:B:575:MET:HG2	1.95	0.48
2:B:1950:093:SAP	2:B:1950:093:HAT2	2.53	0.48
1:A:843:LYS:HA	1:A:932:VAL:CG1	2.43	0.48
1:B:329:LYS:NZ	1:B:361:ASP:HB2	2.27	0.48
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.96	0.48
1:A:786:THR:O	1:A:790:SER:OG	2.29	0.48
1:A:807:HIS:O	1:A:810:ASN:HB2	2.13	0.48
1:B:310:LEU:HD22	1:B:311:SER:H	1.78	0.48
1:B:357:TRP:CD1	1:B:358:ALA:N	2.81	0.48
1:A:395:LEU:C	1:A:395:LEU:HD23	2.38	0.48
1:B:300:ILE:HA	1:B:304:TYR:CD2	2.49	0.48
1:B:311:SER:HB3	1:B:314:GLU:CD	2.39	0.48
1:B:399:LEU:H	1:B:399:LEU:CD2	2.27	0.48
1:A:769:HIS:HB3	1:A:770:HIS:HD2	1.78	0.48
1:B:382:ALA:O	1:B:385:ARG:HB2	2.14	0.48
1:B:823:ASP:OD1	1:B:824:PHE:N	2.46	0.48
1:B:906:GLU:O	1:B:909:GLN:NE2	2.47	0.48
1:B:325:LEU:C	1:B:327:SER:N	2.71	0.48
1:B:783:VAL:HG13	1:B:816:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:C	1:B:370:SER:H	2.22	0.48
1:B:388:GLN:OE1	1:B:388:GLN:HA	2.13	0.48
1:B:888:ALA:O	1:B:889:THR:HG22	2.14	0.48
1:A:729:LEU:HD21	1:A:793:GLY:HA3	1.96	0.48
1:A:737:THR:HB	1:A:741:HIS:CD2	2.48	0.47
1:B:301:VAL:O	1:B:305:PRO:HD2	2.14	0.47
1:A:608:ILE:HG21	1:A:737:THR:HG21	1.96	0.47
1:A:614:LEU:HD21	1:A:636:LEU:CD2	2.44	0.47
1:A:776:PRO:HD2	1:A:779:ILE:O	2.14	0.47
1:B:555:LEU:HB3	1:B:580:LEU:HG	1.96	0.47
1:B:752:VAL:HG12	1:B:808:LEU:HD23	1.96	0.47
1:A:308:TYR:CD1	1:A:310:LEU:HD13	2.49	0.47
1:A:399:LEU:HB3	1:A:400:GLN:HE22	1.78	0.47
1:B:364:ASP:O	1:B:367:GLU:HB3	2.14	0.47
1:A:737:THR:CG2	1:A:741:HIS:CD2	2.98	0.47
1:A:790:SER:CB	1:A:819:LEU:H	2.27	0.47
1:A:329:LYS:H	1:A:329:LYS:HG3	1.32	0.47
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.96	0.47
1:A:737:THR:CG2	1:A:738:SER:N	2.69	0.47
1:B:322:ARG:HG3	1:B:335:PHE:CD1	2.50	0.47
1:A:343:LEU:HD13	1:A:345:ASP:N	2.28	0.47
1:B:312:SER:O	1:B:315:GLN:HG2	2.14	0.47
1:B:408:GLU:CB	1:B:409:ASP:HA	2.18	0.47
1:B:717:ASP:HB2	1:B:729:LEU:HD12	1.97	0.47
1:A:712:MET:CE	1:A:716:MET:HE3	2.45	0.47
1:A:823:ASP:CG	1:A:823:ASP:O	2.58	0.47
1:B:777:TYR:CD1	1:B:777:TYR:N	2.83	0.47
1:B:879:LEU:HD23	1:B:879:LEU:N	2.29	0.47
1:A:332:LEU:HD12	1:A:336:LEU:HD21	1.93	0.46
1:A:747:VAL:CG2	2:A:1949:093:HAK	2.25	0.46
1:A:915:GLU:N	1:A:915:GLU:OE2	2.46	0.46
1:A:291:ALA:O	1:A:294:ARG:NE	2.48	0.46
1:B:696:ILE:O	1:B:743:PHE:HA	2.15	0.46
1:B:697:PHE:HA	1:B:742:GLY:O	2.16	0.46
1:A:402:VAL:O	1:A:405:LEU:HB2	2.15	0.46
1:A:827:ILE:N	1:A:892:ASP:OD2	2.39	0.46
1:A:303:ARG:O	1:A:304:TYR:CD2	2.69	0.46
1:A:708:LEU:HD12	1:A:890:VAL:HG21	1.97	0.46
1:A:747:VAL:HG22	2:A:1949:093:HAE3	1.97	0.46
1:A:814:THR:CG2	1:A:818:LYS:N	2.66	0.46
1:B:678:MET:HA	1:B:679:PRO:HD3	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:764:ASN:HA	1:B:767:ARG:NH1	2.30	0.46
1:A:708:LEU:HD23	1:A:708:LEU:O	2.15	0.46
1:A:922:GLN:HE22	1:B:919:GLN:CB	2.21	0.46
1:B:319:TRP:CG	1:B:322:ARG:CZ	2.98	0.46
1:B:743:PHE:C	1:B:744:LEU:HD23	2.40	0.46
1:B:948:ARG:O	1:B:949:LYS:CB	2.62	0.46
1:A:298:HIS:CE1	1:A:318:VAL:HA	2.39	0.46
1:A:375:HIS:CD2	1:A:376:PRO:N	2.83	0.46
1:A:590:GLY:HA3	1:A:594:LEU:HD12	1.98	0.46
1:B:752:VAL:CG1	1:B:808:LEU:HD23	2.46	0.46
1:A:654:PHE:HB3	1:A:657:ASP:O	2.16	0.46
1:B:642:PHE:HB2	1:B:644:VAL:O	2.16	0.46
1:B:788:ILE:HG13	1:B:860:PHE:HB2	1.96	0.46
1:A:573:HIS:CD2	1:A:573:HIS:C	2.94	0.46
1:A:649:PHE:CD1	1:A:663:THR:O	2.69	0.46
1:A:759:GLU:O	1:A:760:GLY:C	2.56	0.46
1:B:367:GLU:O	1:B:367:GLU:HG3	2.14	0.46
1:B:763:HIS:NE2	1:B:848:ALA:O	2.49	0.46
1:A:332:LEU:HD23	1:A:360:MET:HB2	1.98	0.46
1:A:408:GLU:OE2	1:A:533:LEU:N	2.48	0.46
1:B:302:TYR:CZ	1:B:303:ARG:HG3	2.50	0.46
1:B:756:LEU:HA	1:B:759:GLU:O	2.16	0.46
1:B:776:PRO:HG2	1:B:777:TYR:H	1.81	0.46
1:B:891:PRO:O	1:B:895:LEU:HD12	2.14	0.46
1:A:629:THR:HB	1:A:672:LEU:HD11	1.90	0.46
1:B:360:MET:O	1:B:385:ARG:NH2	2.48	0.46
1:B:625:ARG:HG3	1:B:672:LEU:HD22	1.97	0.46
1:A:785:ASP:O	1:A:789:LYS:HG3	2.16	0.45
1:B:544:ASN:OD1	1:B:547:LEU:HB2	2.16	0.45
1:B:664:LYS:HG3	1:B:685:VAL:HG23	1.98	0.45
