



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:54 AM UTC

PDB ID : 4LSG / pdb_00004lsg
Title : Structure of Mouse P-Glycoprotein
Authors : Chang, G.; Szewczyk, P.
Deposited on : 2013-07-22
Resolution : 3.80 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

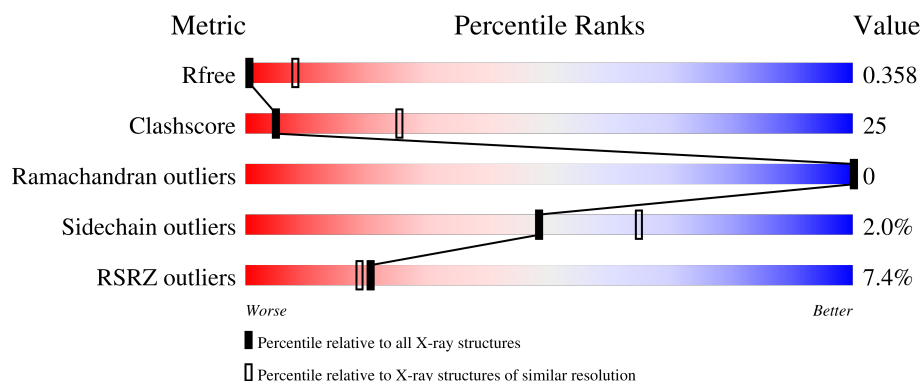
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

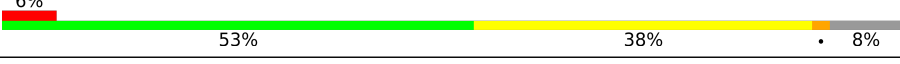
The reported resolution of this entry is 3.80 Å.

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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1284	
1	B	1284	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18352 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9170	5895	1552	1686	37			
1	B	1182	Total	C	N	O	S	0	0	0
			9170	5895	1552	1686	37			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	ALA	CYS	engineered mutation	UNP P21447
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447
B	952	ALA	CYS	engineered mutation	UNP P21447
B	1277	LEU	-	expression tag	UNP P21447
B	1278	GLU	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447
B	1283	HIS	-	expression tag	UNP P21447
B	1284	HIS	-	expression tag	UNP P21447

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Hg	0	0
			6	6		

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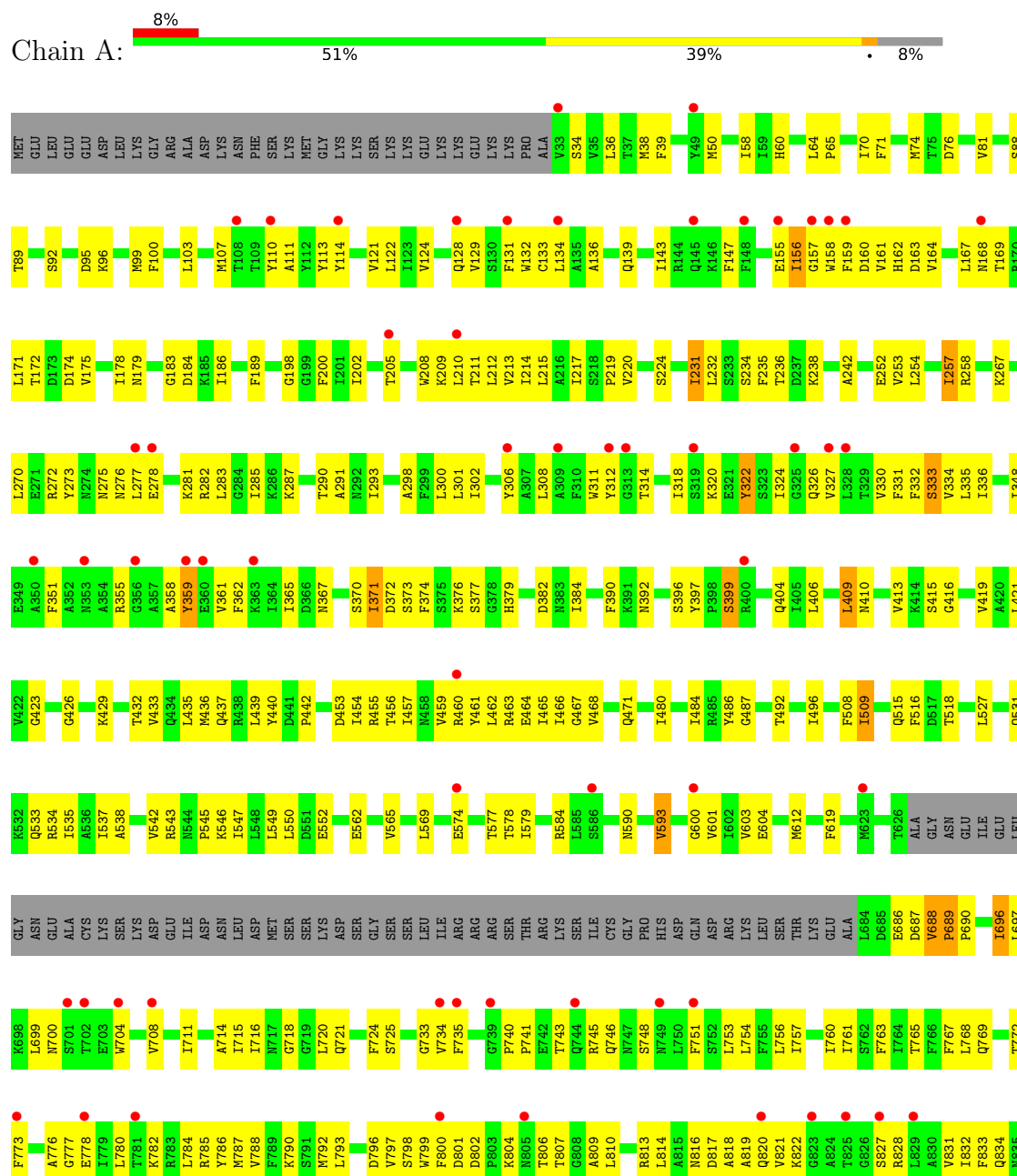
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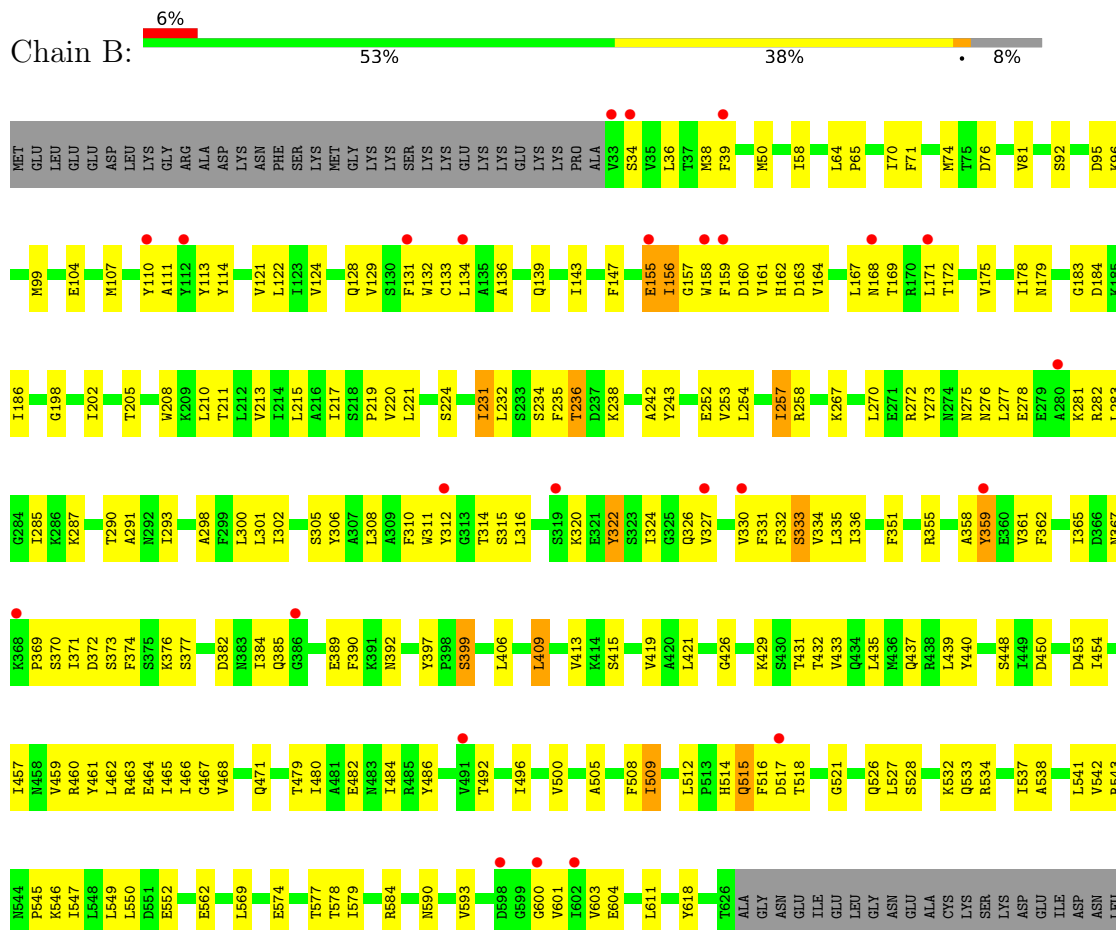
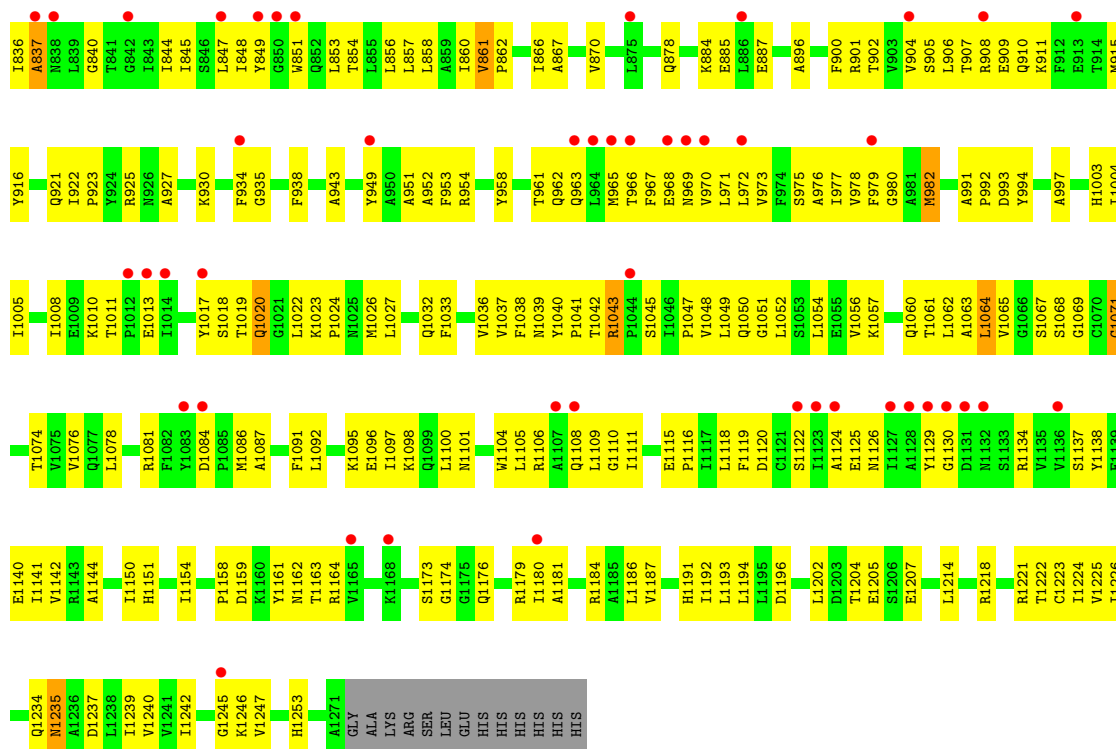
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Hg	0	0
			6	6		

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: Multidrug resistance protein 1A







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.80 19.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.98-3.80) 95.3 (19.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.69 (at 3.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.336 , 0.357 0.336 , 0.358	Depositor DCC
R_{free} test set	4203 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å ²)	133.9	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18352	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: HG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	2/9338 (0.0%)	1.03	34/12625 (0.3%)
1	B	0.45	2/9338 (0.0%)	1.03	38/12625 (0.3%)
All	All	0.45	4/18676 (0.0%)	1.03	72/25250 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	688	VAL	C-N	6.41	1.41	1.33
1	B	688	VAL	C-N	6.26	1.40	1.33
1	B	689	PRO	N-CD	5.33	1.55	1.47
1	A	689	PRO	N-CD	5.29	1.55	1.47

