



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:06 AM UTC

PDB ID : 6S7Q / pdb_00006s7q
Title : Crystal structure of ergothioneine degrading enzyme Ergothionase from *Treponema denticola* in complex with desmethyl-ergothioneine sulfonic acid
Authors : Leisinger, F.; Seebeck, F.P.
Deposited on : 2019-07-05
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

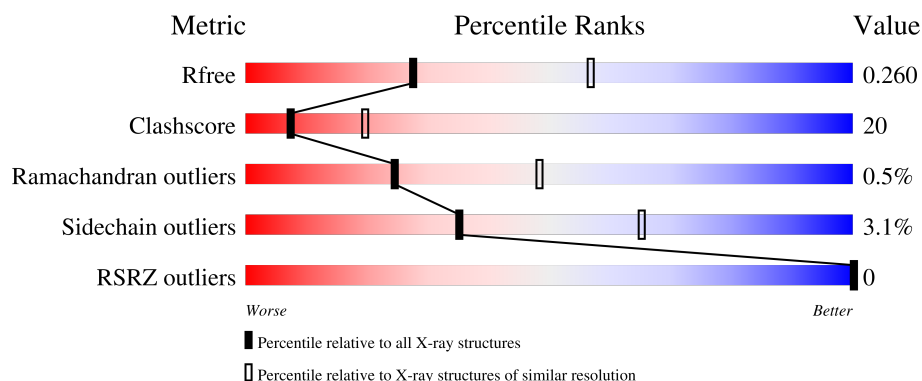
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	 63% 35% 2% 0% 0%
1	B	497	 64% 34% 2% 0% 0%
1	C	497	 62% 37% 1% 0% 0%
1	D	497	 64% 34% 2% 0% 0%
1	E	497	 68% 30% 2% 0% 0%

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Mol	Chain	Length	Quality of chain
1	F	497	 62% 35% .
1	G	497	 62% 35% .
1	H	497	 67% 31% .

2 Entry composition

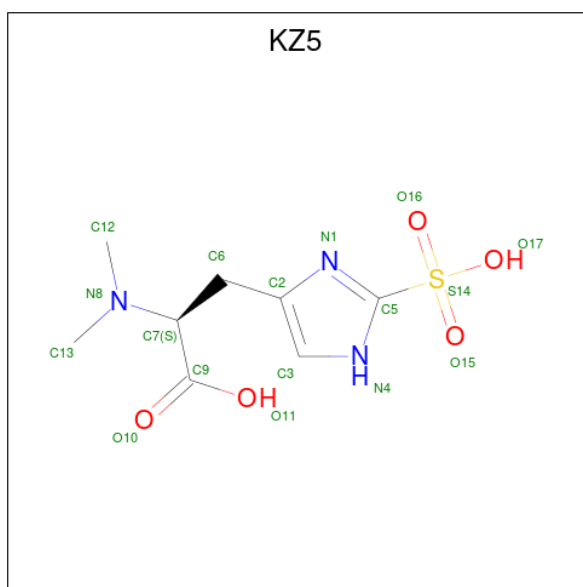
There are 3 unique types of molecules in this entry. The entry contains 31655 atoms, of which 104 are hydrogens and 0 are deuteriums.

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 ergothionase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	B	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	C	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	D	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	E	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	F	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	G	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			
1	H	497	Total	C	N	O	S	0	0	0
			3902	2468	667	742	25			

- Molecule 2 is (2 {S})-2-(dimethylamino)-3-(2-sulfo-1 {H}-imidazol-4-yl)propanoic acid (CCD ID: KZ5) (formula: C₈H₁₃N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	C	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	C	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	D	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	E	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	F	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	G	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0
2	H	1	Total 30	C 8	H 13	N 3	O 5	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	35	Total	O	0	0
			35	35		
3	C	26	Total	O	0	0
			26	26		
3	D	24	Total	O	0	0
			24	24		

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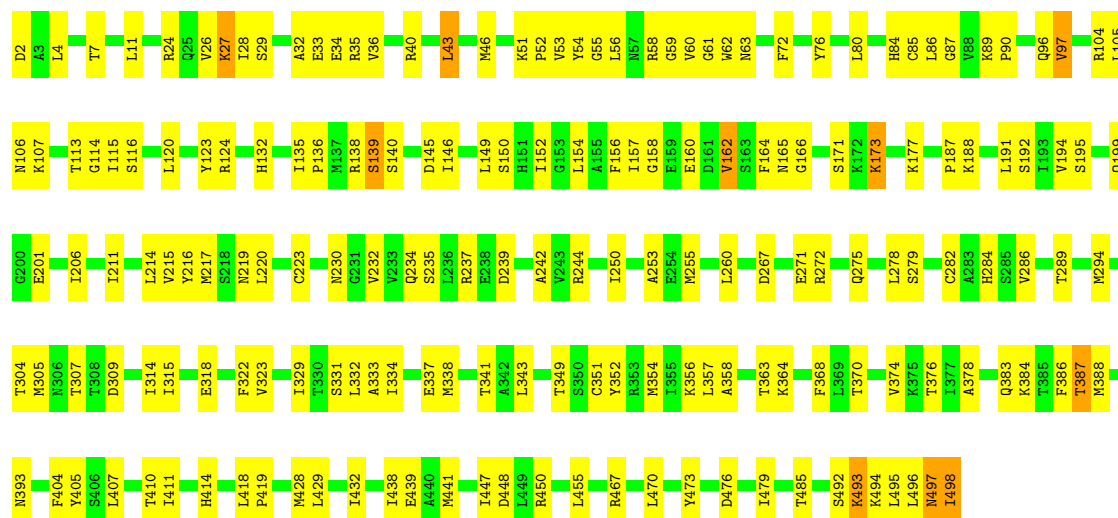
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	25	Total 25	O 25	0	0
3	F	23	Total 23	O 23	0	0
3	G	16	Total 16	O 16	0	0
3	H	14	Total 14	O 14	0	0

3 Residue-property plots [i](#)

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.

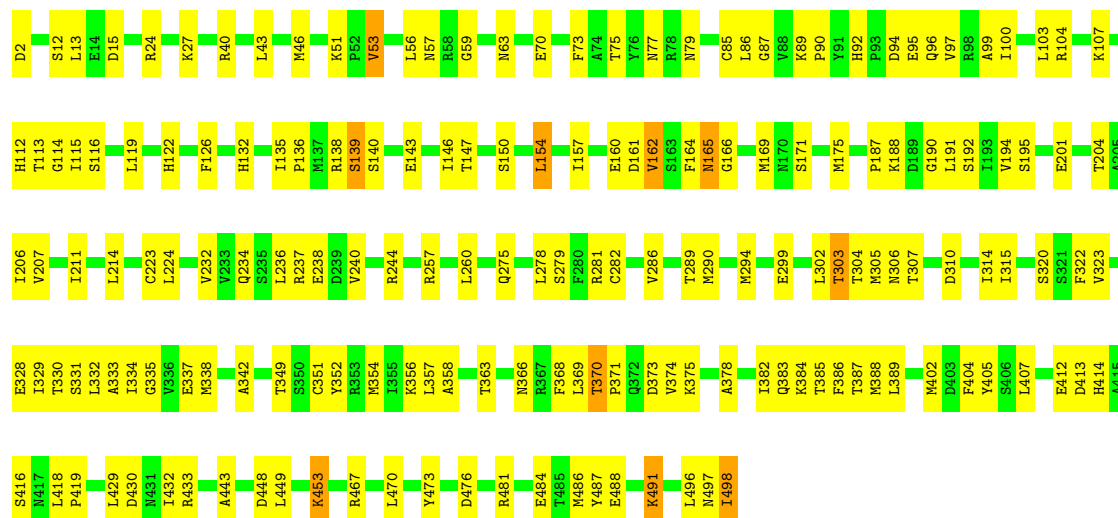
• Molecule 1: ergothionase

Chain A: 



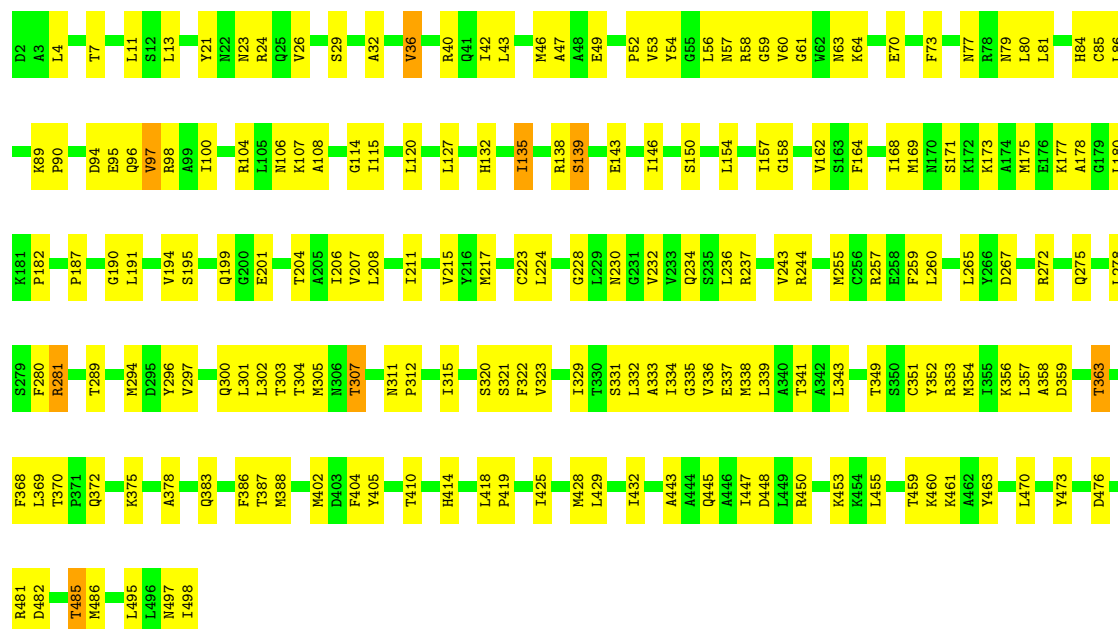
• Molecule 1: ergothionase

Chain B: 