1:B:342:LYS:HG3	1:B:346:GLU:CD	2.41	0.45
1:A:319:TRP:NE1	1:A:322:ARG:NH2	2.53	0.45
1:A:676:ALA:O	1:A:677:LEU:C	2.59	0.45
1:B:594:LEU:N	1:B:594:LEU:HD23	2.30	0.45
1:B:899:LYS:O	1:B:903:LYS:HG3	2.16	0.45
1:B:366:LEU:HD12	1:B:881:LEU:CD2	2.46	0.45
1:A:814:THR:CG2	1:A:818:LYS:HB2	2.47	0.45
1:A:319:TRP:CD1	1:A:322:ARG:NE	2.74	0.45
1:A:734:VAL:CG2	1:A:744:LEU:HD23	2.34	0.45
1:A:878:MET:HA	1:A:881:LEU:HD12	1.99	0.45
1:B:329:LYS:HZ1	1:B:361:ASP:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:VAL:O	1:B:319:TRP:C	2.58	0.45
1:B:339:ILE:CD1	1:B:350:ALA:HB1	2.46	0.45
1:B:939:GLN:HG2	1:B:943:PHE:CZ	2.52	0.45
1:A:718:LYS:O	1:A:722:ARG:CG	2.63	0.45
1:A:723:GLU:N	1:A:723:GLU:OE1	2.50	0.45
1:B:710:LEU:O	1:B:714:THR:OG1	2.34	0.45
1:B:314:GLU:O	1:B:318:VAL:CG1	2.61	0.45
1:B:357:TRP:HD1	1:B:358:ALA:N	2.15	0.45
1:B:821:HIS:N	1:B:821:HIS:CD2	2.85	0.45
1:A:332:LEU:CD1	1:A:336:LEU:HD21	2.47	0.45
1:A:553:TRP:O	1:A:557:ILE:CG1	2.55	0.45
1:A:580:LEU:HD23	1:A:580:LEU:C	2.41	0.44
1:A:689:ALA:CB	1:A:691:HIS:CE1	2.99	0.44
1:A:782:GLU:O	1:A:786:THR:HG23	2.17	0.44
1:A:783:VAL:HG13	1:A:816:ASN:O	2.17	0.44
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.47	0.44
1:B:308:TYR:HD2	1:B:308:TYR:HA	1.69	0.44
1:B:310:LEU:HD13	1:B:311:SER:HG	1.82	0.44
1:B:794:TYR:CD1	1:B:821:HIS:CD2	3.05	0.44
1:A:591:ASN:CG	1:A:592:PHE:H	2.04	0.44
1:A:649:PHE:CE1	1:A:662:ILE:HG13	2.48	0.44
1:A:335:PHE:HE2	1:A:339:ILE:HD12	1.81	0.44
1:A:360:MET:HE2	1:A:360:MET:HB3	1.80	0.44
1:A:896:GLU:OE1	1:A:898:ASP:OD1	2.36	0.44
1:B:366:LEU:CD1	1:B:881:LEU:HD21	2.47	0.44
1:A:303:ARG:C	1:A:304:TYR:HD2	2.26	0.44
1:A:709:ILE:O	1:A:712:MET:HB2	2.17	0.44
1:B:678:MET:HE3	1:B:678:MET:HB3	1.88	0.44
1:B:699:HIS:CD2	1:B:699:HIS:N	2.82	0.44
1:B:739:SER:O	1:B:740:LYS:CG	2.56	0.44
1:A:719:LEU:O	1:A:723:GLU:HG2	2.17	0.44
1:A:726:ASP:C	1:A:727:LEU:HD23	2.43	0.44
1:A:747:VAL:HG23	2:A:1949:093:NAK	2.26	0.44
1:B:302:TYR:CE2	1:B:303:ARG:HG3	2.52	0.44
1:B:600:ASN:HA	1:B:603:LYS:HD3	2.00	0.44
1:B:636:LEU:HD12	1:B:670:THR:HG21	2.00	0.43
1:B:766:PHE:HE1	1:B:817:GLY:HA2	1.83	0.43
1:A:328:HIS:O	1:A:331:ALA:HB3	2.17	0.43
1:A:354:LEU:HD23	1:A:354:LEU:C	2.43	0.43
1:A:811:LEU:N	1:A:811:LEU:HD23	2.33	0.43
1:B:317:LEU:HD12	1:B:317:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:LYS:HE3	1:B:685:VAL:HG21	2.01	0.43
1:A:396:LEU:HD12	1:A:718:LYS:HE3	2.00	0.43
1:A:532:ASN:ND2	1:A:534:CYS:SG	2.89	0.43
1:B:865:TYR:OH	1:B:922:GLN:HG3	2.17	0.43
1:A:319:TRP:NE1	1:A:323:PHE:CZ	2.85	0.43
1:A:344:GLU:O	1:A:348:THR:HG23	2.18	0.43
1:A:625:ARG:HG3	1:A:626:ASN:N	2.27	0.43
1:A:668:MET:N	1:A:668:MET:SD	2.85	0.43
1:A:888:ALA:O	1:A:889:THR:HG23	2.19	0.43
1:B:350:ALA:O	1:B:354:LEU:N	2.44	0.43
1:B:375:HIS:O	1:B:378:VAL:HG22	2.18	0.43
1:B:686:THR:OG1	1:B:691:HIS:HB2	2.18	0.43
2:B:1950:093:HAD	2:B:1950:093:HAE1	2.00	0.43
1:A:652:ILE:HG22	1:A:653:PRO:O	2.19	0.43
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.67	0.43
1:B:575:MET:O	1:B:579:VAL:HG23	2.18	0.43
1:B:704:ARG:H	1:B:704:ARG:HG3	1.60	0.43
1:B:819:LEU:HD12	1:B:819:LEU:C	2.43	0.43
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.85	0.43
1:B:830:ARG:NH2	1:B:903:LYS:HZ1	2.16	0.43
1:B:416:LEU:CG	1:B:582:MET:HE1	2.49	0.43
1:A:381:TYR:O	1:A:385:ARG:HG2	2.18	0.43
1:A:708:LEU:HD23	1:A:708:LEU:C	2.44	0.43
1:A:822:ILE:HD13	1:A:822:ILE:HG21	1.77	0.43
1:A:865:TYR:CD1	1:A:921:LEU:HD23	2.52	0.43
1:B:370:SER:HB3	1:B:371:PRO:HD2	2.01	0.43
1:A:684:PHE:O	1:A:692:GLU:HA	2.17	0.43
1:B:368:LEU:HD22	1:B:373:PHE:CE2	2.54	0.43
1:A:391:ASP:OD2	1:A:391:ASP:N	2.52	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.81	0.43
1:B:343:LEU:CG	1:B:344:GLU:H	2.31	0.43
1:B:885:MET:HE3	1:B:888:ALA:CB	2.49	0.43
1:B:893:ILE:O	1:B:897:PRO:HA	2.18	0.43
1:A:602:ARG:NH1	1:A:606:ARG:HD2	2.33	0.42
1:A:820:PHE:CD2	1:A:820:PHE:N	2.87	0.42
1:A:843:LYS:HE2	1:A:847:GLU:OE2	2.18	0.42
1:A:845:MET:O	1:A:848:ALA:HB3	2.19	0.42
