



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:39 PM UTC

PDB ID : 9DJT / pdb_00009djt
Title : Ternary complex structure of Cereblon-DDB1 bound to WIZ(ZF7) and the molecular glue WIZ-5
Authors : Partridge, J.R.; Ma, X.; Ornelas, E.
Deposited on : 2024-09-06
Resolution : 2.95 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:

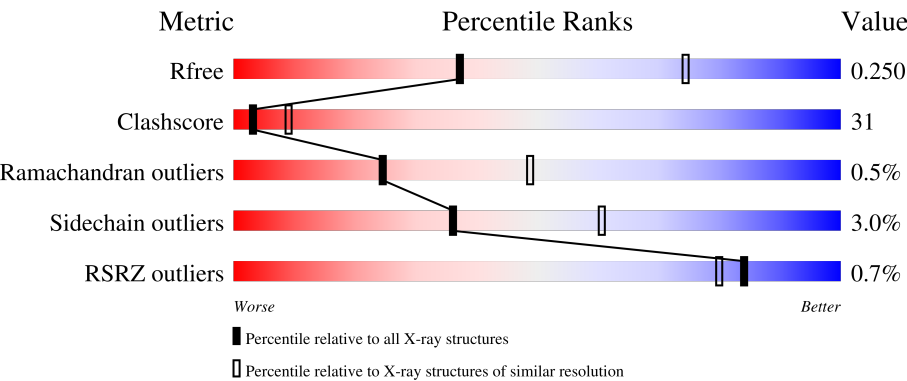
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	373	% 50%38%9%
1	D	373	% 57%35%7%
2	B	836	51%42%
2	E	836	% 52%42%5%
3	C	30	3% 57%17%13%

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Mol	Chain	Length	Quality of chain
3	F	30	 53% 37% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17742 atoms, of which 54 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 Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2651	1700	446	482	23			
1	D	347	Total	C	N	O	S	0	0	0
			2617	1682	436	477	22			

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	801	Total	C	N	O	S	0	0	0
			6058	3852	1007	1165	34			
2	E	795	Total	C	N	O	S	0	0	0
			5881	3747	966	1135	33			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	700	GLY	-	linker	UNP Q16531
B	701	ASN	-	linker	UNP Q16531
B	702	GLY	-	linker	UNP Q16531
B	703	ASN	-	linker	UNP Q16531
B	704	SER	-	linker	UNP Q16531
B	705	GLY	-	linker	UNP Q16531
E	700	GLY	-	linker	UNP Q16531
E	701	ASN	-	linker	UNP Q16531
E	702	GLY	-	linker	UNP Q16531
E	703	ASN	-	linker	UNP Q16531
E	704	SER	-	linker	UNP Q16531
E	705	GLY	-	linker	UNP Q16531

- Molecule 3 is a protein called Protein Wiz.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	S	0	0	0
			176	107	31	35	3			
3	F	27	Total	C	N	O	S	0	0	0
			191	115	35	38	3			

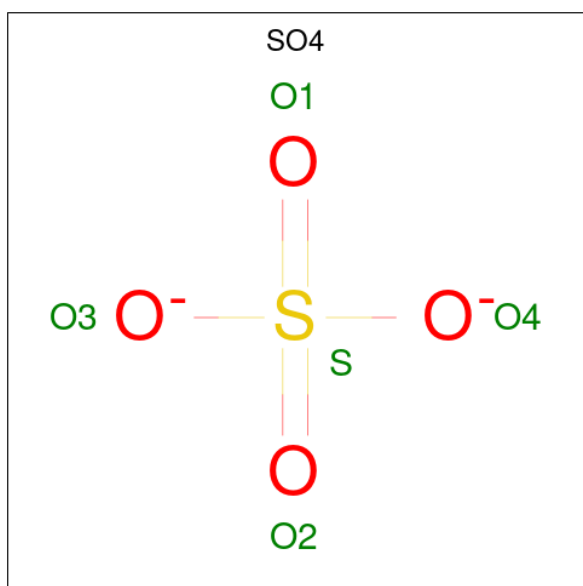
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	866	SER	-	expression tag	UNP O95785
F	866	SER	-	expression tag	UNP O95785

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

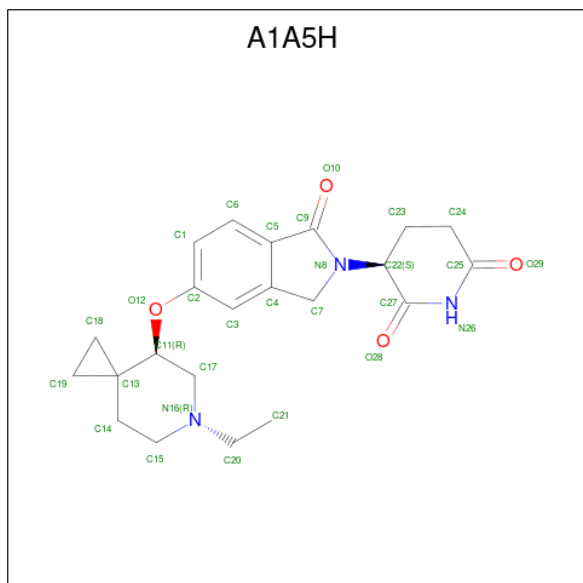
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is (3S)-3-(5-{[(4R)-6-ethyl-6-azaspiro[2.5]octan-4-yl]oxy}-1-oxo-1,3-dihydro-2H-isoindol-2-yl)piperidine-2,6-dione (CCD ID: A1A5H) (formula: C₂₂H₂₇N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O 56 22 27 3 4	27	0
6	D	1	Total C H N O 56 22 27 3 4	27	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total O 6 6	0	0
7	B	16	Total O 16 16	0	0
7	C	1	Total O 1 1	0	0
7	D	7	Total O 7 7	0	0
7	E	11	Total O 11 11	0	0

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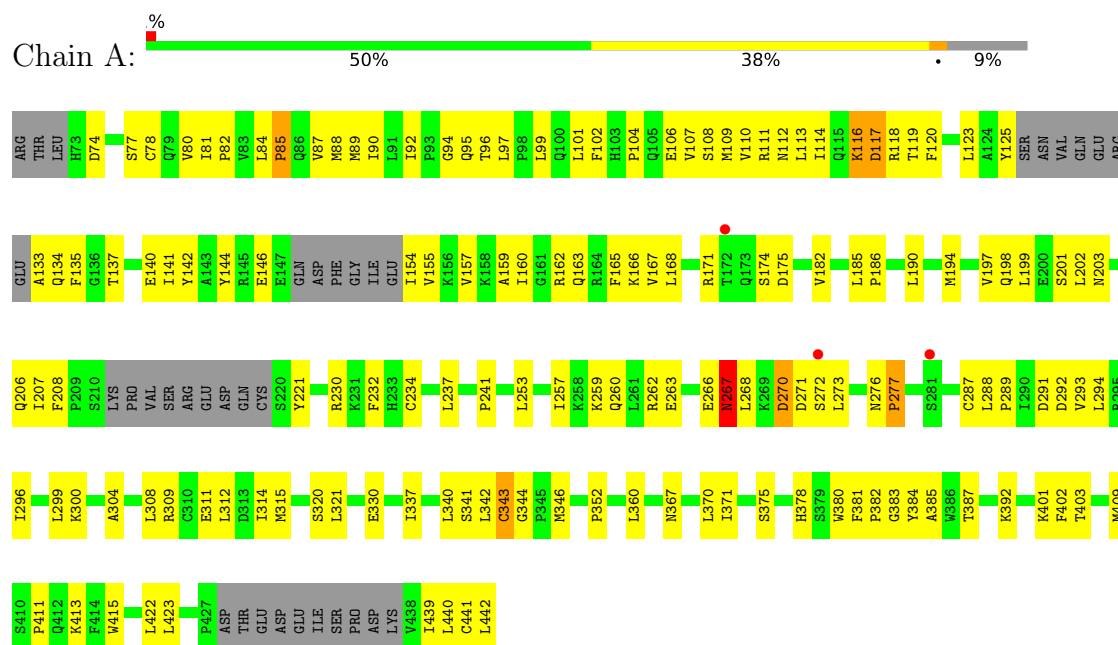
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	O	0	0
			1	1		

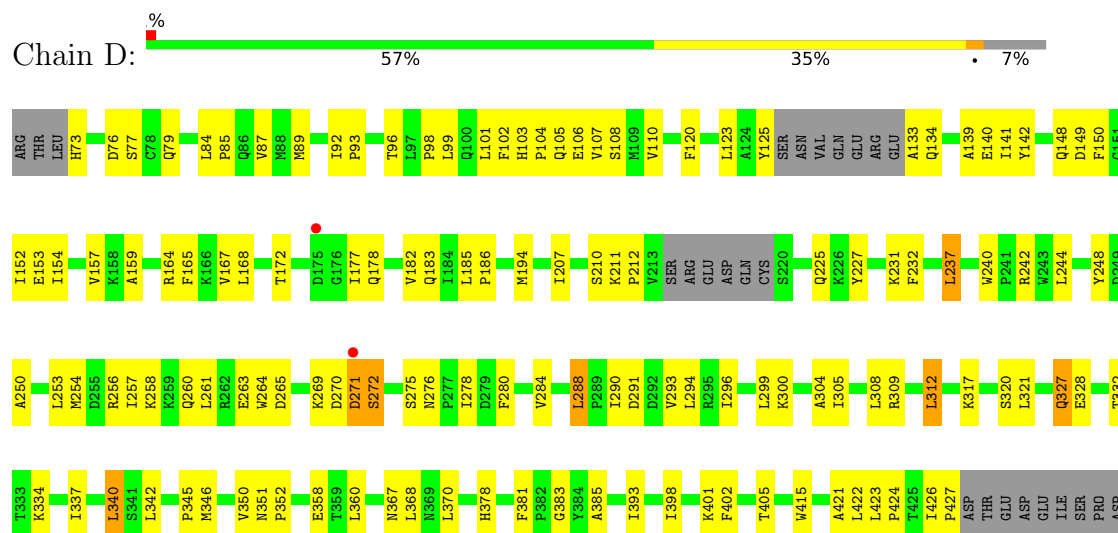
3 Residue-property plots

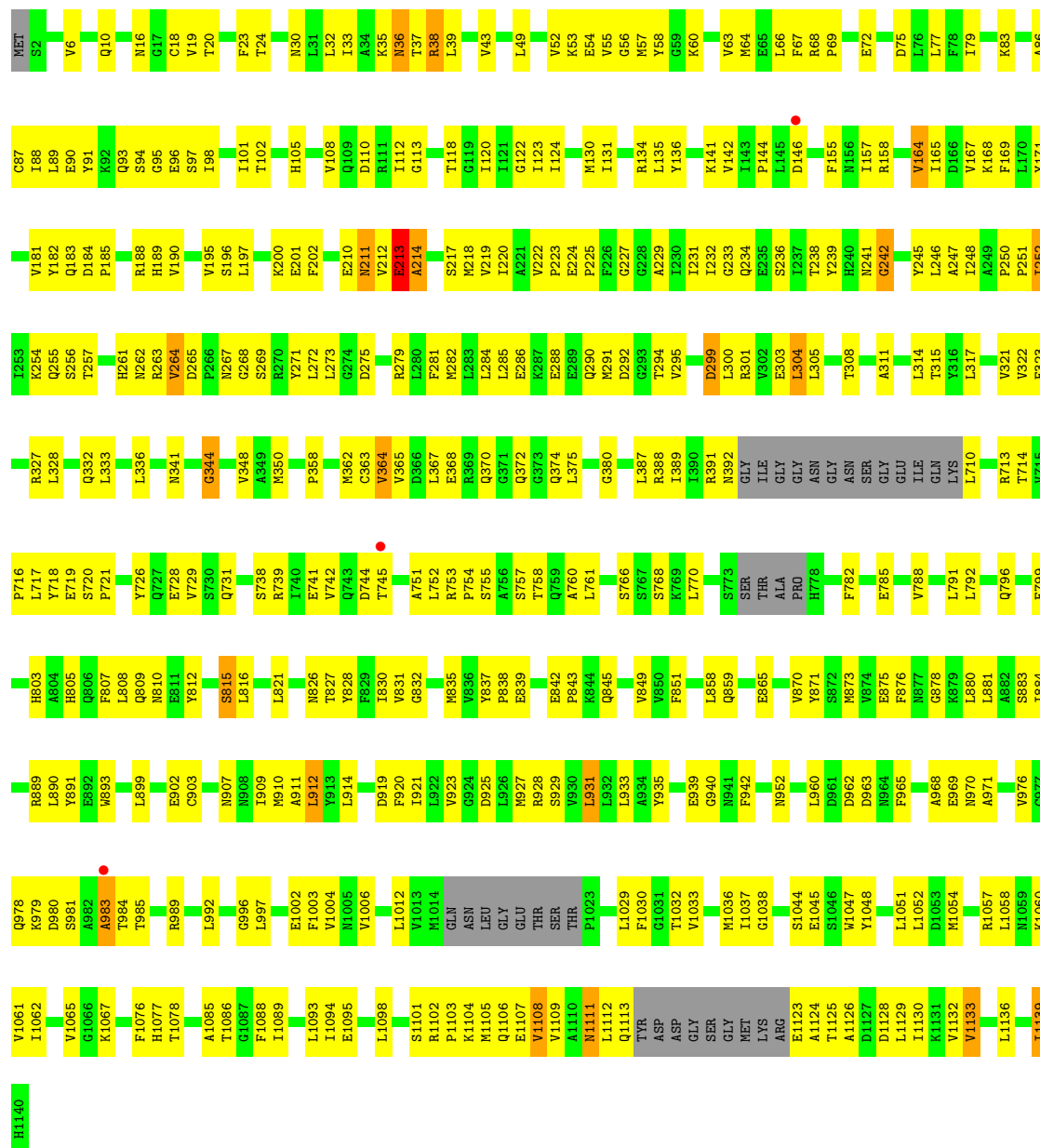
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Protein cereblon





- Molecule 2: DNA damage-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.71Å 145.60Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.95 29.96 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.96-2.95) 98.9 (29.96-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.205 , 0.260 (Not available) , 0.250	Depositor DCC
R_{free} test set	3187 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17742	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.74% 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: SO4, ZN, A1A5H