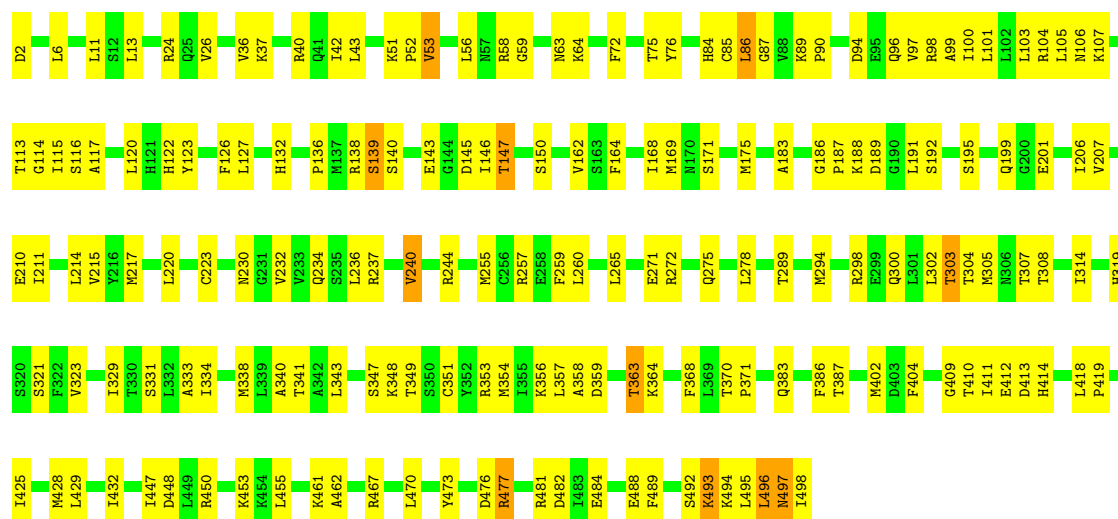
- Molecule 1: ergothionase

Chain C:  62% 37%



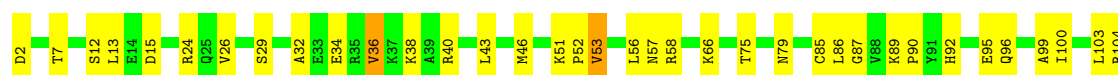
- Molecule 1: ergothionase

Chain D:  64% 34%



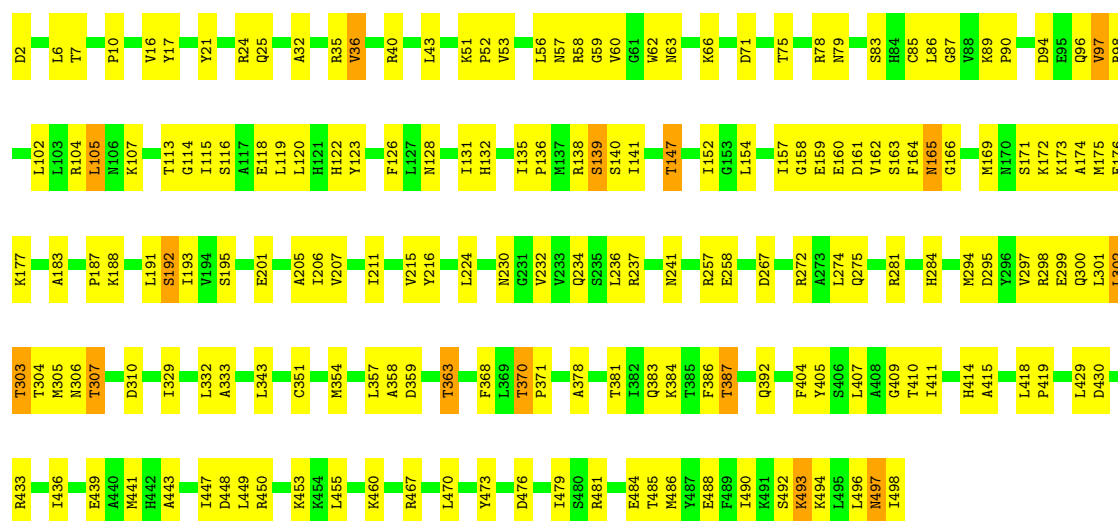
- Molecule 1: ergothionase

Chain E:  68% 30%

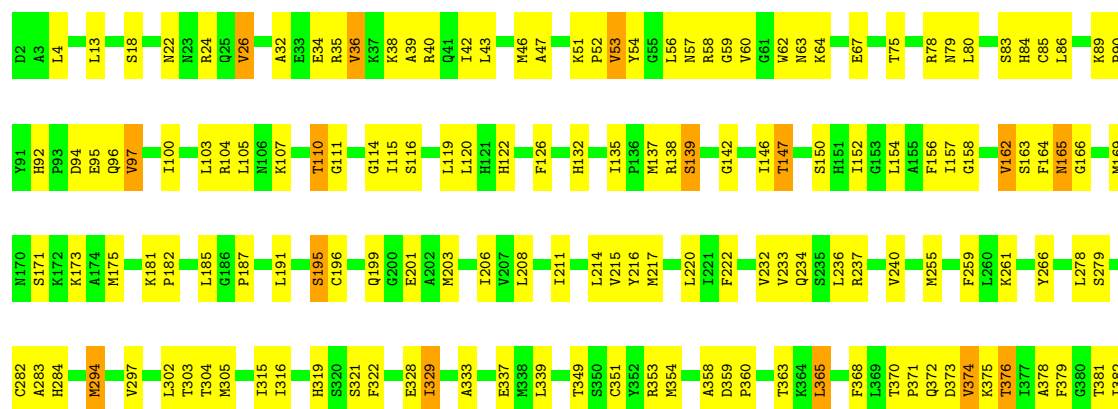


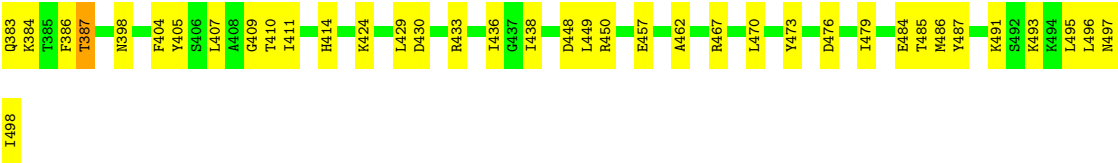


• Molecule 1: ergothionase

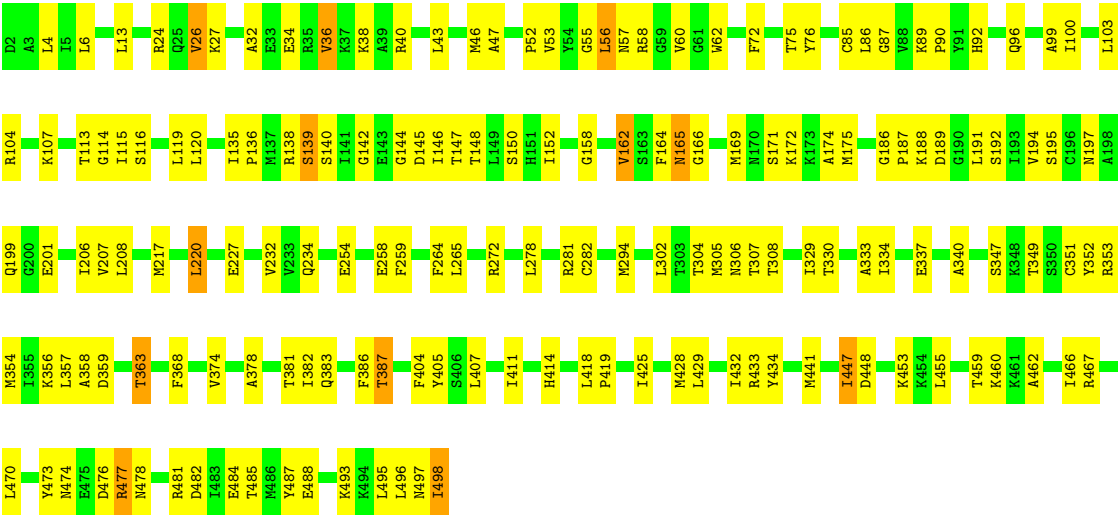


• Molecule 1: ergothionase





● Molecule 1: ergothionase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.76Å 76.94Å 174.84Å 88.56° 81.41° 79.79°	Depositor
Resolution (Å)	49.05 – 2.70 49.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.05-2.70) 79.8 (49.05-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.261 0.226 , 0.260	Depositor DCC
R_{free} test set	5182 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	1.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31655	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KZ5

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	0.13	0/3971	0.33	0/5358
1	B	0.12	0/3971	0.33	0/5358
1	C	0.12	0/3971	0.33	0/5358
1	D	0.11	0/3971	0.33	0/5358
1	E	0.11	0/3971	0.32	0/5358
1	F	0.11	0/3971	0.34	0/5358
1	G	0.11	0/3971	0.32	0/5358
1	H	0.11	0/3971	0.31	0/5358
All	All	0.12	0/31768	0.33	0/42864

There are no bond length outliers.

There are no bond angle outliers.

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	3902	0	3912	177	0
1	B	3902	0	3912	175	0
1	C	3902	0	3911	197	0
1	D	3902	0	3912	180	0
1	E	3902	0	3910	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3902	0	3912	161	0
1	G	3902	0	3912	186	0
1	H	3902	0	3910	154	0
2	A	17	13	0	1	0
2	C	34	26	0	5	0
2	D	17	13	0	4	0
2	E	17	13	0	2	0
2	F	17	13	0	3	0
2	G	17	13	0	4	0
2	H	17	13	0	2	0
3	A	36	0	0	4	0
3	B	35	0	0	1	0
3	C	26	0	0	2	0
3	D	24	0	0	1	0
3	E	25	0	0	4	0
3	F	23	0	0	3	0
3	G	16	0	0	1	0
3	H	14	0	0	2	0
All	All	31551	104	31291	1276	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 20.