1:B:300:ILE:HA	1:B:304:TYR:HD2	1.84	0.42
1:B:300:ILE:HG12	1:B:304:TYR:CD2	2.54	0.42
1:B:717:ASP:OD1	1:B:721:ARG:HG3	2.19	0.42
1:A:673:PHE:HE2	1:A:696:ILE:HG12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HG	1:B:646:PHE:CE2	2.54	0.42
1:B:837:PRO:O	1:B:840:LYS:HE3	2.19	0.42
1:B:912:LEU:HB3	1:B:916:GLU:HB2	2.00	0.42
1:A:841:LEU:HD23	1:A:845:MET:HE2	2.00	0.42
1:B:777:TYR:C	1:B:779:ILE:N	2.75	0.42
1:A:826:TYR:HB3	1:A:830:ARG:O	2.20	0.42
1:A:948:ARG:HD2	1:A:948:ARG:C	2.44	0.42
1:B:656:LEU:HD23	1:B:657:ASP:N	2.35	0.42
1:B:314:GLU:HA	1:B:317:LEU:HD23	2.02	0.42
1:B:614:LEU:HD21	1:B:636:LEU:CD2	2.47	0.42
1:B:888:ALA:O	1:B:889:THR:CB	2.67	0.42
1:A:580:LEU:HD23	1:A:584:LEU:HG	2.02	0.42
1:A:841:LEU:O	1:A:932:VAL:HG21	2.20	0.42
1:A:860:PHE:CE1	1:A:864:CYS:SG	3.13	0.42
1:B:741:HIS:ND1	1:B:741:HIS:N	2.68	0.42
1:A:400:GLN:NE2	1:A:400:GLN:N	2.68	0.41
1:A:747:VAL:HG21	1:A:820:PHE:CZ	2.55	0.41
1:B:375:HIS:CD2	1:B:376:PRO:N	2.88	0.41
1:B:570:GLU:N	1:B:570:GLU:OE1	2.51	0.41
1:B:823:ASP:OD1	1:B:823:ASP:C	2.62	0.41
1:A:375:HIS:NE2	1:A:377:GLN:CB	2.84	0.41
1:A:923:SER:O	1:A:927:VAL:HG22	2.20	0.41
1:B:614:LEU:C	1:B:614:LEU:CD1	2.90	0.41
1:A:403:GLN:NE2	1:A:888:ALA:HA	2.35	0.41
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.75	0.41
1:B:375:HIS:NE2	1:B:377:GLN:CB	2.82	0.41
1:A:293:ILE:O	1:A:297:LEU:HD23	2.20	0.41
1:A:319:TRP:HH2	1:A:346:GLU:HG3	1.85	0.41
1:A:636:LEU:CD1	1:A:670:THR:HG21	2.51	0.41
1:B:368:LEU:HD22	1:B:373:PHE:HE2	1.85	0.41
1:B:933:MET:HA	1:B:934:PRO:HD3	1.89	0.41
1:A:308:TYR:C	1:A:310:LEU:H	2.26	0.41
1:B:639:GLN:OE1	1:B:639:GLN:N	2.54	0.41
1:B:777:TYR:O	1:B:778:GLY:C	2.63	0.41
1:A:709:ILE:HA	1:A:709:ILE:HD13	1.77	0.41
1:B:420:ILE:C	1:B:421:PHE:CD2	2.99	0.41
1:B:608:ILE:HD13	1:B:608:ILE:HA	1.89	0.41
1:B:653:PRO:HB3	1:B:661:TYR:CE1	2.55	0.41
1:B:794:TYR:HB3	1:B:821:HIS:NE2	2.35	0.41
1:A:299:THR:HA	1:A:302:TYR:CZ	2.48	0.41
1:B:582:MET:HB3	1:B:582:MET:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:PHE:CD1	1:B:607:PHE:C	2.98	0.41
1:B:804:GLY:O	1:B:805:ASP:CB	2.69	0.41
1:A:727:LEU:HD23	1:A:727:LEU:N	2.35	0.41
1:B:325:LEU:C	1:B:327:SER:H	2.28	0.41
1:B:400:GLN:HG2	1:B:881:LEU:HD22	2.02	0.41
1:B:575:MET:SD	1:B:575:MET:C	3.04	0.41
1:A:298:HIS:HB3	1:A:302:TYR:CZ	2.51	0.41
1:A:585:LYS:HD2	1:A:585:LYS:HA	1.78	0.41
1:A:828:LEU:O	1:A:830:ARG:NH1	2.54	0.41
1:B:302:TYR:CE2	1:B:303:ARG:NE	2.86	0.41
1:B:302:TYR:HD1	1:B:330:LYS:HB2	1.86	0.41
1:B:307:THR:O	1:B:308:TYR:HD2	2.04	0.41
1:B:333:THR:O	1:B:337:LYS:HG3	2.21	0.41
1:B:639:GLN:C	1:B:641:MET:H	2.29	0.41
1:B:751:THR:HG22	1:B:754:GLU:HG3	2.02	0.41
1:A:313:GLU:C	1:A:315:GLN:N	2.77	0.41
1:A:326:SER:O	1:A:327:SER:C	2.64	0.41
1:A:333:THR:HG21	1:A:364:ASP:OD2	2.21	0.41
2:A:1949:093:CL	2:A:1949:093:NAU	2.91	0.41
1:B:806:ARG:HH22	1:B:823:ASP:H	1.69	0.41
1:B:923:SER:O	1:B:927:VAL:HG22	2.21	0.41
1:A:303:ARG:O	1:A:304:TYR:HD2	2.03	0.40
1:A:400:GLN:OE1	1:A:711:GLN:OE1	2.38	0.40
1:A:580:LEU:HD23	1:A:580:LEU:O	2.21	0.40
1:B:709:ILE:HD13	1:B:709:ILE:HA	1.93	0.40
1:B:850:GLY:O	1:B:854:SER:HB3	2.21	0.40
1:A:641:MET:HE3	1:A:641:MET:HB3	1.79	0.40
1:A:810:ASN:HB3	1:A:811:LEU:HD23	2.03	0.40
1:B:610:GLU:HG3	1:B:644:VAL:H	1.87	0.40
1:A:314:GLU:H	1:A:314:GLU:HG3	1.76	0.40
1:A:379:ARG:O	1:A:383:VAL:HG23	2.21	0.40
1:A:824:PHE:HB3	1:A:827:ILE:HD11	2.03	0.40
1:A:888:ALA:O	1:A:889:THR:CG2	2.70	0.40
1:B:604:GLN:HE21	1:B:653:PRO:HG2	1.86	0.40
1:A:305:PRO:HA	1:A:306:PRO:HD3	1.91	0.40
1:A:674:LYS:HD3	1:A:674:LYS:H	1.86	0.40
1:A:885:MET:O	1:A:888:ALA:HB2	2.21	0.40
1:B:718:LYS:O	1:B:722:ARG:HG3	2.21	0.40
1:A:925:LEU:O	1:A:929:ILE:HG13	2.21	0.40
1:B:368:LEU:C	1:B:370:SER:N	2.77	0.40
1:B:557:ILE:HD11	1:B:736:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LYS:HE3	1:B:652:ILE:HG12	2.04	0.40
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.07	0.13
1:B:391:ASP:OD2	1:B:724:ASN:ND2[8_565]	2.18	0.02