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ILE	N-CA-C	9.10	119.02	110.74
1	B	231	ILE	N-CA-C	8.95	118.88	110.74
1	A	372	ASP	N-CA-C	-8.72	102.00	114.12
1	B	1043	ARG	CA-C-N	-7.35	114.23	121.65
1	B	1043	ARG	C-N-CA	-7.35	114.23	121.65
1	A	935	GLY	N-CA-C	7.05	121.03	112.49
1	A	708	VAL	N-CA-C	-7.01	104.60	113.22
1	B	399	SER	N-CA-C	-6.97	104.38	113.17
1	B	708	VAL	N-CA-C	-6.91	104.72	113.22
1	A	318	ILE	N-CA-C	6.89	116.98	110.30
1	A	1043	ARG	CA-C-N	-6.87	114.72	121.65
1	A	1043	ARG	C-N-CA	-6.87	114.72	121.65
1	A	257	ILE	N-CA-C	6.83	118.41	110.62
1	B	935	GLY	N-CA-C	6.80	120.71	112.49
1	A	399	SER	N-CA-C	-6.79	104.61	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	THR	N-CA-C	6.76	118.31	111.07
1	B	686	GLU	N-CA-C	6.60	116.71	108.19
1	A	689	PRO	N-CA-C	6.59	118.74	110.70
1	B	688	VAL	CA-C-N	-6.59	113.59	120.38
1	B	688	VAL	C-N-CA	-6.59	113.59	120.38
1	B	155	GLU	CB-CA-C	-6.56	108.30	117.23
1	A	377	SER	CB-CA-C	-6.37	109.24	116.63
1	B	324	ILE	N-CA-C	-6.37	106.53	112.83
1	A	324	ILE	N-CA-C	-6.37	106.53	112.83
1	B	1071	GLY	N-CA-C	-6.33	105.74	114.67
1	B	761	ILE	N-CA-C	-6.31	104.34	110.72
1	A	688	VAL	CA-C-N	-6.31	113.88	120.38
1	A	688	VAL	C-N-CA	-6.31	113.88	120.38
1	B	322	TYR	N-CA-C	-6.30	103.50	112.13
1	B	740	PRO	N-CA-C	6.29	118.37	110.70
1	B	169	THR	N-CA-C	-6.25	104.39	111.14
1	A	1071	GLY	N-CA-C	-6.23	105.89	114.67
1	A	169	THR	N-CA-C	-6.21	104.14	111.03
1	B	426	GLY	N-CA-C	6.15	119.78	111.72
1	A	371	ILE	CB-CA-C	-6.11	101.27	111.29
1	B	257	ILE	N-CA-C	6.11	117.58	110.62
1	A	761	ILE	N-CA-C	-6.04	104.62	110.72
1	A	322	TYR	N-CA-C	-6.02	103.88	112.13
1	B	515	GLN	CB-CA-C	-6.00	109.67	116.63
1	B	372	ASP	N-CA-C	-5.98	104.83	114.09
1	A	837	ALA	N-CA-C	5.97	117.79	111.28
1	B	333	SER	N-CA-C	-5.91	105.33	112.54
1	A	333	SER	N-CA-C	-5.90	105.35	112.54
1	A	426	GLY	N-CA-C	5.83	119.36	111.72
1	A	982	MET	N-CA-C	-5.73	104.94	111.07
1	A	515	GLN	CB-CA-C	-5.69	110.03	116.63
1	B	837	ALA	N-CA-C	5.69	117.48	111.28
1	A	134	LEU	N-CA-C	5.67	118.19	111.33
1	B	155	GLU	N-CA-C	5.64	118.09	108.67
1	B	377	SER	CB-CA-C	-5.61	110.13	116.63
1	B	162	HIS	CB-CA-C	-5.53	108.60	116.34
1	A	359	TYR	N-CA-C	5.53	118.23	111.82
1	A	162	HIS	CB-CA-C	-5.51	108.62	116.34
1	B	952	ALA	N-CA-C	5.50	116.96	110.97
1	A	205	THR	N-CA-C	5.46	116.91	111.07
1	B	740	PRO	CA-C-N	-5.44	114.36	119.85
1	B	740	PRO	C-N-CA	-5.44	114.36	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1021	GLY	N-CA-C	5.44	122.02	113.86
1	B	804	LYS	N-CA-C	-5.42	106.34	113.17
1	B	95	ASP	N-CA-C	5.40	118.08	111.82
1	A	367	ASN	CB-CA-C	-5.30	108.89	115.89
1	B	367	ASN	CB-CA-C	-5.28	108.92	115.89
1	B	689	PRO	N-CA-C	5.27	117.12	110.70
1	B	134	LEU	N-CA-C	5.26	117.70	111.33
1	B	359	TYR	N-CA-C	5.23	117.89	111.82
1	B	236	THR	N-CA-C	-5.17	105.54	111.07
1	B	982	MET	N-CA-C	-5.13	105.58	111.07
1	A	952	ALA	N-CA-C	5.11	116.54	110.97
1	A	799	TRP	N-CA-C	-5.09	106.57	112.89
1	A	861	VAL	CB-CA-C	-5.09	108.86	113.70
1	A	95	ASP	N-CA-C	5.08	117.71	111.82
1	A	804	LYS	N-CA-C	-5.05	106.81	113.17

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	9170	0	9338	476	0
1	B	9170	0	9338	456	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	18352	0	18676	926	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 25.