All (1276) 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:E:53:VAL:HB	1:E:56:LEU:HD21	1.27	1.16
1:H:46:MET:HE3	1:H:53:VAL:HG21	1.32	1.11
1:B:53:VAL:HB	1:B:56:LEU:HD21	1.22	1.10
1:C:301:LEU:HG	1:C:305:MET:HE2	1.30	1.10
1:A:53:VAL:HB	1:A:56:LEU:HD21	1.32	1.05
1:B:329:ILE:HD11	1:B:332:LEU:HD23	1.39	1.04
1:B:86:LEU:HB2	1:B:147:THR:HG23	1.41	1.03
1:C:338:MET:HE3	1:D:338:MET:HE3	1.42	1.01
1:F:301:LEU:HG	1:F:305:MET:HE2	1.44	0.99
1:G:383:GLN:O	1:G:387:THR:OG1	1.79	0.99
1:D:448:ASP:OD2	1:D:467:ARG:NH1	1.95	0.98
1:F:53:VAL:HB	1:F:56:LEU:HD21	1.44	0.98
1:F:383:GLN:O	1:F:387:THR:OG1	1.81	0.98
1:A:46:MET:HE3	1:A:53:VAL:HG21	1.46	0.97
1:G:169:MET:SD	1:G:173:LYS:NZ	2.37	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASP:OD2	1:A:467:ARG:NH1	1.98	0.96
1:D:211:ILE:HD13	1:D:429:LEU:HD21	1.46	0.95
1:H:383:GLN:O	1:H:387:THR:OG1	1.82	0.94
1:F:211:ILE:HD13	1:F:429:LEU:HD21	1.50	0.93
1:B:46:MET:HE3	1:B:53:VAL:HG21	1.48	0.92
1:G:363:THR:HG23	1:G:365:LEU:H	1.34	0.92
1:C:211:ILE:HD13	1:C:429:LEU:HD21	1.49	0.92
1:E:46:MET:HE3	1:E:53:VAL:HG21	1.53	0.90
1:C:47:ALA:HB2	1:C:56:LEU:HD21	1.50	0.89
1:E:212:GLU:HB2	1:E:294:MET:HE1	1.54	0.87
1:G:164:PHE:HB3	1:G:169:MET:HE3	1.56	0.87
1:C:42:ILE:O	1:C:46:MET:HG2	1.74	0.87
1:F:329:ILE:HD11	1:F:332:LEU:HD23	1.57	0.87
1:A:27:LYS:HZ2	1:A:28:ILE:H	1.21	0.86
1:C:278:LEU:HD13	1:D:412:GLU:HA	1.56	0.86
1:C:338:MET:HE3	1:D:338:MET:CE	2.04	0.86
1:D:383:GLN:O	1:D:387:THR:OG1	1.94	0.85
1:A:338:MET:HE3	1:B:338:MET:HE3	1.57	0.85
1:F:303:THR:O	1:F:307:THR:OG1	1.93	0.85
1:A:211:ILE:HD13	1:A:429:LEU:HD21	1.59	0.84
1:D:340:ALA:HB1	1:D:428:MET:HE1	1.58	0.84
1:E:53:VAL:CB	1:E:56:LEU:HD21	2.07	0.84
1:H:40:ARG:HH12	1:H:187:PRO:HD2	1.42	0.84
1:B:211:ILE:HD13	1:B:429:LEU:HD21	1.57	0.84
1:C:335:GLY:HA2	1:D:338:MET:HE1	1.58	0.83
1:G:32:ALA:O	1:G:36:VAL:HG23	1.79	0.83
1:F:329:ILE:HD13	1:F:418:LEU:HD22	1.60	0.83
1:A:220:LEU:HD21	1:A:498:ILE:HD12	1.60	0.83
1:B:51:LYS:O	1:B:57:ASN:ND2	2.11	0.82
1:H:477:ARG:HG2	1:H:478:ASN:N	1.95	0.82
1:A:244:ARG:HH22	1:B:304:THR:HG23	1.44	0.81
1:B:53:VAL:CB	1:B:56:LEU:HD21	2.09	0.81
1:E:52:PRO:HA	1:E:57:ASN:HD21	1.43	0.81
1:A:338:MET:HE1	1:B:335:GLY:HA2	1.63	0.81
1:B:53:VAL:HB	1:B:56:LEU:CD2	2.08	0.81
1:B:481:ARG:HG2	1:B:481:ARG:HH11	1.46	0.81
1:D:164:PHE:HB3	1:D:169:MET:HE3	1.62	0.81
1:G:100:ILE:CD1	1:G:199:GLN:HA	2.11	0.80
1:C:32:ALA:O	1:C:36:VAL:HG23	1.81	0.80
1:F:298:ARG:O	1:F:302:LEU:HD23	1.80	0.80
1:A:173:LYS:HE2	1:A:177:LYS:HZ1	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ILE:CD1	1:C:429:LEU:HD21	2.11	0.80
1:A:338:MET:CE	1:B:338:MET:HE3	2.11	0.79
1:B:94:ASP:O	1:B:97:VAL:HG12	1.82	0.79
1:H:100:ILE:CD1	1:H:199:GLN:HA	2.12	0.79
1:A:53:VAL:CB	1:A:56:LEU:HD21	2.11	0.79
1:F:216:TYR:OH	1:F:497:ASN:O	1.99	0.79
1:D:461:LYS:NZ	1:D:498:ILE:HG13	1.98	0.79
1:D:94:ASP:HA	1:D:97:VAL:HG12	1.65	0.79
1:F:131:ILE:HG23	1:F:162:VAL:HG11	1.63	0.79
1:D:211:ILE:CD1	1:D:429:LEU:HD21	2.13	0.78
1:G:42:ILE:O	1:G:46:MET:HG2	1.81	0.78
1:C:98:ARG:NH1	1:C:127:LEU:O	2.16	0.78
1:C:335:GLY:HA2	1:D:338:MET:CE	2.13	0.78
1:H:140:SER:HB3	1:H:419:PRO:HG2	1.65	0.78
1:H:169:MET:HE2	1:H:174:ALA:HB2	1.65	0.78
1:A:329:ILE:HD11	1:A:332:LEU:HD23	1.66	0.77
1:D:96:GLN:HG2	1:D:206:ILE:HG13	1.67	0.77
1:E:191:LEU:HD22	1:E:195:SER:HB2	1.65	0.76
1:C:329:ILE:HD11	1:C:332:LEU:HD23	1.67	0.76
1:G:181:LYS:HG3	1:G:182:PRO:HD2	1.68	0.76
1:E:124:ARG:NH1	1:E:125:ASP:OD1	2.19	0.76
1:B:385:THR:O	1:B:389:LEU:HD13	1.84	0.76
1:D:191:LEU:HD12	1:D:195:SER:HB2	1.67	0.76
1:H:53:VAL:HB	1:H:56:LEU:CD2	2.15	0.75
1:C:304:THR:HG23	1:D:244:ARG:HH22	1.51	0.75
1:G:107:LYS:NZ	1:G:196:CYS:SG	2.57	0.75
1:C:244:ARG:HA	1:D:307:THR:HG21	1.67	0.75
1:C:115:ILE:HG21	1:C:120:LEU:HD21	1.68	0.75
2:E:501:KZ5:C3	1:H:60:VAL:HB	2.17	0.75
1:H:162:VAL:HG21	1:H:171:SER:HA	1.69	0.75
1:C:53:VAL:HG23	1:C:56:LEU:HB3	1.68	0.75
1:H:46:MET:CE	1:H:53:VAL:HG21	2.15	0.75
1:D:340:ALA:CB	1:D:428:MET:HE1	2.17	0.74
1:F:52:PRO:HA	1:F:57:ASN:HD21	1.51	0.74
1:A:173:LYS:HE2	1:A:177:LYS:NZ	2.02	0.74
1:A:43:LEU:HD21	1:A:114:GLY:HA3	1.70	0.74
1:F:211:ILE:CD1	1:F:429:LEU:HD21	2.18	0.74
1:F:173:LYS:HB3	1:F:177:LYS:NZ	2.03	0.73
1:D:453:LYS:HE2	1:D:453:LYS:HA	1.68	0.73
1:H:340:ALA:CB	1:H:428:MET:HE1	2.18	0.73
1:A:211:ILE:HD12	1:A:343:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:VAL:HB	1:E:56:LEU:CD2	2.13	0.73
1:G:162:VAL:HG21	1:G:171:SER:HA	1.70	0.73
1:H:191:LEU:HD12	1:H:195:SER:HB2	1.71	0.73
1:D:94:ASP:HA	1:D:97:VAL:CG1	2.19	0.73
1:D:271:GLU:O	1:D:364:LYS:NZ	2.22	0.73
1:G:142:GLY:O	1:G:329:ILE:HD11	1.88	0.73
1:A:162:VAL:HG21	1:A:171:SER:HA	1.71	0.72
1:A:60:VAL:HB	2:A:501:KZ5:C3	2.18	0.72
1:A:479:ILE:HB	1:D:86:LEU:CD1	2.20	0.72
1:C:77:ASN:O	1:C:81:LEU:HD13	1.89	0.72
1:D:461:LYS:HZ2	1:D:498:ILE:HG13	1.54	0.72
1:D:498:ILE:HG23	1:D:498:ILE:O	1.87	0.72
1:A:214:LEU:HD21	1:A:432:ILE:HG21	1.70	0.72
1:D:85:CYS:O	1:D:86:LEU:HD13	1.89	0.72
1:E:162:VAL:HG21	1:E:171:SER:HA	1.71	0.71
1:G:430:ASP:OD1	1:G:487:TYR:OH	2.08	0.71
1:A:338:MET:HB2	1:B:338:MET:HE2	1.71	0.71
1:B:107:LYS:NZ	1:B:201:GLU:OE1	2.23	0.71
1:G:383:GLN:HA	1:G:386:PHE:CZ	2.26	0.71
1:A:53:VAL:HB	1:A:56:LEU:CD2	2.17	0.70
1:B:329:ILE:HG12	1:B:332:LEU:HB3	1.73	0.70
1:F:97:VAL:HG22	1:F:135:ILE:HD12	1.73	0.70
1:F:96:GLN:HG2	1:F:206:ILE:HG13	1.73	0.70
1:C:36:VAL:HG11	1:C:120:LEU:HD12	1.74	0.70
1:C:372:GLN:HG2	1:C:375:LYS:HD2	1.72	0.70
1:D:84:HIS:C	1:D:86:LEU:HD22	2.16	0.70
1:D:186:GLY:N	1:D:189:ASP:OD2	2.20	0.70
1:H:87:GLY:HA3	1:H:136:PRO:HG2	1.74	0.70
1:B:329:ILE:CD1	1:B:332:LEU:HD23	2.20	0.70
1:G:115:ILE:HD11	1:G:119:LEU:HD13	1.73	0.70
1:B:97:VAL:HG11	1:B:132:HIS:HB3	1.74	0.69
1:C:461:LYS:HB2	1:C:498:ILE:HG13	1.74	0.69
1:H:162:VAL:CG2	1:H:171:SER:HA	2.22	0.69
1:H:477:ARG:NH1	1:H:482:ASP:OD1	2.21	0.69
1:B:412:GLU:OE1	2:C:501:KZ5:O17	2.10	0.69
1:C:100:ILE:CD1	1:C:199:GLN:HA	2.22	0.69
1:A:407:LEU:HD11	1:D:387:THR:HG21	1.75	0.69
1:E:253:ALA:HB2	1:E:284:HIS:CD2	2.28	0.69
1:F:53:VAL:CB	1:F:56:LEU:HD21	2.20	0.69
1:C:191:LEU:HD12	1:C:195:SER:HB2	1.75	0.69
1:A:211:ILE:CD1	1:A:429:LEU:HD21	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ARG:NH2	1:E:187:PRO:HD2	2.08	0.68
1:F:119:LEU:HD13	1:F:193:ILE:HD11	1.75	0.68
1:G:4:LEU:HB2	1:G:24:ARG:HE	1.59	0.68
1:B:94:ASP:HA	1:B:97:VAL:HG12	1.74	0.68
1:C:447:ILE:HG21	1:C:455:LEU:HD21	1.76	0.68
1:E:302:LEU:HD23	1:E:305:MET:CE	2.23	0.68
1:A:338:MET:CE	1:B:335:GLY:HA2	2.23	0.68
1:C:267:ASP:HB3	1:F:71:ASP:OD2	1.92	0.68
1:D:36:VAL:HG11	1:D:120:LEU:HD12	1.75	0.68
1:E:100:ILE:CD1	1:E:199:GLN:HA	2.24	0.68
1:F:267:ASP:O	1:F:272:ARG:NH1	2.26	0.68
1:A:447:ILE:HG21	1:A:455:LEU:HD21	1.74	0.68
1:E:2:ASP:O	1:E:24:ARG:HD2	1.93	0.68
1:H:53:VAL:HB	1:H:56:LEU:HD22	1.73	0.68
1:G:363:THR:OG1	1:G:365:LEU:HD23	1.94	0.67
1:B:315:ILE:HD12	1:B:322:PHE:CD2	2.29	0.67
1:C:97:VAL:HG11	1:C:132:HIS:HB3	1.75	0.67
1:A:4:LEU:HD13	1:A:24:ARG:NH1	2.10	0.67
1:C:53:VAL:HG21	1:C:56:LEU:HD23	1.75	0.67
1:D:492:SER:C	1:D:494:LYS:H	2.03	0.67
1:F:371:PRO:HA	1:F:449:LEU:HD11	1.77	0.67
1:C:453:LYS:HA	1:C:453:LYS:HE2	1.76	0.67
1:B:302:LEU:HD23	1:B:305:MET:CE	2.24	0.66
1:C:40:ARG:NH2	1:C:187:PRO:HD2	2.10	0.66
1:C:211:ILE:HD11	1:C:343:LEU:HD11	1.77	0.66
1:C:244:ARG:HA	1:D:307:THR:CG2	2.25	0.66
1:C:473:TYR:OH	1:C:476:ASP:HA	1.94	0.66
1:G:36:VAL:HG11	1:G:120:LEU:HD12	1.77	0.66
1:C:302:LEU:HD23	1:C:305:MET:HE3	1.78	0.66
1:B:97:VAL:HG23	1:B:135:ILE:HD12	1.77	0.66
1:C:481:ARG:O	1:C:485:THR:HG23	1.96	0.66
1:G:156:PHE:O	1:G:175:MET:HE1	1.95	0.66
1:C:301:LEU:CG	1:C:305:MET:HE2	2.18	0.66
1:D:302:LEU:HD23	1:D:305:MET:CE	2.26	0.66
1:B:481:ARG:HG2	1:B:481:ARG:NH1	2.11	0.66
1:B:211:ILE:CD1	1:B:429:LEU:HD21	2.24	0.65
1:F:378:ALA:HA	1:F:473:TYR:CE2	2.30	0.65
1:G:47:ALA:HB2	1:G:56:LEU:HD21	1.77	0.65
1:G:164:PHE:HB3	1:G:169:MET:CE	2.27	0.65
1:G:370:THR:CG2	1:G:376:THR:HG23	2.27	0.65
1:A:162:VAL:CG2	1:A:171:SER:HA	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:LEU:HA	1:H:272:ARG:NH1	2.11	0.65
1:D:13:LEU:HD23	1:D:305:MET:HE1	1.79	0.65
1:E:357:LEU:O	1:E:363:THR:HG21	1.96	0.65
1:C:211:ILE:HD12	1:C:343:LEU:HD21	1.77	0.65
1:A:2:ASP:O	1:A:24:ARG:HD2	1.96	0.65
1:A:87:GLY:HA3	1:A:136:PRO:HG2	1.79	0.65
1:A:341:THR:HG23	1:B:402:MET:HE1	1.78	0.65
1:C:303:THR:O	1:C:307:THR:OG1	2.15	0.65
1:D:461:LYS:HZ1	1:D:498:ILE:HA	1.62	0.65
1:G:372:GLN:HB3	1:G:376:THR:HG22	1.78	0.65
1:H:115:ILE:HG21	1:H:120:LEU:HD21	1.79	0.65
1:D:52:PRO:HB3	1:D:58:ARG:NH2	2.12	0.64
1:D:333:ALA:HA	1:D:418:LEU:HD13	1.78	0.64
1:A:441:MET:HG3	1:A:470:LEU:HD21	1.78	0.64
1:H:32:ALA:O	1:H:36:VAL:HG23	1.98	0.64
1:F:43:LEU:HD11	1:F:114:GLY:HA3	1.78	0.64
1:C:315:ILE:HD12	1:C:322:PHE:CD2	2.33	0.64
1:E:176:GLU:HG2	3:F:602:HOH:O	1.96	0.64
1:D:329:ILE:HD12	1:D:418:LEU:CD2	2.28	0.64
1:C:244:ARG:O	1:D:307:THR:HG21	1.97	0.64
1:D:467:ARG:HD3	1:D:470:LEU:O	1.98	0.64
1:G:52:PRO:HA	1:G:57:ASN:HD21	1.62	0.64
1:C:96:GLN:HG2	1:C:206:ILE:HG13	1.80	0.64
1:C:329:ILE:HD13	1:C:418:LEU:HD22	1.77	0.64
1:F:94:ASP:HB3	1:F:132:HIS:HD2	1.61	0.64
1:B:40:ARG:HD2	1:B:116:SER:HA	1.79	0.64
1:D:56:LEU:HD13	1:D:187:PRO:HB2	1.80	0.64