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	0.48	0/2713	0.75	6/3693 (0.2%)
1	D	0.49	0/2679	0.74	6/3662 (0.2%)
2	B	0.43	0/6169	0.72	13/8392 (0.2%)
2	E	0.44	0/5989	0.72	10/8171 (0.1%)
3	C	0.44	0/178	0.99	4/240 (1.7%)
3	F	0.47	0/193	0.83	1/259 (0.4%)
All	All	0.45	0/17921	0.73	40/24417 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	ILE	N-CA-C	9.18	119.99	111.45
1	A	186	PRO	CB-CA-C	-8.37	97.76	111.56
2	B	1111	ASN	N-CA-C	8.32	123.45	111.56
2	B	36	ASN	N-CA-C	-8.19	95.86	108.31
2	E	70	LYS	N-CA-C	-7.56	98.83	110.10
1	A	117	ASP	N-CA-C	-7.44	104.72	114.31
2	E	37	THR	N-CA-C	7.28	121.80	112.34
2	B	981	SER	N-CA-C	-6.84	103.88	111.82
2	B	213	GLU	CB-CA-C	-6.74	99.74	109.84
3	F	893	LEU	N-CA-C	6.64	118.40	111.03
2	B	37	THR	N-CA-C	6.64	120.97	112.34
2	B	264	VAL	N-CA-C	6.51	117.13	110.82
2	B	980	ASP	N-CA-C	-6.48	99.82	109.15
2	B	214	ALA	N-CA-C	6.48	120.04	111.75
1	A	266	GLU	N-CA-C	-6.21	97.57	110.80
2	E	855	ASP	N-CA-CB	-6.12	101.84	111.39
3	C	892	HIS	N-CA-C	6.05	119.14	111.69
1	A	116	LYS	N-CA-C	6.05	123.69	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	PHE	N-CA-C	-6.04	99.12	108.31
2	E	70	LYS	CB-CA-C	6.01	119.28	109.90
3	C	870	THR	N-CA-C	5.99	119.55	112.72
2	E	746	SER	N-CA-C	-5.70	106.54	112.93
2	E	36	ASN	N-CA-C	-5.67	99.69	108.31
2	B	217	SER	CB-CA-C	5.64	116.79	109.28
1	D	327	GLN	CB-CA-C	-5.57	102.63	111.48
2	B	264	VAL	CB-CA-C	-5.56	104.75	112.04
2	B	38	ARG	N-CA-CB	-5.48	101.86	110.69
2	B	983	ALA	N-CA-C	-5.46	99.89	108.63
1	D	269	LYS	N-CA-C	-5.42	106.80	113.41
1	D	328	GLU	N-CA-CB	5.42	120.16	110.79
2	B	782	PHE	N-CA-C	-5.35	101.06	109.25
2	E	174	GLN	N-CA-C	5.32	117.49	111.11
1	A	117	ASP	N-CA-CB	5.27	117.91	110.90
1	D	393	ILE	N-CA-CB	-5.24	101.93	110.31
2	E	62	ALA	N-CA-C	-5.22	107.46	113.88
1	A	270	ASP	CB-CA-C	-5.17	109.63	117.07
3	C	870	THR	N-CA-CB	-5.16	103.01	110.70
2	E	984	THR	CB-CA-C	-5.14	102.21	110.74
2	E	886	SER	N-CA-C	5.13	119.41	113.20
3	C	869	LEU	CB-CA-C	5.12	120.11	110.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2651	0	2587	169	0
1	D	2617	0	2488	123	0
2	B	6058	0	5814	399	0
2	E	5881	0	5540	395	0
3	C	176	0	159	9	0
3	F	191	0	176	7	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	D	5	0	0	1	0
6	A	29	27	0	0	0
6	D	29	27	0	0	0
7	A	6	0	0	0	0
7	B	16	0	0	0	0
7	C	1	0	0	1	0
7	D	7	0	0	1	0
7	E	11	0	0	0	0
7	F	1	0	0	0	0
All	All	17688	54	16764	1066	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 31.