All (926) 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:132:TRP:CD1	1:B:183:GLY:HA3	1.53	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:THR:CG2	1:A:1101:ASN:HA	1.50	1.41
1:A:107:MET:HE3	1:A:958:TYR:CD2	1.57	1.40
1:A:132:TRP:CD1	1:A:183:GLY:HA3	1.59	1.36
1:B:1017:TYR:CE2	1:B:1019:THR:HG23	1.65	1.30
1:B:133:CYS:SG	1:B:934:PHE:HD2	1.63	1.21
1:B:132:TRP:HZ2	1:B:179:ASN:ND2	1.39	1.20
1:B:995:ALA:O	1:B:998:THR:HG22	1.41	1.15
1:B:1017:TYR:CE2	1:B:1019:THR:CG2	2.31	1.14
1:A:979:PHE:O	1:A:982:MET:HG2	1.44	1.14
1:A:384:ILE:HG22	1:A:546:LYS:HG3	1.29	1.13
1:B:132:TRP:CD1	1:B:183:GLY:CA	2.32	1.13
1:B:979:PHE:O	1:B:982:MET:HG2	1.46	1.12
1:B:991:ALA:HB1	1:B:992:PRO:HD2	1.29	1.09
1:B:107:MET:SD	1:B:958:TYR:CE2	2.45	1.09
1:B:382:ASP:C	1:B:384:ILE:HD12	1.77	1.08
1:A:1019:THR:HG23	1:A:1101:ASN:HA	1.08	1.08
1:B:300:LEU:HD21	1:B:763:PHE:HB2	1.36	1.07
1:A:132:TRP:CD1	1:A:183:GLY:CA	2.37	1.07
1:A:107:MET:CE	1:A:958:TYR:CD2	2.36	1.06
1:A:107:MET:SD	1:A:954:ARG:CD	2.43	1.06
1:A:300:LEU:HD21	1:A:763:PHE:HB2	1.37	1.06
1:B:970:VAL:HG23	1:B:971:LEU:HD22	1.37	1.06
1:A:133:CYS:SG	1:A:934:PHE:HD2	1.79	1.05
1:A:970:VAL:HG23	1:A:971:LEU:HD22	1.39	1.05
1:B:132:TRP:CZ2	1:B:179:ASN:ND2	2.27	1.02
1:A:1019:THR:HG23	1:A:1101:ASN:CA	1.91	1.01
1:B:1024:PRO:O	1:B:1027:LEU:HD13	1.60	1.00
1:B:133:CYS:SG	1:B:934:PHE:CD2	2.54	0.99
1:A:837:ALA:HB1	1:A:982:MET:HE1	1.42	0.99
1:A:107:MET:SD	1:A:954:ARG:HD2	2.03	0.98
1:B:382:ASP:O	1:B:384:ILE:HD12	1.61	0.98
1:B:1017:TYR:HE2	1:B:1019:THR:HG23	1.29	0.97
1:A:107:MET:HE2	1:A:958:TYR:CB	1.94	0.97
1:B:786:TYR:CE1	1:B:790:LYS:NZ	2.31	0.97
1:B:132:TRP:HD1	1:B:183:GLY:HA3	1.23	0.97
1:A:132:TRP:HZ2	1:A:179:ASN:ND2	1.64	0.96
1:A:107:MET:CE	1:A:958:TYR:CB	2.45	0.93
1:A:107:MET:CE	1:A:958:TYR:CG	2.52	0.92
1:B:213:VAL:HG11	1:B:312:TYR:HD2	1.34	0.92
1:B:132:TRP:CE3	1:B:133:CYS:HA	2.04	0.92
1:A:1019:THR:HG21	1:A:1101:ASN:HA	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TRP:HD1	1:A:183:GLY:HA3	1.17	0.91
1:B:384:ILE:O	1:B:384:ILE:HG22	1.67	0.91
1:B:384:ILE:HG22	1:B:546:LYS:HG3	1.52	0.91
1:A:107:MET:HE3	1:A:958:TYR:HD2	1.19	0.90
1:A:1017:TYR:CE1	1:A:1019:THR:HB	2.05	0.90
1:A:163:ASP:HB2	1:A:167:LEU:HB2	1.53	0.90
1:A:281:LYS:HD3	1:A:782:LYS:HE2	1.54	0.89
1:B:107:MET:SD	1:B:958:TYR:CD2	2.66	0.89
1:B:281:LYS:HD3	1:B:782:LYS:HE2	1.55	0.89
1:B:132:TRP:HE3	1:B:133:CYS:HA	1.34	0.89
1:A:107:MET:HE2	1:A:958:TYR:HB2	1.53	0.89
1:B:163:ASP:HB2	1:B:167:LEU:HB2	1.53	0.88
1:A:132:TRP:HZ2	1:A:179:ASN:HD21	1.17	0.87
1:A:1017:TYR:HE1	1:A:1019:THR:HB	1.40	0.87
1:B:1017:TYR:HE2	1:B:1019:THR:CG2	1.77	0.87
1:A:132:TRP:CE3	1:A:133:CYS:HA	2.10	0.87
1:B:132:TRP:HE3	1:B:133:CYS:CA	1.88	0.86
1:A:107:MET:HE2	1:A:958:TYR:CG	2.08	0.86
1:A:740:PRO:HG2	1:A:741:PRO:HD3	1.57	0.86
1:B:995:ALA:O	1:B:998:THR:CG2	2.23	0.85
1:B:714:ALA:HB1	1:B:833:PHE:HB2	1.60	0.83
1:A:107:MET:SD	1:A:954:ARG:HD3	2.17	0.82
1:B:991:ALA:HB1	1:B:992:PRO:CD	2.10	0.82
1:A:714:ALA:HB1	1:A:833:PHE:HB2	1.61	0.82
1:A:133:CYS:SG	1:A:934:PHE:CD2	2.71	0.82
1:A:878:GLN:HG3	1:A:934:PHE:HE1	1.44	0.82
1:A:1024:PRO:O	1:A:1027:LEU:HD13	1.79	0.82
1:A:270:LEU:HG	1:A:790:LYS:HD2	1.63	0.81
1:A:930:LYS:HD2	1:A:934:PHE:CZ	2.15	0.81
1:A:921:GLN:HE22	1:B:479:THR:HG22	1.45	0.81
1:B:213:VAL:HG11	1:B:312:TYR:CD2	2.16	0.81
1:A:1018:SER:O	1:A:1019:THR:HG22	1.80	0.81
1:B:969:ASN:H	1:B:972:LEU:HD13	1.46	0.80
1:B:688:VAL:C	1:B:690:PRO:HD2	2.06	0.80
1:A:384:ILE:CG2	1:A:546:LYS:HG3	2.11	0.80
1:B:168:ASN:HA	1:B:171:LEU:HB2	1.64	0.80
1:A:159:PHE:CE1	1:A:900:PHE:CD2	2.70	0.79
1:B:837:ALA:HB1	1:B:982:MET:HE1	1.64	0.79
1:A:132:TRP:HE3	1:A:133:CYS:CA	1.95	0.79
1:A:969:ASN:H	1:A:972:LEU:HD13	1.47	0.78
1:B:132:TRP:HB2	1:B:184:ASP:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HG	1:B:790:LYS:HD2	1.66	0.78
1:A:991:ALA:HB1	1:A:992:PRO:HD2	1.65	0.78
1:A:168:ASN:HA	1:A:171:LEU:HB2	1.65	0.77
1:B:132:TRP:HB2	1:B:184:ASP:N	2.00	0.77
1:B:132:TRP:CZ2	1:B:179:ASN:CG	2.62	0.77
1:B:132:TRP:HZ2	1:B:179:ASN:CG	1.92	0.76
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.68	0.76
1:B:688:VAL:HG23	1:B:690:PRO:HD2	1.66	0.76
1:A:966:THR:HG23	1:A:968:GLU:H	1.51	0.75
1:A:1019:THR:CG2	1:A:1101:ASN:CA	2.47	0.75
1:A:132:TRP:HE3	1:A:133:CYS:HA	1.49	0.75
1:B:979:PHE:C	1:B:982:MET:HG2	2.12	0.75
1:A:132:TRP:CZ2	1:A:179:ASN:OD1	2.40	0.74
1:B:700:ASN:O	1:B:704:TRP:N	2.21	0.74
1:A:384:ILE:HG22	1:A:546:LYS:CG	2.15	0.74
1:B:382:ASP:O	1:B:384:ILE:CD1	2.35	0.73
1:A:267:LYS:HA	1:A:270:LEU:HD22	1.69	0.73
1:B:930:LYS:HD2	1:B:934:PHE:CZ	2.23	0.73
1:B:979:PHE:O	1:B:982:MET:CG	2.32	0.73
1:B:966:THR:HG23	1:B:968:GLU:H	1.53	0.73
1:A:700:ASN:O	1:A:704:TRP:N	2.20	0.73
1:A:792:MET:HE1	1:A:810:LEU:HB3	1.71	0.73
1:B:267:LYS:HA	1:B:270:LEU:HD22	1.70	0.73
1:A:979:PHE:C	1:A:982:MET:HG2	2.14	0.73
1:B:65:PRO:HB2	1:B:202:ILE:HD12	1.70	0.73
1:B:370:SER:O	1:B:371:ILE:HG13	1.88	0.72
1:A:463:ARG:O	1:A:543:ARG:NH2	2.21	0.72
1:B:1037:VAL:HG12	1:B:1051:GLY:H	1.54	0.72
1:A:686:GLU:OE1	1:A:813:ARG:NH1	2.22	0.72
1:B:1017:TYR:CD2	1:B:1019:THR:HG23	2.24	0.72
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.70	0.72
1:A:878:GLN:HG3	1:A:934:PHE:CE1	2.25	0.71
1:A:688:VAL:C	1:A:690:PRO:HD2	2.15	0.71
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.72	0.71
1:B:991:ALA:CB	1:B:992:PRO:HD2	2.16	0.71
1:B:1040:TYR:O	1:B:1042:THR:N	2.23	0.71
1:B:687:ASP:HA	1:B:1003:HIS:CE1	2.26	0.71
1:A:60:HIS:ND1	1:A:128:GLN:OE1	2.25	0.70
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.73	0.70
1:B:1017:TYR:CE2	1:B:1019:THR:HG21	2.26	0.70
1:A:1040:TYR:O	1:A:1042:THR:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.56	0.70
1:B:696:ILE:HG13	1:B:697:LEU:H	1.56	0.70
1:B:384:ILE:O	1:B:546:LYS:HG3	1.92	0.69
1:B:696:ILE:HG13	1:B:697:LEU:N	2.05	0.69
1:A:132:TRP:HZ2	1:A:179:ASN:CG	2.01	0.69
1:A:107:MET:CE	1:A:954:ARG:HD2	2.23	0.69
1:A:159:PHE:CE1	1:A:900:PHE:CE2	2.81	0.69
1:A:272:ARG:O	1:A:276:ASN:ND2	2.25	0.69
1:B:272:ARG:O	1:B:276:ASN:ND2	2.24	0.69
1:A:740:PRO:HG2	1:A:741:PRO:CD	2.22	0.69
1:A:1100:LEU:HD23	1:A:1105:LEU:HB2	1.73	0.68
1:B:70:ILE:HD13	1:B:113:TYR:HB3	1.75	0.68
1:A:132:TRP:HB2	1:A:184:ASP:H	1.58	0.68
1:B:969:ASN:HA	1:B:972:LEU:HB2	1.76	0.68
1:A:65:PRO:HB2	1:A:202:ILE:HD12	1.73	0.68
1:A:756:LEU:HA	1:A:760:ILE:HD13	1.75	0.68
1:B:159:PHE:CE1	1:B:900:PHE:CD2	2.82	0.68
1:B:1144:ALA:HA	1:B:1186:LEU:HD11	1.73	0.68
1:A:76:ASP:HB2	1:A:326:GLN:HG2	1.75	0.68
1:A:1048:VAL:HG21	1:A:1074:THR:HG21	1.76	0.68
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.74	0.68
1:B:543:ARG:NH2	1:B:905:SER:O	2.26	0.68
1:A:70:ILE:HD13	1:A:113:TYR:HB3	1.75	0.68
1:A:979:PHE:O	1:A:982:MET:CG	2.32	0.68
1:B:756:LEU:HA	1:B:760:ILE:HD13	1.74	0.68
1:B:306:TYR:HD2	1:B:754:LEU:HD21	1.59	0.67
1:A:107:MET:CE	1:A:958:TYR:HB3	2.24	0.67
1:B:1024:PRO:O	1:B:1027:LEU:CD1	2.41	0.67
1:A:382:ASP:O	1:A:384:ILE:HG12	1.93	0.67
1:B:132:TRP:CZ2	1:B:179:ASN:OD1	2.48	0.67
1:A:851:TRP:O	1:A:853:LEU:N	2.22	0.66
1:A:962:GLN:O	1:A:963:GLN:NE2	2.25	0.66
1:B:995:ALA:C	1:B:998:THR:HG22	2.20	0.66
1:B:696:ILE:HD13	1:B:994:TYR:OH	1.94	0.66
1:A:1110:GLY:HA3	1:A:1193:LEU:HA	1.78	0.65
1:B:787:MET:HE2	1:B:1008:ILE:HD11	1.77	0.65
1:A:306:TYR:HD2	1:A:754:LEU:HD21	1.61	0.65
1:A:220:VAL:HG12	1:A:301:LEU:HD13	1.77	0.65
1:A:132:TRP:CE3	1:A:133:CYS:CA	2.76	0.65
1:A:798:SER:HA	1:A:802:ASP:H	1.62	0.65
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:HB3	1:B:301:LEU:HD12	1.77	0.65
1:A:224:SER:HB3	1:A:301:LEU:HD12	1.78	0.65
1:A:132:TRP:CZ2	1:A:179:ASN:ND2	2.56	0.65
1:B:384:ILE:HG22	1:B:546:LYS:CG	2.27	0.65
1:A:687:ASP:HA	1:A:1003:HIS:CE1	2.31	0.64
1:A:1017:TYR:HD1	1:A:1018:SER:H	1.46	0.64
1:A:1118:LEU:HD21	1:A:1180:ILE:HG21	1.78	0.64
1:A:962:GLN:O	1:A:962:GLN:HG2	1.98	0.64
1:B:1100:LEU:HD23	1:B:1105:LEU:HB2	1.79	0.64
1:B:484:ILE:HG23	1:B:542:VAL:HG21	1.79	0.64
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.79	0.63
1:B:901:ARG:O	1:B:904:VAL:HG12	1.98	0.63
1:B:1048:VAL:HG21	1:B:1074:THR:HG21	1.78	0.63
1:B:543:ARG:HH12	1:B:905:SER:HA	1.64	0.63
1:A:930:LYS:HD2	1:A:934:PHE:CE2	2.33	0.63
1:B:384:ILE:O	1:B:384:ILE:CG2	2.40	0.63
1:A:132:TRP:CZ2	1:A:179:ASN:CG	2.77	0.63
1:A:486:TYR:HB3	1:A:908:ARG:HH21	1.62	0.63
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.80	0.63
1:B:687:ASP:HA	1:B:1003:HIS:HE1	1.63	0.63
1:B:1118:LEU:HD21	1:B:1180:ILE:HG21	1.80	0.62
1:B:50:MET:HG3	1:B:131:PHE:CE1	2.34	0.62
1:A:210:LEU:HB2	1:A:331:PHE:CD2	2.35	0.62
1:B:156:ILE:HG12	1:B:439:LEU:O	2.00	0.62
1:B:820:GLN:HB3	1:B:997:ALA:HA	1.80	0.62
1:B:220:VAL:HG12	1:B:301:LEU:HD13	1.82	0.62
1:A:787:MET:HE2	1:A:1008:ILE:HD11	1.81	0.62
1:B:355:ARG:HG2	1:B:359:TYR:HD2	1.63	0.62
1:A:281:LYS:HB3	1:A:782:LYS:HG3	1.82	0.62
1:B:479:THR:OG1	1:B:482:GLU:N	2.26	0.61
1:A:92:SER:OG	1:A:96:LYS:NZ	2.32	0.61
1:A:921:GLN:HG3	1:B:517:ASP:HB3	1.83	0.61
1:B:369:PRO:O	1:B:371:ILE:HG12	2.00	0.61
1:B:845:ILE:O	1:B:848:ILE:HG12	2.00	0.61
1:A:132:TRP:HB2	1:A:184:ASP:N	2.14	0.61
1:A:796:ASP:OD1	1:A:796:ASP:N	2.34	0.61
1:B:281:LYS:HB3	1:B:782:LYS:HG3	1.81	0.61
1:B:1057:LYS:H	1:B:1060:GLN:HE21	1.47	0.61
1:B:508:PHE:HE2	1:B:534:ARG:HD2	1.66	0.61
1:B:550:LEU:HD23	1:B:569:LEU:HD13	1.83	0.61
1:A:550:LEU:HD23	1:A:569:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1110:GLY:HA3	1:B:1193:LEU:HA	1.82	0.61
1:B:104:GLU:HG3	1:B:107:MET:HE2	1.83	0.61
1:B:686:GLU:OE1	1:B:813:ARG:NH1	2.34	0.60
1:B:382:ASP:C	1:B:384:ILE:CD1	2.67	0.60
1:A:949:TYR:HD1	1:A:953:PHE:HE2	1.48	0.60
1:B:798:SER:HA	1:B:802:ASP:H	1.65	0.60
1:A:849:TYR:HE1	1:A:972:LEU:HD23	1.66	0.60
1:A:107:MET:HE1	1:A:954:ARG:HD2	1.83	0.60
1:A:901:ARG:O	1:A:904:VAL:HG12	2.01	0.60
1:B:76:ASP:HB2	1:B:326:GLN:HG2	1.83	0.60
1:B:308:LEU:HD21	1:B:312:TYR:HE2	1.66	0.60
1:A:786:TYR:O	1:A:790:LYS:HG2	2.02	0.60
1:B:692:SER:OG	1:B:696:ILE:HG23	2.02	0.60
1:A:716:ILE:HD11	1:A:765:THR:HB	1.83	0.60
1:B:132:TRP:HE3	1:B:133:CYS:N	2.00	0.60
1:B:796:ASP:OD1	1:B:796:ASP:N	2.35	0.60
1:B:949:TYR:HD1	1:B:953:PHE:HE2	1.50	0.60
1:A:969:ASN:HA	1:A:972:LEU:HB2	1.84	0.59
1:B:355:ARG:HG2	1:B:359:TYR:CD2	2.37	0.59
1:B:385:GLN:O	1:B:450:ASP:OD1	2.20	0.59
1:A:384:ILE:HG22	1:A:384:ILE:O	2.02	0.59
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.84	0.59
1:B:382:ASP:HA	1:B:384:ILE:HD11	1.84	0.59
1:B:306:TYR:CD2	1:B:754:LEU:HD21	2.38	0.59
1:A:861:VAL:HG11	1:A:980:GLY:HA3	1.85	0.59
1:B:369:PRO:O	1:B:371:ILE:HG23	2.03	0.59