1:F:32:ALA:O	1:F:36:VAL:HG23	1.98	0.64
1:F:53:VAL:HB	1:F:56:LEU:CD2	2.24	0.64
1:H:357:LEU:O	1:H:363:THR:HG21	1.97	0.64
1:C:498:ILE:HD12	1:C:498:ILE:H	1.63	0.64
1:E:253:ALA:HB2	1:E:284:HIS:HD2	1.62	0.63
1:F:172:LYS:HE2	1:F:176:GLU:OE2	1.98	0.63
1:A:43:LEU:HD21	1:A:314:ILE:CD1	2.29	0.63
1:A:497:ASN:O	1:A:498:ILE:HB	1.99	0.63
1:C:53:VAL:CG2	1:C:56:LEU:HB3	2.29	0.63
1:E:405:TYR:CD1	1:H:387:THR:HG23	2.33	0.63
1:G:89:LYS:HB2	1:G:90:PRO:HA	1.80	0.63
1:H:85:CYS:HA	1:H:150:SER:OG	1.98	0.63
1:G:85:CYS:HA	1:G:150:SER:OG	1.98	0.63
1:G:162:VAL:CG2	1:G:171:SER:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:LYS:NZ	1:G:457:GLU:OE1	2.31	0.63
1:A:230:ASN:OD1	1:A:272:ARG:NH2	2.32	0.63
1:F:173:LYS:O	1:F:177:LYS:HG3	1.98	0.63
1:A:40:ARG:NH2	1:A:187:PRO:HD2	2.13	0.63
1:B:498:ILE:HD13	1:B:498:ILE:N	2.14	0.63
1:C:201:GLU:OE2	1:C:304:THR:HG22	1.98	0.63
1:E:162:VAL:CG2	1:E:171:SER:HA	2.28	0.63
1:E:201:GLU:OE2	1:E:304:THR:HG22	1.98	0.63
1:G:169:MET:HB2	1:G:173:LYS:HE3	1.80	0.63
1:F:40:ARG:NH2	1:F:187:PRO:HD2	2.14	0.63
1:G:370:THR:HG22	1:G:372:GLN:H	1.64	0.63
1:A:267:ASP:O	1:A:272:ARG:NH1	2.32	0.63
1:C:98:ARG:HD3	1:C:132:HIS:CE1	2.33	0.63
1:F:6:LEU:HD13	1:F:105:LEU:HD22	1.81	0.63
1:A:357:LEU:O	1:A:363:THR:HG21	2.00	0.62
1:E:214:LEU:HD13	1:E:214:LEU:O	1.98	0.62
1:A:89:LYS:HB2	1:A:90:PRO:HA	1.81	0.62
1:B:2:ASP:O	1:B:24:ARG:HD2	1.99	0.62
1:G:201:GLU:OE1	1:G:305:MET:HA	1.97	0.62
1:D:359:ASP:O	1:D:363:THR:HG23	1.99	0.62
1:H:254:GLU:OE2	1:H:258:GLU:OE2	2.18	0.62
1:A:253:ALA:HB2	1:A:284:HIS:CD2	2.34	0.62
1:B:87:GLY:HA3	1:B:136:PRO:HG2	1.82	0.62
1:D:357:LEU:O	1:D:363:THR:HG21	2.00	0.62
1:H:140:SER:CB	1:H:419:PRO:HG2	2.29	0.62
1:A:43:LEU:CD2	1:A:114:GLY:HA3	2.30	0.62
1:F:383:GLN:HA	1:F:386:PHE:CE2	2.35	0.62
1:C:297:VAL:HG21	1:C:339:LEU:HD11	1.82	0.62
1:A:97:VAL:HG11	1:A:132:HIS:HB3	1.81	0.62
1:A:304:THR:HG23	1:B:244:ARG:HH22	1.65	0.62
1:C:36:VAL:HG11	1:C:120:LEU:CD1	2.30	0.62
1:F:89:LYS:HB2	1:F:90:PRO:HA	1.82	0.62
1:F:329:ILE:HD13	1:F:418:LEU:CD2	2.29	0.62
1:F:492:SER:O	1:F:494:LYS:N	2.33	0.62
1:G:40:ARG:NH2	1:G:187:PRO:HD2	2.14	0.62
1:H:278:LEU:HD12	1:H:282:CYS:SG	2.40	0.62
1:A:27:LYS:NZ	1:A:28:ILE:H	1.97	0.61
1:A:383:GLN:O	1:A:387:THR:HB	2.00	0.61
1:B:405:TYR:CD1	1:C:387:THR:HG23	2.34	0.61
1:A:27:LYS:HZ2	1:A:28:ILE:N	1.95	0.61
1:D:383:GLN:HA	1:D:386:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:GLY:HA2	1:F:171:SER:OG	2.00	0.61
1:G:304:THR:HG21	1:G:329:ILE:HG22	1.82	0.61
1:C:85:CYS:HA	1:C:150:SER:OG	2.01	0.61
1:C:334:ILE:C	1:D:338:MET:HE2	2.25	0.61
1:E:383:GLN:HA	1:E:386:PHE:CE2	2.36	0.61
1:F:7:THR:O	1:F:35:ARG:NH2	2.33	0.61
1:G:56:LEU:HD13	1:G:187:PRO:HB2	1.82	0.61
1:A:40:ARG:HA	1:A:43:LEU:HD23	1.83	0.61
1:F:113:THR:HG23	1:F:310:ASP:OD2	2.00	0.61
1:G:220:LEU:HD21	1:G:462:ALA:HB2	1.82	0.61
1:H:135:ILE:HD11	1:H:152:ILE:HD11	1.83	0.61
1:C:56:LEU:HD13	1:C:187:PRO:HB2	1.82	0.61
1:E:34:GLU:HG3	1:E:38:LYS:NZ	2.16	0.61
1:E:382:ILE:HA	1:H:86:LEU:HD13	1.82	0.61
1:G:126:PHE:HZ	1:G:175:MET:HE3	1.64	0.61
1:A:253:ALA:HB2	1:A:284:HIS:HD2	1.66	0.60
1:D:358:ALA:HB1	1:D:368:PHE:CD1	2.36	0.60
1:C:191:LEU:CD1	1:C:195:SER:HB2	2.32	0.60
1:F:51:LYS:O	1:F:53:VAL:HG23	2.00	0.60
1:H:340:ALA:HB1	1:H:428:MET:HE1	1.83	0.60
1:B:366:ASN:HB3	1:B:370:THR:HG22	1.81	0.60
1:F:383:GLN:HA	1:F:386:PHE:CZ	2.36	0.60
1:G:371:PRO:HG2	1:G:376:THR:HG21	1.83	0.60
1:A:338:MET:HE3	1:B:338:MET:HB2	1.83	0.60
1:A:107:LYS:HD2	1:A:307:THR:O	2.01	0.60
1:F:94:ASP:HB3	1:F:132:HIS:CD2	2.36	0.60
1:G:429:LEU:O	1:G:433:ARG:HG3	2.01	0.60
1:A:216:TYR:HA	1:A:255:MET:HE1	1.84	0.60
1:D:40:ARG:NH2	1:D:187:PRO:HD2	2.16	0.60
1:G:86:LEU:HB2	1:G:147:THR:HG22	1.84	0.60
1:B:40:ARG:NH2	1:B:187:PRO:HD2	2.16	0.60
1:B:150:SER:O	1:B:154:LEU:HD22	2.02	0.60
1:C:4:LEU:HB2	1:C:24:ARG:HE	1.66	0.60
1:C:334:ILE:O	1:D:338:MET:HE2	2.01	0.60
1:D:13:LEU:HD11	1:D:298:ARG:HG3	1.84	0.60
1:D:85:CYS:C	1:D:86:LEU:HD13	2.27	0.60
1:G:34:GLU:HG2	1:G:38:LYS:HE3	1.83	0.60
1:B:51:LYS:NZ	1:B:320:SER:OG	2.34	0.60
1:B:162:VAL:CG2	1:B:171:SER:HA	2.31	0.60
1:B:384:LYS:NZ	2:C:502:KZ5:O17	2.30	0.60
1:E:378:ALA:HA	1:E:473:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:ILE:HD12	1:G:322:PHE:CD2	2.37	0.60
1:B:86:LEU:HB2	1:B:147:THR:CG2	2.26	0.60
1:G:302:LEU:HD23	1:G:305:MET:CE	2.32	0.60
2:F:501:KZ5:O17	1:G:384:LYS:NZ	2.30	0.59
1:B:387:THR:HG23	1:C:405:TYR:CD1	2.38	0.59
1:C:104:ARG:O	1:C:104:ARG:HD3	2.03	0.59
1:D:104:ARG:O	1:D:104:ARG:HD3	2.02	0.59
1:D:113:THR:HG22	1:D:192:SER:OG	2.02	0.59
1:G:470:LEU:HD22	1:G:486:MET:SD	2.42	0.59
1:H:429:LEU:O	1:H:433:ARG:HG3	2.02	0.59
1:A:275:GLN:HG2	1:B:323:VAL:HG11	1.84	0.59
1:D:6:LEU:HD11	1:D:26:VAL:HG21	1.83	0.59
1:D:492:SER:O	1:D:494:LYS:N	2.34	0.59
1:C:201:GLU:OE1	1:C:305:MET:HA	2.03	0.59
1:A:467:ARG:HD3	1:A:470:LEU:O	2.02	0.59
1:B:384:LYS:NZ	2:C:502:KZ5:O16	2.36	0.59
1:C:278:LEU:HD23	1:D:143:GLU:OE2	2.02	0.59
1:E:232:VAL:HG12	1:E:234:GLN:H	1.67	0.59
1:H:36:VAL:HG11	1:H:120:LEU:CD1	2.33	0.59
1:A:338:MET:HE2	1:B:334:ILE:O	2.03	0.59
1:F:358:ALA:HB1	1:F:368:PHE:CD1	2.37	0.59
1:F:404:PHE:CE1	1:F:414:HIS:HA	2.37	0.59
1:G:236:LEU:HD21	1:G:284:HIS:HB3	1.85	0.59
1:E:139:SER:C	1:E:147:THR:HG21	2.27	0.59
1:G:132:HIS:HB2	1:G:163:SER:HB3	1.85	0.59
1:B:43:LEU:CD1	1:B:114:GLY:HA3	2.33	0.59
1:B:107:LYS:HD3	1:B:307:THR:O	2.03	0.59
1:D:84:HIS:O	1:D:86:LEU:HD22	2.03	0.58
1:H:201:GLU:OE2	1:H:304:THR:HG22	2.03	0.58
1:A:338:MET:HE2	1:B:334:ILE:C	2.28	0.58
1:C:244:ARG:CA	1:D:307:THR:HG21	2.33	0.58
1:E:479:ILE:HB	1:H:86:LEU:HD23	1.85	0.58
1:A:354:MET:HG3	1:A:439:GLU:HG3	1.85	0.58
1:C:42:ILE:CG2	1:C:46:MET:HE3	2.32	0.58
1:C:175:MET:HE1	1:C:182:PRO:CA	2.34	0.58
1:E:96:GLN:O	1:E:100:ILE:HG12	2.03	0.58
1:E:104:ARG:O	1:E:104:ARG:HD3	2.03	0.58
1:A:244:ARG:NH2	1:B:304:THR:HG23	2.16	0.58
1:C:173:LYS:HG2	1:C:177:LYS:HZ2	1.68	0.58
1:A:113:THR:HG22	1:A:192:SER:OG	2.02	0.58
1:F:104:ARG:O	1:F:104:ARG:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:381:THR:HG23	2:H:501:KZ5:O15	2.04	0.58
1:C:329:ILE:CD1	1:C:332:LEU:HD23	2.34	0.57
1:D:40:ARG:HD2	1:D:116:SER:HA	1.86	0.57
1:E:32:ALA:O	1:E:36:VAL:HG23	2.04	0.57
1:E:85:CYS:HA	1:E:150:SER:OG	2.03	0.57
1:H:115:ILE:HD11	1:H:119:LEU:HD13	1.85	0.57
1:C:80:LEU:HG	1:C:84:HIS:CE1	2.39	0.57
1:C:169:MET:SD	1:C:173:LYS:NZ	2.76	0.57
1:D:220:LEU:HD21	1:D:462:ALA:HB2	1.86	0.57
1:B:139:SER:HB2	1:B:147:THR:HG21	1.85	0.57
1:E:138:ARG:O	1:E:139:SER:CB	2.52	0.57
1:A:315:ILE:HD12	1:A:322:PHE:CD2	2.40	0.57
1:C:402:MET:CE	1:D:341:THR:HG23	2.34	0.57
1:D:72:PHE:CE2	1:D:76:TYR:HB2	2.39	0.57
1:E:359:ASP:O	1:E:363:THR:HG23	2.04	0.57
1:G:191:LEU:O	1:G:195:SER:HB2	2.05	0.57
1:C:372:GLN:HG2	1:C:375:LYS:CD	2.35	0.57
1:E:100:ILE:HD13	1:E:199:GLN:HA	1.87	0.57
1:F:188:LYS:O	1:F:192:SER:HB3	2.04	0.57
1:G:100:ILE:HD13	1:G:199:GLN:HA	1.85	0.57
1:C:244:ARG:C	1:D:307:THR:HG21	2.30	0.57
1:C:275:GLN:HB3	1:C:281:ARG:NH1	2.19	0.57
1:F:493:LYS:HD3	1:F:496:LEU:HD11	1.87	0.57
1:G:35:ARG:HA	1:G:38:LYS:HZ2	1.69	0.57
1:G:383:GLN:HA	1:G:386:PHE:CE2	2.40	0.57
1:B:2:ASP:O	1:B:24:ARG:NH2	2.26	0.57
1:E:126:PHE:CZ	1:E:175:MET:HE2	2.40	0.57
1:G:35:ARG:HA	1:G:38:LYS:NZ	2.20	0.56
1:G:135:ILE:HD11	1:G:152:ILE:CG1	2.35	0.56
1:H:4:LEU:HB2	1:H:24:ARG:HE	1.70	0.56
1:B:51:LYS:O	1:B:53:VAL:HG23	2.03	0.56
1:B:104:ARG:O	1:B:104:ARG:HD3	2.04	0.56
1:B:162:VAL:HG21	1:B:171:SER:HA	1.85	0.56
1:E:113:THR:HG23	1:E:310:ASP:OD2	2.05	0.56
1:E:156:PHE:O	1:E:175:MET:HE1	2.05	0.56
1:F:358:ALA:HB1	1:F:368:PHE:HD1	1.69	0.56
1:H:56:LEU:HD23	1:H:57:ASN:H	1.71	0.56
1:A:383:GLN:HA	1:A:386:PHE:CZ	2.40	0.56
1:F:59:GLY:HA3	1:F:63:ASN:O	2.05	0.56
1:B:302:LEU:O	1:B:306:ASN:ND2	2.36	0.56
1:C:146:ILE:HA	1:C:194:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASN:HB2	1:C:450:ARG:CZ	2.36	0.56
1:A:323:VAL:HG11	1:B:275:GLN:HG2	1.87	0.56
1:C:304:THR:HG21	1:C:329:ILE:CD1	2.36	0.56
1:D:493:LYS:O	1:D:496:LEU:HB2	2.05	0.56
1:A:11:LEU:HD13	1:A:106:ASN:ND2	2.21	0.56
3:A:614:HOH:O	1:D:89:LYS:HG2	2.05	0.56
1:C:164:PHE:HB3	1:C:169:MET:HE3	1.88	0.56
1:E:265:LEU:HA	1:E:272:ARG:NH1	2.20	0.56
1:F:43:LEU:CD1	1:F:114:GLY:HA3	2.36	0.56
1:F:173:LYS:HB3	1:F:177:LYS:HZ3	1.69	0.56
1:F:115:ILE:HG21	1:F:120:LEU:HD21	1.87	0.56
1:C:329:ILE:HG12	1:C:332:LEU:HB3	1.87	0.56
1:F:2:ASP:O	1:F:24:ARG:HD2	2.05	0.56
1:F:351:CYS:HA	1:F:354:MET:HE3	1.88	0.56
1:A:96:GLN:HG2	1:A:206:ILE:HG13	1.88	0.56
1:B:384:LYS:NZ	2:C:502:KZ5:S14	2.80	0.56
1:F:105:LEU:HD23	1:F:105:LEU:C	2.31	0.56
1:H:138:ARG:O	1:H:139:SER:CB	2.54	0.56
1:A:27:LYS:HZ3	1:A:124:ARG:HH11	1.54	0.55
1:B:191:LEU:HD12	1:B:195:SER:HB2	1.88	0.55
1:B:232:VAL:CG1	1:B:234:GLN:HG3	2.36	0.55
1:C:338:MET:HE2	1:D:338:MET:HB2	1.87	0.55
1:G:51:LYS:O	1:G:53:VAL:HG23	2.06	0.55
1:A:278:LEU:HD13	1:B:143:GLU:OE2	2.05	0.55
1:B:278:LEU:HD22	1:B:282:CYS:SG	2.45	0.55
1:G:278:LEU:HD12	1:G:282:CYS:SG	2.46	0.55
1:C:46:MET:HE1	1:C:321:SER:H	1.71	0.55
1:E:309:ASP:HB2	1:E:327:PHE:HA	1.88	0.55
1:F:21:TYR:OH	1:F:206:ILE:HD12	2.06	0.55
1:G:97:VAL:HG11	1:G:132:HIS:HB3	1.88	0.55
1:H:358:ALA:HB1	1:H:368:PHE:CD1	2.40	0.55
1:B:232:VAL:HG12	1:B:234:GLN:H	1.71	0.55