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	539/696 (77%)	505 (94%)	30 (6%)	4 (1%)	18	51
1	B	540/696 (78%)	517 (96%)	20 (4%)	3 (1%)	21	54
All	All	1079/1392 (78%)	1022 (95%)	50 (5%)	7 (1%)	21	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	A	305	PRO
1	B	408	GLU
1	A	304	TYR
1	A	591	ASN
1	B	889	THR
1	A	679	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/612 (80%)	392 (80%)	98 (20%)	1	7
1	B	490/612 (80%)	386 (79%)	104 (21%)	1	6
All	All	980/1224 (80%)	778 (79%)	202 (21%)	1	7

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	LEU
1	A	317	LEU
1	A	328	HIS
1	A	332	LEU
1	A	333	THR
1	A	335	PHE
1	A	339	ILE
1	A	341	TRP
1	A	343	LEU
1	A	347	VAL
1	A	351	LEU
1	A	354	LEU
1	A	361	ASP
1	A	363	GLU
1	A	368	LEU
1	A	370	SER
1	A	373	PHE
1	A	378	VAL
1	A	396	LEU
1	A	400	GLN
1	A	409	ASP
1	A	415	HIS
1	A	416	LEU
1	A	417	HIS
1	A	419	CYS
1	A	532	ASN
1	A	533	LEU