1:A:355:ARG:HG2	1:A:359:TYR:HD2	1.67	0.59
1:B:210:LEU:HB2	1:B:331:PHE:CD2	2.38	0.59
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.35	0.58
1:B:471:GLN:N	1:B:471:GLN:OE1	2.36	0.58
1:B:1039:ASN:ND2	1:B:1047:PRO:HG3	2.18	0.58
1:A:50:MET:HG3	1:A:131:PHE:CE1	2.39	0.58
1:A:278:GLU:HA	1:A:782:LYS:HD3	1.86	0.58
1:A:845:ILE:O	1:A:848:ILE:HG12	2.03	0.58
1:B:132:TRP:CH2	1:B:179:ASN:OD1	2.56	0.58
1:B:849:TYR:HE1	1:B:972:LEU:HD23	1.68	0.58
1:B:484:ILE:HG21	1:B:496:ILE:HG13	1.86	0.58
1:B:527:LEU:HD23	1:B:527:LEU:H	1.69	0.58
1:B:994:TYR:O	1:B:994:TYR:CD2	2.56	0.58
1:A:355:ARG:HG2	1:A:359:TYR:CD2	2.39	0.58
1:B:306:TYR:CZ	1:B:724:PHE:HE1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:MET:HG3	1:B:131:PHE:HE1	1.67	0.58
1:B:777:GLY:HA3	1:B:822:LYS:HG3	1.86	0.58
1:B:308:LEU:HD21	1:B:312:TYR:CE2	2.39	0.58
1:A:753:LEU:O	1:A:757:ILE:HB	2.04	0.57
1:A:1193:LEU:HD12	1:A:1218:ARG:HB3	1.85	0.57
1:B:1214:LEU:O	1:B:1218:ARG:HG2	2.04	0.57
1:A:362:PHE:HA	1:A:365:ILE:HB	1.85	0.57
1:A:1100:LEU:HD11	1:A:1104:TRP:HZ3	1.68	0.57
1:B:122:LEU:HD13	1:B:943:ALA:HB2	1.85	0.57
1:A:371:ILE:O	1:A:371:ILE:HG13	2.04	0.57
1:A:711:ILE:O	1:A:715:ILE:HG12	2.04	0.57
1:B:753:LEU:O	1:B:757:ILE:HB	2.04	0.57
1:B:786:TYR:O	1:B:790:LYS:HG2	2.04	0.57
1:A:132:TRP:HD1	1:A:183:GLY:CA	1.97	0.57
1:A:837:ALA:HB1	1:A:982:MET:CE	2.24	0.57
1:B:906:LEU:HG	1:B:909:GLU:HG3	1.86	0.57
1:A:361:VAL:O	1:A:365:ILE:N	2.25	0.57
1:A:466:ILE:HG23	1:A:549:LEU:HD13	1.87	0.57
1:B:1052:LEU:HD13	1:B:1242:ILE:HD13	1.86	0.57
1:A:211:THR:HG23	1:A:331:PHE:CE2	2.40	0.57
1:A:1176:GLN:OE1	1:A:1176:GLN:N	2.37	0.57
1:A:484:ILE:HG21	1:A:496:ILE:HG13	1.87	0.57
1:A:1039:ASN:ND2	1:A:1047:PRO:HG3	2.20	0.57
1:A:1122:SER:HB3	1:A:1125:GLU:HG2	1.86	0.57
1:B:359:TYR:HA	1:B:362:PHE:HB2	1.86	0.57
1:B:979:PHE:HA	1:B:982:MET:HG2	1.87	0.57
1:B:1037:VAL:HG22	1:B:1087:ALA:HB3	1.87	0.57
1:B:1130:GLY:HA2	1:B:1134:ARG:HB2	1.87	0.56
1:A:471:GLN:N	1:A:471:GLN:OE1	2.36	0.56
1:B:849:TYR:CE1	1:B:972:LEU:HD23	2.40	0.56
1:B:961:THR:HA	1:B:965:MET:HB3	1.86	0.56
1:A:257:ILE:HG12	1:A:800:PHE:CD1	2.40	0.56
1:A:777:GLY:HA3	1:A:822:LYS:HG3	1.86	0.56
1:B:382:ASP:HA	1:B:384:ILE:CD1	2.35	0.56
1:B:480:ILE:HG12	1:B:518:THR:HG23	1.87	0.56
1:B:711:ILE:O	1:B:715:ILE:HG12	2.04	0.56
1:B:994:TYR:HA	1:B:997:ALA:HB3	1.87	0.56
1:A:966:THR:CG2	1:A:968:GLU:HG2	2.36	0.56
1:B:716:ILE:HD11	1:B:765:THR:HB	1.88	0.56
1:B:856:LEU:HD21	1:B:951:ALA:HB1	1.86	0.56
1:A:816:ASN:O	1:A:820:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PHE:CE1	1:B:900:PHE:CE2	2.93	0.56
1:B:1100:LEU:HD11	1:B:1104:TRP:HZ3	1.71	0.56
1:A:384:ILE:CG2	1:A:546:LYS:CG	2.81	0.56
1:A:527:LEU:H	1:A:527:LEU:HD23	1.70	0.56
1:B:966:THR:CG2	1:B:968:GLU:HG2	2.36	0.56
1:A:331:PHE:O	1:A:334:VAL:HB	2.06	0.55
1:A:390:PHE:HE2	1:A:432:THR:HB	1.71	0.55
1:A:111:ALA:HA	1:A:114:TYR:CE2	2.41	0.55
1:A:508:PHE:HE2	1:A:534:ARG:HD2	1.69	0.55
1:A:834:GLN:HA	1:A:837:ALA:HB3	1.89	0.55
1:A:1061:THR:HA	1:A:1223:CYS:SG	2.46	0.55
1:A:853:LEU:HD11	1:A:973:VAL:HG22	1.87	0.55
1:B:466:ILE:HG23	1:B:549:LEU:HD13	1.87	0.55
1:B:1063:ALA:HB3	1:B:1239:ILE:HA	1.87	0.55
1:A:147:PHE:CD1	1:A:365:ILE:HG23	2.42	0.55
1:A:306:TYR:CD2	1:A:754:LEU:HD21	2.42	0.55
1:A:486:TYR:O	1:A:907:THR:OG1	2.20	0.55
1:A:155:GLU:OE1	1:A:373:SER:OG	2.23	0.55
1:A:442:PRO:HG2	1:A:455:ARG:HH21	1.71	0.55
1:A:1052:LEU:HD13	1:A:1242:ILE:HD13	1.89	0.55
1:B:361:VAL:O	1:B:365:ILE:N	2.26	0.55
1:B:978:VAL:O	1:B:982:MET:N	2.38	0.55
1:B:1129:TYR:CE2	1:B:1184:ARG:HD2	2.42	0.55
1:A:437:GLN:HB2	1:A:439:LEU:HD23	1.88	0.55
1:A:906:LEU:HG	1:A:909:GLU:HG3	1.89	0.55
1:B:905:SER:C	1:B:907:THR:H	2.13	0.55
1:B:81:VAL:HG22	1:B:99:MET:HB3	1.89	0.55
1:A:308:LEU:HD21	1:A:312:TYR:HE2	1.71	0.54
1:A:765:THR:O	1:A:769:GLN:HG2	2.08	0.54
1:A:885:GLU:HB3	1:A:923:PRO:HG3	1.89	0.54
1:A:1129:TYR:CE2	1:A:1184:ARG:HD2	2.42	0.54
1:B:816:ASN:O	1:B:820:GLN:HG2	2.07	0.54
1:A:1048:VAL:HG23	1:A:1049:LEU:HD22	1.88	0.54
1:A:1110:GLY:N	1:A:1192:ILE:O	2.41	0.54
1:B:834:GLN:HA	1:B:837:ALA:HB3	1.89	0.54
1:A:107:MET:HE1	1:A:958:TYR:HB3	1.88	0.54
1:A:978:VAL:O	1:A:982:MET:N	2.41	0.54
1:A:156:ILE:HG12	1:A:439:LEU:O	2.08	0.54
1:A:308:LEU:CD2	1:A:312:TYR:CE2	2.91	0.54
1:B:468:VAL:HG22	1:B:549:LEU:HB2	1.90	0.54
1:B:979:PHE:CA	1:B:982:MET:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:SD	1:A:954:ARG:CG	2.95	0.54
1:A:186:ILE:HD11	1:A:351:PHE:CD1	2.43	0.54
1:B:533:GLN:O	1:B:537:ILE:HG13	2.08	0.54
1:A:39:PHE:CE1	1:A:355:ARG:HA	2.43	0.54
1:A:308:LEU:HD21	1:A:312:TYR:CE2	2.43	0.54
1:B:1120:ASP:HB2	1:B:1164:ARG:HH21	1.72	0.54
1:A:461:TYR:O	1:A:465:ILE:HG12	2.08	0.53
1:B:111:ALA:HA	1:B:114:TYR:CE2	2.42	0.53
1:A:231:ILE:HG21	1:A:290:THR:HB	1.90	0.53
1:A:543:ARG:NH2	1:A:904:VAL:O	2.40	0.53
1:A:1120:ASP:HB2	1:A:1164:ARG:HH21	1.72	0.53
1:B:993:ASP:O	1:B:994:TYR:HB3	2.09	0.53
1:B:1110:GLY:N	1:B:1192:ILE:O	2.41	0.53
1:A:100:PHE:CE2	1:A:962:GLN:HB2	2.42	0.53
1:A:234:SER:O	1:A:238:LYS:HG3	2.08	0.53
1:B:132:TRP:CG	1:B:183:GLY:CA	2.91	0.53
1:A:129:VAL:HG21	1:A:938:PHE:HB3	1.90	0.53
1:A:492:THR:OG1	1:B:910:GLN:OE1	2.20	0.53
1:B:278:GLU:HA	1:B:782:LYS:HD3	1.90	0.53
1:B:543:ARG:NH1	1:B:905:SER:HA	2.22	0.53
1:A:209:LYS:O	1:A:213:VAL:HG23	2.09	0.53
1:A:1010:LYS:HG2	1:A:1011:THR:H	1.74	0.53
1:A:1106:ARG:HA	1:A:1109:LEU:HD12	1.90	0.53
1:B:1048:VAL:HG23	1:B:1049:LEU:HD22	1.90	0.53
1:A:359:TYR:HA	1:A:362:PHE:HB2	1.89	0.53
1:A:1130:GLY:HA2	1:A:1134:ARG:HB2	1.89	0.53
1:A:687:ASP:HA	1:A:1003:HIS:HE1	1.72	0.53
1:B:1010:LYS:HG2	1:B:1011:THR:H	1.74	0.53
1:A:797:VAL:HG21	1:A:1013:GLU:OE2	2.08	0.53
1:A:905:SER:C	1:A:907:THR:H	2.17	0.53
1:A:1235:ASN:OD1	1:A:1235:ASN:N	2.39	0.53
1:B:258:ARG:HH21	1:B:801:ASP:HA	1.74	0.53
1:B:267:LYS:O	1:B:270:LEU:HB2	2.09	0.53
1:B:362:PHE:HA	1:B:365:ILE:HB	1.89	0.53
1:B:797:VAL:HG21	1:B:1013:GLU:OE2	2.08	0.53
1:B:1176:GLN:OE1	1:B:1176:GLN:N	2.38	0.53
1:A:453:ASP:OD1	1:A:454:ILE:N	2.42	0.52
1:A:612:MET:HA	1:A:619:PHE:HB2	1.92	0.52
1:A:884:LYS:O	1:A:887:GLU:HB3	2.09	0.52
1:B:147:PHE:CD1	1:B:365:ILE:HG23	2.44	0.52
1:A:1043:ARG:HH12	1:A:1086:MET:HE1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:HB2	1:B:110:TYR:HE1	1.74	0.52
1:B:1151:HIS:HA	1:B:1154:ILE:HB	1.91	0.52
1:A:107:MET:SD	1:A:954:ARG:HG2	2.50	0.52
1:A:308:LEU:CD2	1:A:312:TYR:HE2	2.22	0.52
1:A:740:PRO:CD	1:A:741:PRO:HD2	2.39	0.52
1:B:257:ILE:HG12	1:B:800:PHE:CD1	2.44	0.52
1:B:331:PHE:O	1:B:334:VAL:HB	2.10	0.52
1:B:437:GLN:HB2	1:B:439:LEU:HD23	1.90	0.52
1:B:765:THR:O	1:B:769:GLN:HG2	2.08	0.52
1:A:50:MET:HG3	1:A:131:PHE:HE1	1.73	0.52
1:A:1037:VAL:HG22	1:A:1087:ALA:HB3	1.92	0.52
1:B:234:SER:O	1:B:238:LYS:HG3	2.09	0.52
1:A:1023:LYS:HB2	1:A:1026:MET:HG3	1.91	0.52
1:B:970:VAL:HG23	1:B:971:LEU:CD2	2.25	0.52
1:B:406:LEU:HD12	1:B:600:GLY:O	2.10	0.52
1:B:906:LEU:HA	1:B:909:GLU:HG2	1.92	0.52
1:A:1064:LEU:HB3	1:A:1226:ILE:HA	1.92	0.52
1:B:39:PHE:CE1	1:B:355:ARG:HA	2.45	0.52
1:B:878:GLN:HG3	1:B:934:PHE:HE1	1.75	0.52
1:A:306:TYR:CZ	1:A:724:PHE:HE1	2.27	0.52
1:A:1181:ALA:HA	1:A:1184:ARG:HE	1.73	0.52
1:B:231:ILE:HG21	1:B:290:THR:HB	1.92	0.52
1:B:155:GLU:OE1	1:B:373:SER:OG	2.25	0.52
1:B:382:ASP:CA	1:B:384:ILE:HD12	2.40	0.52
1:B:1106:ARG:HA	1:B:1109:LEU:HD12	1.91	0.52
1:B:186:ILE:HD11	1:B:351:PHE:CD1	2.46	0.51
1:B:461:TYR:O	1:B:465:ILE:HG12	2.10	0.51
1:B:1060:GLN:HB2	1:B:1237:ASP:CG	2.35	0.51
1:B:480:ILE:HG12	1:B:518:THR:CG2	2.41	0.51
1:B:562:GLU:OE1	1:B:584:ARG:NH1	2.43	0.51
1:A:798:SER:OG	1:A:1041:PRO:HG2	2.11	0.51
1:A:1033:PHE:HD1	1:A:1036:VAL:HG21	1.75	0.51
1:B:215:LEU:O	1:B:219:PRO:HD3	2.10	0.51
1:A:242:ALA:HB2	1:A:283:LEU:HD12	1.93	0.51
1:A:1018:SER:C	1:A:1019:THR:HG22	2.36	0.51
1:A:1026:MET:HE3	1:A:1095:LYS:HD3	1.92	0.51
1:A:74:MET:HB2	1:A:110:TYR:HE1	1.74	0.51
1:A:236:THR:HA	1:A:287:LYS:HE2	1.92	0.51
1:A:740:PRO:CG	1:A:741:PRO:CD	2.89	0.51
1:B:806:THR:O	1:B:810:LEU:HG	2.10	0.51
1:B:107:MET:HA	1:B:110:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:ALA:HB2	1:B:1161:TYR:HB3	1.92	0.51
1:A:100:PHE:HE2	1:A:962:GLN:HB2	1.76	0.51
1:A:534:ARG:HA	1:A:537:ILE:HD12	1.93	0.51
1:B:995:ALA:O	1:B:999:VAL:HG23	2.11	0.51
1:A:518:THR:HG23	1:A:518:THR:O	2.11	0.51
1:A:1018:SER:O	1:A:1019:THR:CG2	2.55	0.51
1:A:132:TRP:HE3	1:A:133:CYS:N	2.08	0.50
1:B:1033:PHE:HD1	1:B:1036:VAL:HG21	1.76	0.50
1:A:384:ILE:HD13	1:A:384:ILE:N	2.26	0.50
1:B:211:THR:HG23	1:B:331:PHE:CE2	2.47	0.50
1:B:467:GLY:HA3	1:B:545:PRO:HG3	1.93	0.50
1:B:998:THR:HG23	1:B:999:VAL:N	2.26	0.50
1:A:39:PHE:HE1	1:A:358:ALA:HB3	1.76	0.50
1:A:267:LYS:O	1:A:270:LEU:HB2	2.11	0.50
1:A:374:PHE:HD1	1:A:376:LYS:H	1.58	0.50
1:B:242:ALA:HB2	1:B:283:LEU:HD12	1.93	0.50
1:B:975:SER:O	1:B:978:VAL:HG12	2.11	0.50
1:B:132:TRP:CD1	1:B:183:GLY:HA2	2.39	0.50
1:B:453:ASP:OD1	1:B:454:ILE:N	2.44	0.50
1:A:200:PHE:CE2	1:A:215:LEU:HD21	2.46	0.50
1:A:132:TRP:O	1:A:136:ALA:HB3	2.12	0.50
1:A:840:GLY:O	1:A:844:ILE:HG12	2.12	0.50
1:B:994:TYR:O	1:B:994:TYR:CG	2.64	0.50
1:A:384:ILE:HD11	1:A:461:TYR:OH	2.11	0.50
1:A:927:ALA:HA	1:A:930:LYS:HG2	1.93	0.50
1:A:1038:PHE:HB3	1:A:1049:LEU:HD23	1.94	0.50
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.94	0.50
1:A:159:PHE:CZ	1:A:900:PHE:CE2	3.00	0.49
1:A:902:THR:HA	1:A:908:ARG:HE	1.76	0.49
1:B:236:THR:HA	1:B:287:LYS:HE2	1.94	0.49
1:A:122:LEU:HD13	1:A:943:ALA:HB2	1.94	0.49
1:A:533:GLN:O	1:A:537:ILE:HG13	2.12	0.49
1:A:1124:ALA:HB2	1:A:1161:TYR:HB3	1.94	0.49
1:B:415:SER:HA	1:B:577:THR:HG22	1.94	0.49
1:B:884:LYS:O	1:B:887:GLU:HB3	2.12	0.49
1:A:258:ARG:HH21	1:A:801:ASP:HA	1.77	0.49
1:A:979:PHE:CA	1:A:982:MET:HG2	2.42	0.49
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.93	0.49
1:A:406:LEU:HD12	1:A:600:GLY:O	2.13	0.49
1:A:562:GLU:OE1	1:A:584:ARG:NH1	2.44	0.49
1:A:910:GLN:OE1	1:B:492:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:HA	1:B:285:ILE:HG22	1.94	0.49
1:B:845:ILE:HG22	1:B:849:TYR:CE1	2.47	0.49
1:B:927:ALA:HA	1:B:930:LYS:HG2	1.93	0.49
1:A:819:ALA:O	1:A:822:LYS:HB3	2.12	0.49
1:A:851:TRP:C	1:A:853:LEU:H	2.18	0.49
1:A:1100:LEU:HD11	1:A:1104:TRP:CZ3	2.48	0.49
1:B:1032:GLN:HB2	1:B:1091:PHE:HB2	1.93	0.49
1:B:1235:ASN:OD1	1:B:1235:ASN:N	2.40	0.49
1:A:1214:LEU:O	1:A:1218:ARG:HG2	2.13	0.49
1:B:178:ILE:HG12	1:B:358:ALA:HB2	1.94	0.49
1:B:1064:LEU:HB3	1:B:1226:ILE:HA	1.94	0.49
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.95	0.49
1:A:74:MET:HB2	1:A:110:TYR:CE1	2.48	0.49
1:A:107:MET:HA	1:A:110:TYR:HD2	1.77	0.49