1:H:358:ALA:HB1	1:H:368:PHE:HD1	1.72	0.55
1:A:220:LEU:CD2	1:A:498:ILE:HD12	2.35	0.55
1:D:211:ILE:CD1	1:D:343:LEU:HD11	2.36	0.55
1:E:43:LEU:HD11	1:E:114:GLY:HA3	1.88	0.55
1:F:496:LEU:O	1:F:497:ASN:HB2	2.06	0.55
1:G:54:TYR:OH	1:G:60:VAL:HG13	2.06	0.55
1:G:201:GLU:OE2	1:G:304:THR:HG22	2.06	0.55
1:G:62:TRP:HA	1:G:411:ILE:HD12	1.87	0.55
1:G:216:TYR:HA	1:G:255:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:LYS:HB2	1:H:90:PRO:HA	1.89	0.55
1:A:32:ALA:HA	1:A:35:ARG:NH1	2.21	0.55
1:E:333:ALA:HA	1:E:418:LEU:HD13	1.87	0.55
1:G:158:GLY:HA2	1:G:171:SER:OG	2.05	0.55
1:H:169:MET:HE2	1:H:174:ALA:CB	2.36	0.55
1:B:112:HIS:ND1	1:B:314:ILE:O	2.34	0.55
1:B:382:ILE:HA	1:C:86:LEU:HD13	1.88	0.55
1:C:372:GLN:HG2	1:C:375:LYS:CG	2.36	0.55
1:E:232:VAL:CG1	1:E:234:GLN:HG3	2.37	0.55
1:B:113:THR:HG22	1:B:192:SER:OG	2.07	0.55
1:C:455:LEU:HB2	1:C:460:LYS:HE3	1.88	0.55
1:D:43:LEU:HD11	1:D:114:GLY:HA3	1.89	0.55
1:E:405:TYR:CG	1:H:387:THR:HG23	2.42	0.55
1:F:329:ILE:HG12	1:F:332:LEU:HB3	1.89	0.55
1:G:115:ILE:HD11	1:G:119:LEU:CD1	2.36	0.55
1:H:497:ASN:O	1:H:498:ILE:HB	2.07	0.55
1:D:37:LYS:HE2	1:D:117:ALA:CB	2.37	0.55
1:E:92:HIS:HD2	1:E:135:ILE:HG22	1.71	0.55
1:F:131:ILE:CG2	1:F:162:VAL:HG11	2.33	0.55
1:H:142:GLY:O	1:H:329:ILE:HD11	2.07	0.55
1:B:201:GLU:OE2	1:B:304:THR:HG22	2.07	0.54
1:G:104:ARG:HD3	1:G:104:ARG:O	2.07	0.54
1:G:126:PHE:CZ	1:G:175:MET:HE3	2.43	0.54
1:H:191:LEU:CD1	1:H:195:SER:HB2	2.36	0.54
1:C:349:THR:HG22	1:C:353:ARG:NH1	2.22	0.54
1:C:402:MET:HE1	1:D:341:THR:HG23	1.89	0.54
1:E:13:LEU:HD23	1:E:305:MET:HE1	1.89	0.54
1:E:274:LEU:HD23	1:E:275:GLN:HG3	1.89	0.54
1:H:34:GLU:HG2	1:H:38:LYS:HE3	1.88	0.54
1:A:384:LYS:NZ	2:D:501:KZ5:O15	2.40	0.54
1:D:52:PRO:HB3	1:D:58:ARG:CZ	2.37	0.54
1:H:104:ARG:O	1:H:104:ARG:HD3	2.08	0.54
1:B:201:GLU:OE1	1:B:305:MET:HA	2.08	0.54
1:B:329:ILE:HD11	1:B:332:LEU:CD2	2.26	0.54
1:C:372:GLN:HG2	1:C:375:LYS:HB2	1.90	0.54
1:D:94:ASP:CA	1:D:97:VAL:HG12	2.37	0.54
1:G:96:GLN:HG2	1:G:206:ILE:HG13	1.89	0.54
1:B:138:ARG:O	1:B:139:SER:CB	2.55	0.54
1:C:255:MET:HG2	1:C:259:PHE:CE2	2.42	0.54
1:D:162:VAL:O	1:D:168:ILE:HA	2.08	0.54
1:G:107:LYS:HD2	1:G:196:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:LYS:HA	1:H:175:MET:HE3	1.88	0.54
1:A:214:LEU:HD21	1:A:432:ILE:CG2	2.36	0.54
1:B:303:THR:O	1:B:307:THR:HG23	2.07	0.54
1:E:87:GLY:HA3	1:E:136:PRO:HG2	1.88	0.54
1:A:56:LEU:HB3	1:A:188:LYS:HB2	1.89	0.54
1:A:164:PHE:O	1:A:166:GLY:N	2.40	0.54
1:B:96:GLN:HG2	1:B:206:ILE:HG13	1.90	0.54
1:C:54:TYR:OH	1:C:61:GLY:N	2.26	0.54
1:C:280:PHE:HE1	1:C:356:LYS:HB2	1.71	0.54
1:C:443:ALA:O	1:C:447:ILE:HG12	2.08	0.54
1:E:51:LYS:O	1:E:53:VAL:HG23	2.07	0.54
1:H:36:VAL:HG11	1:H:120:LEU:HD12	1.89	0.54
1:B:138:ARG:O	1:B:139:SER:HB3	2.06	0.54
1:C:143:GLU:OE2	1:D:278:LEU:HD13	2.08	0.54
1:F:104:ARG:NH2	1:F:192:SER:O	2.30	0.54
1:G:279:SER:OG	1:G:353:ARG:HG3	2.08	0.54
1:H:359:ASP:O	1:H:363:THR:HG23	2.08	0.54
1:B:89:LYS:HB2	1:B:90:PRO:HA	1.90	0.54
1:D:138:ARG:O	1:D:139:SER:CB	2.55	0.54
1:E:207:VAL:HG13	1:E:425:ILE:HG21	1.90	0.54
1:E:278:LEU:HD22	1:E:282:CYS:SG	2.48	0.54
1:G:43:LEU:CD1	1:G:114:GLY:HA3	2.38	0.54
1:H:138:ARG:O	1:H:139:SER:HB3	2.08	0.54
1:C:383:GLN:HA	1:C:386:PHE:CZ	2.41	0.54
1:E:304:THR:HG21	1:E:329:ILE:HG22	1.90	0.54
1:F:381:THR:HG23	2:G:501:KZ5:O15	2.08	0.54
1:G:103:LEU:C	1:G:107:LYS:HE3	2.33	0.54
1:A:51:LYS:O	1:A:53:VAL:HG23	2.08	0.53
1:C:356:LYS:NZ	1:D:413:ASP:OD2	2.39	0.53
1:D:461:LYS:NZ	1:D:498:ILE:HA	2.23	0.53
1:A:201:GLU:OE1	1:A:304:THR:HG22	2.08	0.53
1:B:94:ASP:C	1:B:97:VAL:HG12	2.33	0.53
1:D:89:LYS:HB2	1:D:90:PRO:HA	1.90	0.53
1:F:98:ARG:HH11	1:F:132:HIS:CE1	2.27	0.53
1:F:230:ASN:OD1	1:F:272:ARG:NH2	2.41	0.53
1:H:92:HIS:HD2	1:H:135:ILE:HG22	1.72	0.53
1:H:302:LEU:O	1:H:306:ASN:ND2	2.37	0.53
1:A:384:LYS:NZ	2:D:501:KZ5:O17	2.37	0.53
1:C:43:LEU:CD1	1:C:114:GLY:HA3	2.38	0.53
1:D:122:HIS:CE1	1:D:183:ALA:HB2	2.43	0.53
1:H:474:ASN:OD1	3:H:601:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:O	1:D:211:ILE:HG12	2.09	0.53
1:G:211:ILE:O	1:G:215:VAL:HG23	2.08	0.53
1:A:383:GLN:HA	1:A:386:PHE:CE2	2.43	0.53
1:C:104:ARG:HD3	1:C:104:ARG:C	2.33	0.53
1:D:473:TYR:OH	1:D:476:ASP:HA	2.08	0.53
1:E:66:LYS:HD2	1:H:374:VAL:HG22	1.91	0.53
1:E:316:ILE:HD12	1:E:316:ILE:N	2.23	0.53
1:F:135:ILE:HD11	1:F:152:ILE:HD11	1.90	0.53
1:B:59:GLY:HA3	1:B:63:ASN:O	2.09	0.53
1:B:140:SER:HB3	1:B:419:PRO:HG2	1.90	0.53
1:C:52:PRO:HA	1:C:57:ASN:HD21	1.73	0.53
1:C:89:LYS:HB2	1:C:90:PRO:HA	1.89	0.53
1:D:86:LEU:HD23	1:D:147:THR:HG22	1.88	0.53
1:D:145:ASP:OD2	1:D:199:GLN:HB3	2.08	0.53
2:F:501:KZ5:O16	1:G:384:LYS:NZ	2.42	0.53
1:G:103:LEU:O	1:G:107:LYS:HE3	2.08	0.53
1:H:100:ILE:HD12	1:H:199:GLN:HA	1.91	0.53
1:C:357:LEU:O	1:C:363:THR:HG21	2.09	0.53
1:F:448:ASP:OD2	1:F:467:ARG:NH1	2.42	0.53
1:B:94:ASP:CA	1:B:97:VAL:HG12	2.39	0.53
1:C:244:ARG:HH22	1:D:304:THR:HG23	1.74	0.53
1:D:329:ILE:HD12	1:D:418:LEU:HD22	1.89	0.53
1:D:351:CYS:HA	1:D:354:MET:HE3	1.90	0.53
1:F:97:VAL:HG11	1:F:132:HIS:HB3	1.90	0.53
1:H:232:VAL:HG12	1:H:234:GLN:H	1.74	0.53
1:C:473:TYR:CZ	1:C:476:ASP:HA	2.43	0.53
1:F:86:LEU:HB2	1:F:147:THR:HG22	1.91	0.53
1:G:372:GLN:CG	1:G:375:LYS:HB3	2.39	0.53
1:A:138:ARG:O	1:A:139:SER:CB	2.57	0.53
1:B:470:LEU:HD22	1:B:486:MET:SD	2.49	0.53
1:F:274:LEU:HD23	1:F:275:GLN:HG3	1.90	0.53
1:G:39:ALA:HA	1:G:316:ILE:HD11	1.91	0.53
1:G:409:GLY:O	1:G:410:THR:OG1	2.24	0.53
1:A:27:LYS:NZ	1:A:124:ARG:HH11	2.07	0.52
1:A:138:ARG:O	1:A:139:SER:HB3	2.09	0.52
1:A:278:LEU:HD22	1:A:282:CYS:SG	2.49	0.52
1:D:489:PHE:O	1:D:492:SER:OG	2.22	0.52
1:E:7:THR:HG22	1:E:29:SER:HB3	1.91	0.52
1:F:484:GLU:O	1:F:488:GLU:HG2	2.09	0.52
1:A:7:THR:HG22	1:A:29:SER:CB	2.40	0.52
1:F:453:LYS:HE2	1:F:453:LYS:HA	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG21	1:A:329:ILE:CD1	2.39	0.52
1:E:2:ASP:N	3:E:604:HOH:O	2.43	0.52
1:E:52:PRO:HA	1:E:57:ASN:ND2	2.21	0.52
1:F:232:VAL:HG12	1:F:234:GLN:H	1.74	0.52
1:G:64:LYS:HE3	1:G:411:ILE:HD13	1.91	0.52
1:C:138:ARG:O	1:C:139:SER:CB	2.58	0.52
1:C:158:GLY:HA2	1:C:171:SER:OG	2.10	0.52
1:C:162:VAL:CG1	1:C:171:SER:HB3	2.39	0.52
1:E:95:GLU:OE1	1:E:95:GLU:N	2.33	0.52
1:F:40:ARG:HD2	1:F:116:SER:HA	1.91	0.52
1:A:46:MET:HE1	1:A:53:VAL:HG11	1.90	0.52
1:D:232:VAL:HG12	1:D:234:GLN:H	1.73	0.52
1:E:441:MET:HG3	1:E:470:LEU:HD21	1.91	0.52
1:B:146:ILE:HD12	2:C:501:KZ5:N4	2.24	0.52
1:D:51:LYS:O	1:D:53:VAL:HG23	2.08	0.52
1:D:207:VAL:HG13	1:D:425:ILE:HG21	1.92	0.52
1:F:86:LEU:HD11	1:G:381:THR:HB	1.92	0.52
1:H:113:THR:HG22	1:H:192:SER:OG	2.08	0.52
1:C:64:LYS:NZ	3:C:602:HOH:O	2.43	0.52
1:F:169:MET:CE	1:F:173:LYS:HB2	2.40	0.52
1:A:341:THR:HG23	1:B:402:MET:CE	2.39	0.52
1:B:383:GLN:HA	1:B:386:PHE:CE2	2.45	0.52
1:C:46:MET:HE1	1:C:321:SER:N	2.25	0.52
1:C:315:ILE:HD12	1:C:322:PHE:HD2	1.75	0.52
1:G:333:ALA:O	1:G:337:GLU:HG3	2.10	0.52
1:G:354:MET:SD	1:G:438:ILE:HG22	2.50	0.52
1:B:378:ALA:HA	1:B:473:TYR:CE2	2.45	0.52
1:D:492:SER:C	1:D:494:LYS:N	2.68	0.52
1:E:375:LYS:NZ	1:H:75:THR:HB	2.25	0.52
1:F:104:ARG:HD3	1:F:104:ARG:C	2.34	0.52
1:G:42:ILE:CG2	1:G:46:MET:HE3	2.39	0.52
1:A:271:GLU:O	1:A:364:LYS:NZ	2.37	0.51
1:A:376:THR:HG23	1:A:476:ASP:CG	2.35	0.51
1:B:46:MET:HE1	1:B:53:VAL:HG11	1.92	0.51
1:D:85:CYS:HA	1:D:150:SER:OG	2.09	0.51
1:F:36:VAL:HG11	1:F:120:LEU:HD12	1.91	0.51
1:G:328:GLU:OE1	1:G:414:HIS:ND1	2.40	0.51
1:H:40:ARG:NH1	1:H:187:PRO:HD2	2.17	0.51
1:H:96:GLN:HG2	1:H:206:ILE:HG13	1.92	0.51
1:A:7:THR:HG22	1:A:29:SER:HB3	1.90	0.51
1:A:140:SER:HB3	1:A:419:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ILE:HD12	1:B:322:PHE:HD2	1.73	0.51
1:C:108:ALA:HB1	1:C:115:ILE:HG21	1.91	0.51
1:C:138:ARG:O	1:C:139:SER:HB3	2.11	0.51
1:D:302:LEU:HD23	1:D:305:MET:HE2	1.91	0.51
1:F:138:ARG:O	1:F:139:SER:CB	2.58	0.51
1:G:97:VAL:HG22	1:G:135:ILE:HD12	1.91	0.51
1:H:6:LEU:HD21	1:H:26:VAL:HB	1.93	0.51
1:H:96:GLN:O	1:H:100:ILE:HG12	2.10	0.51
1:E:279:SER:OG	1:E:353:ARG:HG3	2.10	0.51
1:F:141:ILE:O	1:F:415:ALA:HB1	2.11	0.51
1:F:301:LEU:CG	1:F:305:MET:HE2	2.29	0.51
1:D:99:ALA:O	1:D:103:LEU:HG	2.10	0.51
1:E:188:LYS:CG	1:E:191:LEU:HD12	2.41	0.51
1:E:303:THR:O	1:E:307:THR:HG23	2.11	0.51
1:G:46:MET:HE1	1:G:321:SER:H	1.75	0.51
1:A:54:TYR:CE1	1:A:60:VAL:HA	2.45	0.51
1:B:188:LYS:O	1:B:192:SER:HB2	2.11	0.51
1:D:191:LEU:CD1	1:D:195:SER:HB2	2.38	0.51
1:E:36:VAL:HG11	1:E:120:LEU:HD12	1.91	0.51
1:E:493:LYS:HD3	1:E:496:LEU:HD12	1.92	0.51
1:F:169:MET:HE3	1:F:173:LYS:HB2	1.91	0.51
1:G:373:ASP:C	1:G:375:LYS:H	2.18	0.51
1:G:315:ILE:HD12	1:G:322:PHE:HD2	1.76	0.51
1:H:455:LEU:HD12	1:H:460:LYS:HE3	1.93	0.51
1:A:275:GLN:HG2	1:B:323:VAL:CG1	2.40	0.51
1:A:388:MET:HE3	3:D:622:HOH:O	2.11	0.51
1:B:374:VAL:HG23	1:B:375:LYS:HG3	1.92	0.51
1:C:207:VAL:HG13	1:C:425:ILE:HG21	1.92	0.51
1:E:43:LEU:CD1	1:E:114:GLY:HA3	2.40	0.51
1:G:4:LEU:HB2	1:G:24:ARG:NE	2.26	0.51
1:G:42:ILE:HG22	1:G:46:MET:HE3	1.93	0.51
1:B:115:ILE:HD11	1:B:119:LEU:CD1	2.40	0.51
1:D:358:ALA:HB1	1:D:368:PHE:HD1	1.75	0.51
1:E:7:THR:HG22	1:E:29:SER:CB	2.41	0.51
1:E:53:VAL:CG1	1:E:56:LEU:HD21	2.40	0.51
1:F:164:PHE:O	1:F:165:ASN:C	2.54	0.51
1:A:43:LEU:HD21	1:A:314:ILE:HD11	1.91	0.51
1:A:329:ILE:HG12	1:A:332:LEU:HB3	1.92	0.51