All (1066) 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)
2:E:130:MET:CE	2:E:142:VAL:HG13	1.46	1.44
1:A:207:ILE:HG23	2:B:188:ARG:NH2	1.61	1.16
1:A:401:LYS:HE2	1:A:413:LYS:HD3	1.17	1.16
1:A:194:MET:O	1:A:198:GLN:HG3	1.44	1.14
2:B:1098:LEU:HD11	2:B:1133:VAL:HG11	1.25	1.13
2:E:130:MET:HE3	2:E:142:VAL:CG1	1.76	1.13
2:E:910:MET:HE2	2:E:912:LEU:HD11	1.31	1.13
2:E:157:ILE:HG13	2:E:202:PHE:CE2	1.86	1.10
1:A:340:LEU:HD23	1:A:381:PHE:HD1	1.15	1.09
1:D:125:TYR:CD1	1:D:133:ALA:N	2.21	1.08
2:E:1058:LEU:HD21	2:E:1097:PHE:HB2	1.28	1.08
1:A:101:LEU:HD12	1:A:106:GLU:HB3	1.34	1.07
1:A:207:ILE:HG23	2:B:188:ARG:HH22	0.94	1.07
2:E:130:MET:CE	2:E:142:VAL:CG1	2.29	1.07
1:A:207:ILE:HG21	2:B:165:ILE:HD12	1.36	1.05
2:B:102:THR:HG21	2:B:1067:LYS:HG3	1.05	1.05
1:A:260:GLN:O	1:A:263:GLU:HG2	1.57	1.04
2:B:768:SER:OG	2:B:808:LEU:HD21	1.56	1.03
2:B:928:ARG:HD2	2:B:969:GLU:OE1	1.60	1.01
3:F:881:THR:HG23	3:F:884:GLY:H	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:MET:HE1	2:B:195:VAL:HG11	1.44	1.00
1:A:340:LEU:HD23	1:A:381:PHE:CD1	1.95	1.00
1:A:165:PHE:HB2	1:A:182:VAL:HG13	1.41	1.00
2:B:392:ASN:HA	2:B:710:LEU:HG	1.42	0.99
2:B:102:THR:HG21	2:B:1067:LYS:CG	1.91	0.99
2:B:1098:LEU:HD11	2:B:1133:VAL:CG1	1.92	0.98
2:E:996:GLY:O	2:E:997:LEU:HD23	1.63	0.98
2:E:157:ILE:HG13	2:E:202:PHE:CZ	2.00	0.97
1:A:383:GLY:HA3	1:A:409:MET:HE1	1.46	0.96
1:D:305:ILE:HG21	2:E:927:MET:HE1	1.44	0.96
2:B:1098:LEU:CD1	2:B:1133:VAL:HG11	1.96	0.96
2:E:23:PHE:H	2:E:30:ASN:HD22	1.10	0.95
1:A:401:LYS:HE2	1:A:413:LYS:CD	1.95	0.95
2:B:102:THR:CG2	2:B:1067:LYS:HG3	1.96	0.95
2:E:43:VAL:HG23	2:E:52:VAL:HG21	1.45	0.95
1:D:165:PHE:HB2	1:D:182:VAL:HG13	1.49	0.94
1:D:168:LEU:HD21	1:D:183:GLN:HB2	1.46	0.94
2:B:19:VAL:HG22	2:B:64:MET:HE3	1.48	0.93
2:E:1051:LEU:HD12	2:E:1094:ILE:HD12	1.51	0.92
2:E:1083:GLU:HG3	2:E:1084:PRO:HD2	1.49	0.92
2:E:157:ILE:CG1	2:E:202:PHE:CE2	2.53	0.92
2:E:215:GLU:HB3	2:E:234:GLN:HG3	1.50	0.91
2:E:238:THR:HG22	2:E:247:ALA:CB	2.00	0.91
3:C:870:THR:HA	3:C:885:LEU:HD12	1.52	0.91
2:E:102:THR:HG21	2:E:1066:GLY:H	1.34	0.91
1:A:135:PHE:CE2	1:A:300:LYS:HD3	2.05	0.91
2:B:741:GLU:HG2	2:B:751:ALA:HA	1.52	0.90
2:E:157:ILE:HD12	2:E:202:PHE:CD2	2.08	0.89
1:A:401:LYS:CE	1:A:413:LYS:HD3	2.01	0.89
2:B:168:LYS:HG3	2:B:219:VAL:HG23	1.55	0.89
2:B:1057:ARG:HH22	2:B:1112:LEU:HB2	1.37	0.89
2:B:928:ARG:HH11	2:B:928:ARG:HG2	1.37	0.88
2:E:1055:GLN:HE21	2:E:1089:ILE:HG23	1.38	0.88
3:C:871:THR:HG22	3:C:878:CYS:SG	2.12	0.88
2:E:24:THR:H	2:E:30:ASN:HD21	1.21	0.88
2:B:252:ILE:HD12	2:B:252:ILE:H	1.38	0.87
2:E:69:PRO:HD2	2:E:72:GLU:HG3	1.55	0.87
2:B:815:SER:HB2	2:B:873:MET:HE2	1.55	0.86
1:A:207:ILE:HG21	2:B:188:ARG:HH12	1.38	0.86
1:A:340:LEU:CD2	1:A:381:PHE:CD1	2.59	0.86
2:E:24:THR:HA	2:E:91:TYR:HD2	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD13	1:A:314:ILE:HD13	1.58	0.86
2:B:181:VAL:HG22	2:B:190:VAL:HG22	1.58	0.86
2:B:1105:MET:HE2	2:B:1130:ILE:HD11	1.58	0.85
2:E:318:ASP:O	2:E:321:VAL:HG22	1.76	0.85
2:B:729:VAL:HG21	2:B:827:THR:HG21	1.56	0.85
2:E:130:MET:HE1	2:E:142:VAL:HG22	1.59	0.84
2:E:1134:GLU:O	2:E:1137:THR:HG22	1.77	0.84
1:A:101:LEU:CD1	1:A:106:GLU:HB3	2.07	0.84
1:A:207:ILE:CG2	2:B:188:ARG:HH22	1.86	0.84
2:B:374:GLN:HG2	2:B:391:ARG:HB3	1.58	0.84
1:A:84:LEU:HD23	1:A:120:PHE:CD2	2.13	0.83
1:D:101:LEU:CD2	1:D:110:VAL:HG21	2.09	0.82
2:E:130:MET:SD	2:E:195:VAL:HG11	2.18	0.82
2:E:740:ILE:O	2:E:752:LEU:HD23	1.78	0.82
2:E:340:SER:HB3	2:E:346:TYR:HE1	1.43	0.82
2:E:130:MET:HE1	2:E:142:VAL:CG2	2.09	0.82
2:E:43:VAL:HG23	2:E:52:VAL:CG2	2.10	0.82
2:E:102:THR:CG2	2:E:1066:GLY:H	1.92	0.81
1:D:225:GLN:OE1	2:E:838:PRO:HB3	1.80	0.81
2:B:1109:VAL:HG12	2:B:1129:LEU:HD12	1.63	0.81
2:E:376:VAL:HG22	2:E:389:ILE:HG13	1.61	0.80
2:E:24:THR:HA	2:E:91:TYR:CD2	2.15	0.80
2:B:53:LYS:HD2	2:B:98:ILE:HG22	1.64	0.80
2:B:251:PRO:O	2:B:254:LYS:HG2	1.83	0.79
1:A:135:PHE:HE2	1:A:300:LYS:HD3	1.45	0.79
2:B:231:ILE:HB	2:B:238:THR:HG23	1.66	0.78
1:A:199:LEU:HB2	1:A:202:LEU:HD23	1.65	0.78
2:E:826:ASN:ND2	2:E:852:GLN:HE22	1.82	0.78
2:B:891:TYR:HB3	2:B:899:LEU:HD22	1.65	0.78
1:D:104:PRO:HA	1:D:107:VAL:CG1	2.14	0.78
2:B:130:MET:HE3	2:B:142:VAL:HG13	1.65	0.78
1:D:327:GLN:O	1:D:327:GLN:HG2	1.83	0.78
2:E:130:MET:HE3	2:E:142:VAL:HG13	0.80	0.78
2:E:232:ILE:HG12	2:E:237:ILE:HG12	1.66	0.77
2:B:1105:MET:CE	2:B:1130:ILE:HD11	2.13	0.77
2:E:1050:LEU:HD23	2:E:1054:MET:HG2	1.66	0.77
2:E:133:LEU:HD22	2:E:143:ILE:HD11	1.66	0.77
2:B:168:LYS:HG3	2:B:219:VAL:CG2	2.15	0.76
2:B:67:PHE:HZ	2:B:88:ILE:HD13	1.49	0.76
1:D:84:LEU:O	1:D:87:VAL:HG13	1.83	0.76
2:B:890:LEU:HD12	2:B:891:TYR:H	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:889:ARG:HH21	2:E:904:ASN:HD21	1.31	0.76
2:B:392:ASN:OD1	2:B:710:LEU:HD11	1.86	0.76
2:E:238:THR:HG22	2:E:247:ALA:HB1	1.67	0.76
2:E:130:MET:HE1	2:E:142:VAL:CG1	2.16	0.76
2:B:1057:ARG:NH2	2:B:1112:LEU:HB2	2.00	0.76
1:D:125:TYR:HD1	1:D:133:ALA:N	1.79	0.75
2:B:839:GLU:OE1	2:B:839:GLU:N	2.17	0.75
1:D:305:ILE:HG21	2:E:927:MET:CE	2.16	0.75
2:E:89:LEU:CD2	2:E:102:THR:HG22	2.16	0.75
1:A:259:LYS:HZ3	1:A:262:ARG:HH21	1.34	0.75
2:B:188:ARG:HD2	2:B:214:ALA:O	1.86	0.75
2:E:1054:MET:O	2:E:1058:LEU:HD12	1.86	0.75
2:E:90:GLU:CB	2:E:101:ILE:HD11	2.17	0.75
1:D:317:LYS:O	1:D:426:ILE:HG12	1.86	0.74
2:E:157:ILE:CD1	2:E:202:PHE:CE2	2.69	0.74
2:B:859:GLN:OE1	2:B:859:GLN:HA	1.85	0.74
2:B:24:THR:HA	2:B:91:TYR:CD2	2.23	0.74
1:A:95:GLN:O	1:A:160:ILE:HD12	1.88	0.74
2:E:23:PHE:H	2:E:30:ASN:ND2	1.85	0.74
2:B:891:TYR:HB3	2:B:899:LEU:CD2	2.17	0.74
2:E:1098:LEU:HD11	2:E:1134:GLU:HG3	1.69	0.74
3:C:871:THR:HA	3:C:877:ALA:O	1.88	0.73
1:D:92:ILE:HG23	1:D:299:LEU:HD11	1.70	0.73
1:A:199:LEU:CB	1:A:202:LEU:HD23	2.17	0.73
2:B:282:MET:HB3	2:B:305:LEU:HD11	1.70	0.73
2:E:1058:LEU:CD2	2:E:1097:PHE:HB2	2.14	0.73
2:B:842:GLU:HG3	2:B:843:PRO:HD2	1.71	0.73
2:B:996:GLY:O	2:B:997:LEU:HD23	1.88	0.73
2:B:158:ARG:HB2	2:B:158:ARG:CZ	2.18	0.72
2:B:53:LYS:HD2	2:B:98:ILE:CG2	2.18	0.72
2:B:252:ILE:HD12	2:B:252:ILE:N	2.03	0.72
2:E:248:ILE:HG12	2:E:250:PRO:HD3	1.69	0.72
1:D:248:TYR:HD2	2:E:927:MET:HE3	1.52	0.72
2:E:1050:LEU:O	2:E:1054:MET:HG2	1.89	0.72
2:B:252:ILE:H	2:B:252:ILE:CD1	2.03	0.72
2:E:927:MET:HE2	2:E:953:TRP:HZ3	1.53	0.72
2:B:1058:LEU:HB3	2:B:1062:ILE:CD1	2.20	0.71
2:E:741:GLU:HG2	2:E:751:ALA:HA	1.71	0.71
2:E:189:HIS:ND1	2:E:210:GLU:O	2.22	0.71
2:B:1098:LEU:HD21	2:B:1133:VAL:HG12	1.70	0.71
2:B:1054:MET:O	2:B:1058:LEU:HG	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1109:VAL:HG12	2:B:1129:LEU:CD1	2.20	0.71
2:E:364:VAL:HG22	2:E:375:LEU:HD13	1.71	0.71
2:B:983:ALA:HA	2:B:989:ARG:HG2	1.71	0.71
2:E:927:MET:HE2	2:E:953:TRP:CZ3	2.26	0.71
1:A:84:LEU:HD11	1:A:101:LEU:HD11	1.72	0.71
2:B:807:PHE:CZ	2:B:831:VAL:HG11	2.25	0.71
2:B:881:LEU:CD2	2:B:921:ILE:HD13	2.21	0.71
2:E:996:GLY:C	2:E:997:LEU:HD23	2.16	0.71
2:B:815:SER:HB2	2:B:873:MET:CE	2.21	0.70
2:B:821:LEU:HD11	2:B:880:LEU:HB2	1.73	0.70
2:B:1012:LEU:HD13	2:B:1029:LEU:HD11	1.72	0.70
2:E:102:THR:HG21	2:E:1066:GLY:N	2.07	0.70
2:E:13:THR:OG1	2:E:355:ASN:HA	1.90	0.70
1:A:165:PHE:CB	1:A:182:VAL:HG13	2.19	0.70
2:E:238:THR:HG22	2:E:247:ALA:HB2	1.74	0.70
1:D:250:ALA:O	1:D:254:MET:HG3	1.91	0.69
1:A:194:MET:O	1:A:198:GLN:CG	2.34	0.69
2:E:199:GLU:O	2:E:201:GLU:HG2	1.92	0.69
1:D:291:ASP:OD2	1:D:293:VAL:HG22	1.93	0.69
2:E:1055:GLN:HE22	2:E:1089:ILE:HA	1.57	0.69
3:F:881:THR:HG23	3:F:884:GLY:N	2.05	0.69
1:A:125:TYR:N	1:A:133:ALA:HB3	2.06	0.69
2:B:890:LEU:HD12	2:B:891:TYR:N	2.08	0.69
2:E:6:VAL:HG12	2:E:1040:VAL:HG22	1.74	0.69
2:E:24:THR:H	2:E:30:ASN:ND2	1.91	0.69
2:B:821:LEU:HD22	2:B:878:GLY:O	1.92	0.69
2:E:943:GLU:HA	2:E:943:GLU:OE1	1.91	0.68
1:A:241:PRO:HB3	2:B:812:TYR:CZ	2.28	0.68
3:C:870:THR:HA	3:C:885:LEU:CD1	2.22	0.68
1:D:141:ILE:HG23	1:D:157:VAL:CG2	2.24	0.68
2:E:744:ASP:OD2	2:E:750:THR:HG23	1.94	0.68
2:B:184:ASP:HB2	2:B:185:PRO:HD2	1.75	0.68
2:B:1101:SER:O	2:B:1105:MET:HG3	1.93	0.68
1:A:346:MET:O	1:A:346:MET:HG2	1.92	0.68
2:E:1132:VAL:O	2:E:1136:LEU:HD12	1.94	0.68
2:B:246:LEU:HD21	2:B:299:ASP:HA	1.75	0.68
2:E:69:PRO:HD2	2:E:72:GLU:CG	2.23	0.68
1:A:207:ILE:HG21	2:B:165:ILE:CD1	2.20	0.68
1:A:259:LYS:NZ	1:A:262:ARG:HH21	1.92	0.68
1:A:146:GLU:HG2	1:A:155:VAL:HG22	1.74	0.68
1:D:194:MET:HA	1:D:194:MET:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:LEU:HG	2:B:79:ILE:CD1	2.24	0.68
2:B:388:ARG:CD	2:B:714:THR:HG22	2.24	0.68
2:B:1109:VAL:CG1	2:B:1129:LEU:HD12	2.24	0.68
1:D:256:ARG:NH1	5:D:502:SO4:O3	2.27	0.68
2:B:69:PRO:HD2	2:B:72:GLU:HG3	1.76	0.68
2:B:717:LEU:HD12	2:B:721:PRO:HG3	1.76	0.67
2:B:43:VAL:HG23	2:B:52:VAL:HG21	1.75	0.67
2:B:729:VAL:HG21	2:B:827:THR:CG2	2.23	0.67
1:D:194:MET:HG3	1:D:231:LYS:O	1.94	0.67
2:B:388:ARG:HD2	2:B:714:THR:HG22	1.76	0.67
1:D:442:LEU:HD23	2:E:908:ASN:O	1.94	0.67
2:E:32:LEU:CD2	2:E:41:ILE:HG12	2.24	0.67
2:E:803:HIS:CD2	2:E:858:LEU:HG	2.30	0.67
1:A:207:ILE:CG2	2:B:188:ARG:HH12	2.06	0.67
2:E:98:ILE:O	2:E:98:ILE:HD12	1.93	0.67
2:B:171:TYR:CD2	2:B:223:PRO:HA	2.30	0.67
1:A:82:PRO:HG3	1:A:113:LEU:HD21	1.75	0.67
2:E:105:HIS:C	2:E:152:LEU:HD12	2.20	0.67
2:E:760:ALA:HA	2:E:801:VAL:CG2	2.24	0.67
2:B:112:ILE:HD12	2:B:113:GLY:H	1.58	0.67
2:E:157:ILE:CG1	2:E:202:PHE:CZ	2.75	0.67
2:E:31:LEU:HD22	2:E:317:LEU:HD21	1.77	0.67
2:B:978:GLN:HG3	2:B:979:LYS:O	1.95	0.66
2:B:93:GLN:HB2	2:B:98:ILE:HG12	1.77	0.66
2:B:305:LEU:HD23	2:B:336:LEU:HD22	1.76	0.66
1:D:401:LYS:HB2	1:D:415:TRP:CZ3	2.30	0.66
2:E:889:ARG:HD3	2:E:891:TYR:CZ	2.30	0.66
2:E:1030:PHE:CZ	2:E:1038:GLY:HA3	2.31	0.66
1:A:289:PRO:N	1:A:346:MET:HE1	2.11	0.66
2:B:321:VAL:CG1	2:B:333:LEU:HD22	2.26	0.66
1:D:101:LEU:HD23	1:D:110:VAL:HG21	1.76	0.66
2:E:124:ILE:HG12	2:E:131:ILE:HG12	1.77	0.66
2:B:39:LEU:HB3	2:B:55:VAL:HG13	1.78	0.66
1:A:117:ASP:OD1	1:A:119:THR:N	2.28	0.66
2:B:16:ASN:ND2	2:B:36:ASN:H	1.93	0.66
2:B:881:LEU:HD21	2:B:921:ILE:HD13	1.77	0.66
1:D:165:PHE:CB	1:D:182:VAL:HG13	2.23	0.66
1:A:111:ARG:O	1:A:114:ILE:HG22	1.95	0.66
1:A:206:GLN:NE2	1:A:206:GLN:HA	2.09	0.66
2:E:932:LEU:HD22	2:E:965:PHE:CZ	2.31	0.66
2:E:385:GLY:HA3	2:E:719:GLU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:C	1:A:135:PHE:HD1	2.04	0.65
2:E:101:ILE:HD12	2:E:101:ILE:O	1.96	0.65
2:E:248:ILE:HG12	2:E:250:PRO:CD	2.26	0.65
2:E:1127:ASP:HA	2:E:1130:ILE:HD12	1.79	0.65
1:A:289:PRO:CA	1:A:346:MET:HE1	2.27	0.65
2:B:291:MET:CA	2:B:291:MET:HE3	2.26	0.65
2:E:874:VAL:HG11	2:E:916:THR:HG23	1.79	0.65
2:B:291:MET:HE3	2:B:291:MET:O	1.96	0.65
2:B:996:GLY:HA2	2:B:1086:THR:HG23	1.78	0.65
2:E:824:ASP:OD1	2:E:825:PRO:HD2	1.96	0.65
1:A:74:ASP:HB2	1:A:77:SER:HB2	1.78	0.64
1:A:114:ILE:HG12	1:A:144:TYR:CD2	2.32	0.64
1:D:104:PRO:HA	1:D:107:VAL:HG12	1.77	0.64
2:E:1105:MET:O	2:E:1109:VAL:HG22	1.97	0.64
1:A:194:MET:HE2	1:A:194:MET:HA	1.78	0.64
1:D:73:HIS:CD2	1:D:79:GLN:HE21	2.16	0.64
1:D:120:PHE:CE1	1:D:139:ALA:HB3	2.32	0.64
2:B:1129:LEU:O	2:B:1132:VAL:HG22	1.97	0.64
2:E:75:ASP:O	2:E:76:LEU:HD23	1.97	0.64
2:B:94:SER:O	2:B:96:GLU:N	2.30	0.64
2:B:1098:LEU:H	2:B:1098:LEU:HD12	1.63	0.64
2:E:210:GLU:O	2:E:211:ASN:ND2	2.31	0.64
2:B:285:LEU:HD22	2:B:300:LEU:HD23	1.80	0.64
2:E:378:CYS:HB3	2:E:721:PRO:HB2	1.78	0.64
2:E:1083:GLU:CG	2:E:1084:PRO:HD2	2.25	0.64
2:E:304:LEU:C	2:E:304:LEU:HD23	2.22	0.63
2:B:910:MET:HE2	2:B:912:LEU:HD21	1.80	0.63
2:B:1105:MET:HE1	2:B:1130:ILE:CG1	2.28	0.63
1:A:84:LEU:O	1:A:87:VAL:HG22	1.99	0.63
2:E:1130:ILE:HG22	2:E:1134:GLU:OE1	1.98	0.63
2:B:57:MET:HE1	2:B:79:ILE:HG12	1.79	0.63
2:B:768:SER:HB2	2:B:770:LEU:HD23	1.80	0.63
2:B:875:GLU:OE2	2:B:878:GLY:N	2.27	0.63
2:E:39:LEU:HB3	2:E:55:VAL:HG12	1.80	0.63
2:E:317:LEU:HB2	2:E:321:VAL:HG23	1.80	0.63
2:E:1051:LEU:HD12	2:E:1094:ILE:CD1	2.28	0.63
2:E:1011:SER:OG	2:E:1013:VAL:HG22	1.99	0.63
2:B:1125:THR:HG22	2:B:1126:ALA:H	1.63	0.62
2:E:39:LEU:HB3	2:E:55:VAL:CG1	2.29	0.62
2:E:952:ASN:ND2	2:E:969:GLU:OE1	2.30	0.62
2:B:809:GLN:O	2:B:810:ASN:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ASP:HB2	2:B:185:PRO:CD	2.29	0.62
2:B:890:LEU:HB2	2:B:942:PHE:HZ	1.63	0.62