1:A:139:GLN:O	1:A:143:ILE:HG12	2.12	0.49
1:B:34:SER:HA	1:B:38:MET:HB2	1.94	0.49
1:B:1023:LYS:HB2	1:B:1026:MET:HG3	1.95	0.49
1:A:715:ILE:HD12	1:A:836:ILE:HG13	1.94	0.49
1:B:590:ASN:OD1	1:B:590:ASN:N	2.40	0.49
1:A:34:SER:HA	1:A:38:MET:HB2	1.94	0.49
1:A:257:ILE:HG12	1:A:800:PHE:CG	2.48	0.49
1:A:857:LEU:HD11	1:A:977:ILE:HG13	1.95	0.49
1:B:518:THR:HG23	1:B:518:THR:O	2.13	0.49
1:A:252:GLU:HG3	1:A:253:VAL:N	2.27	0.49
1:A:468:VAL:HG22	1:A:549:LEU:HB2	1.94	0.49
1:A:1084:ASP:HB3	1:A:1098:LYS:NZ	2.27	0.49
1:B:311:TRP:HZ3	1:B:748:SER:HA	1.78	0.49
1:B:756:LEU:O	1:B:760:ILE:HB	2.12	0.49
1:A:132:TRP:HB2	1:A:184:ASP:HB3	1.94	0.48
1:A:979:PHE:HA	1:A:982:MET:HG2	1.94	0.48
1:A:1024:PRO:O	1:A:1027:LEU:CD1	2.56	0.48
1:B:270:LEU:CG	1:B:790:LYS:HD2	2.41	0.48
1:B:852:GLN:HG3	1:B:955:PHE:CE2	2.48	0.48
1:A:413:VAL:HG11	1:A:419:VAL:HG11	1.95	0.48
1:B:128:GLN:O	1:B:131:PHE:HB3	2.13	0.48
1:B:486:TYR:O	1:B:907:THR:OG1	2.26	0.48
1:B:902:THR:HA	1:B:908:ARG:HE	1.78	0.48
1:A:806:THR:O	1:A:810:LEU:HG	2.13	0.48
1:B:39:PHE:HE1	1:B:358:ALA:HB3	1.78	0.48
1:B:471:GLN:HB3	1:B:552:GLU:HB2	1.95	0.48
1:B:819:ALA:O	1:B:822:LYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1084:ASP:HB3	1:B:1098:LYS:NZ	2.29	0.48
1:A:178:ILE:HG12	1:A:358:ALA:HB2	1.94	0.48
1:A:790:LYS:N	1:A:790:LYS:HD3	2.29	0.48
1:B:74:MET:HB2	1:B:110:TYR:CE1	2.48	0.48
1:B:252:GLU:HG3	1:B:253:VAL:N	2.28	0.48
1:B:1038:PHE:CD2	1:B:1049:LEU:HD23	2.48	0.48
1:A:71:PHE:HA	1:A:74:MET:HG2	1.94	0.48
1:A:132:TRP:CD1	1:A:183:GLY:HA2	2.42	0.48
1:A:333:SER:HA	1:A:336:ILE:HG12	1.95	0.48
1:B:71:PHE:HA	1:B:74:MET:HG2	1.95	0.48
1:A:282:ARG:HA	1:A:285:ILE:HG22	1.96	0.48
1:A:733:GLY:HA2	1:A:967:PHE:HB2	1.95	0.48
1:A:756:LEU:O	1:A:760:ILE:HB	2.12	0.48
1:B:689:PRO:N	1:B:690:PRO:CD	2.76	0.48
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.67	0.48
1:A:849:TYR:CE1	1:A:972:LEU:HD23	2.46	0.48
1:A:1040:TYR:OH	1:A:1074:THR:HG22	2.13	0.48
1:B:534:ARG:HA	1:B:537:ILE:HD12	1.96	0.48
1:A:1071:GLY:H	1:A:1074:THR:HG23	1.79	0.48
1:B:374:PHE:HD1	1:B:376:LYS:H	1.59	0.48
1:B:384:ILE:CG2	1:B:546:LYS:CG	2.91	0.48
1:B:397:TYR:C	1:B:399:SER:H	2.21	0.48
1:B:786:TYR:CD1	1:B:790:LYS:NZ	2.71	0.48
1:B:1017:TYR:CZ	1:B:1019:THR:HG21	2.49	0.48
1:B:1181:ALA:HA	1:B:1184:ARG:HE	1.78	0.48
1:A:1038:PHE:HB3	1:A:1049:LEU:HB2	1.96	0.48
1:B:421:LEU:HD13	1:B:579:ILE:HG13	1.96	0.48
1:B:480:ILE:CG1	1:B:518:THR:CG2	2.91	0.48
1:B:330:VAL:O	1:B:333:SER:HB2	2.14	0.47
1:B:976:ALA:HA	1:B:979:PHE:CD2	2.50	0.47
1:B:1176:GLN:O	1:B:1180:ILE:HG13	2.14	0.47
1:A:397:TYR:C	1:A:399:SER:H	2.22	0.47
1:A:467:GLY:HA3	1:A:545:PRO:HG3	1.95	0.47
1:A:1060:GLN:HB2	1:A:1237:ASP:CG	2.39	0.47
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	1.96	0.47
1:B:132:TRP:O	1:B:136:ALA:HB3	2.14	0.47
1:B:156:ILE:HG22	1:B:160:ASP:OD2	2.14	0.47
1:B:332:PHE:O	1:B:335:LEU:HB2	2.14	0.47
1:B:333:SER:HA	1:B:336:ILE:HG12	1.95	0.47
1:B:463:ARG:NH1	1:B:903:VAL:HG22	2.29	0.47
1:B:1057:LYS:HB2	1:B:1060:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:O	1:A:788:VAL:HG23	2.15	0.47
1:A:1033:PHE:HB2	1:A:1054:LEU:H	1.78	0.47
1:B:172:THR:O	1:B:175:VAL:HG22	2.14	0.47
1:B:370:SER:O	1:B:371:ILE:CG1	2.58	0.47
1:B:1040:TYR:OH	1:B:1074:THR:HG22	2.13	0.47
1:A:768:LEU:O	1:A:772:THR:HG23	2.14	0.47
1:A:784:LEU:HG	1:A:821:VAL:HG21	1.96	0.47
1:A:806:THR:HG23	1:A:809:ALA:H	1.78	0.47
1:B:314:THR:HG22	1:B:735:PHE:HE2	1.80	0.47
1:A:721:GLN:O	1:A:724:PHE:HB3	2.15	0.47
1:B:139:GLN:O	1:B:143:ILE:HG12	2.15	0.47
1:B:1137:SER:HB3	1:B:1140:GLU:HB3	1.96	0.47
1:A:215:LEU:O	1:A:219:PRO:HD3	2.14	0.47
1:A:813:ARG:HD3	1:A:817:ASP:OD2	2.14	0.47
1:B:208:TRP:O	1:B:211:THR:OG1	2.31	0.47
1:A:175:VAL:HA	1:A:178:ILE:HG13	1.96	0.47
1:A:311:TRP:HB2	1:A:751:PHE:CD1	2.50	0.47
1:A:332:PHE:CD1	1:A:335:LEU:HD12	2.49	0.47
1:A:785:ARG:HG2	1:A:814:LEU:O	2.15	0.47
1:A:818:ALA:HA	1:A:821:VAL:HG22	1.96	0.47
1:A:878:GLN:CG	1:A:934:PHE:HE1	2.20	0.47
1:A:1234:GLN:HA	1:A:1253:HIS:CD2	2.50	0.47
1:B:92:SER:OG	1:B:96:LYS:NZ	2.46	0.47
1:B:688:VAL:HG23	1:B:690:PRO:CD	2.42	0.47
1:B:785:ARG:HG2	1:B:814:LEU:O	2.15	0.47
1:B:999:VAL:HG12	1:B:1003:HIS:NE2	2.29	0.47
1:B:1038:PHE:HB3	1:B:1049:LEU:HB2	1.96	0.47
1:B:1038:PHE:HD2	1:B:1049:LEU:HD23	1.80	0.47
1:A:311:TRP:HZ3	1:A:748:SER:HA	1.80	0.47
1:A:320:LYS:HB3	1:A:322:TYR:CD1	2.49	0.47
1:A:862:PRO:O	1:A:866:ILE:HG13	2.14	0.47
1:B:129:VAL:HG21	1:B:938:PHE:HB3	1.96	0.47
1:B:538:ALA:O	1:B:542:VAL:HG23	2.15	0.47
1:B:1051:GLY:HA3	1:B:1246:LYS:NZ	2.29	0.47
1:A:696:ILE:HG13	1:A:828:ARG:HH21	1.80	0.47
1:A:1092:LEU:HD21	1:A:1100:LEU:HD13	1.97	0.47
1:B:293:ILE:HG12	1:B:767:PHE:HD1	1.79	0.47
1:B:306:TYR:HE2	1:B:754:LEU:HD11	1.79	0.47
1:B:466:ILE:HG12	1:B:547:ILE:HD12	1.97	0.47
1:B:806:THR:HG23	1:B:809:ALA:H	1.80	0.47
1:B:1071:GLY:H	1:B:1074:THR:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1202:LEU:HB3	1:B:1207:GLU:HG2	1.97	0.47
1:A:172:THR:O	1:A:175:VAL:HG22	2.15	0.47
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.80	0.47
1:A:1137:SER:HB3	1:A:1140:GLU:HB3	1.96	0.47
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.15	0.47
1:B:312:TYR:O	1:B:316:LEU:HG	2.14	0.47
1:B:813:ARG:HD3	1:B:817:ASP:OD2	2.15	0.47
1:B:840:GLY:O	1:B:844:ILE:HG12	2.14	0.47
1:B:949:TYR:CD1	1:B:953:PHE:HE2	2.30	0.47
1:B:1032:GLN:HB3	1:B:1091:PHE:HD1	1.80	0.47
1:B:1062:LEU:HD12	1:B:1224:ILE:HG23	1.96	0.47
1:A:327:VAL:HB	1:A:331:PHE:CE1	2.50	0.46
1:A:993:ASP:O	1:A:994:TYR:C	2.58	0.46
1:B:1038:PHE:HB3	1:B:1049:LEU:HD23	1.97	0.46
1:B:1050:GLN:H	1:B:1245:GLY:HA3	1.80	0.46
1:A:1104:TRP:HE1	1:A:1108:GLN:HE22	1.62	0.46
1:B:856:LEU:O	1:B:860:ILE:HG12	2.14	0.46
1:B:862:PRO:O	1:B:866:ILE:HG13	2.14	0.46
1:A:435:LEU:HD23	1:A:440:TYR:HB2	1.97	0.46
1:A:725:SER:HB3	1:A:975:SER:OG	2.15	0.46
1:A:965:MET:HE3	1:A:970:VAL:CG1	2.45	0.46
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.97	0.46
1:A:1142:VAL:HA	1:A:1161:TYR:OH	2.15	0.46
1:B:107:MET:HA	1:B:110:TYR:CD2	2.50	0.46
1:B:129:VAL:HG11	1:B:934:PHE:O	2.16	0.46
1:B:132:TRP:CE3	1:B:133:CYS:N	2.82	0.46
1:B:358:ALA:O	1:B:362:PHE:N	2.48	0.46
1:B:688:VAL:CG2	1:B:690:PRO:HD2	2.41	0.46
1:B:768:LEU:O	1:B:772:THR:HG23	2.15	0.46
1:B:930:LYS:HD2	1:B:934:PHE:CE2	2.49	0.46
1:A:159:PHE:CD1	1:A:900:PHE:CD2	3.02	0.46
1:A:949:TYR:CD1	1:A:953:PHE:HE2	2.31	0.46
1:A:1159:ASP:HB3	1:A:1162:ASN:HB2	1.98	0.46
1:A:132:TRP:CE3	1:A:133:CYS:N	2.84	0.46
1:B:1122:SER:HB3	1:B:1125:GLU:HG2	1.98	0.46
1:A:856:LEU:O	1:A:860:ILE:HG12	2.14	0.46
1:B:306:TYR:CD1	1:B:332:PHE:HE1	2.33	0.46
1:B:480:ILE:CG1	1:B:518:THR:HG23	2.44	0.46
1:B:721:GLN:O	1:B:724:PHE:HB3	2.16	0.46
1:B:922:ILE:HB	1:B:923:PRO:HD3	1.98	0.46
1:A:453:ASP:HB3	1:A:456:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:VAL:HG23	1:A:604:GLU:H	1.81	0.46
1:A:1038:PHE:CD2	1:A:1049:LEU:HD23	2.51	0.46
1:B:315:SER:O	1:B:320:LYS:HG3	2.15	0.46
1:B:784:LEU:O	1:B:788:VAL:HG23	2.16	0.46
1:B:896:ALA:HB2	1:B:916:TYR:HE2	1.81	0.46
1:A:254:LEU:HB2	1:A:807:THR:HG23	1.98	0.46
1:A:327:VAL:O	1:A:331:PHE:HD1	1.99	0.46
1:A:332:PHE:O	1:A:335:LEU:HB2	2.15	0.46
1:A:421:LEU:HD13	1:A:579:ILE:HG13	1.98	0.46
1:A:921:GLN:NE2	1:B:479:THR:HG22	2.22	0.46
1:B:715:ILE:HD12	1:B:836:ILE:HG13	1.97	0.46
1:A:590:ASN:OD1	1:A:590:ASN:N	2.39	0.46
1:B:1196:ASP:CG	1:B:1226:ILE:HD11	2.41	0.46
1:A:1091:PHE:CE2	1:A:1096:GLU:HG2	2.51	0.46
1:B:351:PHE:O	1:B:355:ARG:HB2	2.16	0.46
1:B:784:LEU:HG	1:B:821:VAL:HG21	1.98	0.46
1:B:818:ALA:HA	1:B:821:VAL:HG22	1.98	0.46
1:A:689:PRO:N	1:A:690:PRO:CD	2.80	0.45
1:A:740:PRO:HD2	1:A:741:PRO:HD2	1.98	0.45
1:A:1158:PRO:O	1:A:1163:THR:OG1	2.34	0.45
1:B:147:PHE:CE2	1:B:171:LEU:HB3	2.51	0.45
1:B:459:VAL:O	1:B:463:ARG:HG2	2.16	0.45
1:B:1064:LEU:HB3	1:B:1226:ILE:HG22	1.96	0.45
1:A:107:MET:HA	1:A:110:TYR:CD2	2.52	0.45
1:A:208:TRP:O	1:A:212:LEU:HG	2.16	0.45
1:A:538:ALA:O	1:A:542:VAL:HG23	2.16	0.45
1:A:1032:GLN:HB3	1:A:1091:PHE:HD1	1.80	0.45
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.40	0.45
1:B:460:ARG:HA	1:B:906:LEU:HD13	1.98	0.45
1:A:392:ASN:N	1:A:409:LEU:O	2.49	0.45
1:A:487:GLY:O	1:A:907:THR:HG21	2.15	0.45
1:A:906:LEU:HA	1:A:909:GLU:HG2	1.98	0.45
1:A:198:GLY:O	1:A:202:ILE:HG13	2.16	0.45
1:A:285:ILE:HB	1:A:778:GLU:CD	2.41	0.45
1:A:697:LEU:HD23	1:A:828:ARG:CZ	2.46	0.45
1:B:332:PHE:CD1	1:B:335:LEU:HD12	2.51	0.45
1:B:1068:SER:OG	1:B:1069:GLY:N	2.49	0.45
1:B:232:LEU:HA	1:B:232:LEU:HD23	1.66	0.45
1:B:697:LEU:HD23	1:B:828:ARG:CZ	2.47	0.45
1:A:81:VAL:HG22	1:A:99:MET:HB3	1.99	0.45
1:A:509:ILE:HD13	1:A:516:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LEU:HG	1:A:1104:TRP:CE2	2.52	0.45
1:B:132:TRP:HD1	1:B:183:GLY:CA	2.04	0.45
1:B:332:PHE:HD1	1:B:335:LEU:HD12	1.82	0.45
1:B:460:ARG:O	1:B:464:GLU:HG3	2.16	0.45
1:B:699:LEU:HD11	1:B:1005:ILE:HG12	1.99	0.45
1:B:733:GLY:HA2	1:B:967:PHE:HB2	1.99	0.45
1:B:852:GLN:HG3	1:B:955:PHE:HE2	1.81	0.45
1:B:1022:LEU:HG	1:B:1104:TRP:NE1	2.31	0.45
1:B:1043:ARG:HH12	1:B:1086:MET:HE1	1.82	0.45
1:A:147:PHE:CE2	1:A:171:LEU:HB3	2.52	0.45
1:A:156:ILE:HG22	1:A:160:ASP:OD2	2.16	0.45
1:A:231:ILE:HG23	1:A:235:PHE:CD2	2.52	0.45
1:A:688:VAL:HG23	1:A:690:PRO:HD2	1.99	0.45
1:B:397:TYR:O	1:B:399:SER:N	2.48	0.45
1:A:358:ALA:O	1:A:362:PHE:N	2.50	0.45
1:A:1057:LYS:O	1:A:1060:GLN:HG2	2.17	0.45
1:B:861:VAL:HB	1:B:862:PRO:HD3	1.98	0.45
1:B:1120:ASP:OD1	1:B:1120:ASP:N	2.50	0.45
1:A:129:VAL:HG11	1:A:934:PHE:O	2.16	0.45
1:A:327:VAL:HB	1:A:331:PHE:HE1	1.82	0.45
1:A:845:ILE:HG22	1:A:849:TYR:CE1	2.52	0.45
1:A:1239:ILE:HD13	1:A:1253:HIS:N	2.32	0.45
1:B:463:ARG:HH12	1:B:903:VAL:HG22	1.82	0.45
1:A:468:VAL:HB	1:A:904:VAL:HG21	1.99	0.45
1:B:175:VAL:HA	1:B:178:ILE:HG13	1.99	0.45
1:B:281:LYS:HD2	1:B:778:GLU:HG2	1.98	0.45
1:B:382:ASP:CA	1:B:384:ILE:CD1	2.95	0.45
1:B:1142:VAL:HA	1:B:1161:TYR:OH	2.16	0.45
1:A:306:TYR:HE2	1:A:754:LEU:HD11	1.82	0.44
1:A:813:ARG:O	1:A:817:ASP:HB2	2.17	0.44
1:B:603:VAL:HG23	1:B:604:GLU:N	2.33	0.44
1:B:780:LEU:O	1:B:784:LEU:HB2	2.17	0.44
1:A:100:PHE:HA	1:A:103:LEU:HB2	1.98	0.44
1:A:423:GLY:HA3	1:A:429:LYS:HD2	1.98	0.44
1:A:861:VAL:HB	1:A:862:PRO:HD3	2.00	0.44
1:B:257:ILE:HG12	1:B:800:PHE:CG	2.51	0.44
1:B:1005:ILE:HA	1:B:1008:ILE:HG22	1.99	0.44
1:B:1234:GLN:HA	1:B:1253:HIS:CD2	2.52	0.44
1:A:330:VAL:O	1:A:333:SER:HB2	2.17	0.44
1:B:311:TRP:HB2	1:B:751:PHE:CD1	2.52	0.44
1:A:158:TRP:CD1	1:A:159:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:PHE:O	1:A:410:ASN:HA	2.18	0.44
1:A:415:SER:HA	1:A:577:THR:HG22	1.99	0.44