1:B:164:PHE:O	1:B:166:GLY:N	2.44	0.51
1:C:43:LEU:HD11	1:C:114:GLY:HA3	1.91	0.51
1:C:333:ALA:O	1:C:337:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:CYS:HA	1:C:354:MET:HE3	1.93	0.51
1:F:447:ILE:HG21	1:F:455:LEU:HD11	1.93	0.51
1:G:35:ARG:HD2	1:G:110:THR:O	2.10	0.51
1:B:279:SER:HA	1:B:349:THR:HG23	1.92	0.51
1:D:107:LYS:HE3	1:D:307:THR:O	2.11	0.51
1:E:115:ILE:HG21	1:E:120:LEU:HD21	1.93	0.51
1:E:191:LEU:CD2	1:E:195:SER:HB2	2.36	0.51
1:E:433:ARG:HD3	1:E:491:LYS:HB3	1.93	0.51
1:F:138:ARG:O	1:F:139:SER:HB3	2.09	0.51
1:G:43:LEU:HD11	1:G:114:GLY:HA3	1.92	0.51
1:B:107:LYS:HE2	1:B:305:MET:O	2.10	0.50
1:C:81:LEU:HD11	1:C:190:GLY:HA2	1.91	0.50
1:F:78:ARG:HH12	1:F:159:GLU:CD	2.19	0.50
1:F:140:SER:HB3	1:F:419:PRO:HG2	1.92	0.50
1:F:169:MET:HE2	1:F:174:ALA:N	2.26	0.50
1:G:138:ARG:O	1:G:139:SER:CB	2.59	0.50
1:A:55:GLY:HA3	1:A:191:LEU:CD2	2.41	0.50
1:A:279:SER:N	1:B:413:ASP:OD1	2.44	0.50
1:B:333:ALA:O	1:B:337:GLU:HG3	2.11	0.50
1:C:13:LEU:HD21	1:C:305:MET:HE1	1.93	0.50
1:C:461:LYS:CB	1:C:498:ILE:HG13	2.40	0.50
1:E:184:LYS:HD2	3:E:601:HOH:O	2.11	0.50
1:B:164:PHE:O	1:B:165:ASN:C	2.54	0.50
1:D:409:GLY:O	1:D:410:THR:OG1	2.29	0.50
2:F:501:KZ5:S14	1:G:384:LYS:NZ	2.85	0.50
1:D:104:ARG:HD3	1:D:104:ARG:C	2.37	0.50
1:E:354:MET:SD	1:E:438:ILE:HG22	2.51	0.50
1:F:154:LEU:O	1:F:157:ILE:HG12	2.12	0.50
1:F:295:ASP:OD1	1:F:298:ARG:NH1	2.43	0.50
1:A:56:LEU:HA	3:A:608:HOH:O	2.11	0.50
1:A:104:ARG:O	1:A:104:ARG:HD3	2.11	0.50
1:B:476:ASP:OD2	1:C:79:ASN:HB3	2.10	0.50
1:E:164:PHE:O	1:E:165:ASN:C	2.54	0.50
1:E:348:LYS:HG3	1:H:405:TYR:OH	2.11	0.50
1:F:83:SER:HA	1:G:479:ILE:HD12	1.94	0.50
1:F:173:LYS:HB3	1:F:177:LYS:HZ2	1.76	0.50
1:A:59:GLY:HA3	1:A:63:ASN:O	2.11	0.50
1:A:497:ASN:O	1:A:498:ILE:CB	2.60	0.50
1:D:138:ARG:O	1:D:139:SER:HB3	2.12	0.50
1:E:443:ALA:O	1:E:447:ILE:HG12	2.12	0.50
1:F:53:VAL:CG1	1:F:56:LEU:HD21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:384:LYS:NZ	2:G:501:KZ5:O17	2.45	0.50
1:G:297:VAL:HG21	1:G:339:LEU:HD11	1.93	0.50
1:H:164:PHE:O	1:H:165:ASN:C	2.54	0.50
1:H:383:GLN:HA	1:H:386:PHE:CZ	2.46	0.50
1:H:383:GLN:HA	1:H:386:PHE:CE2	2.46	0.50
1:A:54:TYR:OH	1:A:61:GLY:N	2.30	0.50
1:B:43:LEU:HD12	1:B:114:GLY:HA3	1.93	0.50
1:E:89:LYS:HB2	1:E:90:PRO:HA	1.93	0.50
1:B:115:ILE:HD11	1:B:119:LEU:HD13	1.94	0.50
1:B:358:ALA:HB1	1:B:368:PHE:HD1	1.76	0.50
1:D:211:ILE:HD11	1:D:343:LEU:HD11	1.94	0.50
1:F:357:LEU:O	1:F:363:THR:HG21	2.12	0.50
1:F:405:TYR:HB2	1:G:387:THR:HG21	1.93	0.50
1:H:477:ARG:HG2	1:H:478:ASN:H	1.76	0.50
1:A:33:GLU:O	1:A:36:VAL:HG22	2.12	0.50
1:A:55:GLY:HA3	1:A:191:LEU:HD23	1.94	0.50
1:B:302:LEU:HD23	1:B:305:MET:HE3	1.93	0.50
1:H:278:LEU:N	1:H:278:LEU:HD22	2.27	0.50
1:B:484:GLU:O	1:B:488:GLU:HG2	2.12	0.49
1:C:482:ASP:O	1:C:486:MET:HG2	2.12	0.49
1:D:162:VAL:HG13	1:D:171:SER:HB3	1.93	0.49
1:F:302:LEU:HD22	1:F:305:MET:HE3	1.94	0.49
1:C:223:CYS:HB3	1:C:260:LEU:HD21	1.93	0.49
1:E:496:LEU:O	1:E:497:ASN:HB2	2.11	0.49
1:G:360:PRO:HA	1:G:363:THR:HG22	1.93	0.49
1:A:467:ARG:HA	1:A:470:LEU:O	2.12	0.49
1:B:433:ARG:HD3	1:B:491:LYS:HB2	1.94	0.49
1:D:105:LEU:HD13	1:D:123:TYR:HB2	1.93	0.49
1:D:349:THR:HG22	1:D:353:ARG:NH1	2.27	0.49
1:F:79:ASN:HB3	1:G:476:ASP:OD2	2.13	0.49
1:G:56:LEU:HD13	1:G:187:PRO:CB	2.41	0.49
1:H:330:THR:O	1:H:334:ILE:HG12	2.12	0.49
1:B:351:CYS:HA	1:B:354:MET:HE3	1.94	0.49
1:C:265:LEU:HA	1:C:272:ARG:HH11	1.77	0.49
1:F:135:ILE:HD11	1:F:152:ILE:CG1	2.42	0.49
1:G:370:THR:OG1	1:G:378:ALA:HB3	2.12	0.49
1:C:359:ASP:O	1:C:363:THR:HG23	2.12	0.49
1:D:329:ILE:HD12	1:D:418:LEU:HD23	1.94	0.49
1:H:43:LEU:CD1	1:H:114:GLY:HA3	2.43	0.49
1:A:232:VAL:HG12	1:A:234:GLN:H	1.77	0.49
1:B:358:ALA:HB1	1:B:368:PHE:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:TYR:CD1	1:H:387:THR:CG2	2.95	0.49
1:G:370:THR:HG23	1:G:371:PRO:HD2	1.95	0.49
1:A:338:MET:CB	1:B:338:MET:HE2	2.41	0.49
1:B:85:CYS:HA	1:B:150:SER:OG	2.13	0.49
1:B:191:LEU:CD1	1:B:195:SER:HB2	2.42	0.49
1:H:40:ARG:NH2	1:H:116:SER:HB3	2.27	0.49
1:H:208:LEU:CD2	1:H:294:MET:HG2	2.42	0.49
1:A:53:VAL:CG1	1:A:56:LEU:HD21	2.42	0.49
1:A:211:ILE:O	1:A:215:VAL:HG23	2.13	0.49
1:C:70:GLU:HG2	1:C:73:PHE:CE2	2.48	0.49
1:C:175:MET:HE1	1:C:182:PRO:HA	1.94	0.49
1:D:383:GLN:HA	1:D:386:PHE:CE2	2.48	0.49
1:F:122:HIS:CE1	1:F:183:ALA:HB2	2.48	0.49
1:F:302:LEU:HD22	1:F:305:MET:CE	2.43	0.49
1:A:135:ILE:HD11	1:A:152:ILE:CG1	2.43	0.49
1:D:140:SER:OG	1:D:419:PRO:HG2	2.13	0.49
1:B:164:PHE:HB3	1:B:169:MET:HE3	1.94	0.49
1:F:387:THR:HG21	1:G:405:TYR:HB2	1.93	0.49
1:H:158:GLY:HA2	1:H:171:SER:OG	2.13	0.49
1:H:351:CYS:HA	1:H:354:MET:HE3	1.95	0.49
1:A:40:ARG:HH21	1:A:187:PRO:HD2	1.77	0.48
1:B:224:LEU:HB3	1:B:443:ALA:HB1	1.95	0.48
1:F:236:LEU:O	1:F:257:ARG:HD3	2.13	0.48
1:G:405:TYR:O	1:G:407:LEU:HD22	2.13	0.48
1:H:115:ILE:HD11	1:H:119:LEU:CD1	2.42	0.48
1:A:211:ILE:CD1	1:A:343:LEU:HD21	2.41	0.48
1:G:378:ALA:HA	1:G:473:TYR:CE2	2.48	0.48
1:H:146:ILE:HA	1:H:194:VAL:HB	1.95	0.48
1:A:97:VAL:HG22	1:A:135:ILE:HD12	1.96	0.48
1:B:154:LEU:O	1:B:157:ILE:HG12	2.13	0.48
1:H:493:LYS:HB3	1:H:496:LEU:HD12	1.95	0.48
1:C:302:LEU:HA	1:C:305:MET:HE3	1.94	0.48
1:D:42:ILE:CD1	1:D:319:HIS:HA	2.43	0.48
1:E:13:LEU:CD2	1:E:305:MET:HE1	2.43	0.48
1:E:201:GLU:OE1	1:E:305:MET:HA	2.13	0.48
1:E:383:GLN:HA	1:E:386:PHE:CZ	2.48	0.48
1:G:42:ILE:CD1	1:G:319:HIS:HA	2.44	0.48
1:G:132:HIS:O	1:G:163:SER:N	2.31	0.48
1:G:297:VAL:HG21	1:G:339:LEU:CD1	2.44	0.48
1:A:315:ILE:HD12	1:A:322:PHE:HD2	1.78	0.48
1:B:383:GLN:HA	1:B:386:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:ALA:N	1:D:498:ILE:HD11	2.29	0.48
1:E:66:LYS:HD2	1:H:374:VAL:CG2	2.43	0.48
1:E:139:SER:OG	1:E:147:THR:HG23	2.13	0.48
1:C:338:MET:HB2	1:D:338:MET:HE3	1.95	0.48
1:C:358:ALA:HB1	1:C:368:PHE:CD1	2.48	0.48
1:D:201:GLU:OE2	1:D:304:THR:HG22	2.13	0.48
1:E:169:MET:SD	1:E:173:LYS:NZ	2.78	0.48
1:F:201:GLU:OE2	1:F:304:THR:HG22	2.14	0.48
1:F:493:LYS:HD3	1:F:496:LEU:CD1	2.43	0.48
1:G:164:PHE:O	1:G:165:ASN:C	2.57	0.48
1:H:349:THR:HG22	1:H:353:ARG:NH1	2.28	0.48
1:B:329:ILE:HD13	1:B:418:LEU:HD22	1.95	0.48
1:E:381:THR:OG1	2:E:501:KZ5:O16	2.26	0.48
1:B:214:LEU:HD11	1:B:432:ILE:HG21	1.95	0.48
1:D:484:GLU:O	1:D:488:GLU:HG2	2.13	0.48
1:E:86:LEU:HD13	1:H:382:ILE:HA	1.94	0.48
1:E:404:PHE:CE1	1:E:414:HIS:HA	2.49	0.48
1:G:135:ILE:HD11	1:G:152:ILE:HG13	1.96	0.48
1:G:372:GLN:O	1:G:376:THR:HG23	2.14	0.48
1:C:224:LEU:CD2	1:C:459:THR:HB	2.44	0.48
1:C:243:VAL:O	1:D:307:THR:HG23	2.14	0.48
1:D:13:LEU:CD2	1:D:305:MET:HE1	2.43	0.48
1:H:27:LYS:NZ	1:H:27:LYS:HB3	2.27	0.48
1:H:43:LEU:HD11	1:H:114:GLY:HA3	1.95	0.48
1:B:113:THR:OG1	1:B:310:ASP:OD2	2.21	0.48
1:D:140:SER:HB3	1:D:419:PRO:HG2	1.96	0.48
1:D:495:LEU:O	1:D:498:ILE:CG2	2.61	0.48
1:G:358:ALA:HB1	1:G:368:PHE:HD1	1.77	0.48
1:C:211:ILE:O	1:C:215:VAL:HG23	2.14	0.47
1:D:94:ASP:CG	1:D:132:HIS:HD1	2.22	0.47
1:E:66:LYS:HB3	1:H:374:VAL:HG22	1.95	0.47
1:E:349:THR:HG22	1:E:353:ARG:NH1	2.29	0.47
1:G:232:VAL:HG12	1:G:234:GLN:H	1.79	0.47
1:H:405:TYR:O	1:H:407:LEU:HD12	2.14	0.47
1:A:384:LYS:NZ	2:D:501:KZ5:S14	2.87	0.47
1:B:43:LEU:HD11	1:B:114:GLY:HA3	1.95	0.47
1:C:304:THR:HG21	1:C:329:ILE:HG13	1.96	0.47
1:A:329:ILE:HD13	1:A:418:LEU:HD22	1.95	0.47
1:A:410:THR:HB	1:B:356:LYS:HE2	1.96	0.47
1:C:497:ASN:O	1:C:498:ILE:C	2.57	0.47
1:D:497:ASN:HB2	1:D:498:ILE:H	1.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LEU:HD12	1:E:120:LEU:HD22	1.95	0.47
1:F:481:ARG:O	1:F:485:THR:HG23	2.13	0.47
1:G:36:VAL:HG11	1:G:120:LEU:CD1	2.43	0.47
1:A:323:VAL:CG1	1:B:275:GLN:HG2	2.45	0.47
1:B:77:ASN:OD1	1:B:190:GLY:N	2.33	0.47
1:D:126:PHE:CE1	1:D:175:MET:HE2	2.50	0.47
1:D:477:ARG:NH1	1:D:482:ASP:OD2	2.47	0.47
1:G:4:LEU:O	1:G:26:VAL:HA	2.14	0.47
1:G:135:ILE:HD11	1:G:152:ILE:HD11	1.96	0.47
1:G:146:ILE:HD12	2:G:501:KZ5:N4	2.29	0.47
1:G:302:LEU:HA	1:G:305:MET:HE2	1.96	0.47
1:A:378:ALA:HA	1:A:473:TYR:CE2	2.49	0.47
1:A:414:HIS:CE1	1:B:286:VAL:HG22	2.50	0.47
1:B:315:ILE:HD12	1:B:322:PHE:CE2	2.49	0.47
1:B:333:ALA:CB	1:B:416:SER:HB2	2.45	0.47
1:C:297:VAL:HG21	1:C:339:LEU:CD1	2.43	0.47
1:E:104:ARG:HD3	1:E:104:ARG:C	2.39	0.47
1:G:85:CYS:C	1:G:86:LEU:HG	2.39	0.47
1:H:455:LEU:HD12	1:H:460:LYS:CE	2.45	0.47
1:A:149:LEU:HD12	1:A:194:VAL:O	2.15	0.47
1:C:59:GLY:HA3	1:C:63:ASN:O	2.14	0.47
1:G:370:THR:HG21	1:G:376:THR:O	2.15	0.47
1:A:52:PRO:HB3	1:A:58:ARG:CZ	2.45	0.47
1:B:104:ARG:HD3	1:B:104:ARG:C	2.39	0.47
1:C:46:MET:CE	1:C:320:SER:HA	2.45	0.47
1:C:265:LEU:HA	1:C:272:ARG:NH1	2.29	0.47
1:D:140:SER:CB	1:D:419:PRO:HG2	2.44	0.47
1:D:237:ARG:HB2	1:D:240:VAL:HG23	1.97	0.47
1:D:447:ILE:HG21	1:D:455:LEU:HD21	1.96	0.47
1:E:34:GLU:HG3	1:E:38:LYS:HZ2	1.79	0.47
1:E:164:PHE:O	1:E:166:GLY:N	2.48	0.47
1:F:89:LYS:HE2	1:G:484:GLU:OE1	2.15	0.47
1:F:299:GLU:O	1:F:303:THR:HG22	2.15	0.47
1:F:359:ASP:O	1:F:363:THR:HG23	2.13	0.47
1:G:169:MET:HB2	1:G:173:LYS:CE	2.45	0.47
1:G:358:ALA:HB1	1:G:368:PHE:CD1	2.49	0.47
1:H:217:MET:HG2	1:H:495:LEU:HB2	1.96	0.47
1:H:447:ILE:HG21	1:H:455:LEU:HD11	1.96	0.47
1:C:154:LEU:O	1:C:157:ILE:HG12	2.15	0.47
1:C:410:THR:O	1:D:356:LYS:HE2	2.15	0.47
1:E:56:LEU:HD23	1:E:56:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:PHE:O	1:G:166:GLY:N	2.48	0.47