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Mol	Chain	Res	Type
1	A	549	ASN
1	A	556	SER
1	A	561	GLU
1	A	569	ASP
1	A	573	HIS
1	A	575	MET
1	A	578	MET
1	A	581	LYS
1	A	602	ARG
1	A	611	LEU
1	A	612	VAL
1	A	614	LEU
1	A	617	LEU
1	A	618	VAL
1	A	625	ARG
1	A	629	THR
1	A	634	LYS
1	A	638	GLU
1	A	639	GLN
1	A	641	MET
1	A	644	VAL
1	A	645	ASN
1	A	649	PHE
1	A	656	LEU
1	A	657	ASP
1	A	662	ILE
1	A	663	THR
1	A	668	MET
1	A	670	THR
1	A	674	LYS
1	A	677	LEU
1	A	678	MET
1	A	682	LEU
1	A	683	THR
1	A	688	ILE
1	A	702	ASP
1	A	705	GLN
1	A	706	ASP
1	A	710	LEU
1	A	722	ARG
1	A	723	GLU
1	A	725	LEU

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Mol	Chain	Res	Type
1	A	747	VAL
1	A	748	ASP
1	A	750	CYS
1	A	751	THR
1	A	759	GLU
1	A	773	ASP
1	A	782	GLU
1	A	788	ILE
1	A	790	SER
1	A	808	LEU
1	A	811	LEU
1	A	813	LEU
1	A	822	ILE
1	A	835	MET
1	A	839	MET
1	A	842	SER
1	A	877	VAL
1	A	878	MET
1	A	889	THR
1	A	895	LEU
1	A	896	GLU
1	A	898	ASP
1	A	913	THR
1	A	920	HIS
1	A	927	VAL
1	A	930	THR
1	A	937	VAL
1	A	940	ILE
1	A	944	THR
1	B	293	ILE
1	B	295	ASP
1	B	297	LEU
1	B	298	HIS
1	B	300	ILE
1	B	302	TYR
1	B	308	TYR
1	B	310	LEU
1	B	313	GLU
1	B	316	ASP
1	B	317	LEU
1	B	318	VAL
1	B	321	PHE

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Mol	Chain	Res	Type
1	B	322	ARG
1	B	332	LEU
1	B	335	PHE
1	B	336	LEU
1	B	340	ASN
1	B	344	GLU
1	B	346	GLU
1	B	347	VAL
1	B	366	LEU
1	B	367	GLU
1	B	378	VAL
1	B	392	GLU
1	B	398	LEU
1	B	399	LEU
1	B	413	ILE
1	B	419	CYS
1	B	535	THR
1	B	539	GLN
1	B	540	ARG
1	B	543	THR
1	B	544	ASN
1	B	546	THR
1	B	547	LEU
1	B	549	ASN
1	B	556	SER
1	B	569	ASP
1	B	570	GLU
1	B	573	HIS
1	B	579	VAL
1	B	580	LEU
1	B	591	ASN
1	B	594	LEU
1	B	606	ARG
1	B	611	LEU
1	B	614	LEU
1	B	624	ASN
1	B	631	LYS
1	B	634	LYS
1	B	635	LEU
1	B	639	GLN
1	B	640	ASP
1	B	641	MET

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Mol	Chain	Res	Type
1	B	643	LYS
1	B	644	VAL
1	B	645	ASN
1	B	656	LEU
1	B	663	THR
1	B	670	THR
1	B	677	LEU
1	B	678	MET
1	B	681	LYS
1	B	685	VAL
1	B	691	HIS
1	B	699	HIS
1	B	704	ARG
1	B	708	LEU
1	B	710	LEU
1	B	714	THR
1	B	715	LEU
1	B	725	LEU
1	B	741	HIS
1	B	750	CYS
1	B	758	ARG
1	B	765	PHE
1	B	779	ILE
1	B	786	THR
1	B	788	ILE
1	B	800	LEU
1	B	811	LEU
1	B	812	LEU
1	B	813	LEU
1	B	814	THR
1	B	819	LEU
1	B	822	ILE
1	B	827	ILE
1	B	835	MET
1	B	839	MET
1	B	852	ILE
1	B	854	SER
1	B	855	GLU
1	B	866	THR
1	B	876	ASN
1	B	877	VAL
1	B	879	LEU

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Mol	Chain	Res	Type
1	B	889	THR
1	B	913	THR
1	B	927	VAL
1	B	932	VAL
1	B	940	ILE
1	B	945	GLN
1	B	948	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	328	HIS
1	A	349	GLN
1	A	375	HIS
1	A	403	GLN
1	A	412	HIS
1	A	549	ASN
1	A	573	HIS
1	A	639	GLN
1	A	645	ASN
1	A	648	ASN
1	A	691	HIS
1	A	699	HIS
1	A	711	GLN
1	A	741	HIS
1	A	769	HIS
1	A	770	HIS
1	A	807	HIS
1	A	810	ASN
1	A	870	HIS
1	A	922	GLN
1	B	349	GLN
1	B	403	GLN
1	B	568	GLN
1	B	573	HIS
1	B	604	GLN
1	B	633	GLN
1	B	711	GLN
1	B	724	ASN
1	B	807	HIS
1	B	870	HIS