1:A:820:GLN:HB3	1:A:997:ALA:HA	1.99	0.44
1:A:856:LEU:HD21	1:A:951:ALA:HB1	1.98	0.44
1:B:1054:LEU:HD11	1:B:1240:VAL:HG11	1.99	0.44
1:B:1158:PRO:O	1:B:1163:THR:OG1	2.34	0.44
1:A:460:ARG:O	1:A:464:GLU:HG3	2.17	0.44
1:A:603:VAL:HG23	1:A:604:GLU:N	2.32	0.44
1:A:773:PHE:HA	1:A:776:ALA:HB3	2.00	0.44
1:A:849:TYR:C	1:A:851:TRP:H	2.26	0.44
1:A:1081:ARG:HB2	1:A:1105:LEU:HD23	1.98	0.44
1:B:1193:LEU:HD12	1:B:1218:ARG:HB3	1.99	0.44
1:A:780:LEU:O	1:A:784:LEU:HB2	2.18	0.44
1:A:925:ARG:HA	1:B:514:HIS:ND1	2.32	0.44
1:B:603:VAL:HG23	1:B:604:GLU:H	1.81	0.44
1:B:718:GLY:HA2	1:B:837:ALA:HB2	2.00	0.44
1:A:211:THR:HG23	1:A:331:PHE:CD2	2.53	0.44
1:A:459:VAL:O	1:A:463:ARG:HG2	2.17	0.44
1:A:810:LEU:O	1:A:813:ARG:HB2	2.17	0.44
1:B:158:TRP:CD1	1:B:159:PHE:N	2.86	0.44
1:B:308:LEU:CD2	1:B:312:TYR:CE2	3.01	0.44
1:A:1068:SER:OG	1:A:1069:GLY:N	2.50	0.44
1:B:790:LYS:HD3	1:B:790:LYS:N	2.32	0.44
1:A:902:THR:OG1	1:A:908:ARG:HB2	2.18	0.44
1:B:232:LEU:HD11	1:B:291:ALA:HA	2.00	0.44
1:B:306:TYR:CD1	1:B:332:PHE:CE1	3.06	0.44
1:B:390:PHE:HE2	1:B:432:THR:HB	1.82	0.44
1:A:128:GLN:O	1:A:131:PHE:HB3	2.18	0.43
1:A:718:GLY:HA2	1:A:837:ALA:HB2	2.00	0.43
1:A:854:THR:HG22	1:A:858:LEU:HD23	1.99	0.43
1:A:970:VAL:HG23	1:A:971:LEU:CD2	2.27	0.43
1:A:1063:ALA:HB3	1:A:1239:ILE:HG13	1.98	0.43
1:A:1221:ARG:HD3	1:A:1221:ARG:HA	1.85	0.43
1:B:231:ILE:HG23	1:B:235:PHE:CD2	2.53	0.43
1:B:521:GLY:N	1:B:526:GLN:OE1	2.33	0.43
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	2.00	0.43
1:B:132:TRP:CG	1:B:183:GLY:HA2	2.52	0.43
1:B:243:TYR:CE2	1:B:815:ALA:HB2	2.54	0.43
1:B:810:LEU:O	1:B:813:ARG:HB2	2.17	0.43
1:B:878:GLN:HG3	1:B:934:PHE:CE1	2.54	0.43
1:B:1239:ILE:HD13	1:B:1253:HIS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CE2	1:A:277:LEU:HD11	2.53	0.43
1:A:379:HIS:HB3	1:A:457:ILE:HA	1.99	0.43
1:B:275:ASN:O	1:B:278:GLU:HB3	2.18	0.43
1:B:419:VAL:HG12	1:B:578:THR:O	2.18	0.43
1:B:1039:ASN:OD1	1:B:1045:SER:OG	2.36	0.43
1:A:293:ILE:HG12	1:A:767:PHE:HD1	1.83	0.43
1:A:382:ASP:C	1:A:384:ILE:HG12	2.43	0.43
1:A:419:VAL:HG12	1:A:578:THR:O	2.18	0.43
1:A:1020:GLN:HB2	1:A:1101:ASN:N	2.33	0.43
1:B:285:ILE:HB	1:B:778:GLU:CD	2.42	0.43
1:B:316:LEU:HA	1:B:320:LYS:HB2	2.00	0.43
1:B:574:GLU:O	1:B:574:GLU:HG3	2.18	0.43
1:B:1022:LEU:HG	1:B:1104:TRP:CE2	2.54	0.43
1:A:314:THR:HG22	1:A:735:PHE:HE2	1.82	0.43
1:A:1039:ASN:OD1	1:A:1045:SER:OG	2.36	0.43
1:B:285:ILE:HB	1:B:778:GLU:OE2	2.19	0.43
1:B:435:LEU:HD23	1:B:440:TYR:HB2	2.00	0.43
1:B:508:PHE:O	1:B:512:LEU:HB2	2.19	0.43
1:B:734:VAL:HG21	1:B:746:GLN:HG3	2.00	0.43
1:A:466:ILE:HG12	1:A:547:ILE:HD12	1.99	0.43
1:B:1100:LEU:HD11	1:B:1104:TRP:CZ3	2.51	0.43
1:A:200:PHE:HE2	1:A:215:LEU:HD21	1.82	0.43
1:A:1050:GLN:O	1:A:1246:LYS:HD2	2.18	0.43
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	2.00	0.43
1:B:392:ASN:N	1:B:409:LEU:O	2.52	0.43
1:B:979:PHE:HA	1:B:982:MET:CG	2.48	0.43
1:B:1150:ILE:HB	1:B:1179:ARG:HB3	2.00	0.43
1:A:111:ALA:HA	1:A:114:TYR:HE2	1.83	0.43
1:A:232:LEU:HD11	1:A:291:ALA:HA	2.01	0.43
1:A:419:VAL:HG23	1:A:593:VAL:HG13	2.00	0.43
1:B:221:LEU:HD23	1:B:301:LEU:HB3	2.01	0.43
1:B:1033:PHE:HB2	1:B:1054:LEU:H	1.83	0.43
1:A:281:LYS:HD2	1:A:778:GLU:HG2	2.00	0.43
1:A:574:GLU:HG3	1:A:574:GLU:O	2.18	0.43
1:A:699:LEU:HD11	1:A:1005:ILE:HG12	2.00	0.43
1:A:867:ALA:HA	1:A:870:VAL:HG12	2.01	0.43
1:B:121:VAL:HA	1:B:124:VAL:HG22	2.01	0.43
1:B:413:VAL:HG11	1:B:419:VAL:HG11	2.01	0.43
1:B:431:THR:O	1:B:435:LEU:HG	2.19	0.43
1:B:1061:THR:N	1:B:1237:ASP:OD1	2.48	0.43
1:A:1062:LEU:HD12	1:A:1224:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ARG:O	1:B:817:ASP:HB2	2.18	0.43
1:A:962:GLN:O	1:A:963:GLN:HG2	2.19	0.42
1:A:992:PRO:O	1:A:994:TYR:N	2.51	0.42
1:A:1074:THR:O	1:A:1078:LEU:HG	2.18	0.42
1:B:611:LEU:HD23	1:B:618:TYR:CG	2.54	0.42
1:B:965:MET:HE3	1:B:970:VAL:CG1	2.49	0.42
1:A:471:GLN:HB3	1:A:552:GLU:HB2	2.00	0.42
1:B:1091:PHE:CE2	1:B:1096:GLU:HG2	2.54	0.42
1:A:211:THR:HG22	1:A:334:VAL:HG21	2.01	0.42
1:A:716:ILE:O	1:A:720:LEU:HB2	2.19	0.42
1:A:797:VAL:O	1:A:797:VAL:HG13	2.19	0.42
1:A:965:MET:HE3	1:A:970:VAL:HG13	2.01	0.42
1:A:1101:ASN:HB3	1:A:1104:TRP:HB3	2.01	0.42
1:B:111:ALA:HA	1:B:114:TYR:HE2	1.82	0.42
1:B:389:GLU:HB2	1:B:448:SER:HB3	2.01	0.42
1:B:900:PHE:O	1:B:903:VAL:HG12	2.19	0.42
1:B:946:TYR:O	1:B:950:ALA:N	2.48	0.42
1:B:1173:SER:OG	1:B:1174:GLY:N	2.52	0.42
1:A:285:ILE:HB	1:A:778:GLU:OE2	2.19	0.42
1:A:298:ALA:O	1:A:302:ILE:HG13	2.19	0.42
1:A:396:SER:HB2	1:A:404:GLN:HA	2.00	0.42
1:A:457:ILE:HD11	1:A:462:LEU:HD13	2.02	0.42
1:A:734:VAL:HG21	1:A:746:GLN:HG3	2.01	0.42
1:A:1181:ALA:HA	1:A:1184:ARG:NE	2.33	0.42
1:B:429:LYS:HB2	1:B:429:LYS:HE2	1.78	0.42
1:B:703:GLU:HB3	1:B:783:ARG:HD2	2.00	0.42
1:A:155:GLU:HB3	1:A:156:ILE:H	1.56	0.42
1:A:745:ARG:HD2	1:A:745:ARG:HA	1.83	0.42
1:A:1038:PHE:HD2	1:A:1049:LEU:HD23	1.84	0.42
1:B:500:VAL:O	1:B:505:ALA:N	2.46	0.42
1:B:961:THR:O	1:B:961:THR:HG22	2.20	0.42
1:B:1057:LYS:H	1:B:1060:GLN:NE2	2.16	0.42
1:A:107:MET:HE1	1:A:958:TYR:CB	2.42	0.42
1:A:278:GLU:OE2	1:A:782:LYS:NZ	2.43	0.42
1:A:911:LYS:O	1:A:915:MET:HG3	2.20	0.42
1:A:1043:ARG:HH12	1:A:1086:MET:CE	2.32	0.42
1:A:1173:SER:OG	1:A:1174:GLY:N	2.53	0.42
1:B:713:CYS:SG	1:B:768:LEU:HB3	2.60	0.42
1:B:725:SER:HB3	1:B:975:SER:OG	2.19	0.42
1:A:189:PHE:CZ	1:A:348:ILE:HD11	2.55	0.42
1:A:711:ILE:HD11	1:A:832:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ILE:HD13	1:B:516:PHE:CE1	2.54	0.42
1:B:972:LEU:O	1:B:975:SER:HB2	2.20	0.42
1:A:71:PHE:HE1	1:A:953:PHE:CZ	2.37	0.42
1:A:270:LEU:CG	1:A:790:LYS:HD2	2.41	0.42
1:A:531:GLN:O	1:A:535:ILE:HG13	2.20	0.42
1:A:896:ALA:HB2	1:A:916:TYR:HE2	1.84	0.42
1:B:132:TRP:CB	1:B:184:ASP:H	2.27	0.42
1:A:1091:PHE:HE2	1:A:1096:GLU:HG2	1.85	0.42
1:A:1191:HIS:CD2	1:A:1221:ARG:HE	2.38	0.42
1:B:163:ASP:OD2	1:B:167:LEU:HD13	2.20	0.42
1:B:1175:GLY:O	1:B:1179:ARG:HG3	2.20	0.42
1:B:1218:ARG:C	1:B:1220:GLY:H	2.27	0.42
1:A:777:GLY:CA	1:A:822:LYS:HG3	2.50	0.42
1:A:922:ILE:HB	1:A:923:PRO:HD3	2.01	0.42
1:A:1120:ASP:OD1	1:A:1120:ASP:N	2.53	0.42
1:B:688:VAL:HG21	1:B:1006:ARG:NH1	2.35	0.42
1:B:821:VAL:HG11	1:B:1004:ILE:HG21	2.02	0.42
1:A:110:TYR:O	1:A:114:TYR:HD2	2.03	0.41
1:A:121:VAL:HA	1:A:124:VAL:HG22	2.02	0.41
1:A:163:ASP:OD2	1:A:167:LEU:HD13	2.20	0.41
1:A:406:LEU:HD11	1:A:409:LEU:HG	2.02	0.41
1:A:853:LEU:HD21	1:A:973:VAL:HG22	2.01	0.41
1:B:198:GLY:O	1:B:202:ILE:HG13	2.20	0.41
1:B:797:VAL:O	1:B:797:VAL:HG13	2.20	0.41
1:A:821:VAL:HG11	1:A:1004:ILE:HG21	2.01	0.41
1:A:930:LYS:CD	1:A:934:PHE:CE2	3.00	0.41
1:B:273:TYR:CE2	1:B:277:LEU:HD11	2.54	0.41
1:B:684:LEU:HD22	1:B:809:ALA:HB2	2.02	0.41
1:B:903:VAL:HG23	1:B:909:GLU:OE2	2.20	0.41
1:B:911:LYS:O	1:B:915:MET:HG3	2.20	0.41
1:B:1011:THR:HG23	1:B:1011:THR:O	2.20	0.41
1:B:1063:ALA:HB3	1:B:1239:ILE:HG13	2.02	0.41
1:A:157:GLY:O	1:A:161:VAL:HG22	2.20	0.41
1:B:867:ALA:HA	1:B:870:VAL:HG12	2.02	0.41
1:B:1005:ILE:O	1:B:1008:ILE:HG22	2.21	0.41
1:A:132:TRP:CD1	1:A:184:ASP:H	2.38	0.41
1:A:132:TRP:CH2	1:A:179:ASN:OD1	2.72	0.41
1:A:1138:TYR:O	1:A:1141:ILE:HG12	2.20	0.41
1:A:1202:LEU:HB3	1:A:1207:GLU:HG2	2.01	0.41
1:B:132:TRP:CD1	1:B:184:ASP:H	2.39	0.41
1:B:515:GLN:O	1:B:518:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HA	1:A:217:ILE:HG12	2.03	0.41
1:A:969:ASN:N	1:A:972:LEU:HD13	2.25	0.41
1:A:1115:GLU:HA	1:A:1116:PRO:HD2	1.87	0.41
1:A:1234:GLN:HG2	1:A:1253:HIS:CD2	2.55	0.41
1:B:971:LEU:HD13	1:B:971:LEU:HA	1.92	0.41
1:B:1050:GLN:O	1:B:1246:LYS:HD2	2.21	0.41
1:A:1011:THR:HG23	1:A:1011:THR:O	2.20	0.41
1:A:1054:LEU:HD11	1:A:1240:VAL:HG11	2.02	0.41
1:B:320:LYS:HB3	1:B:322:TYR:CD1	2.55	0.41
1:B:468:VAL:HB	1:B:904:VAL:HG21	2.01	0.41
1:B:1074:THR:O	1:B:1078:LEU:HG	2.20	0.41
1:A:174:ASP:O	1:A:178:ILE:HG13	2.21	0.41
1:A:716:ILE:CD1	1:A:765:THR:HB	2.48	0.41
1:A:845:ILE:HD13	1:A:845:ILE:HA	1.95	0.41
1:A:1119:PHE:O	1:A:1126:ASN:ND2	2.44	0.41
1:B:716:ILE:O	1:B:720:LEU:HB2	2.21	0.41
1:A:1067:SER:OG	1:A:1068:SER:N	2.53	0.41
1:B:157:GLY:O	1:B:161:VAL:HG22	2.20	0.41
1:B:217:ILE:HD12	1:B:305:SER:HA	2.02	0.41
1:B:310:PHE:HD1	1:B:310:PHE:HA	1.69	0.41
1:B:528:SER:O	1:B:532:LYS:HG3	2.21	0.41
1:B:773:PHE:HA	1:B:776:ALA:HB3	2.01	0.41
1:B:846:SER:HA	1:B:849:TYR:CD2	2.55	0.41
1:B:1070:CYS:C	1:B:1072:LYS:H	2.28	0.41
1:B:1139:GLU:CD	1:B:1139:GLU:H	2.29	0.41
1:B:1181:ALA:HA	1:B:1184:ARG:NE	2.35	0.41
1:A:370:SER:OG	1:A:371:ILE:N	2.54	0.41
1:A:970:VAL:HG23	1:A:971:LEU:N	2.36	0.41
1:B:110:TYR:O	1:B:114:TYR:HD2	2.03	0.41
1:B:257:ILE:HG21	1:B:800:PHE:CD1	2.56	0.41
1:B:298:ALA:O	1:B:302:ILE:HG13	2.20	0.41
1:B:696:ILE:CG1	1:B:828:ARG:HH21	2.33	0.41
1:B:1061:THR:HA	1:B:1223:CYS:SG	2.61	0.41
1:B:1234:GLN:HG2	1:B:1253:HIS:NE2	2.36	0.41
1:A:416:GLY:H	1:A:577:THR:HG22	1.86	0.41
1:A:480:ILE:HG12	1:A:518:THR:HG23	2.02	0.41
1:A:857:LEU:HD13	1:A:976:ALA:HB3	2.02	0.41
1:A:1192:ILE:HA	1:A:1222:THR:O	2.21	0.41
1:A:1234:GLN:HG2	1:A:1253:HIS:NE2	2.35	0.41
1:A:1005:ILE:HA	1:A:1008:ILE:HG22	2.03	0.40
1:A:1017:TYR:CD1	1:A:1018:SER:N	2.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:ILE:HA	1:A:1194:LEU:HB2	2.02	0.40
1:B:969:ASN:CA	1:B:972:LEU:HB2	2.49	0.40
1:A:163:ASP:O	1:A:164:VAL:HG22	2.21	0.40
1:A:436:MET:HE3	1:A:466:ILE:HD11	2.04	0.40
1:A:793:LEU:HD12	1:A:793:LEU:HA	1.94	0.40
1:B:163:ASP:O	1:B:164:VAL:HG22	2.22	0.40
1:B:827:SER:O	1:B:831:VAL:HG23	2.21	0.40
1:A:397:TYR:O	1:A:399:SER:N	2.47	0.40
1:B:1081:ARG:HB2	1:B:1105:LEU:HD23	2.03	0.40
1:A:257:ILE:HG21	1:A:800:PHE:CD1	2.56	0.40
1:A:537:ILE:HD11	1:A:565:VAL:HG13	2.03	0.40
1:A:1019:THR:HG21	1:A:1101:ASN:CA	2.35	0.40
1:B:254:LEU:HB2	1:B:807:THR:HG23	2.03	0.40
1:B:902:THR:OG1	1:B:908:ARG:HB2	2.22	0.40
1:A:88:SER:OG	1:A:89:THR:N	2.55	0.40
1:A:275:ASN:O	1:A:278:GLU:HB3	2.21	0.40
1:A:351:PHE:O	1:A:355:ARG:HB2	2.20	0.40
1:A:827:SER:O	1:A:831:VAL:HG23	2.21	0.40
1:A:971:LEU:HD13	1:A:971:LEU:HA	1.88	0.40
1:B:217:ILE:HG21	1:B:308:LEU:HD22	2.04	0.40
1:B:327:VAL:HB	1:B:331:PHE:CE1	2.57	0.40
1:B:745:ARG:HA	1:B:745:ARG:HD2	1.84	0.40
1:B:1053:SER:O	1:B:1054:LEU:HD13	2.22	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	1178/1284 (92%)	1069 (91%)	109 (9%)	0	100	100
1	B	1178/1284 (92%)	1069 (91%)	109 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2356/2568 (92%)	2138 (91%)	218 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	975/1064 (92%)	955 (98%)	20 (2%)	47	64
1	B	975/1064 (92%)	956 (98%)	19 (2%)	50	66
All	All	1950/2128 (92%)	1911 (98%)	39 (2%)	48	65