1:H:164:PHE:O	1:H:166:GLY:N	2.47	0.47
1:A:352:TYR:O	1:A:356:LYS:HG2	2.15	0.47
1:B:304:THR:HG21	1:B:329:ILE:CD1	2.45	0.47
1:B:357:LEU:O	1:B:363:THR:HG21	2.15	0.47
1:C:56:LEU:HD13	1:C:187:PRO:CB	2.45	0.47
1:D:87:GLY:HA3	1:D:136:PRO:HG2	1.95	0.47
1:F:224:LEU:HB3	1:F:443:ALA:HB1	1.97	0.47
1:G:78:ARG:HB2	1:G:185:LEU:HD12	1.96	0.47
1:A:338:MET:SD	1:B:338:MET:HE3	2.55	0.47
1:E:138:ARG:O	1:E:139:SER:HB3	2.14	0.47
1:F:470:LEU:HD22	1:F:486:MET:SD	2.54	0.47
1:G:105:LEU:HD12	1:G:120:LEU:HD22	1.95	0.47
1:H:497:ASN:O	1:H:498:ILE:CB	2.62	0.47
1:D:11:LEU:HD11	1:D:106:ASN:CG	2.41	0.46
1:E:52:PRO:HB3	1:E:58:ARG:CZ	2.45	0.46
1:E:115:ILE:HD11	1:E:119:LEU:HD13	1.96	0.46
1:E:135:ILE:HD11	1:E:152:ILE:CG1	2.44	0.46
1:G:278:LEU:N	1:G:278:LEU:HD22	2.29	0.46
1:G:491:LYS:O	1:G:491:LYS:HG2	2.15	0.46
1:H:378:ALA:HA	1:H:473:TYR:CE2	2.49	0.46
1:A:286:VAL:HG11	1:A:349:THR:OG1	2.15	0.46
1:A:447:ILE:CG2	1:A:455:LEU:HD21	2.43	0.46
1:D:146:ILE:HD12	2:D:501:KZ5:N4	2.31	0.46
1:E:36:VAL:HG11	1:E:120:LEU:CD1	2.44	0.46
1:H:441:MET:HG3	1:H:470:LEU:HD21	1.98	0.46
1:E:140:SER:HB3	1:E:419:PRO:HG2	1.95	0.46
1:G:398:ASN:O	1:G:424:LYS:NZ	2.40	0.46
1:B:223:CYS:HB3	1:B:260:LEU:HD21	1.97	0.46
1:C:232:VAL:HG12	1:C:234:GLN:H	1.80	0.46
1:F:405:TYR:O	1:F:407:LEU:HD12	2.15	0.46
1:G:52:PRO:HB3	1:G:58:ARG:CZ	2.45	0.46
1:A:201:GLU:OE2	1:A:305:MET:HA	2.15	0.46
1:A:404:PHE:CE1	1:A:414:HIS:HA	2.50	0.46
1:C:383:GLN:HA	1:C:386:PHE:CE2	2.51	0.46
1:F:392:GLN:OE1	1:G:138:ARG:NH1	2.47	0.46
1:B:27:LYS:NZ	1:B:27:LYS:HB3	2.30	0.46
1:B:146:ILE:HA	1:B:194:VAL:HB	1.97	0.46
1:B:370:THR:HG21	1:B:373:ASP:HA	1.97	0.46
1:C:115:ILE:HG23	1:C:120:LEU:HD11	1.97	0.46
1:D:37:LYS:HE2	1:D:117:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:MET:CE	1:G:203:MET:HE3	2.45	0.46
1:G:351:CYS:HA	1:G:354:MET:HE3	1.98	0.46
1:A:496:LEU:O	1:A:497:ASN:HB3	2.16	0.46
1:C:80:LEU:O	1:C:84:HIS:ND1	2.49	0.46
1:C:404:PHE:CE1	1:C:414:HIS:HA	2.51	0.46
1:D:230:ASN:HB2	1:D:450:ARG:CZ	2.46	0.46
1:E:214:LEU:HD21	1:E:436:ILE:CD1	2.46	0.46
1:F:232:VAL:CG1	1:F:234:GLN:HG3	2.45	0.46
1:H:478:ASN:ND2	1:H:481:ARG:NH1	2.64	0.46
1:C:211:ILE:HD13	1:C:429:LEU:CD2	2.35	0.46
1:E:52:PRO:CA	1:E:57:ASN:HD21	2.22	0.46
1:G:236:LEU:HD23	1:G:284:HIS:CG	2.51	0.46
1:H:220:LEU:HD23	1:H:220:LEU:O	2.15	0.46
1:E:139:SER:OG	1:E:147:THR:CG2	2.64	0.46
1:H:55:GLY:HA3	1:H:191:LEU:CD2	2.45	0.46
1:A:492:SER:O	1:A:494:LYS:N	2.49	0.46
1:B:95:GLU:OE2	1:B:95:GLU:N	2.38	0.46
1:C:7:THR:HG22	1:C:29:SER:HB2	1.98	0.46
1:E:355:ILE:HA	3:E:611:HOH:O	2.15	0.46
1:F:105:LEU:HD12	1:F:123:TYR:HB3	1.97	0.46
1:F:191:LEU:HD12	1:F:195:SER:HB2	1.97	0.46
1:G:450:ARG:NH1	3:G:601:HOH:O	2.27	0.46
1:C:115:ILE:CG2	1:C:120:LEU:HD11	2.46	0.45
1:C:311:ASN:HA	1:C:312:PRO:C	2.41	0.45
1:D:59:GLY:HA3	1:D:63:ASN:O	2.16	0.45
1:H:145:ASP:OD2	1:H:199:GLN:HB3	2.15	0.45
1:A:54:TYR:HH	1:A:61:GLY:H	1.56	0.45
1:D:495:LEU:O	1:D:498:ILE:HG21	2.16	0.45
1:E:214:LEU:HD21	1:E:436:ILE:HD11	1.98	0.45
1:F:107:LYS:HE3	1:F:307:THR:O	2.17	0.45
1:F:230:ASN:HB2	1:F:450:ARG:CZ	2.47	0.45
1:G:59:GLY:HA3	1:G:63:ASN:O	2.16	0.45
1:H:169:MET:HE2	1:H:174:ALA:CA	2.46	0.45
1:H:186:GLY:N	1:H:189:ASP:OD2	2.35	0.45
1:A:145:ASP:HB2	1:A:149:LEU:HG	1.98	0.45
1:C:211:ILE:CD1	1:C:343:LEU:HD11	2.44	0.45
1:E:89:LYS:HE2	1:H:484:GLU:OE1	2.16	0.45
1:C:94:ASP:HB3	1:C:132:HIS:HD2	1.82	0.45
1:E:119:LEU:HD13	1:E:193:ILE:HD11	1.97	0.45
1:E:375:LYS:HD3	1:H:72:PHE:HE1	1.81	0.45
1:F:476:ASP:OD2	1:G:79:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:SER:O	1:G:22:ASN:HB2	2.16	0.45
1:G:237:ARG:HB2	1:G:240:VAL:HG23	1.97	0.45
1:G:349:THR:HG22	1:G:353:ARG:NH1	2.32	0.45
1:H:52:PRO:HB3	1:H:58:ARG:NH2	2.32	0.45
1:B:369:LEU:O	1:B:449:LEU:HD11	2.16	0.45
1:C:289:THR:HG23	1:D:331:SER:OG	2.17	0.45
1:C:329:ILE:HD13	1:C:418:LEU:CD2	2.44	0.45
1:C:356:LYS:HE2	1:D:410:THR:O	2.16	0.45
1:E:298:ARG:O	1:E:302:LEU:HG	2.15	0.45
1:E:315:ILE:HG22	1:E:318:GLU:H	1.81	0.45
1:F:87:GLY:HA3	1:F:136:PRO:HG2	1.99	0.45
1:H:434:TYR:CD1	1:H:487:TYR:HB2	2.51	0.45
1:B:70:GLU:HG2	1:B:73:PHE:CE2	2.52	0.45
1:E:316:ILE:HD12	1:E:316:ILE:H	1.79	0.45
1:H:278:LEU:HD22	1:H:278:LEU:H	1.82	0.45
1:A:338:MET:SD	1:B:338:MET:CE	3.05	0.45
1:D:94:ASP:O	1:D:98:ARG:HG3	2.17	0.45
1:F:36:VAL:HG11	1:F:120:LEU:CD1	2.46	0.45
1:F:409:GLY:O	1:F:410:THR:OG1	2.34	0.45
1:A:107:LYS:NZ	1:A:309:ASP:OD2	2.50	0.45
1:A:123:TYR:CE2	1:A:156:PHE:HE2	2.35	0.45
1:C:378:ALA:HA	1:C:473:TYR:CE2	2.51	0.45
1:C:455:LEU:N	1:C:455:LEU:HD12	2.32	0.45
1:D:43:LEU:CD1	1:D:114:GLY:HA3	2.46	0.45
1:D:232:VAL:CG1	1:D:234:GLN:HG3	2.47	0.45
1:E:126:PHE:HZ	1:E:175:MET:CE	2.29	0.45
1:A:158:GLY:HA2	1:A:171:SER:OG	2.17	0.45
1:B:154:LEU:HA	1:B:157:ILE:HG12	1.99	0.45
1:B:204:THR:HG21	1:B:332:LEU:HD11	1.99	0.45
1:B:214:LEU:HD11	1:B:432:ILE:CG2	2.47	0.45
1:B:453:LYS:HD2	1:B:453:LYS:HA	1.55	0.45
1:D:300:GLN:O	1:D:303:THR:HG23	2.17	0.45
1:D:498:ILE:O	1:D:498:ILE:CG2	2.58	0.45
1:H:333:ALA:O	1:H:337:GLU:HG3	2.16	0.45
1:A:230:ASN:HB2	1:A:450:ARG:CZ	2.47	0.45
1:D:2:ASP:O	1:D:24:ARG:HD2	2.17	0.45
1:E:46:MET:HE1	1:E:53:VAL:HG11	1.98	0.45
1:E:433:ARG:NH2	3:E:605:HOH:O	2.44	0.45
1:G:62:TRP:CD2	1:G:409:GLY:HA3	2.52	0.45
1:G:138:ARG:O	1:G:139:SER:HB3	2.17	0.45
1:C:352:TYR:O	1:C:356:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ILE:HB	1:H:86:LEU:CD2	2.47	0.44
1:F:405:TYR:CD1	1:G:387:THR:HG23	2.52	0.44
1:F:460:LYS:HD2	3:F:621:HOH:O	2.17	0.44
1:G:94:ASP:HB3	1:G:132:HIS:ND1	2.32	0.44
1:G:233:VAL:HG21	1:G:266:TYR:CE1	2.52	0.44
1:G:363:THR:O	1:G:365:LEU:CD2	2.65	0.44
1:H:62:TRP:HA	1:H:411:ILE:HD12	1.98	0.44
1:A:493:LYS:HD3	1:A:496:LEU:HD11	1.99	0.44
1:B:122:HIS:O	1:B:126:PHE:HB2	2.18	0.44
1:B:232:VAL:HG12	1:B:234:GLN:HG3	1.97	0.44
1:C:4:LEU:HB2	1:C:24:ARG:NE	2.32	0.44
1:A:146:ILE:HA	1:A:194:VAL:HB	1.98	0.44
1:A:289:THR:HG23	1:B:331:SER:OG	2.18	0.44
1:B:207:VAL:O	1:B:211:ILE:HG12	2.18	0.44
1:E:301:LEU:HD13	1:E:332:LEU:HD21	1.99	0.44
1:G:42:ILE:HD12	1:G:316:ILE:HD13	1.99	0.44
1:B:236:LEU:O	1:B:257:ARG:HD3	2.17	0.44
1:B:352:TYR:O	1:B:356:LYS:HG2	2.18	0.44
1:C:323:VAL:HG11	1:D:275:GLN:HG2	1.99	0.44
1:D:211:ILE:O	1:D:215:VAL:HG23	2.18	0.44
1:D:236:LEU:O	1:D:257:ARG:HD3	2.17	0.44
1:D:255:MET:HG2	1:D:259:PHE:CE2	2.52	0.44
1:A:40:ARG:HD2	1:A:116:SER:HA	2.00	0.44
1:B:79:ASN:HB3	1:C:476:ASP:OD2	2.17	0.44
1:F:164:PHE:O	1:F:166:GLY:N	2.50	0.44
1:G:214:LEU:HD11	1:G:436:ILE:HD11	1.99	0.44
1:H:100:ILE:HD13	1:H:199:GLN:HA	1.93	0.44
1:H:220:LEU:HD11	1:H:498:ILE:HD12	1.99	0.44
1:D:371:PRO:HG3	1:D:473:TYR:O	2.17	0.44
1:F:10:PRO:HA	1:F:306:ASN:CG	2.42	0.44
1:F:118:GLU:OE1	1:F:183:ALA:HA	2.17	0.44
1:F:441:MET:HG3	1:F:470:LEU:HD21	1.99	0.44
1:D:101:LEU:HB2	1:D:127:LEU:HD21	1.98	0.44
1:E:146:ILE:HD12	2:H:501:KZ5:C5	2.48	0.44
1:E:220:LEU:HD21	1:E:462:ALA:HB2	1.99	0.44
1:E:405:TYR:HB2	1:H:387:THR:HG21	1.99	0.44
1:F:25:GLN:OE1	1:F:128:ASN:HB3	2.17	0.44
1:G:304:THR:HG21	1:G:329:ILE:CG2	2.47	0.44
1:A:85:CYS:C	1:A:86:LEU:HG	2.43	0.44
1:C:21:TYR:CD1	1:C:95:GLU:HG2	2.52	0.44
1:E:126:PHE:CE1	1:E:175:MET:HE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:TYR:CD1	1:G:387:THR:CG2	3.00	0.44
1:F:405:TYR:CG	1:G:387:THR:HG23	2.53	0.44
1:H:145:ASP:CG	1:H:199:GLN:HB3	2.42	0.44
1:H:498:ILE:O	1:H:498:ILE:HG23	2.16	0.44
1:A:354:MET:SD	1:A:439:GLU:HA	2.58	0.44
1:B:328:GLU:OE1	1:B:414:HIS:ND1	2.47	0.44
1:D:162:VAL:CG1	1:D:171:SER:HB3	2.48	0.44
1:E:302:LEU:HD23	1:E:305:MET:HE2	1.96	0.44
1:F:354:MET:HG3	1:F:439:GLU:HG3	1.99	0.44
1:F:405:TYR:HB2	1:G:387:THR:CG2	2.48	0.44
1:G:92:HIS:CE1	1:G:137:MET:HG2	2.53	0.44
1:G:154:LEU:O	1:G:157:ILE:HG12	2.17	0.44
1:H:4:LEU:HB2	1:H:24:ARG:NE	2.32	0.44
1:A:304:THR:HG21	1:A:329:ILE:HG13	2.00	0.43
1:A:329:ILE:CD1	1:A:332:LEU:HD23	2.42	0.43
1:B:371:PRO:HG3	1:B:473:TYR:O	2.18	0.43
1:C:204:THR:HG21	1:C:332:LEU:HD11	2.00	0.43
1:C:338:MET:CG	1:D:334:ILE:HD12	2.48	0.43
1:F:94:ASP:OD2	1:F:163:SER:HB3	2.18	0.43
1:H:144:GLY:N	1:H:197:ASN:OD1	2.47	0.43
1:A:405:TYR:O	1:A:407:LEU:HD22	2.18	0.43
1:B:497:ASN:O	1:B:498:ILE:HB	2.18	0.43
1:C:237:ARG:HD2	3:C:620:HOH:O	2.17	0.43
1:E:328:GLU:OE1	1:E:330:THR:OG1	2.34	0.43
1:G:359:ASP:O	1:G:363:THR:HG22	2.18	0.43
1:H:227:GLU:HB3	1:H:264:PHE:HE2	1.84	0.43
1:B:92:HIS:HD2	1:B:135:ILE:HG22	1.82	0.43
1:B:430:ASP:OD1	1:B:487:TYR:OH	2.25	0.43
1:D:164:PHE:HB3	1:D:169:MET:CE	2.42	0.43
1:D:473:TYR:CZ	1:D:476:ASP:HA	2.53	0.43
1:A:105:LEU:HD12	1:A:120:LEU:HD22	2.01	0.43
1:A:188:LYS:O	1:A:192:SER:HB2	2.18	0.43
1:A:250:ILE:HG12	3:A:605:HOH:O	2.17	0.43
1:A:479:ILE:HB	1:D:86:LEU:HD12	2.00	0.43
1:B:13:LEU:HD23	1:B:305:MET:HE1	2.00	0.43
1:B:496:LEU:O	1:B:498:ILE:HD13	2.18	0.43
1:D:104:ARG:HD2	1:D:123:TYR:CZ	2.53	0.43
1:H:47:ALA:HB2	1:H:56:LEU:HD11	2.00	0.43
1:H:404:PHE:CE1	1:H:414:HIS:HA	2.53	0.43
1:A:331:SER:HA	1:B:289:THR:HG23	2.01	0.43
1:E:214:LEU:HD13	1:E:214:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:LYS:HZ3	1:H:75:THR:HB	1.83	0.43
1:G:40:ARG:HD2	1:G:116:SER:HA	1.99	0.43
1:G:379:PHE:HB3	1:G:382:ILE:CG2	2.48	0.43
1:H:453:LYS:HA	1:H:453:LYS:HD3	1.84	0.43
1:C:97:VAL:CG2	1:C:135:ILE:HG22	2.49	0.43