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Mol	Chain	Res	Type
1	B	876	ASN
1	B	919	GLN
1	B	939	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	093	B	1950	-	25,25,25	4.65	17 (68%)	33,36,36	5.71	18 (54%)
2	093	A	1949	-	25,25,25	4.46	15 (60%)	33,36,36	5.22	17 (51%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	093	B	1950	-	-	15/19/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	093	A	1949	-	-	7/19/19/19	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	093	CAJ-CAI	10.39	1.59	1.38
2	A	1949	093	CAJ-CAI	9.86	1.58	1.38
2	A	1949	093	CAQ-NAR	8.61	1.45	1.32
2	B	1950	093	CAQ-NAR	8.49	1.45	1.32
2	B	1950	093	CAJ-NAK	8.23	1.60	1.37
2	A	1949	093	CAJ-NAK	8.05	1.59	1.37
2	A	1949	093	SAN-NAU	7.86	1.73	1.61
2	B	1950	093	SAN-NAU	7.48	1.72	1.61
2	B	1950	093	CAG-CAF	6.33	1.49	1.39
2	A	1949	093	CAQ-NAK	6.16	1.51	1.36
2	B	1950	093	CAQ-NAK	6.11	1.51	1.36
2	A	1949	093	CAG-CAF	5.63	1.48	1.39
2	B	1950	093	CAD-CAC	5.59	1.47	1.38
2	B	1950	093	CAI-SAP	-5.37	1.61	1.74
2	A	1949	093	CAD-CAC	4.99	1.46	1.38
2	A	1949	093	CAI-SAP	-4.95	1.62	1.74
2	B	1950	093	CAS-NAR	4.10	1.47	1.38
2	A	1949	093	CAS-NAR	3.88	1.46	1.38
2	A	1949	093	OAO-SAN	3.72	1.47	1.43
2	B	1950	093	CAT-CAS	3.54	1.54	1.49
2	B	1950	093	CAF-SAN	3.47	1.82	1.77
2	B	1950	093	OAO-SAN	3.47	1.47	1.43
2	B	1950	093	OAM-SAN	3.32	1.47	1.43
2	B	1950	093	CAC-CAB	3.00	1.44	1.38
2	A	1949	093	CAF-SAN	2.83	1.81	1.77
2	B	1950	093	CAB-CAF	-2.79	1.36	1.40
2	A	1949	093	OAM-SAN	2.76	1.46	1.43
2	A	1949	093	CAT-CAS	2.75	1.53	1.49
2	A	1949	093	CAB-CAF	-2.74	1.36	1.40
2	A	1949	093	CAC-CAB	2.57	1.44	1.38
2	B	1950	093	CAB-CL	2.46	1.79	1.73
2	B	1950	093	OAL-CAS	-2.00	1.18	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1950	093	CAQ-SAP-CAI	27.30	105.35	88.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	093	CAQ-SAP-CAI	24.72	103.75	88.35
2	A	1949	093	OAO-SAN-OAM	-8.88	108.74	119.52
2	B	1950	093	OAO-SAN-OAM	-7.10	110.90	119.52
2	B	1950	093	CAT-CAS-NAR	6.79	124.91	114.84
2	B	1950	093	CAG-CAH-CAI	-5.72	112.77	120.36
2	A	1949	093	CAG-CAH-CAI	-5.62	112.89	120.36
2	B	1950	093	CAE-CAJ-CAI	-5.51	124.50	130.98
2	A	1949	093	CAE-CAJ-CAI	-5.49	124.53	130.98
2	B	1950	093	CAB-CAF-SAN	-5.44	119.44	123.19
2	B	1950	093	CAF-CAB-CL	-5.27	117.70	121.52
2	B	1950	093	CAI-CAJ-NAK	4.34	112.26	105.70
2	A	1949	093	CAT-CAS-NAR	3.72	120.35	114.84
2	A	1949	093	CAF-CAB-CL	-3.71	118.83	121.52
2	A	1949	093	CAW-CAV-NAU	3.66	118.88	110.90
2	A	1949	093	CAH-CAI-SAP	3.60	126.49	117.32
2	B	1950	093	OAL-CAS-NAR	-3.53	116.88	123.63
2	B	1950	093	CAD-CAH-CAI	3.41	126.26	120.84
2	A	1949	093	CAI-CAJ-NAK	3.25	110.61	105.70
2	A	1949	093	CAB-CAF-SAN	-3.17	121.01	123.19
2	A	1949	093	OAM-SAN-NAU	3.09	111.85	107.03
2	A	1949	093	CAV-NAU-SAN	-2.91	111.52	120.27
2	B	1950	093	CAW-CAV-NAU	2.85	117.10	110.90
2	B	1950	093	OAO-SAN-NAU	2.80	111.39	107.03
2	B	1950	093	CAV-NAU-SAN	-2.78	111.92	120.27
2	B	1950	093	CAS-NAR-CAQ	2.62	123.33	117.26
2	A	1949	093	OAO-SAN-NAU	2.62	111.10	107.03
2	A	1949	093	CAD-CAH-CAI	2.58	124.94	120.84
2	B	1950	093	CAH-CAI-SAP	2.53	123.75	117.32
2	A	1949	093	CAD-CAH-CAG	2.43	122.06	119.25
2	B	1950	093	CAC-CAD-CAH	-2.35	118.28	120.80
2	A	1949	093	OAM-SAN-CAF	-2.15	104.14	107.68
2	B	1950	093	CAC-CAB-CL	2.12	122.59	118.42
2	B	1950	093	CAJ-CAI-SAP	-2.07	106.13	111.50
2	A	1949	093	OAO-SAN-CAF	2.05	111.06	107.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1949	093	NAK-CAQ-NAR-CAS
2	B	1950	093	NAK-CAQ-NAR-CAS
2	B	1950	093	SAP-CAQ-NAR-CAS

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Mol	Chain	Res	Type	Atoms
2	B	1950	093	OAL-CAS-NAR-CAQ
2	B	1950	093	CAT-CAS-NAR-CAQ
2	B	1950	093	NAU-CAV-CAW-OAX
2	B	1950	093	CAV-NAU-SAN-OAM
2	B	1950	093	CAV-NAU-SAN-OAO
2	B	1950	093	CAG-CAF-SAN-OAM
2	B	1950	093	CAV-NAU-SAN-CAF
2	A	1949	093	CAG-CAF-SAN-OAM
2	A	1949	093	CAG-CAH-CAI-CAJ
2	B	1950	093	CAG-CAF-SAN-NAU
2	A	1949	093	CAD-CAH-CAI-CAJ
2	B	1950	093	CAG-CAH-CAI-CAJ
2	A	1949	093	SAP-CAQ-NAR-CAS
2	B	1950	093	CAB-CAF-SAN-OAM
2	B	1950	093	CAD-CAH-CAI-CAJ
2	B	1950	093	CAG-CAH-CAI-SAP
2	A	1949	093	CAB-CAF-SAN-OAM
2	A	1949	093	CAG-CAH-CAI-SAP
2	B	1950	093	CAD-CAH-CAI-SAP