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	58	ILE
1	A	64	LEU
1	A	156	ILE
1	A	409	LEU
1	A	509	ILE
1	A	593	VAL
1	A	601	VAL
1	A	696	ILE
1	A	743	THR
1	A	847	LEU
1	A	961	THR
1	A	1020	GLN
1	A	1056	VAL
1	A	1064	LEU
1	A	1065	VAL
1	A	1187	VAL
1	A	1225	VAL
1	A	1235	ASN
1	A	1247	VAL

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Mol	Chain	Res	Type
1	B	36	LEU
1	B	58	ILE
1	B	64	LEU
1	B	156	ILE
1	B	409	LEU
1	B	509	ILE
1	B	541	LEU
1	B	593	VAL
1	B	601	VAL
1	B	743	THR
1	B	847	LEU
1	B	1056	VAL
1	B	1064	LEU
1	B	1065	VAL
1	B	1187	VAL
1	B	1225	VAL
1	B	1235	ASN
1	B	1242	ILE
1	B	1247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	154	GLN
1	A	168	ASN
1	A	179	ASN
1	A	544	ASN
1	A	700	ASN
1	A	747	ASN
1	A	749	ASN
1	A	820	GLN
1	A	918	GLN
1	A	942	GLN
1	A	986	GLN
1	A	1077	GLN
1	A	1114	GLN
1	A	1253	HIS
1	B	83	ASN
1	B	128	GLN
1	B	154	GLN
1	B	168	ASN