1:D:87:VAL:CG2	1:D:123:LEU:HB2	2.28	0.62
2:E:121:ILE:HD12	2:E:167:VAL:HG12	1.80	0.62
2:B:927:MET:HA	2:B:952:ASN:O	2.00	0.62
2:E:184:ASP:HB2	2:E:185:PRO:HD2	1.80	0.62
2:E:1050:LEU:HD23	2:E:1054:MET:CG	2.29	0.62
2:B:1136:LEU:O	2:B:1139:ILE:HG22	2.00	0.62
2:E:171:TYR:CD2	2:E:223:PRO:HA	2.34	0.62
2:E:1059:ASN:ND2	2:E:1070:HIS:HB3	2.15	0.62
2:E:1109:VAL:HG12	2:E:1129:LEU:HD12	1.82	0.62
2:B:255:GLN:CB	2:B:279:ARG:NH1	2.62	0.62
2:E:981:SER:O	2:E:983:ALA:HB2	1.98	0.62
1:D:280:PHE:O	1:D:284:VAL:HG23	2.00	0.61
2:B:1030:PHE:CZ	2:B:1038:GLY:HA3	2.35	0.61
1:D:96:THR:O	1:D:98:PRO:HD3	2.00	0.61
3:C:869:LEU:O	3:C:885:LEU:HD12	2.00	0.61
1:A:112:ASN:O	1:A:116:LYS:HG3	2.00	0.61
2:B:33:ILE:HD11	2:B:323:PHE:CZ	2.36	0.61
2:B:883:SER:O	2:B:884:ILE:HD13	2.01	0.61
2:B:57:MET:HE1	2:B:79:ILE:HG21	1.82	0.61
2:B:713:ARG:NH1	2:B:799:PHE:HD2	1.98	0.61
1:D:257:ILE:HG12	1:D:312:LEU:HD13	1.83	0.61
2:B:130:MET:HE1	2:B:195:VAL:CG1	2.27	0.61
2:E:263:ARG:HH11	2:E:266:PRO:HA	1.65	0.61
2:B:57:MET:CE	2:B:79:ILE:HG12	2.30	0.61
2:B:1048:TYR:CD1	2:B:1089:ILE:HD11	2.35	0.61
2:B:755:SER:H	2:B:758:THR:HB	1.66	0.61
2:E:996:GLY:HA2	2:E:1086:THR:O	2.01	0.61
2:B:374:GLN:CG	2:B:391:ARG:HB3	2.31	0.60
2:E:248:ILE:CD1	2:E:250:PRO:HG3	2.31	0.60
1:A:207:ILE:HG23	2:B:188:ARG:CZ	2.29	0.60
1:D:210:SER:O	1:D:212:PRO:HD3	2.01	0.60
2:E:944:GLU:C	2:E:945:ILE:HD13	2.26	0.60
2:E:1104:LYS:O	2:E:1108:VAL:HG13	2.00	0.60
1:A:288:LEU:C	1:A:346:MET:HE1	2.26	0.60
2:B:108:VAL:O	2:B:141:LYS:HE3	2.01	0.60
2:B:1102:ARG:N	2:B:1103:PRO:HD2	2.16	0.60
1:D:271:ASP:O	1:D:272:SER:C	2.44	0.60
2:E:32:LEU:HD22	2:E:41:ILE:HG12	1.81	0.60
2:B:832:GLY:N	2:B:873:MET:HE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:891:TYR:CG	2:B:899:LEU:HD22	2.35	0.60
2:E:821:LEU:HD21	2:E:830:ILE:HD11	1.84	0.60
2:B:282:MET:CB	2:B:305:LEU:HD11	2.30	0.60
1:D:87:VAL:HG21	1:D:123:LEU:HB2	1.83	0.60
2:E:807:PHE:HB3	2:E:811:GLU:OE1	2.00	0.60
2:E:1102:ARG:HA	2:E:1105:MET:HG3	1.83	0.60
2:B:91:TYR:OH	2:B:98:ILE:HD13	2.01	0.60
2:E:130:MET:CE	2:E:142:VAL:HG22	2.31	0.60
2:E:118:THR:OG1	2:E:134:ARG:NH2	2.32	0.60
2:B:1054:MET:HE3	2:B:1058:LEU:HD21	1.83	0.60
2:E:130:MET:SD	2:E:197:LEU:HD21	2.42	0.60
2:E:178:ILE:HD12	2:E:178:ILE:C	2.27	0.60
2:E:967:GLY:HA3	2:E:975:PHE:CZ	2.36	0.60
2:B:134:ARG:NH1	2:B:164:VAL:HG22	2.17	0.60
2:B:255:GLN:HG3	2:B:279:ARG:HH12	1.67	0.60
1:D:385:ALA:O	1:D:402:PHE:HA	2.01	0.60
2:B:362:MET:HE2	2:B:375:LEU:HD21	1.83	0.59
2:E:910:MET:HE2	2:E:912:LEU:CD1	2.20	0.59
2:B:291:MET:HE3	2:B:291:MET:HA	1.84	0.59
2:B:768:SER:HG	2:B:808:LEU:HD21	1.64	0.59
2:E:134:ARG:HD2	2:E:134:ARG:C	2.27	0.59
2:E:248:ILE:HG12	2:E:250:PRO:HG3	1.84	0.59
2:B:1125:THR:HG22	2:B:1126:ALA:N	2.17	0.59
1:A:375:SER:O	1:A:385:ALA:HB1	2.02	0.59
2:B:317:LEU:HD12	2:B:321:VAL:HG12	1.85	0.59
2:B:766:SER:HB2	2:B:808:LEU:HD12	1.84	0.59
2:E:807:PHE:CZ	2:E:831:VAL:HG11	2.37	0.59
1:A:92:ILE:HG23	1:A:299:LEU:HD21	1.85	0.59
2:B:102:THR:HG23	2:B:102:THR:O	2.02	0.59
1:A:94:GLY:C	1:A:160:ILE:HD11	2.28	0.59
1:A:401:LYS:HE2	1:A:413:LYS:NZ	2.18	0.59
2:B:223:PRO:C	2:B:225:PRO:HD2	2.27	0.59
2:E:315:THR:HG22	2:E:323:PHE:HB3	1.85	0.59
2:B:87:CYS:SG	2:B:89:LEU:HD21	2.43	0.59
2:B:921:ILE:HB	2:B:933:LEU:HB2	1.84	0.59
2:E:120:ILE:N	2:E:120:ILE:HD12	2.18	0.59
2:B:928:ARG:HG2	2:B:928:ARG:NH1	2.09	0.58
2:E:156:ASN:O	2:E:157:ILE:CG2	2.51	0.58
2:B:197:LEU:H	2:B:197:LEU:HD12	1.68	0.58
2:B:372:GLN:HA	2:B:372:GLN:OE1	2.03	0.58
1:D:260:GLN:O	1:D:263:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:766:SER:HB2	2:E:805:HIS:NE2	2.18	0.58
1:D:305:ILE:CG2	2:E:927:MET:HE1	2.28	0.58
2:E:215:GLU:CB	2:E:234:GLN:HG3	2.27	0.58
2:E:321:VAL:HA	2:E:334:VAL:O	2.03	0.58
2:B:891:TYR:CB	2:B:899:LEU:HD22	2.32	0.58
2:B:925:ASP:OD1	2:B:929:SER:HB2	2.04	0.58
2:B:1047:TRP:O	2:B:1051:LEU:HD23	2.02	0.58
2:B:88:ILE:C	2:B:89:LEU:HD23	2.28	0.58
2:B:1044:SER:O	2:B:1047:TRP:N	2.36	0.58
2:B:10:GLN:HB3	2:B:1037:ILE:HB	1.84	0.58
2:B:255:GLN:CB	2:B:279:ARG:HH12	2.15	0.58
2:B:870:VAL:HG22	2:B:884:ILE:CD1	2.32	0.58
1:D:260:GLN:OE1	1:D:334:LYS:NZ	2.36	0.58
2:E:157:ILE:CD1	2:E:202:PHE:CD2	2.84	0.58
2:E:803:HIS:HD2	2:E:858:LEU:HD12	1.69	0.58
2:B:308:THR:HB	2:B:332:GLN:OE1	2.04	0.58
2:B:830:ILE:HG22	2:B:873:MET:SD	2.43	0.58
2:E:793:ILE:HG22	2:E:802:LEU:HB2	1.84	0.58
2:B:93:GLN:HA	2:B:97:SER:O	2.03	0.58
2:B:255:GLN:HB2	2:B:279:ARG:NH1	2.18	0.58
1:D:276:ASN:OD1	1:D:278:ILE:N	2.36	0.58
2:E:157:ILE:HD12	2:E:202:PHE:CE2	2.33	0.58
2:E:1059:ASN:HD21	2:E:1070:HIS:HB3	1.68	0.58
1:D:98:PRO:O	1:D:99:LEU:HD23	2.04	0.58
2:E:21:GLY:HA3	2:E:66:LEU:CD1	2.34	0.58
2:E:314:LEU:HD21	2:E:324:VAL:HG13	1.86	0.58
2:E:1102:ARG:N	2:E:1103:PRO:HD2	2.19	0.58
2:B:55:VAL:CG2	2:B:1065:VAL:HG21	2.34	0.58
2:B:910:MET:CE	2:B:912:LEU:HD21	2.34	0.58
2:B:94:SER:HB3	2:B:97:SER:HB3	1.86	0.57
2:E:106:GLY:N	2:E:152:LEU:HD12	2.19	0.57
2:E:803:HIS:HD2	2:E:858:LEU:CD1	2.15	0.57
2:E:220:ILE:HB	2:E:230:ILE:HB	1.87	0.57
2:E:275:ASP:CG	2:E:279:ARG:HB2	2.29	0.57
2:E:1029:LEU:CD2	2:E:1039:LEU:HD12	2.34	0.57
2:E:760:ALA:HA	2:E:801:VAL:HG23	1.84	0.57
2:E:961:ASP:OD1	2:E:963:ASP:N	2.22	0.57
1:A:140:GLU:OE1	1:A:162:ARG:NH2	2.35	0.57
2:B:255:GLN:CG	2:B:279:ARG:HH12	2.16	0.57
3:C:881:THR:HG22	7:C:1001:HOH:O	2.04	0.57
2:E:1127:ASP:HA	2:E:1130:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:879:PHE:CZ	3:F:888:HIS:HB2	2.40	0.57
2:B:39:LEU:HB3	2:B:55:VAL:CG1	2.34	0.57
2:B:213:GLU:OE2	2:B:233:GLY:HA3	2.04	0.57
2:E:356:LEU:HB3	2:E:359:ILE:HD11	1.87	0.57
1:A:296:ILE:O	1:A:300:LYS:HG3	2.04	0.57
2:B:392:ASN:OD1	2:B:710:LEU:CD1	2.53	0.57
2:E:171:TYR:CG	2:E:223:PRO:HA	2.39	0.57
2:E:358:PRO:HD2	2:E:380:GLY:HA2	1.85	0.57
2:E:767:SER:O	2:E:767:SER:OG	2.20	0.57
2:E:847:ARG:HG2	2:E:865:GLU:HA	1.86	0.57
2:B:1058:LEU:HB3	2:B:1062:ILE:HD13	1.86	0.57
1:D:327:GLN:O	1:D:327:GLN:CG	2.49	0.57
1:D:340:LEU:HD22	1:D:381:PHE:HD2	1.70	0.57
2:E:21:GLY:HA3	2:E:66:LEU:HD12	1.86	0.57
1:A:221:TYR:OH	2:B:838:PRO:HB2	2.05	0.56
2:B:49:LEU:HD13	2:B:333:LEU:HD11	1.85	0.56
2:E:1047:TRP:O	2:E:1051:LEU:HD23	2.05	0.56
1:A:84:LEU:HD23	1:A:120:PHE:CG	2.40	0.56
1:A:289:PRO:HA	1:A:346:MET:HE1	1.88	0.56
2:E:874:VAL:HG11	2:E:916:THR:CG2	2.35	0.56
2:B:1076:PHE:HE1	2:B:1078:THR:CG2	2.18	0.56
2:B:1098:LEU:CG	2:B:1133:VAL:HG11	2.35	0.56
2:B:256:SER:HB3	2:B:275:ASP:OD2	2.05	0.56
2:B:832:GLY:N	2:B:873:MET:CE	2.68	0.56
2:B:263:ARG:HG3	2:B:271:TYR:CE1	2.41	0.56
2:E:947:ARG:HH21	2:E:949:PHE:HZ	1.53	0.56
1:A:342:LEU:O	1:A:343:CYS:C	2.49	0.56
2:B:118:THR:OG1	2:B:134:ARG:NH2	2.29	0.56
2:B:218:MET:HB3	2:B:232:ILE:HB	1.88	0.56
1:D:423:LEU:HD12	1:D:424:PRO:HD2	1.87	0.56
2:E:1023:PRO:HG2	2:E:1024:THR:HG22	1.87	0.56
1:A:190:LEU:HD12	2:B:927:MET:HE3	1.88	0.56
1:A:380:TRP:O	1:A:382:PRO:HD3	2.05	0.56
2:B:36:ASN:OD1	2:B:60:LYS:HG2	2.06	0.56
2:B:979:LYS:HA	2:B:992:LEU:HD23	1.88	0.56
2:B:1044:SER:HB2	2:B:1047:TRP:HD1	1.70	0.56
2:B:1058:LEU:HB3	2:B:1062:ILE:HD11	1.87	0.56
1:D:134:GLN:HB2	1:D:167:VAL:HG22	1.88	0.56
2:E:218:MET:HE1	2:E:261:HIS:HB3	1.88	0.56
2:E:801:VAL:HG23	2:E:801:VAL:O	2.06	0.56
1:D:383:GLY:O	1:D:405:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1051:LEU:HB2	2:E:1089:ILE:CD1	2.36	0.55
2:B:63:VAL:O	2:B:79:ILE:HA	2.05	0.55
2:B:909:ILE:HD12	2:B:910:MET:C	2.31	0.55
2:B:387:LEU:HG	2:B:717:LEU:HD11	1.88	0.55
2:E:157:ILE:CD1	2:E:202:PHE:CZ	2.89	0.55
1:A:84:LEU:HD13	1:A:85:PRO:HD2	1.88	0.55
2:B:317:LEU:HD12	2:B:321:VAL:CG1	2.37	0.55
1:D:248:TYR:HD2	2:E:927:MET:CE	2.18	0.55
2:E:156:ASN:O	2:E:157:ILE:HG23	2.06	0.55
1:D:141:ILE:HG23	1:D:157:VAL:HG23	1.89	0.55
1:A:370:LEU:HD23	1:A:387:THR:HB	1.89	0.55
2:B:1012:LEU:HD13	2:B:1029:LEU:CD1	2.37	0.55
2:E:826:ASN:HD22	2:E:852:GLN:HE22	1.54	0.55
1:A:134:GLN:O	1:A:135:PHE:HD1	1.90	0.55
2:B:181:VAL:CG2	2:B:190:VAL:HG22	2.34	0.55
1:A:207:ILE:CG2	2:B:188:ARG:NH1	2.70	0.55
1:A:260:GLN:HB2	1:A:315:MET:HE1	1.89	0.55
2:B:301:ARG:NH1	2:B:303:GLU:OE2	2.40	0.55
2:E:1051:LEU:HB3	2:E:1089:ILE:HD13	1.88	0.55
2:B:134:ARG:HH11	2:B:164:VAL:HG22	1.71	0.55
1:D:164:ARG:NH2	1:D:186:PRO:O	2.40	0.55
1:D:248:TYR:O	1:D:305:ILE:HD12	2.07	0.55
2:E:1101:SER:OG	2:E:1103:PRO:HG2	2.06	0.55
2:B:212:VAL:HG22	2:B:213:GLU:H	1.72	0.55
2:B:227:GLY:O	2:B:239:TYR:OH	2.22	0.55
2:B:248:ILE:HG13	2:B:250:PRO:HD3	1.89	0.55
1:D:101:LEU:HD21	1:D:110:VAL:HG21	1.89	0.55
1:A:146:GLU:CG	1:A:155:VAL:HG22	2.36	0.54
1:A:197:VAL:HG12	1:A:234:CYS:HB3	1.89	0.54
2:E:1093:LEU:O	2:E:1096:SER:OG	2.24	0.54
1:A:199:LEU:HD22	2:B:327:ARG:HD3	1.88	0.54
2:B:57:MET:CE	2:B:79:ILE:HG21	2.37	0.54
2:B:224:GLU:N	2:B:225:PRO:HD2	2.21	0.54
2:E:981:SER:C	2:E:983:ALA:HB2	2.33	0.54
2:B:285:LEU:HD22	2:B:300:LEU:CD2	2.36	0.54
2:B:1111:ASN:HA	2:B:1123:GLU:CB	2.37	0.54
1:D:92:ILE:HG22	1:D:93:PRO:HD2	1.90	0.54
2:E:138:GLY:CA	2:E:162:LEU:HD13	2.37	0.54
2:E:371:GLY:O	2:E:1014:MET:HG3	2.07	0.54
2:B:321:VAL:HG11	2:B:333:LEU:HD22	1.90	0.54
1:D:148:GLN:HA	1:D:153:GLU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:THR:CA	2:E:91:TYR:HD2	2.16	0.54
2:E:309:SER:O	2:E:310:ILE:C	2.51	0.54
2:E:340:SER:CB	2:E:346:TYR:HE1	2.17	0.54
2:E:366:ASP:OD2	2:E:371:GLY:N	2.40	0.54
2:B:744:ASP:OD1	2:B:745:THR:N	2.41	0.54
2:E:75:ASP:C	2:E:76:LEU:HD23	2.32	0.54
2:E:1030:PHE:CE1	2:E:1038:GLY:HA3	2.42	0.54
1:A:241:PRO:HB3	2:B:812:TYR:OH	2.08	0.54
2:B:1095:GLU:O	2:B:1098:LEU:HD12	2.07	0.54
1:A:167:VAL:C	1:A:168:LEU:HD23	2.32	0.54
1:A:370:LEU:HD21	1:A:401:LYS:HD2	1.89	0.54
1:A:385:ALA:O	1:A:402:PHE:HA	2.07	0.54
2:E:174:GLN:HG3	2:E:175:ALA:H	1.72	0.54
2:B:292:ASP:OD1	2:B:294:THR:N	2.33	0.54
2:B:939:GLU:HA	2:B:939:GLU:OE2	2.08	0.54
2:B:18:CYS:SG	2:B:315:THR:HG23	2.48	0.53
2:B:63:VAL:HG11	2:B:122:GLY:HA3	1.89	0.53
2:B:165:ILE:CD1	2:B:188:ARG:HH12	2.20	0.53
2:B:753:ARG:HB2	2:B:754:PRO:HD2	1.90	0.53
1:D:99:LEU:HB2	1:D:157:VAL:CG1	2.38	0.53
2:B:358:PRO:HD2	2:B:380:GLY:HA2	1.90	0.53
2:B:43:VAL:HG23	2:B:52:VAL:CG2	2.37	0.53
2:E:5:TYR:HB2	2:E:1043:LEU:HD11	1.91	0.53
2:E:361:ASP:OD2	2:E:723:LYS:HA	2.08	0.53
2:E:1105:MET:HA	2:E:1108:VAL:HG22	1.90	0.53
2:B:94:SER:N	2:B:97:SER:O	2.42	0.53
2:B:291:MET:HA	2:B:291:MET:CE	2.39	0.53
2:E:931:LEU:HD12	2:E:932:LEU:N	2.23	0.53
2:B:134:ARG:NH1	2:B:164:VAL:CG2	2.72	0.53
2:B:142:VAL:HG11	2:B:155:PHE:CZ	2.44	0.53
2:E:212:VAL:HG22	2:E:213:GLU:H	1.73	0.53
2:E:55:VAL:HG21	2:E:1065:VAL:HG21	1.89	0.53
2:E:65:GLU:O	2:E:77:LEU:HD12	2.07	0.53
2:E:107:ASN:HD21	2:E:109:GLN:HB2	1.72	0.53
2:B:57:MET:HE1	2:B:79:ILE:CB	2.38	0.53
2:E:1055:GLN:NE2	2:E:1090:ASP:H	2.06	0.53
1:A:135:PHE:CE1	1:A:166:LYS:HG3	2.44	0.53
1:A:207:ILE:HG21	2:B:188:ARG:NH1	2.16	0.53
2:B:223:PRO:HD3	2:B:271:TYR:OH	2.09	0.53
2:E:963:ASP:O	2:E:978:GLN:HA	2.09	0.53
2:E:996:GLY:HA2	2:E:1086:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:MET:CE	2:B:195:VAL:HG11	2.27	0.53
2:B:245:TYR:HE1	2:B:247:ALA:HB2	1.74	0.53
2:B:889:ARG:HD3	2:B:891:TYR:CZ	2.44	0.53
1:A:352:PRO:HG3	1:A:378:HIS:ND1	2.24	0.52
2:B:245:TYR:CE1	2:B:247:ALA:HB2	2.43	0.52
2:B:1051:LEU:HD12	2:B:1094:ILE:HD12	1.91	0.52
2:E:90:GLU:H	2:E:101:ILE:HD12	1.74	0.52
2:E:370:GLN:O	2:E:1014:MET:HE2	2.09	0.52
1:D:317:LYS:HD3	1:D:438:VAL:CG1	2.39	0.52
1:A:340:LEU:CD2	1:A:381:PHE:HB3	2.39	0.52
2:B:830:ILE:HD12	2:B:880:LEU:HD13	1.91	0.52
2:B:1062:ILE:H	2:B:1062:ILE:HD12	1.74	0.52
2:E:59:GLY:HA2	2:E:1073:TRP:CZ3	2.44	0.52
2:E:1055:GLN:NE2	2:E:1089:ILE:HA	2.22	0.52
2:B:881:LEU:HD22	2:B:921:ILE:HD13	1.90	0.52
1:A:401:LYS:HE2	1:A:413:LYS:CE	2.40	0.52
2:B:288:GLU:O	2:B:295:VAL:HG13	2.08	0.52
1:A:340:LEU:HD21	1:A:381:PHE:HB3	1.91	0.52
2:B:213:GLU:OE2	2:B:234:GLN:N	2.42	0.52
1:D:270:ASP:O	1:D:272:SER:N	2.43	0.52
2:E:272:LEU:HD21	2:E:322:VAL:HG21	1.92	0.52
2:E:359:ILE:HD12	2:E:1035:GLY:HA2	1.91	0.52
2:B:57:MET:HE1	2:B:79:ILE:CG1	2.40	0.52
2:B:920:PHE:HE2	2:B:962:ASP:HB3	1.75	0.52
1:A:271:ASP:O	1:A:272:SER:C	2.52	0.52
2:B:261:HIS:HA	2:B:272:LEU:O	2.10	0.52
2:B:363:CYS:O	2:B:375:LEU:HD12	2.10	0.52
1:D:99:LEU:HB2	1:D:157:VAL:HG12	1.92	0.52
1:A:82:PRO:CG	1:A:113:LEU:HD21	2.40	0.51
2:B:832:GLY:H	2:B:873:MET:HE2	1.74	0.51