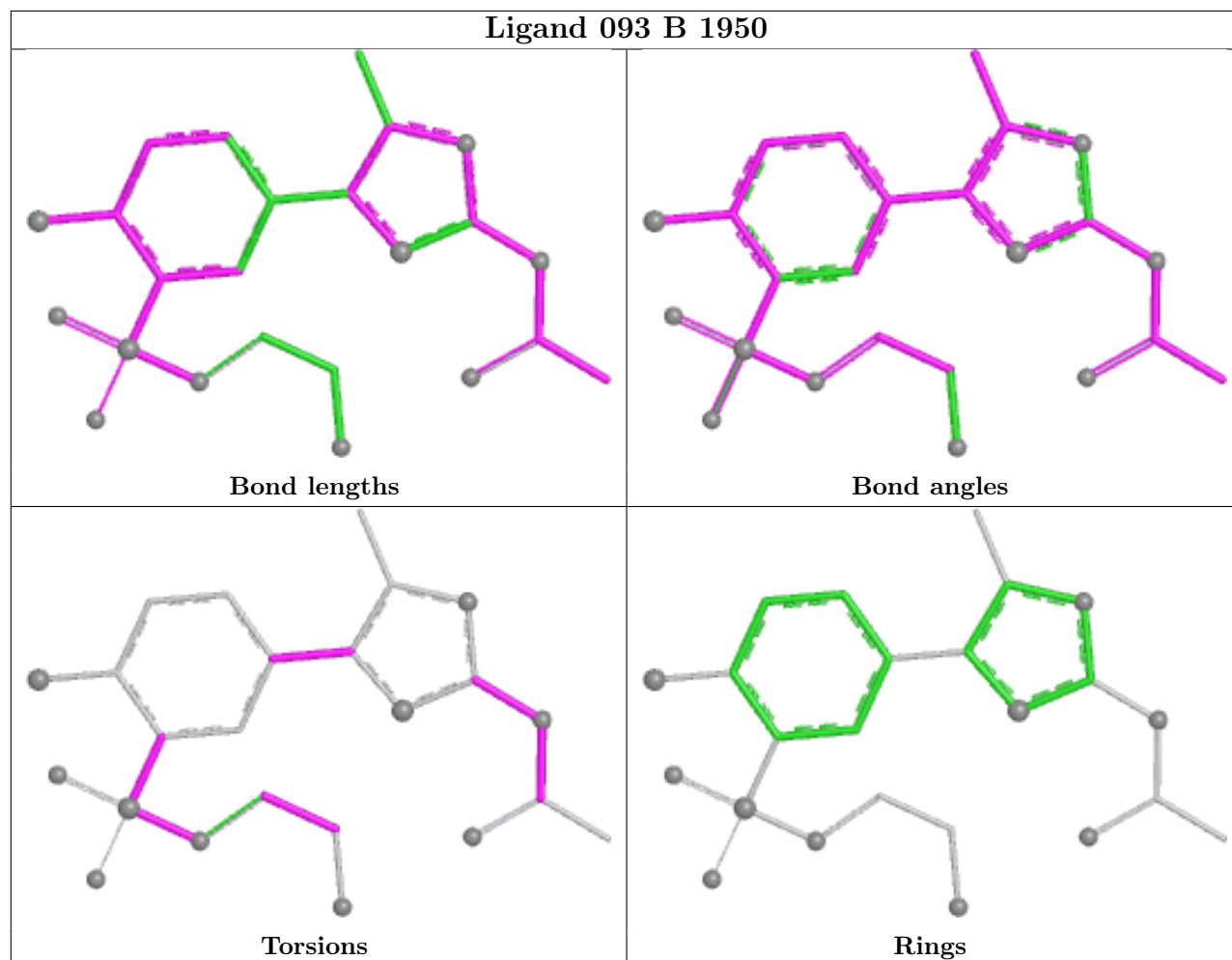
There are no ring outliers.

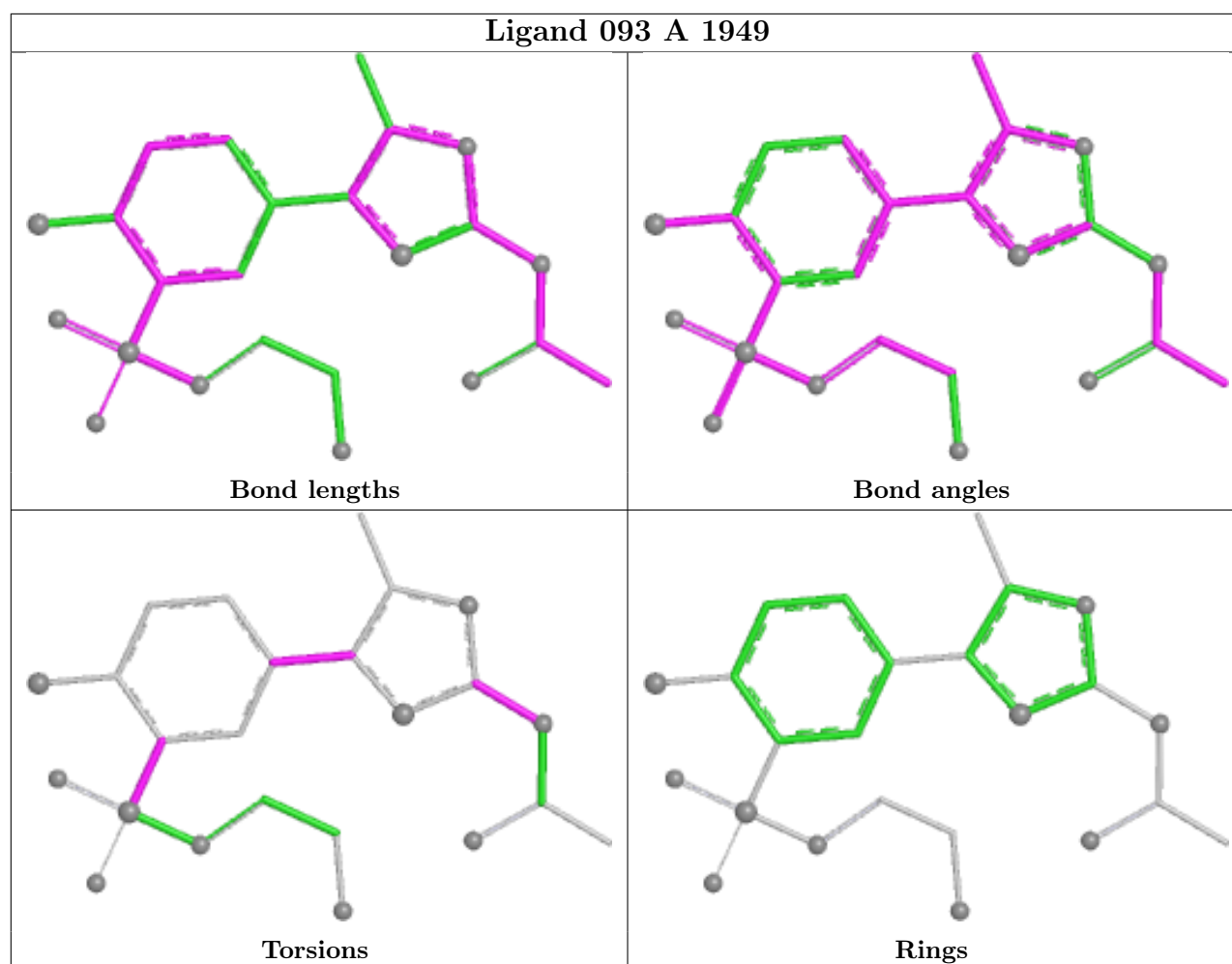
2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1950	093	6	0
2	A	1949	093	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.