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	700	ASN
1	B	747	ASN
1	B	749	ASN
1	B	918	GLN
1	B	942	GLN
1	B	986	GLN
1	B	1060	GLN
1	B	1114	GLN
1	B	1253	HIS

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	1182/1284 (92%)	0.59	105 (8%)	15 16	48, 98, 147, 186	0
1	B	1182/1284 (92%)	0.51	71 (6%)	27 22	50, 103, 148, 189	0
All	All	2364/2568 (92%)	0.55	176 (7%)	20 19	48, 100, 147, 189	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	GLY	8.1
1	A	312	TYR	6.8
1	A	749	ASN	6.4
1	A	1123	ILE	6.0
1	A	1083	TYR	5.7
1	A	309	ALA	5.5
1	B	600	GLY	5.4
1	B	908	ARG	5.3
1	B	168	ASN	5.2
1	A	908	ARG	5.1
1	A	158	TRP	5.0
1	A	1127	ILE	4.9
1	A	623	MET	4.6
1	B	386	GLY	4.5
1	B	1221	ARG	4.3
1	B	970	VAL	4.3
1	A	1128	ALA	4.3
1	A	969	ASN	4.2
1	A	460	ARG	4.2
1	B	1129	TYR	4.1
1	B	1119	PHE	4.0
1	B	134	LEU	4.0
1	A	313	GLY	3.9
1	A	1107	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1124	ALA	3.8
1	A	934	PHE	3.8
1	B	802	ASP	3.8
1	B	926	ASN	3.8
1	A	1132	ASN	3.7
1	A	704	TRP	3.6
1	A	155	GLU	3.6
1	B	916	TYR	3.6
1	B	155	GLU	3.6
1	A	842	GLY	3.5
1	B	33	VAL	3.4
1	A	128	GLN	3.4
1	A	1129	TYR	3.4
1	B	359	TYR	3.3
1	B	934	PHE	3.3
1	A	1168	LYS	3.3
1	A	359	TYR	3.3
1	A	825	THR	3.3
1	B	875	LEU	3.3
1	A	751	PHE	3.2
1	A	838	ASN	3.2
1	B	1226	ILE	3.1
1	A	744	GLN	3.1
1	A	400	ARG	3.1
1	B	901	ARG	3.1
1	A	1084	ASP	3.1
1	B	829	LEU	3.1
1	A	1013	GLU	3.0
1	A	829	LEU	3.0
1	A	325	GLY	3.0
1	B	1110	GLY	3.0
1	B	280	ALA	3.0
1	A	837	ALA	3.0
1	A	966	THR	3.0
1	B	1132	ASN	2.9
1	A	278	GLU	2.9
1	A	979	PHE	2.9
1	B	598	ASP	2.9
1	A	849	TYR	2.9
1	A	168	ASN	2.9
1	A	356	GLY	2.9
1	B	933	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	2.9
1	B	796	ASP	2.8
1	A	851	TRP	2.8
1	A	145	GLN	2.8
1	A	735	PHE	2.7
1	B	1196	ASP	2.7
1	A	850	GLY	2.7
1	B	34	SER	2.7
1	A	904	VAL	2.6
1	A	600	GLY	2.6
1	A	1130	GLY	2.6
1	A	134	LEU	2.6
1	A	875	LEU	2.6
1	B	1220	GLY	2.6
1	B	517	ASP	2.6
1	A	306	TYR	2.6
1	A	1131	ASP	2.6
1	B	1131	ASP	2.6
1	A	131	PHE	2.6
1	A	33	VAL	2.6
1	B	171	LEU	2.6
1	B	839	LEU	2.5
1	A	913	GLU	2.5
1	A	773	PHE	2.5
1	A	708	VAL	2.5
1	A	148	PHE	2.5
1	B	817	ASP	2.5
1	A	1044	PRO	2.5
1	A	847	LEU	2.5
1	B	704	TRP	2.5
1	A	328	LEU	2.5
1	B	158	TRP	2.4
1	A	350	ALA	2.4
1	B	920	LEU	2.4
1	A	108	THR	2.4
1	A	1017	TYR	2.4
1	B	994	TYR	2.4
1	A	205	THR	2.4
1	B	319	SER	2.4
1	B	876	SER	2.4
1	B	1118	LEU	2.4
1	B	942	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	965	MET	2.4
1	A	159	PHE	2.4
1	B	874	MET	2.4
1	A	327	VAL	2.4
1	A	574	GLU	2.4
1	A	972	LEU	2.4
1	B	602	ILE	2.4
1	A	968	GLU	2.4
1	A	363	LYS	2.4
1	A	781	THR	2.3
1	B	1014	ILE	2.3
1	B	368	LYS	2.3
1	B	39	PHE	2.3
1	B	747	ASN	2.3
1	A	210	LEU	2.3
1	A	110	TYR	2.3
1	A	1165	VAL	2.3
1	B	773	PHE	2.3
1	B	312	TYR	2.3
1	B	969	ASN	2.2
1	B	691	ALA	2.2
1	B	852	GLN	2.2
1	A	701	SER	2.2
1	B	836	ILE	2.2
1	A	114	TYR	2.2
1	A	886	LEU	2.2
1	B	900	PHE	2.2
1	A	970	VAL	2.2
1	A	157	GLY	2.2
1	A	1122	SER	2.2
1	A	949	TYR	2.2
1	B	131	PHE	2.2
1	B	838	ASN	2.2
1	A	277	LEU	2.2
1	B	837	ALA	2.1
1	B	159	PHE	2.1
1	A	778	GLU	2.1
1	A	702	THR	2.1
1	A	963	GLN	2.1
1	A	1108	GLN	2.1
1	A	1014	ILE	2.1
1	B	491	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	930	LYS	2.1
1	B	878	GLN	2.1
1	B	1020	GLN	2.1
1	A	739	GLY	2.1
1	B	1055	GLU	2.1
1	B	834	GLN	2.1
1	A	805	ASN	2.1
1	B	327	VAL	2.1
1	A	1245	GLY	2.1
1	B	966	THR	2.1
1	A	964	LEU	2.1
1	A	49	TYR	2.0
1	B	110	TYR	2.0
1	B	112	TYR	2.0
1	A	586	SER	2.0
1	A	734	VAL	2.0
1	A	1136	VAL	2.0
1	B	1165	VAL	2.0
1	A	353	ASN	2.0
1	A	1012	PRO	2.0
1	A	1180	ILE	2.0
1	A	319	SER	2.0
1	A	800	PHE	2.0
1	A	827	SER	2.0
1	A	820	GLN	2.0
1	B	330	VAL	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	HG	B	1302	1/1	-0.17	0.38	109,109,109,109	1
2	HG	A	1302	1/1	0.81	0.22	166,166,166,166	1
2	HG	A	1306	1/1	0.84	0.08	146,146,146,146	0
2	HG	A	1304	1/1	0.85	0.15	146,146,146,146	0
2	HG	B	1301	1/1	0.88	0.07	146,146,146,146	0
2	HG	A	1303	1/1	0.91	0.08	146,146,146,146	0
2	HG	B	1306	1/1	0.91	0.05	146,146,146,146	0
2	HG	B	1303	1/1	0.92	0.06	146,146,146,146	0
2	HG	A	1301	1/1	0.92	0.06	146,146,146,146	0
2	HG	B	1304	1/1	0.94	0.18	146,146,146,146	0
2	HG	A	1305	1/1	0.96	0.03	146,146,146,146	0
2	HG	B	1305	1/1	0.99	0.04	146,146,146,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.