1:D:185:LEU:HB3	1:D:186:PRO:HD2	1.93	0.51
2:E:81:THR:OG1	2:E:85:ASN:HB2	2.10	0.51
1:A:439:ILE:HG22	1:A:440:LEU:N	2.25	0.51
2:B:871:TYR:CD2	2:B:912:LEU:HD13	2.45	0.51
2:B:963:ASP:O	2:B:978:GLN:HA	2.10	0.51
2:E:356:LEU:HD13	2:E:1037:ILE:HD11	1.92	0.51
2:B:1002:GLU:CB	2:B:1032:THR:HG21	2.41	0.51
2:E:248:ILE:HG12	2:E:250:PRO:CG	2.40	0.51
1:A:165:PHE:HB2	1:A:182:VAL:CG1	2.27	0.51
1:D:321:LEU:HB2	1:D:332:THR:HG22	1.91	0.51
1:A:92:ILE:HD12	1:A:92:ILE:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:MET:HB2	2:B:845:GLN:HG3	1.92	0.51
1:D:290:ILE:HA	1:D:424:PRO:HG3	1.92	0.51
1:A:94:GLY:HA2	1:A:160:ILE:HD11	1.93	0.51
2:B:77:LEU:HG	2:B:79:ILE:HD13	1.92	0.51
1:D:254:MET:HE1	1:D:275:SER:O	2.11	0.51
2:B:83:LYS:HE2	2:B:1077:HIS:HB2	1.92	0.51
2:B:285:LEU:CD2	2:B:300:LEU:HD23	2.40	0.51
2:E:340:SER:HB3	2:E:346:TYR:CE1	2.34	0.51
2:E:377:THR:OG1	2:E:388:ARG:HB2	2.10	0.51
2:E:805:HIS:HB2	2:E:858:LEU:HD12	1.91	0.51
2:E:921:ILE:O	2:E:932:LEU:HD12	2.11	0.51
1:A:340:LEU:HD22	1:A:381:PHE:CD1	2.46	0.51
2:B:130:MET:HE3	2:B:142:VAL:CG1	2.38	0.51
2:B:1029:LEU:HA	2:B:1038:GLY:O	2.11	0.51
2:E:32:LEU:HD21	2:E:41:ILE:HG12	1.93	0.51
1:A:370:LEU:HD21	1:A:401:LYS:CD	2.40	0.51
1:D:257:ILE:O	1:D:261:LEU:HG	2.11	0.51
2:B:1104:LYS:HA	2:B:1107:GLU:HG2	1.91	0.51
1:D:153:GLU:C	1:D:154:ILE:HD13	2.36	0.51
2:E:1102:ARG:O	2:E:1106:GLN:HG2	2.11	0.51
1:A:80:VAL:C	1:A:81:ILE:HG13	2.36	0.50
1:A:125:TYR:O	1:A:133:ALA:N	2.44	0.50
2:B:83:LYS:HE2	2:B:1077:HIS:CB	2.41	0.50
2:B:389:ILE:N	2:B:389:ILE:HD12	2.25	0.50
1:D:77:SER:OG	1:D:79:GLN:OE1	2.28	0.50
2:E:935:TYR:O	2:E:937:PRO:HD3	2.11	0.50
2:B:188:ARG:CD	2:B:214:ALA:O	2.57	0.50
2:B:791:LEU:HD12	2:B:792:LEU:N	2.27	0.50
2:E:283:LEU:HD13	2:E:302:VAL:HG22	1.93	0.50
2:B:984:THR:OG1	2:B:985:THR:N	2.44	0.50
1:A:84:LEU:HD13	1:A:109:MET:HE1	1.92	0.50
1:A:99:LEU:HB2	1:A:157:VAL:CG2	2.42	0.50
1:A:259:LYS:NZ	1:A:262:ARG:NH2	2.60	0.50
2:B:32:LEU:HD12	2:B:32:LEU:N	2.27	0.50
2:B:130:MET:CE	2:B:142:VAL:HG13	2.39	0.50
1:D:442:LEU:HD23	1:D:442:LEU:H	1.77	0.50
1:A:165:PHE:CB	1:A:182:VAL:CG1	2.89	0.50
2:B:10:GLN:O	2:B:1036:MET:HG2	2.12	0.50
2:B:1106:GLN:HA	2:B:1109:VAL:HG22	1.92	0.50
2:E:268:GLY:O	2:E:285:LEU:HD22	2.11	0.50
1:D:103:HIS:CE1	1:D:105:GLN:H	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:HD12	1:D:278:ILE:H	1.76	0.50
1:A:199:LEU:CD2	2:B:327:ARG:HD3	2.42	0.50
2:E:104:ALA:HB1	2:E:152:LEU:HG	1.94	0.50
2:B:110:ASP:HB2	2:B:136:TYR:CE2	2.47	0.50
2:B:322:VAL:CG2	2:B:336:LEU:HD11	2.42	0.50
1:D:103:HIS:O	1:D:107:VAL:HG12	2.12	0.50
1:D:240:TRP:HZ2	2:E:913:TYR:CE1	2.30	0.50
2:E:847:ARG:HH12	2:E:849:VAL:CG2	2.25	0.50
2:B:876:PHE:CG	2:B:876:PHE:O	2.61	0.49
2:E:736:LEU:HG	2:E:816:LEU:HD22	1.94	0.49
2:E:1000:LEU:O	2:E:1074:ARG:NH1	2.45	0.49
1:A:168:LEU:HD23	1:A:168:LEU:N	2.27	0.49
2:B:201:GLU:HG2	2:B:202:PHE:N	2.27	0.49
2:B:262:ASN:CG	2:B:315:THR:HA	2.37	0.49
1:D:346:MET:HE3	1:D:358:GLU:HB3	1.95	0.49
2:E:2:SER:HB3	2:E:964:ASN:ND2	2.28	0.49
2:E:272:LEU:CD2	2:E:322:VAL:HG21	2.42	0.49
2:B:713:ARG:NH1	2:B:799:PHE:CD2	2.79	0.49
2:E:120:ILE:HD12	2:E:120:ILE:H	1.77	0.49
2:E:1051:LEU:CB	2:E:1089:ILE:HD13	2.41	0.49
2:B:284:LEU:N	2:B:284:LEU:HD12	2.28	0.49
1:D:248:TYR:OH	2:E:910:MET:HG2	2.12	0.49
2:E:803:HIS:HD2	2:E:858:LEU:HG	1.76	0.49
2:B:181:VAL:HG22	2:B:190:VAL:CG2	2.37	0.49
1:D:342:LEU:N	1:D:342:LEU:HD23	2.26	0.49
2:E:157:ILE:HD12	2:E:202:PHE:CG	2.48	0.49
2:E:178:ILE:HD12	2:E:178:ILE:O	2.12	0.49
2:E:741:GLU:HA	2:E:752:LEU:CD2	2.43	0.49
1:A:84:LEU:CD1	1:A:101:LEU:HD11	2.40	0.49
1:A:320:SER:HB3	1:A:330:GLU:OE2	2.13	0.49
2:E:223:PRO:HG2	2:E:267:ASN:C	2.37	0.49
2:B:928:ARG:CD	2:B:969:GLU:OE1	2.47	0.49
2:E:19:VAL:HG22	2:E:64:MET:HE3	1.94	0.49
2:E:248:ILE:CG1	2:E:250:PRO:HG3	2.43	0.49
2:E:765:VAL:HG12	2:E:806:GLN:HB3	1.94	0.49
2:B:739:ARG:NH1	2:B:757:SER:OG	2.46	0.49
1:D:256:ARG:HH11	2:E:841:ALA:HB3	1.77	0.49
2:E:171:TYR:HB2	2:E:222:VAL:O	2.13	0.49
2:E:1083:GLU:HG3	2:E:1084:PRO:CD	2.33	0.49
1:A:199:LEU:HB3	1:A:202:LEU:HD23	1.94	0.49
2:B:939:GLU:OE2	2:B:939:GLU:CA	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:HG21	1:D:142:TYR:OH	2.13	0.48
2:E:348:VAL:HG13	2:E:348:VAL:O	2.13	0.48
2:E:724:ILE:HA	2:E:734:GLY:O	2.12	0.48
2:E:174:GLN:HG3	2:E:175:ALA:N	2.28	0.48
1:A:237:LEU:HD21	2:B:328:LEU:HD21	1.95	0.48
2:E:810:ASN:HD22	2:E:837:TYR:HE1	1.61	0.48
2:E:815:SER:OG	2:E:832:GLY:HA3	2.13	0.48
1:A:165:PHE:C	1:A:185:LEU:HD13	2.39	0.48
1:A:221:TYR:HH	2:B:838:PRO:HB2	1.78	0.48
2:E:158:ARG:O	2:E:202:PHE:CE2	2.67	0.48
2:E:265:ASP:HB2	2:E:267:ASN:OD1	2.14	0.48
2:B:6:VAL:HG23	2:B:1088:PHE:HD1	1.79	0.48
2:E:282:MET:N	2:E:303:GLU:O	2.36	0.48
2:E:1098:LEU:HD12	2:E:1133:VAL:HG12	1.95	0.48
2:B:264:VAL:HG12	2:B:265:ASP:N	2.27	0.48
2:E:167:VAL:HG22	2:E:168:LYS:N	2.29	0.48
2:E:803:HIS:HD2	2:E:858:LEU:CG	2.26	0.48
2:E:1055:GLN:NE2	2:E:1089:ILE:HG23	2.18	0.48
2:E:1103:PRO:O	2:E:1106:GLN:HB2	2.12	0.48
1:A:253:LEU:HD11	1:A:309:ARG:HG3	1.96	0.48
2:B:1054:MET:CE	2:B:1058:LEU:HD21	2.43	0.48
2:E:10:GLN:OE1	2:E:10:GLN:HA	2.13	0.48
2:E:246:LEU:HD23	2:E:297:LEU:HD11	1.96	0.48
2:E:1132:VAL:O	2:E:1135:GLU:HB3	2.14	0.48
1:A:88:MET:O	1:A:88:MET:HG3	2.14	0.48
2:B:86:ALA:O	2:B:105:HIS:HA	2.13	0.48
2:E:845:GLN:HG3	2:E:845:GLN:O	2.13	0.48
2:B:225:PRO:HG3	2:B:267:ASN:O	2.13	0.48
2:B:304:LEU:HD12	2:B:305:LEU:N	2.29	0.48
2:B:1105:MET:CE	2:B:1130:ILE:CD1	2.90	0.48
2:B:1106:GLN:HA	2:B:1109:VAL:CG2	2.44	0.48
2:B:285:LEU:CD2	2:B:300:LEU:CD2	2.92	0.47
2:B:805:HIS:CD2	2:B:851:PHE:CZ	3.02	0.47
2:E:55:VAL:HG22	2:E:56:GLY:N	2.29	0.47
2:E:766:SER:HB3	2:E:808:LEU:HD22	1.95	0.47
2:B:66:LEU:CD2	2:B:77:LEU:HD13	2.44	0.47
2:B:311:ALA:HB1	2:B:314:LEU:CD1	2.44	0.47
2:E:23:PHE:N	2:E:30:ASN:HD22	1.93	0.47
2:E:80:LEU:HD12	2:E:85:ASN:O	2.13	0.47
2:E:984:THR:HG22	2:E:985:THR:HG23	1.96	0.47
2:E:1058:LEU:O	2:E:1061:VAL:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1061:VAL:HG22	2:B:1062:ILE:HD12	1.97	0.47
2:E:378:CYS:CB	2:E:721:PRO:HB2	2.44	0.47
1:A:89:MET:HG2	1:A:90:ILE:N	2.30	0.47
1:D:321:LEU:HB3	1:D:422:LEU:HD22	1.95	0.47
2:E:803:HIS:CD2	2:E:858:LEU:CG	2.96	0.47
2:B:134:ARG:C	2:B:134:ARG:HD2	2.40	0.47
2:B:849:VAL:HG11	2:B:851:PHE:CZ	2.50	0.47
2:B:1112:LEU:HD13	2:B:1113:GLN:N	2.30	0.47
2:B:196:SER:O	2:B:200:LYS:N	2.47	0.47
2:B:890:LEU:HB2	2:B:942:PHE:CZ	2.47	0.47
2:B:826:ASN:HB2	2:B:828:TYR:CZ	2.50	0.47
2:B:1030:PHE:CE2	2:B:1038:GLY:HA3	2.49	0.47
1:D:237:LEU:HD23	2:E:358:PRO:HG3	1.97	0.47
2:E:215:GLU:OE1	2:E:215:GLU:HA	2.14	0.47
2:E:218:MET:HE2	2:E:232:ILE:HD13	1.96	0.47
2:E:1061:VAL:HG23	2:E:1062:ILE:HD13	1.97	0.47
3:C:879:PHE:CE2	3:C:885:LEU:HA	2.50	0.47
1:D:102:PHE:CD1	1:D:102:PHE:C	2.93	0.47
2:E:10:GLN:CB	2:E:1037:ILE:HD12	2.45	0.47
2:E:304:LEU:HD23	2:E:304:LEU:O	2.15	0.47
2:E:744:ASP:HB3	2:E:750:THR:HG23	1.96	0.47
1:A:92:ILE:HD12	1:A:92:ILE:N	2.28	0.47
1:A:292:ASP:O	1:A:296:ILE:HG13	2.15	0.47
2:B:210:GLU:O	2:B:211:ASN:ND2	2.48	0.47
1:D:401:LYS:HD2	1:D:415:TRP:CH2	2.50	0.47
2:E:1029:LEU:HD23	2:E:1039:LEU:HD12	1.97	0.47
1:D:165:PHE:HB2	1:D:182:VAL:CG1	2.34	0.47
2:E:279:ARG:HB3	2:E:281:PHE:CE1	2.49	0.47
2:B:123:ILE:HG13	2:B:169:PHE:CE2	2.50	0.46
2:B:859:GLN:OE1	2:B:859:GLN:CA	2.62	0.46
1:D:423:LEU:HD12	1:D:424:PRO:CD	2.45	0.46
2:E:13:THR:OG1	2:E:355:ASN:OD1	2.32	0.46
2:E:826:ASN:ND2	2:E:852:GLN:NE2	2.59	0.46
1:A:267:ASN:HB3	1:A:268:LEU:H	1.48	0.46
2:B:1052:LEU:HA	2:B:1052:LEU:HD23	1.51	0.46
1:A:94:GLY:CA	1:A:160:ILE:HD11	2.46	0.46
2:B:291:MET:HE3	2:B:291:MET:C	2.39	0.46
2:E:224:GLU:O	2:E:225:PRO:C	2.58	0.46
1:A:84:LEU:HD13	1:A:84:LEU:HA	1.83	0.46
2:B:157:ILE:HG23	2:B:201:GLU:HA	1.96	0.46
2:B:322:VAL:HG21	2:B:336:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:285:LEU:HD12	2:E:300:LEU:CD2	2.46	0.46
2:E:362:MET:HE2	2:E:1031:GLY:N	2.31	0.46
2:E:1050:LEU:HD23	2:E:1050:LEU:C	2.41	0.46
1:A:165:PHE:HA	1:A:185:LEU:HD13	1.97	0.46
1:A:439:ILE:HG22	1:A:440:LEU:H	1.80	0.46
2:B:365:VAL:HG12	2:B:367:LEU:CD1	2.46	0.46
1:D:296:ILE:O	1:D:300:LYS:HG3	2.15	0.46
1:A:257:ILE:HG12	1:A:312:LEU:HG	1.98	0.46
2:B:57:MET:HE1	2:B:79:ILE:CG2	2.44	0.46
1:D:106:GLU:O	1:D:110:VAL:HG23	2.16	0.46
2:B:970:ASN:HA	2:B:971:ALA:HA	1.62	0.46
2:B:1098:LEU:HD21	2:B:1133:VAL:CG1	2.41	0.46
2:E:263:ARG:CG	2:E:265:ASP:O	2.64	0.46
2:E:881:LEU:HD21	2:E:921:ILE:HD13	1.97	0.46
1:A:293:VAL:HG23	1:A:294:LEU:N	2.30	0.46
1:A:403:THR:HG22	1:A:413:LYS:HG2	1.97	0.46
3:C:879:PHE:CD2	3:C:885:LEU:HA	2.51	0.46
1:D:367:ASN:O	1:D:368:LEU:HD23	2.16	0.46
2:E:24:THR:HG23	2:E:30:ASN:ND2	2.31	0.46
2:E:271:TYR:HB2	2:E:283:LEU:HB3	1.98	0.46
2:E:817:VAL:HG12	2:E:830:ILE:HB	1.97	0.46
2:B:53:LYS:CD	2:B:98:ILE:HG22	2.41	0.46
2:B:118:THR:HG1	2:B:134:ARG:HH22	1.58	0.46
2:B:935:TYR:CE1	2:B:940:GLY:HA2	2.51	0.46
1:A:367:ASN:OD1	1:A:392:LYS:HE2	2.16	0.45
2:B:731:GLN:O	2:B:796:GLN:HG2	2.16	0.45
2:B:1128:ASP:O	2:B:1132:VAL:HG13	2.16	0.45
2:E:387:LEU:HB2	2:E:715:VAL:HB	1.97	0.45
2:E:891:TYR:HB3	2:E:899:LEU:HD22	1.98	0.45
2:B:171:TYR:CG	2:B:223:PRO:HA	2.51	0.45
1:D:149:ASP:N	1:D:152:ILE:O	2.49	0.45
2:E:824:ASP:OD1	2:E:825:PRO:CD	2.64	0.45
2:E:917:LYS:HB2	2:E:917:LYS:HE2	1.56	0.45
2:E:1024:THR:OG1	2:E:1041:THR:HG21	2.16	0.45
1:A:343:CYS:SG	1:A:344:GLY:N	2.89	0.45
1:D:103:HIS:ND1	1:D:104:PRO:N	2.65	0.45
1:D:141:ILE:HD12	1:D:141:ILE:H	1.80	0.45
2:E:124:ILE:CG1	2:E:131:ILE:HG12	2.46	0.45
2:E:929:SER:HB3	2:E:949:PHE:CE1	2.51	0.45
2:E:961:ASP:OD1	2:E:961:ASP:C	2.59	0.45
2:B:57:MET:SD	2:B:79:ILE:HG21	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:ARG:HH11	2:B:799:PHE:HD2	1.58	0.45
1:D:256:ARG:NH1	2:E:841:ALA:HB3	2.30	0.45
2:E:357:GLY:HA2	2:E:358:PRO:C	2.41	0.45
3:F:888:HIS:O	3:F:891:SER:HB3	2.16	0.45
1:A:384:TYR:HE2	1:A:411:PRO:O	1.99	0.45
2:B:362:MET:HG3	2:B:375:LEU:HD11	1.98	0.45
1:D:253:LEU:HD13	1:D:309:ARG:HG3	1.98	0.45
2:E:1029:LEU:HD21	2:E:1039:LEU:HD12	1.98	0.45
2:B:269:SER:HA	2:B:285:LEU:HB2	1.99	0.45
2:B:1093:LEU:HD12	2:B:1093:LEU:HA	1.81	0.45
2:E:131:ILE:HG22	2:E:143:ILE:HD12	1.99	0.45
2:E:1086:THR:O	2:E:1086:THR:HG23	2.16	0.45
1:A:287:CYS:O	1:A:346:MET:HE3	2.16	0.45
1:D:305:ILE:CG2	2:E:927:MET:CE	2.91	0.45
1:D:350:VAL:O	1:D:350:VAL:HG13	2.16	0.45
2:E:23:PHE:N	2:E:30:ASN:ND2	2.59	0.45
2:E:970:ASN:HA	2:E:971:ALA:HA	1.63	0.45
1:A:321:LEU:HD23	1:A:422:LEU:HD13	1.98	0.45
2:E:223:PRO:C	2:E:225:PRO:HD2	2.42	0.45
2:E:348:VAL:O	2:E:348:VAL:CG1	2.64	0.45
2:E:1051:LEU:CB	2:E:1089:ILE:CD1	2.95	0.45
2:B:358:PRO:HA	2:B:1033:VAL:O	2.16	0.45
1:D:232:PHE:HB2	1:D:242:ARG:HG2	1.98	0.45
2:E:889:ARG:CD	2:E:891:TYR:CZ	2.98	0.45
2:B:33:ILE:CD1	2:B:323:PHE:CZ	3.00	0.45
2:B:35:LYS:O	2:B:36:ASN:C	2.59	0.45
2:E:246:LEU:CD2	2:E:297:LEU:CD1	2.95	0.45
2:E:843:PRO:HB2	2:E:869:ALA:HB2	1.99	0.45
1:A:84:LEU:HB3	1:A:87:VAL:CG1	2.47	0.44
2:B:222:VAL:HG21	2:B:239:TYR:HE2	1.82	0.44
2:E:252:ILE:HG13	2:E:281:PHE:HE2	1.82	0.44
2:E:261:HIS:HA	2:E:272:LEU:O	2.17	0.44
1:A:114:ILE:HD12	1:A:114:ILE:HA	1.72	0.44
1:A:311:GLU:O	1:A:315:MET:HG3	2.16	0.44
2:B:291:MET:CA	2:B:291:MET:CE	2.95	0.44
2:B:838:PRO:HD2	2:B:839:GLU:OE1	2.17	0.44
2:E:123:ILE:HD12	2:E:169:PHE:CD2	2.53	0.44
2:E:263:ARG:HG3	2:E:265:ASP:O	2.18	0.44
2:E:945:ILE:HD13	2:E:945:ILE:N	2.30	0.44
1:A:197:VAL:HG23	2:B:1003:PHE:CE2	2.52	0.44
1:A:276:ASN:O	1:A:277:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:PHE:N	2:B:30:ASN:OD1	2.48	0.44
2:B:90:GLU:HG2	2:B:91:TYR:N	2.31	0.44
2:B:165:ILE:CD1	2:B:188:ARG:NH1	2.81	0.44
2:B:768:SER:O	2:B:770:LEU:HD22	2.17	0.44
2:B:1126:ALA:O	2:B:1129:LEU:N	2.50	0.44
2:E:961:ASP:OD1	2:E:962:ASP:N	2.51	0.44
1:A:137:THR:HG23	1:A:163:GLN:O	2.17	0.44
2:B:182:TYR:CZ	2:B:189:HIS:HB2	2.52	0.44
2:B:742:VAL:O	2:B:742:VAL:HG13	2.16	0.44
1:A:96:THR:HB	1:A:142:TYR:OH	2.16	0.44
1:D:288:LEU:HB3	1:D:290:ILE:HG23	1.99	0.44
2:E:248:ILE:HD11	2:E:250:PRO:HG3	1.98	0.44
2:E:315:THR:CG2	2:E:323:PHE:HB3	2.46	0.44
2:E:334:VAL:HB	2:E:347:VAL:CG1	2.47	0.44
2:E:824:ASP:OD2	2:E:828:TYR:OH	2.33	0.44
2:E:1051:LEU:HA	2:E:1054:MET:HB2	2.00	0.44