Ligand 093 B 1950





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	545/696 (78%)	0.32	15 (2%) 55 32	32, 55, 105, 116	0
1	B	546/696 (78%)	0.08	12 (2%) 62 37	43, 65, 116, 123	0
All	All	1091/1392 (78%)	0.20	27 (2%) 58 35	32, 61, 107, 123	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	TYR	5.2
1	B	343	LEU	4.0
1	A	305	PRO	3.5
1	B	293	ILE	3.1
1	A	322	ARG	3.1
1	A	295	ASP	3.1
1	A	785	ASP	3.0
1	A	324	TYR	3.0
1	B	298	HIS	2.9
1	A	699	HIS	2.9
1	A	298	HIS	2.7
1	A	306	PRO	2.7
1	A	303	ARG	2.6
1	B	341	TRP	2.5
1	A	676	ALA	2.4
1	B	306	PRO	2.3
1	A	890	VAL	2.2
1	B	308	TYR	2.2
1	B	305	PRO	2.1
1	B	301	VAL	2.1
1	A	340	ASN	2.1
1	A	310	LEU	2.1
1	B	422	PRO	2.1
1	A	759	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	420	ILE	2.1
1	B	567	LYS	2.1
1	B	317	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

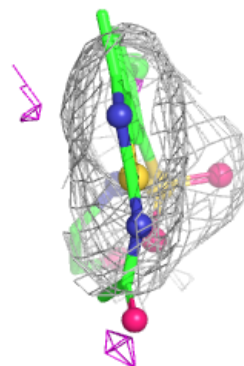
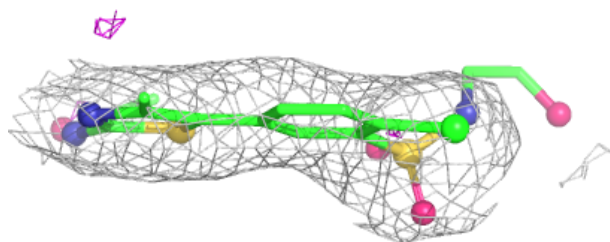
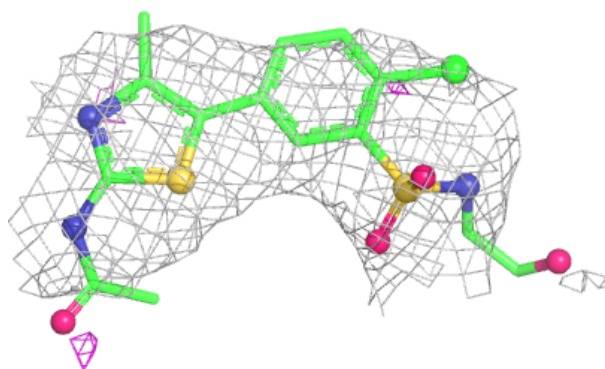
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	093	B	1950	24/24	0.88	0.17	101,108,117,119	0
2	093	A	1949	24/24	0.89	0.16	87,97,104,107	0

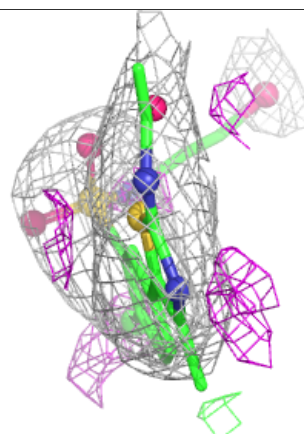
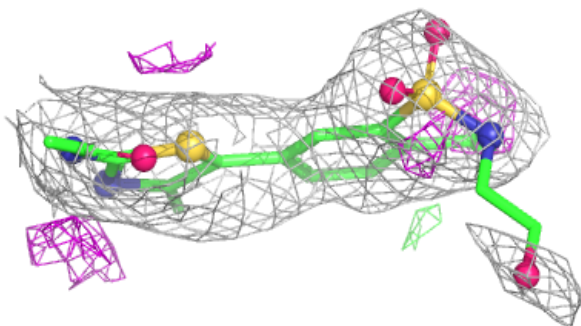
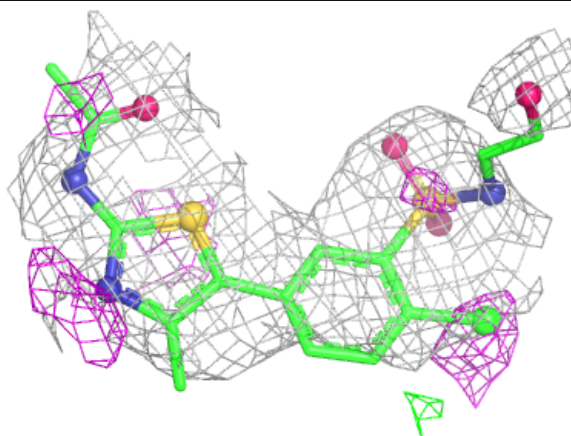
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 093 B 1950:

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

**Electron density around 093 A 1949:**

$2mF_o-DF_c$ (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.