1:A:125:TYR:C	1:A:133:ALA:CB	2.91	0.44
1:A:140:GLU:OE1	1:A:162:ARG:NE	2.48	0.44
2:E:58:TYR:O	2:E:1068:ILE:HG21	2.18	0.44
2:E:239:TYR:CD1	2:E:240:HIS:N	2.86	0.44
2:E:928:ARG:NH1	2:E:950:ASN:HB3	2.31	0.44
1:A:166:LYS:HB2	1:A:185:LEU:HD11	2.00	0.44
2:B:220:ILE:O	2:B:229:ALA:HA	2.18	0.44
2:B:1105:MET:HE1	2:B:1130:ILE:HG12	1.99	0.44
1:D:264:TRP:O	1:D:265:ASP:HB2	2.16	0.44
1:D:352:PRO:HG3	1:D:378:HIS:CD2	2.53	0.44
1:D:370:LEU:HD21	1:D:415:TRP:HH2	1.83	0.44
1:A:96:THR:HA	1:A:159:ALA:O	2.17	0.44
1:A:197:VAL:CG1	1:A:197:VAL:O	2.66	0.44
2:B:241:ASN:O	2:B:242:GLY:C	2.61	0.44
2:B:1044:SER:O	2:B:1045:GLU:C	2.61	0.44
1:D:103:HIS:ND1	1:D:103:HIS:C	2.76	0.44
2:E:10:GLN:HB3	2:E:1037:ILE:HD12	2.00	0.44
2:E:66:LEU:HD23	2:E:77:LEU:HD13	2.00	0.44
1:A:96:THR:HG22	1:A:160:ILE:HD13	1.99	0.44
1:A:194:MET:HG3	1:A:232:PHE:HA	2.00	0.44
2:B:120:ILE:HG23	2:B:135:LEU:HD23	1.99	0.44
2:B:1061:VAL:HG11	2:B:1108:VAL:HG12	2.00	0.44
2:B:1105:MET:HE1	2:B:1130:ILE:HD11	1.97	0.44
2:E:66:LEU:O	2:E:67:PHE:HB3	2.18	0.44
2:E:66:LEU:CD2	2:E:77:LEU:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:932:LEU:HD22	2:E:965:PHE:HZ	1.78	0.44
2:E:1007:PHE:CD1	2:E:1030:PHE:HB3	2.53	0.44
2:E:1100:ILE:HD12	2:E:1104:LYS:CB	2.48	0.44
1:A:117:ASP:C	1:A:118:ARG:HG3	2.44	0.43
1:A:125:TYR:CA	1:A:133:ALA:HB3	2.47	0.43
2:B:1058:LEU:N	2:B:1058:LEU:HD23	2.34	0.43
2:E:131:ILE:CG2	2:E:143:ILE:HD12	2.48	0.43
2:E:288:GLU:O	2:E:295:VAL:HA	2.18	0.43
2:E:760:ALA:CB	2:E:801:VAL:HG23	2.48	0.43
2:E:816:LEU:HD13	2:E:831:VAL:HG22	1.99	0.43
2:E:847:ARG:NH1	2:E:849:VAL:CG2	2.81	0.43
1:A:102:PHE:CD1	1:A:102:PHE:C	2.96	0.43
2:B:362:MET:HE2	2:B:375:LEU:CD2	2.48	0.43
2:B:716:PRO:HB2	2:B:718:TYR:CE1	2.54	0.43
2:B:821:LEU:HD23	2:B:821:LEU:HA	1.64	0.43
2:B:1051:LEU:N	2:B:1051:LEU:HD22	2.32	0.43
2:E:855:ASP:OD1	2:E:855:ASP:N	2.50	0.43
2:E:1129:LEU:HD23	2:E:1129:LEU:HA	1.63	0.43
2:B:53:LYS:HE2	2:B:98:ILE:O	2.18	0.43
2:B:1101:SER:HB3	2:B:1103:PRO:HD2	2.01	0.43
2:E:316:TYR:CD1	2:E:316:TYR:C	2.95	0.43
1:A:101:LEU:HG	1:A:110:VAL:HG21	2.00	0.43
1:A:401:LYS:HB2	1:A:415:TRP:CZ3	2.53	0.43
2:B:282:MET:HG2	2:B:284:LEU:HD11	2.00	0.43
2:B:909:ILE:HD11	2:B:923:VAL:HG12	2.00	0.43
1:D:370:LEU:HD21	1:D:401:LYS:HD2	2.00	0.43
1:D:370:LEU:HD21	1:D:415:TRP:CH2	2.54	0.43
2:E:10:GLN:OE1	2:E:10:GLN:CA	2.67	0.43
1:D:351:ASN:OD1	1:D:351:ASN:C	2.62	0.43
2:B:766:SER:HB2	2:B:808:LEU:CD1	2.47	0.43
1:D:140:GLU:O	1:D:159:ALA:HA	2.19	0.43
2:E:24:THR:HG22	2:E:91:TYR:CD2	2.53	0.43
1:A:208:PHE:CZ	1:A:230:ARG:CB	3.02	0.43
1:A:296:ILE:CG2	1:A:300:LYS:HE3	2.49	0.43
2:E:196:SER:HB3	2:E:199:GLU:HG2	2.00	0.43
2:E:232:ILE:CG1	2:E:237:ILE:HG12	2.43	0.43
1:A:174:SER:O	1:A:175:ASP:C	2.62	0.43
2:B:24:THR:HG23	2:B:30:ASN:ND2	2.34	0.43
2:B:364:VAL:C	2:B:365:VAL:HG23	2.44	0.43
2:B:368:GLU:CB	2:B:370:GLN:HG2	2.49	0.43
1:D:442:LEU:CD2	2:E:908:ASN:O	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:ILE:HG21	2:E:167:VAL:HG13	2.00	0.43
3:F:872:CYS:CA	3:F:885:LEU:HD21	2.49	0.43
2:B:252:ILE:HG22	2:B:281:PHE:HE1	1.83	0.43
2:E:312:GLU:OE1	2:E:312:GLU:HA	2.19	0.43
2:E:1059:ASN:HD21	2:E:1070:HIS:CG	2.37	0.43
1:A:260:GLN:OE1	1:A:315:MET:HE2	2.18	0.42
1:A:291:ASP:OD2	1:A:423:LEU:HD12	2.19	0.42
2:B:213:GLU:HG3	2:B:236:SER:OG	2.19	0.42
2:B:286:GLU:OE1	2:B:301:ARG:HG3	2.19	0.42
2:B:902:GLU:HG2	2:B:903:CYS:SG	2.59	0.42
2:B:914:LEU:CD1	2:B:923:VAL:HG22	2.49	0.42
1:D:367:ASN:C	1:D:368:LEU:HD23	2.44	0.42
2:E:218:MET:HE2	2:E:232:ILE:CD1	2.48	0.42
1:A:97:LEU:HD21	1:A:159:ALA:HB3	2.00	0.42
2:B:68:ARG:HE	2:B:75:ASP:N	2.17	0.42
2:B:225:PRO:CG	2:B:267:ASN:O	2.66	0.42
1:D:76:ASP:OD1	1:D:76:ASP:O	2.37	0.42
2:E:10:GLN:HB3	2:E:1037:ILE:HB	2.01	0.42
2:E:246:LEU:HD21	2:E:299:ASP:HA	2.02	0.42
2:E:1059:ASN:HD21	2:E:1070:HIS:CB	2.31	0.42
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.90	0.42
1:A:309:ARG:NE	1:A:442:LEU:OXT	2.43	0.42
2:B:257:THR:O	2:B:275:ASP:HA	2.19	0.42
2:B:739:ARG:HH21	2:B:788:VAL:HG11	1.84	0.42
2:E:812:TYR:HD1	2:E:814:LEU:HD23	1.84	0.42
1:A:194:MET:HE2	1:A:194:MET:CA	2.48	0.42
2:B:726:TYR:CE2	2:B:728:GLU:HB2	2.54	0.42
2:B:766:SER:CB	2:B:808:LEU:CD1	2.98	0.42
2:B:1002:GLU:HB2	2:B:1032:THR:HG21	2.01	0.42
1:D:337:ILE:HG23	1:D:360:LEU:HD11	2.01	0.42
1:D:440:LEU:HD23	1:D:440:LEU:HA	1.88	0.42
2:E:132:GLY:O	2:E:133:LEU:HD12	2.19	0.42
2:E:273:LEU:HD11	2:E:283:LEU:HB2	2.00	0.42
2:E:1133:VAL:HA	2:E:1136:LEU:HD13	2.01	0.42
1:A:401:LYS:CE	1:A:413:LYS:NZ	2.82	0.42
2:B:1112:LEU:O	2:B:1124:ALA:N	2.52	0.42
1:D:253:LEU:CD1	1:D:309:ARG:HG3	2.49	0.42
1:D:345:PRO:O	1:D:360:LEU:HA	2.19	0.42
2:E:57:MET:HE2	2:E:57:MET:HB3	1.60	0.42
2:E:138:GLY:HA2	2:E:162:LEU:HD13	2.00	0.42
2:E:764:SER:OG	2:E:803:HIS:NE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:719:GLU:HB2	2:B:738:SER:O	2.19	0.42
2:B:883:SER:HB2	2:B:911:ALA:HB3	2.01	0.42
2:E:744:ASP:CB	2:E:750:THR:HG23	2.49	0.42
2:E:1047:TRP:HE3	2:E:1051:LEU:HD21	1.85	0.42
1:A:271:ASP:C	1:A:273:LEU:N	2.77	0.42
2:B:55:VAL:HG22	2:B:56:GLY:N	2.35	0.42
2:B:387:LEU:HA	2:B:387:LEU:HD23	1.81	0.42
2:B:870:VAL:HG22	2:B:884:ILE:HD11	1.99	0.42
2:B:907:ASN:HD22	2:B:931:LEU:HD11	1.83	0.42
2:B:965:PHE:O	2:B:976:VAL:HA	2.19	0.42
2:E:59:GLY:HA2	2:E:1073:TRP:CE3	2.55	0.42
2:E:120:ILE:H	2:E:120:ILE:CD1	2.32	0.42
2:E:218:MET:HB2	2:E:232:ILE:HB	2.01	0.42
2:E:803:HIS:CD2	2:E:858:LEU:HD12	2.53	0.42
1:A:106:GLU:O	1:A:110:VAL:HG23	2.20	0.42
2:B:32:LEU:CD2	2:B:77:LEU:HD22	2.49	0.42
2:B:1062:ILE:HD12	2:B:1062:ILE:N	2.34	0.42
1:D:321:LEU:HD12	1:D:332:THR:CG2	2.50	0.42
3:F:871:THR:HA	3:F:877:ALA:O	2.19	0.42
2:B:223:PRO:HD2	2:B:268:GLY:HA3	2.00	0.42
1:D:172:THR:OG1	1:D:178:GLN:NE2	2.53	0.42
1:D:258:LYS:HB3	1:D:258:LYS:HE3	1.86	0.42
1:D:320:SER:OG	1:D:427:PRO:HG3	2.20	0.42
2:E:131:ILE:HG22	2:E:133:LEU:HD13	2.00	0.42
1:A:165:PHE:CA	1:A:185:LEU:HD13	2.50	0.42
2:E:138:GLY:O	2:E:139:LEU:HD12	2.20	0.42
2:E:849:VAL:HG11	2:E:851:PHE:CZ	2.55	0.42
2:B:101:ILE:O	2:B:101:ILE:HG13	2.20	0.41
2:B:290:GLN:HA	2:B:290:GLN:OE1	2.20	0.41
1:D:346:MET:HE2	1:D:346:MET:HB3	1.89	0.41
2:E:120:ILE:N	2:E:120:ILE:CD1	2.83	0.41
2:E:165:ILE:HG12	2:E:181:VAL:HG12	2.01	0.41
2:E:868:GLY:HA3	2:E:884:ILE:HG22	2.01	0.41
2:E:960:LEU:HA	2:E:960:LEU:HD23	1.67	0.41
1:A:118:ARG:O	1:A:141:ILE:HG13	2.20	0.41
2:B:142:VAL:O	2:B:144:PRO:HD3	2.20	0.41
2:B:167:VAL:O	2:B:167:VAL:HG13	2.20	0.41
2:B:183:GLN:OE1	2:B:188:ARG:HG3	2.20	0.41
2:B:741:GLU:OE2	2:B:751:ALA:HB2	2.20	0.41
2:B:909:ILE:HD12	2:B:910:MET:O	2.20	0.41
2:B:985:THR:O	2:B:989:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:ARG:HD2	2:E:266:PRO:HA	2.02	0.41
2:E:1050:LEU:HD23	2:E:1050:LEU:O	2.20	0.41
1:A:78:CYS:HA	1:A:182:VAL:O	2.20	0.41
1:A:135:PHE:CD2	1:A:300:LYS:HD3	2.53	0.41
1:A:346:MET:O	1:A:346:MET:CG	2.64	0.41
2:B:64:MET:HG3	2:B:79:ILE:HD11	2.01	0.41
2:B:321:VAL:HG22	2:B:350:MET:SD	2.59	0.41
2:B:341:ASN:OD1	2:B:344:GLY:N	2.49	0.41
1:D:76:ASP:OD1	1:D:183:GLN:OE1	2.38	0.41
1:D:300:LYS:HE2	1:D:300:LYS:HB3	1.89	0.41
2:E:24:THR:HG22	2:E:91:TYR:CE2	2.56	0.41
2:E:155:PHE:CD1	2:E:155:PHE:C	2.97	0.41
2:B:146:ASP:OD1	2:B:146:ASP:O	2.37	0.41
2:B:272:LEU:O	2:B:273:LEU:HD23	2.20	0.41
2:B:960:LEU:HD23	2:B:960:LEU:HA	1.61	0.41
1:D:105:GLN:O	1:D:177:ILE:HD11	2.19	0.41
2:E:24:THR:HG23	2:E:30:ASN:CG	2.45	0.41
2:E:89:LEU:HD22	2:E:102:THR:HG22	2.00	0.41
1:A:337:ILE:CD1	1:A:360:LEU:HD11	2.50	0.41
2:B:112:ILE:HD12	2:B:113:GLY:N	2.31	0.41
1:D:89:MET:HE1	7:D:602:HOH:O	2.21	0.41
2:E:33:ILE:HD11	2:E:323:PHE:CZ	2.56	0.41
1:A:190:LEU:CD1	2:B:927:MET:HE3	2.50	0.41
2:B:124:ILE:HG12	2:B:131:ILE:HG12	2.01	0.41
2:B:262:ASN:HB2	2:B:314:LEU:O	2.21	0.41
2:B:928:ARG:HG2	2:B:928:ARG:O	2.20	0.41
2:B:1076:PHE:CE1	2:B:1078:THR:HG22	2.56	0.41
1:D:207:ILE:HB	2:E:165:ILE:HD12	2.03	0.41
2:E:40:GLU:HG2	2:E:54:GLU:HG3	2.01	0.41
2:E:1007:PHE:HD1	2:E:1030:PHE:HB3	1.85	0.41
2:E:1112:LEU:HD12	2:E:1112:LEU:HA	1.76	0.41
1:A:201:SER:OG	1:A:202:LEU:HD22	2.20	0.41
3:C:869:LEU:O	3:C:885:LEU:CD1	2.68	0.41
1:D:87:VAL:HG23	1:D:123:LEU:HB2	2.00	0.41
1:D:165:PHE:CB	1:D:182:VAL:CG1	2.94	0.41
2:E:121:ILE:HD11	2:E:166:ASP:HA	2.03	0.41
2:E:178:ILE:C	2:E:178:ILE:CD1	2.93	0.41
2:E:1010:GLY:O	2:E:1027:SER:OG	2.31	0.41
2:E:1090:ASP:O	2:E:1093:LEU:N	2.53	0.41
2:E:1136:LEU:O	2:E:1139:ILE:HG12	2.20	0.41
1:A:199:LEU:HB3	1:A:202:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD23	2:B:327:ARG:NH1	2.35	0.41
1:A:440:LEU:N	1:A:440:LEU:HD22	2.35	0.41
2:B:718:TYR:CD1	2:B:718:TYR:N	2.89	0.41
2:B:752:LEU:HD23	2:B:752:LEU:HA	1.82	0.41
1:D:398:ILE:HD13	1:D:421:ALA:HB1	2.03	0.41
2:E:310:ILE:HG21	2:E:328:LEU:HD22	2.02	0.41
3:F:872:CYS:HB2	3:F:885:LEU:HD21	2.03	0.41
1:A:90:ILE:N	1:A:90:ILE:CD1	2.84	0.41
1:A:104:PRO:O	1:A:107:VAL:HG22	2.20	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.83	0.41
2:B:907:ASN:ND2	2:B:931:LEU:HD21	2.36	0.41
2:B:1058:LEU:O	2:B:1060:LYS:N	2.54	0.41
1:D:280:PHE:CE1	1:D:284:VAL:HG21	2.55	0.41
2:E:246:LEU:HD23	2:E:297:LEU:CD1	2.50	0.41
2:E:272:LEU:HD12	2:E:282:MET:SD	2.61	0.41
2:E:789:HIS:HE1	2:E:812:TYR:CE1	2.39	0.41
2:B:1002:GLU:HB3	2:B:1032:THR:HG21	2.03	0.41
2:B:1105:MET:HE1	2:B:1130:ILE:CD1	2.51	0.41
2:B:1128:ASP:OD1	2:B:1128:ASP:N	2.32	0.41
2:E:263:ARG:HB2	2:E:271:TYR:CE1	2.56	0.41
2:E:801:VAL:CG2	2:E:801:VAL:O	2.69	0.41
2:E:931:LEU:HD12	2:E:932:LEU:H	1.86	0.41
2:E:1101:SER:C	2:E:1103:PRO:HD2	2.46	0.41
2:B:803:HIS:CD2	2:B:858:LEU:HB2	2.56	0.40
2:B:997:LEU:N	2:B:1086:THR:HG22	2.36	0.40
1:D:381:PHE:CD1	1:D:381:PHE:N	2.89	0.40
2:E:192:THR:OG1	2:E:205:GLY:HA3	2.21	0.40
2:E:926:LEU:HD12	2:E:926:LEU:HA	1.72	0.40
2:B:273:LEU:HB2	2:B:281:PHE:HB2	2.03	0.40
2:B:760:ALA:O	2:B:761:LEU:C	2.64	0.40
2:B:770:LEU:HD13	2:B:770:LEU:HA	1.79	0.40
2:B:810:ASN:ND2	2:B:837:TYR:CD1	2.89	0.40
1:D:227:TYR:CZ	1:D:231:LYS:HD2	2.55	0.40
2:E:1105:MET:O	2:E:1109:VAL:HG13	2.21	0.40
1:A:198:GLN:HB3	1:A:203:ASN:HD21	1.86	0.40
2:B:38:ARG:HH21	2:B:54:GLU:CD	2.30	0.40
2:B:58:TYR:OH	2:B:1093:LEU:HD13	2.21	0.40
2:B:245:TYR:CD1	2:B:245:TYR:C	2.99	0.40
2:B:741:GLU:HG2	2:B:751:ALA:CA	2.37	0.40
2:B:968:ALA:CB	2:B:1004:VAL:HB	2.51	0.40
2:E:10:GLN:OE1	2:E:11:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:904:ASN:HB3	2:E:906:TYR:CE1	2.56	0.40
2:E:1009:HIS:CE1	2:E:1028:VAL:HG22	2.57	0.40
1:A:304:ALA:O	1:A:308:LEU:HG	2.21	0.40
2:B:803:HIS:CD2	2:B:858:LEU:CB	3.04	0.40
2:B:816:LEU:HD13	2:B:831:VAL:HG22	2.03	0.40
2:B:893:TRP:CE3	2:B:893:TRP:HA	2.56	0.40
2:B:997:LEU:O	2:B:1085:ALA:HA	2.22	0.40
2:B:1057:ARG:HD2	2:B:1108:VAL:O	2.21	0.40
1:D:304:ALA:O	1:D:308:LEU:HG	2.21	0.40
2:E:133:LEU:CD2	2:E:143:ILE:HD11	2.43	0.40
2:E:157:ILE:HD13	2:E:157:ILE:HG21	1.92	0.40
2:E:276:MET:O	2:E:310:ILE:HD12	2.21	0.40
2:E:314:LEU:HD23	2:E:314:LEU:HA	1.88	0.40
2:E:879:LYS:HB3	2:E:891:TYR:O	2.21	0.40
1:A:88:MET:O	1:A:89:MET:HB2	2.22	0.40
1:A:89:MET:C	1:A:90:ILE:HD12	2.47	0.40
1:A:270:ASP:C	1:A:272:SER:N	2.79	0.40
2:B:123:ILE:HG13	2:B:169:PHE:HE2	1.87	0.40
2:E:93:GLN:NE2	2:E:95:GLY:O	2.55	0.40
2:E:275:ASP:OD2	2:E:279:ARG:HB2	2.21	0.40
2:E:955:SER:OG	2:E:1004:VAL:O	2.29	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	328/373 (88%)	302 (92%)	23 (7%)	3 (1%)	14	34
1	D	339/373 (91%)	304 (90%)	32 (9%)	3 (1%)	14	34
2	B	791/836 (95%)	727 (92%)	61 (8%)	3 (0%)	30	53
2	E	783/836 (94%)	724 (92%)	57 (7%)	2 (0%)	36	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	24/30 (80%)	22 (92%)	2 (8%)	0	100	100
3	F	25/30 (83%)	25 (100%)	0	0	100	100
All	All	2290/2478 (92%)	2104 (92%)	175 (8%)	11 (0%)	24	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	CYS
2	B	95	GLY
1	D	272	SER
1	A	85	PRO
1	A	267	ASN
2	B	242	GLY
1	D	271	ASP
2	B	344	GLY
2	E	225	PRO
2	E	825	PRO
1	D	85	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	288/340 (85%)	280 (97%)	8 (3%)	38	62
1	D	272/340 (80%)	264 (97%)	8 (3%)	37	61
2	B	643/727 (88%)	623 (97%)	20 (3%)	35	59
2	E	609/727 (84%)	593 (97%)	16 (3%)	40	65
3	C	19/26 (73%)	17 (90%)	2 (10%)	6	19
3	F	21/26 (81%)	20 (95%)	1 (5%)	23	48
All	All	1852/2186 (85%)	1797 (97%)	55 (3%)	36	60

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	154	ILE
1	A	171	ARG
1	A	267	ASN
1	A	277	PRO
1	A	341	SER
1	A	371	ILE
1	A	441	CYS
2	B	20	THR
2	B	164	VAL
2	B	211	ASN
2	B	213	GLU
2	B	252	ILE
2	B	299	ASP
2	B	304	LEU
2	B	348	VAL
2	B	364	VAL
2	B	720	SER
2	B	785	GLU
2	B	815	SER
2	B	865	GLU
2	B	912	LEU
2	B	919	ASP
2	B	931	LEU
2	B	1006	VAL
2	B	1108	VAL
2	B	1133	VAL
2	B	1139	ILE
3	C	878	CYS
3	C	885	LEU
1	D	108	SER
1	D	211	LYS
1	D	237	LEU
1	D	244	LEU
1	D	288	LEU
1	D	294	LEU
1	D	312	LEU
1	D	340	LEU
2	E	15	VAL
2	E	37	THR
2	E	97	SER
2	E	125	ASP
2	E	195	VAL

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Mol	Chain	Res	Type
2	E	265	ASP
2	E	296	THR
2	E	729	VAL
2	E	827	THR
2	E	880	LEU
2	E	917	LYS
2	E	981	SER
2	E	1039	LEU
2	E	1046	SER
2	E	1127	ASP
2	E	1133	VAL
3	F	873	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	206	GLN
1	A	297	GLN
2	B	211	ASN
2	B	727	GLN
2	B	743	GLN
2	B	826	ASN
2	B	905	HIS
2	B	907	ASN
2	B	941	ASN
2	B	950	ASN
2	B	991	HIS
2	B	1034	ASN
2	B	1070	HIS
1	D	73	HIS
1	D	163	GLN
1	D	178	GLN
1	D	198	GLN
1	D	233	HIS
2	E	30	ASN
2	E	85	ASN
2	E	107	ASN
2	E	156	ASN
2	E	211	ASN
2	E	370	GLN
2	E	727	GLN

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Mol	Chain	Res	Type
2	E	826	ASN
2	E	852	GLN
2	E	1055	GLN
2	E	1056	ASN
2	E	1059	ASN
2	E	1140	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1A5H	A	503	-	33,33,33	0.44	0	44,50,50	0.55	0
5	SO4	A	502	-	4,4,4	0.94	0	6,6,6	0.31	0
6	A1A5H	D	503	-	33,33,33	0.35	0	44,50,50	0.66	1 (2%)
5	SO4	D	502	-	4,4,4	0.88	0	6,6,6	0.23	0

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
6	A1A5H	D	503	-	-	3/10/55/55	0/5/5/5
6	A1A5H	A	503	-	-	4/10/55/55	0/5/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	503	A1A5H	C11-C17-N16	2.09	114.70	110.91

There are no chirality outliers.

All (7) torsion outliers are listed below:

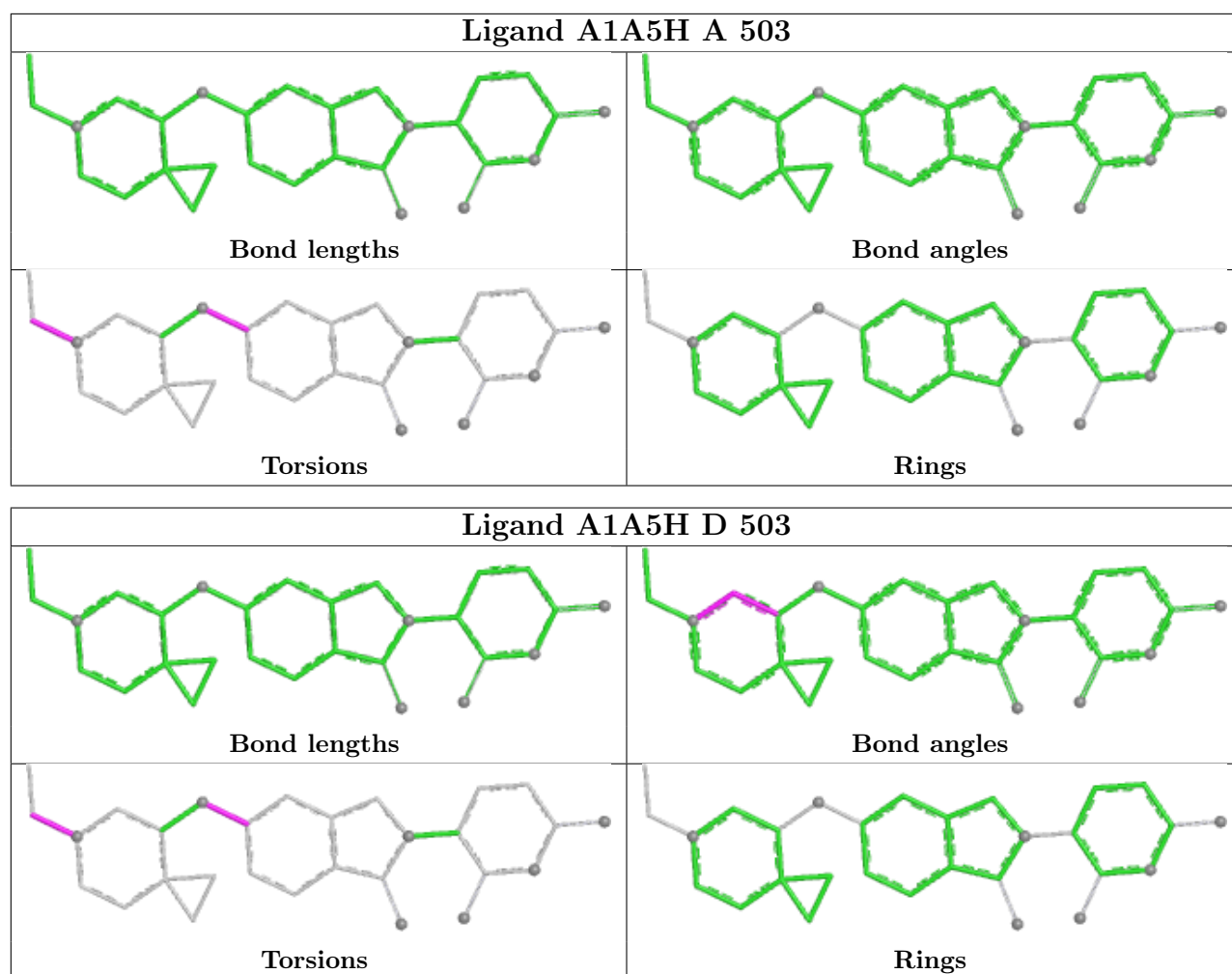
Mol	Chain	Res	Type	Atoms
6	A	503	A1A5H	C21-C20-N16-C17
6	A	503	A1A5H	C21-C20-N16-C15
6	A	503	A1A5H	C3-C2-O12-C11
6	A	503	A1A5H	C1-C2-O12-C11
6	D	503	A1A5H	C1-C2-O12-C11
6	D	503	A1A5H	C3-C2-O12-C11
6	D	503	A1A5H	C21-C20-N16-C17

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	SO4	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/373 (90%)	-0.20	3 (0%) 81 76	74, 96, 150, 182	0
1	D	347/373 (93%)	-0.16	2 (0%) 85 82	76, 96, 154, 199	0
2	B	801/836 (95%)	-0.24	3 (0%) 88 86	69, 98, 144, 189	0
2	E	795/836 (95%)	-0.20	8 (1%) 79 74	73, 102, 148, 194	0
3	C	26/30 (86%)	-0.05	1 (3%) 44 36	90, 102, 113, 117	0
3	F	27/30 (90%)	-0.08	0 100 100	89, 101, 124, 134	0
All	All	2334/2478 (94%)	-0.20	17 (0%) 84 80	69, 99, 149, 199	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	847	ARG	3.5
1	D	175	ASP	2.7
1	A	272	SER	2.6
2	E	291	MET	2.5
2	B	146	ASP	2.4
2	E	202	PHE	2.4
2	E	1054	MET	2.4
2	E	148	ASP	2.4
1	A	281	SER	2.3
1	A	172	THR	2.3
2	E	16	ASN	2.3
2	E	1112	LEU	2.3
1	D	271	ASP	2.2
2	B	745	THR	2.1
2	E	1076	PHE	2.1
3	C	885	LEU	2.1
2	B	983	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

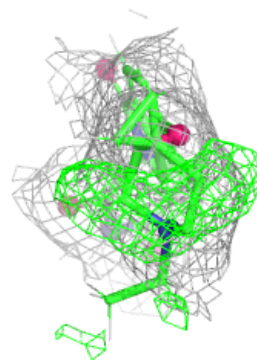
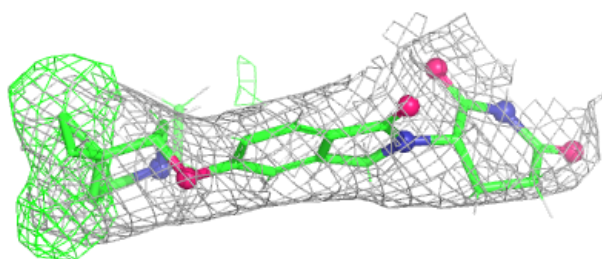
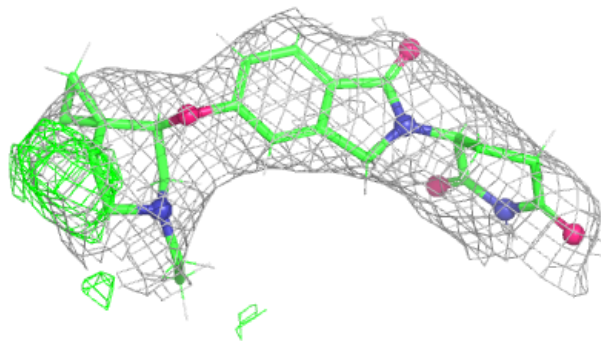
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	A1A5H	A	503	29/29	0.86	0.13	90,111,140,143	27
5	SO4	D	502	5/5	0.88	0.14	119,119,127,128	0
6	A1A5H	D	503	29/29	0.88	0.11	89,112,133,141	27
5	SO4	A	502	5/5	0.94	0.09	99,104,109,112	0
4	ZN	D	501	1/1	0.99	0.08	102,102,102,102	0
4	ZN	A	501	1/1	1.00	0.04	92,92,92,92	0
4	ZN	F	900	1/1	1.00	0.04	101,101,101,101	0
4	ZN	C	900	1/1	1.00	0.03	97,97,97,97	0

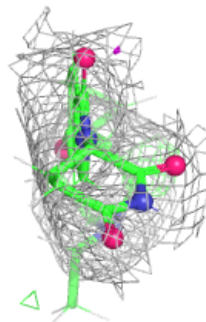
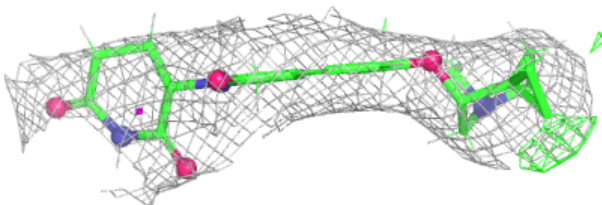
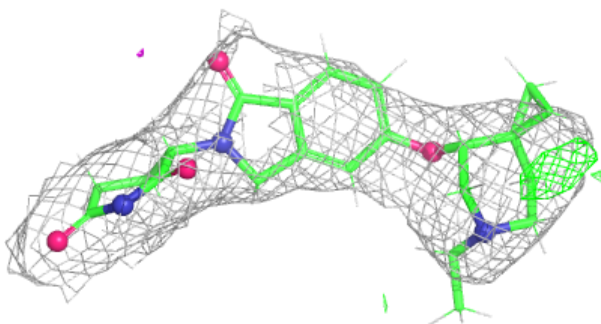
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1A5H A 503:

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

**Electron density around A1A5H D 503:**

$2mF_o-DF_c$ (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.