1:D:115:ILE:HG21	1:D:120:LEU:HD21	2.01	0.43
1:E:462:ALA:O	1:E:466:ILE:HG13	2.18	0.43
1:F:85:CYS:C	1:F:86:LEU:HG	2.43	0.43
1:H:220:LEU:HB2	1:H:259:PHE:CE2	2.53	0.43
1:A:104:ARG:HD3	1:A:104:ARG:C	2.44	0.43
1:B:237:ARG:HB2	1:B:240:VAL:HG23	2.00	0.43
1:B:448:ASP:OD2	1:B:467:ARG:NH1	2.52	0.43
1:D:404:PHE:CE1	1:D:414:HIS:HA	2.53	0.43
1:D:453:LYS:HE2	1:D:453:LYS:CA	2.43	0.43
1:E:79:ASN:HB3	1:H:476:ASP:OD2	2.17	0.43
1:F:83:SER:O	1:F:86:LEU:HD11	2.19	0.43
1:B:40:ARG:HH21	1:B:187:PRO:HD2	1.84	0.43
1:D:40:ARG:CZ	1:D:116:SER:HB3	2.48	0.43
1:E:191:LEU:HD22	1:E:195:SER:CB	2.44	0.43
1:F:333:ALA:HA	1:F:418:LEU:HD13	2.01	0.43
1:G:80:LEU:HG	1:G:84:HIS:CE1	2.53	0.43
1:G:217:MET:HG2	1:G:495:LEU:HB2	1.99	0.43
1:H:220:LEU:HD23	1:H:220:LEU:C	2.43	0.43
1:H:227:GLU:OE2	1:H:459:THR:OG1	2.27	0.43
1:A:72:PHE:CD2	1:A:76:TYR:HB2	2.54	0.43
1:A:354:MET:SD	1:A:438:ILE:HG22	2.59	0.43
1:C:336:VAL:HA	1:C:339:LEU:HD12	2.00	0.43
1:D:115:ILE:HB	1:D:192:SER:OG	2.19	0.43
1:E:56:LEU:HB3	1:E:188:LYS:HB2	2.01	0.43
1:F:387:THR:CG2	1:G:405:TYR:CD1	3.02	0.43
1:H:347:SER:HB3	1:H:432:ILE:HG12	2.01	0.43
1:H:462:ALA:O	1:H:466:ILE:HG13	2.18	0.43
1:D:314:ILE:HG12	1:D:321:SER:HB3	2.01	0.43
1:E:315:ILE:HD12	1:E:322:PHE:CD2	2.54	0.43
1:G:222:PHE:CZ	1:G:283:ALA:HB3	2.54	0.43
1:H:115:ILE:CG2	1:H:120:LEU:HD11	2.49	0.43
1:H:448:ASP:OD2	1:H:467:ARG:NH1	2.52	0.43
1:A:191:LEU:HD12	1:A:195:SER:HB2	2.01	0.42
1:C:175:MET:HE1	1:C:182:PRO:N	2.34	0.42
1:C:323:VAL:CG1	1:D:275:GLN:HG2	2.49	0.42
1:F:139:SER:OG	1:F:147:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:GLN:O	1:G:100:ILE:HG12	2.19	0.42
1:G:181:LYS:CG	1:G:182:PRO:HD2	2.45	0.42
1:H:139:SER:OG	1:H:148:THR:HG23	2.19	0.42
1:H:281:ARG:HB2	3:H:603:HOH:O	2.18	0.42
1:A:80:LEU:HG	1:A:84:HIS:CE1	2.54	0.42
1:A:217:MET:HG2	1:A:495:LEU:HB2	2.00	0.42
1:B:56:LEU:HD23	1:B:56:LEU:H	1.82	0.42
1:C:418:LEU:HB3	1:C:419:PRO:HD3	2.01	0.42
1:D:37:LYS:HE2	1:D:117:ALA:HB2	2.01	0.42
1:G:122:HIS:HD2	1:G:175:MET:HE2	1.84	0.42
1:G:236:LEU:CD2	1:G:284:HIS:HB3	2.48	0.42
1:C:217:MET:HG2	1:C:495:LEU:HB2	2.00	0.42
1:C:428:MET:O	1:C:432:ILE:HG13	2.19	0.42
1:F:407:LEU:HD12	1:F:407:LEU:N	2.34	0.42
1:F:479:ILE:CD1	1:G:83:SER:HA	2.49	0.42
1:G:40:ARG:CZ	1:G:116:SER:HB3	2.49	0.42
1:G:404:PHE:CE1	1:G:414:HIS:HA	2.54	0.42
1:C:49:GLU:O	1:C:49:GLU:HG2	2.19	0.42
1:C:107:LYS:HE3	1:C:307:THR:O	2.19	0.42
1:C:162:VAL:HG13	1:C:171:SER:HB3	2.01	0.42
1:C:162:VAL:O	1:C:168:ILE:HA	2.19	0.42
1:C:372:GLN:HG3	1:C:375:LYS:H	1.84	0.42
1:F:436:ILE:HD11	1:F:490:ILE:HG21	2.01	0.42
1:G:360:PRO:HA	1:G:363:THR:CG2	2.50	0.42
1:H:107:LYS:NZ	1:H:201:GLU:OE1	2.52	0.42
1:H:201:GLU:OE2	1:H:304:THR:CG2	2.67	0.42
1:A:160:GLU:CD	1:D:481:ARG:HH22	2.27	0.42
1:A:407:LEU:HD22	1:A:407:LEU:N	2.33	0.42
1:B:405:TYR:O	1:B:407:LEU:HD22	2.20	0.42
3:B:513:HOH:O	1:C:388:MET:HE3	2.19	0.42
1:E:418:LEU:HB3	1:E:419:PRO:HD3	2.01	0.42
1:F:52:PRO:HB3	1:F:58:ARG:NH2	2.34	0.42
1:F:98:ARG:HH11	1:F:132:HIS:HE1	1.67	0.42
1:H:55:GLY:HA3	1:H:191:LEU:HD23	2.01	0.42
1:A:115:ILE:HG21	1:A:120:LEU:HD21	2.01	0.42
1:C:369:LEU:HB3	1:C:445:GLN:HG2	2.02	0.42
1:C:402:MET:HE3	1:D:341:THR:HG23	2.01	0.42
1:E:311:ASN:HA	1:E:312:PRO:C	2.45	0.42
1:E:312:PRO:HB2	1:E:321:SER:HB2	2.00	0.42
1:F:17:TYR:OH	1:F:205:ALA:O	2.37	0.42
1:G:39:ALA:CA	1:G:316:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:LEU:HD23	1:H:305:MET:HE1	2.02	0.42
1:H:52:PRO:HB3	1:H:58:ARG:CZ	2.49	0.42
1:B:94:ASP:HA	1:B:97:VAL:CG1	2.43	0.42
1:B:160:GLU:OE2	1:B:161:ASP:N	2.48	0.42
1:C:369:LEU:HB3	1:C:445:GLN:CG	2.50	0.42
1:D:188:LYS:O	1:D:192:SER:HB2	2.19	0.42
1:G:58:ARG:CD	1:G:67:GLU:HG2	2.50	0.42
1:G:94:ASP:HB3	1:G:132:HIS:HD1	1.84	0.42
1:G:232:VAL:CG1	1:G:234:GLN:HG3	2.50	0.42
1:G:278:LEU:HD22	1:G:278:LEU:H	1.84	0.42
1:G:448:ASP:OD2	1:G:467:ARG:NH1	2.53	0.42
1:H:220:LEU:HD21	1:H:462:ALA:CB	2.49	0.42
1:H:329:ILE:HD12	1:H:418:LEU:HD22	2.02	0.42
1:B:330:THR:O	1:B:334:ILE:HG12	2.20	0.42
1:C:296:TYR:CZ	1:C:300:GLN:HG3	2.54	0.42
1:D:145:ASP:CG	1:D:199:GLN:HB3	2.45	0.42
1:F:126:PHE:CE1	1:F:175:MET:HE2	2.55	0.42
1:F:418:LEU:HB3	1:F:419:PRO:HD3	2.01	0.42
1:G:370:THR:HG22	1:G:372:GLN:N	2.31	0.42
1:B:99:ALA:O	1:B:103:LEU:HG	2.20	0.42
1:B:388:MET:SD	1:B:389:LEU:HD12	2.60	0.42
1:B:473:TYR:OH	1:B:476:ASP:HA	2.19	0.42
1:C:97:VAL:CG2	1:C:135:ILE:CG2	2.98	0.42
1:C:275:GLN:HG2	1:D:323:VAL:CG1	2.50	0.42
1:C:470:LEU:HD22	1:C:486:MET:SD	2.60	0.42
1:E:12:SER:O	1:E:15:ASP:HB2	2.20	0.42
1:E:158:GLY:HA2	1:E:171:SER:OG	2.19	0.42
1:F:16:VAL:HA	1:F:102:LEU:CD2	2.49	0.42
1:F:281:ARG:HB2	3:F:616:HOH:O	2.20	0.42
1:H:428:MET:O	1:H:432:ILE:HG13	2.19	0.42
1:A:62:TRP:HA	1:A:411:ILE:HD12	2.02	0.42
1:C:372:GLN:HG2	1:C:375:LYS:CB	2.49	0.42
1:D:495:LEU:C	1:D:496:LEU:O	2.63	0.42
1:F:62:TRP:HA	1:F:411:ILE:HD12	2.02	0.42
1:F:241:ASN:OD1	1:F:284:HIS:NE2	2.53	0.42
1:F:384:LYS:NZ	2:G:501:KZ5:S14	2.93	0.42
1:G:42:ILE:HD11	1:G:319:HIS:HA	2.02	0.42
1:G:493:LYS:HB3	1:G:496:LEU:HD12	2.02	0.42
1:H:36:VAL:HG11	1:H:120:LEU:HD11	2.02	0.42
1:B:12:SER:O	1:B:15:ASP:HB2	2.20	0.41
1:E:126:PHE:CZ	1:E:175:MET:CE	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:VAL:O	1:F:211:ILE:HG12	2.20	0.41
1:A:154:LEU:O	1:A:157:ILE:HG12	2.20	0.41
1:A:351:CYS:HA	1:A:354:MET:HE3	2.01	0.41
1:C:278:LEU:HD12	1:C:278:LEU:N	2.35	0.41
1:C:341:THR:HG23	1:D:402:MET:HE1	2.01	0.41
1:F:66:LYS:HD2	1:G:374:VAL:HG22	2.02	0.41
1:G:365:LEU:HD12	1:G:449:LEU:HB3	2.02	0.41
1:H:72:PHE:CD2	1:H:76:TYR:HB2	2.55	0.41
1:B:404:PHE:CE1	1:B:414:HIS:HA	2.56	0.41
1:C:11:LEU:HD11	1:C:106:ASN:CG	2.45	0.41
1:E:34:GLU:HG3	1:E:38:LYS:HZ1	1.86	0.41
1:E:89:LYS:HA	1:E:90:PRO:O	2.20	0.41
1:E:230:ASN:HB2	1:E:450:ARG:CZ	2.49	0.41
1:G:104:ARG:HD3	1:G:104:ARG:C	2.45	0.41
1:H:220:LEU:HD21	1:H:462:ALA:HB2	2.02	0.41
1:A:211:ILE:HD11	1:A:343:LEU:HD11	2.03	0.41
1:B:96:GLN:O	1:B:100:ILE:HG13	2.19	0.41
1:D:307:THR:HG22	1:D:308:THR:N	2.34	0.41
1:D:455:LEU:HD12	1:D:455:LEU:N	2.36	0.41
1:E:96:GLN:HG2	1:E:206:ILE:HG13	2.01	0.41
1:H:278:LEU:H	1:H:278:LEU:CD2	2.33	0.41
1:H:307:THR:HG22	1:H:308:THR:N	2.35	0.41
1:A:333:ALA:O	1:A:337:GLU:HG3	2.20	0.41
1:B:302:LEU:HD23	1:B:305:MET:HE2	2.01	0.41
1:C:236:LEU:O	1:C:257:ARG:HD3	2.21	0.41
1:D:493:LYS:HB3	1:D:496:LEU:HD12	2.02	0.41
1:E:303:THR:HG22	1:E:304:THR:N	2.35	0.41
1:G:46:MET:HE1	1:G:321:SER:N	2.34	0.41
1:G:107:LYS:NZ	1:G:196:CYS:HG	2.16	0.41
1:A:85:CYS:HA	1:A:150:SER:OG	2.20	0.41
1:A:358:ALA:HB1	1:A:368:PHE:HD1	1.85	0.41
1:A:455:LEU:N	1:A:455:LEU:HD12	2.35	0.41
1:B:40:ARG:NH1	1:B:114:GLY:O	2.50	0.41
1:B:56:LEU:HB3	1:B:188:LYS:HB2	2.03	0.41
1:C:85:CYS:C	1:C:86:LEU:HG	2.44	0.41
1:C:275:GLN:HB3	1:C:281:ARG:HH11	1.86	0.41
1:C:453:LYS:HE2	1:C:453:LYS:CA	2.45	0.41
1:D:96:GLN:O	1:D:100:ILE:HG13	2.21	0.41
1:E:405:TYR:HB2	1:H:387:THR:CG2	2.50	0.41
1:G:208:LEU:CD2	1:G:294:MET:HG2	2.50	0.41
1:H:40:ARG:CZ	1:H:116:SER:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLN:HB2	1:D:323:VAL:HB	2.03	0.41
1:E:188:LYS:HG3	1:E:191:LEU:HD12	2.01	0.41
1:E:368:PHE:CD1	1:E:380:GLY:HA2	2.56	0.41
1:F:160:GLU:OE2	1:F:161:ASP:N	2.46	0.41
1:A:242:ALA:N	3:A:605:HOH:O	2.53	0.41
1:A:473:TYR:OH	1:A:476:ASP:HA	2.20	0.41
1:C:178:ALA:HB3	1:C:180:LEU:CD2	2.51	0.41
1:C:404:PHE:CZ	1:D:348:LYS:HD3	2.56	0.41
1:C:448:ASP:OD1	1:C:463:TYR:OH	2.30	0.41
1:G:473:TYR:OH	1:G:476:ASP:HA	2.20	0.41
1:A:135:ILE:HD11	1:A:152:ILE:HG13	2.02	0.41
1:A:334:ILE:HD12	1:B:338:MET:CG	2.50	0.41
1:C:52:PRO:HB3	1:C:58:ARG:CZ	2.51	0.41
1:C:228:GLY:HA2	1:C:447:ILE:HD13	2.03	0.41
1:D:210:GLU:OE1	1:D:210:GLU:HA	2.20	0.41
1:D:347:SER:HB3	1:D:432:ILE:HG12	2.03	0.41
1:E:139:SER:O	1:E:147:THR:HG21	2.21	0.41
1:F:135:ILE:HD11	1:F:152:ILE:HG13	2.03	0.41
1:F:300:GLN:O	1:F:303:THR:HG23	2.21	0.41
1:F:370:THR:HA	1:F:378:ALA:HB2	2.03	0.41
1:G:35:ARG:HG2	1:G:111:GLY:HA3	2.03	0.41
1:G:95:GLU:OE1	1:G:95:GLU:N	2.43	0.41
1:G:220:LEU:HD13	1:G:259:PHE:CG	2.55	0.41
1:G:278:LEU:H	1:G:278:LEU:CD2	2.34	0.41
1:H:104:ARG:HD3	1:H:104:ARG:C	2.45	0.41
1:H:484:GLU:O	1:H:488:GLU:HG2	2.21	0.41
1:C:208:LEU:CD2	1:C:294:MET:HG2	2.50	0.41
1:C:331:SER:HA	1:D:289:THR:HG23	2.02	0.41
1:C:335:GLY:HA2	1:D:338:MET:HE2	2.01	0.41
1:E:222:PHE:CZ	1:E:283:ALA:HB3	2.56	0.41
1:F:126:PHE:HZ	1:F:175:MET:HE3	1.85	0.41
1:F:297:VAL:HG13	1:F:332:LEU:CD1	2.51	0.41
1:A:145:ASP:OD2	1:A:199:GLN:N	2.54	0.40
1:A:393:ASN:HB3	1:A:428:MET:HE3	2.03	0.40
1:B:51:LYS:NZ	1:B:320:SER:HG	2.19	0.40
1:B:126:PHE:HZ	1:B:175:MET:HE2	1.86	0.40
1:C:453:LYS:C	1:C:455:LEU:HD12	2.47	0.40
1:F:211:ILE:HD12	1:F:343:LEU:HD21	2.03	0.40
1:G:13:LEU:HD23	1:G:305:MET:HE1	2.02	0.40
1:H:99:ALA:O	1:H:103:LEU:HG	2.21	0.40
1:H:207:VAL:HG13	1:H:425:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:455:LEU:HB2	1:H:460:LYS:HE3	2.02	0.40
1:A:315:ILE:HG22	1:A:318:GLU:H	1.85	0.40
1:C:23:ASN:HA	1:C:98:ARG:NH2	2.36	0.40
1:C:232:VAL:CG1	1:C:234:GLN:HG3	2.50	0.40
1:D:496:LEU:O	1:D:497:ASN:C	2.65	0.40
1:E:56:LEU:HG	1:E:57:ASN:H	1.86	0.40
1:E:99:ALA:O	1:E:103:LEU:HG	2.20	0.40
1:A:219:ASN:HB2	1:A:255:MET:HE2	2.04	0.40
1:A:237:ARG:NH2	1:A:239:ASP:OD2	2.33	0.40
1:D:64:LYS:HE3	1:D:411:ILE:HD13	2.02	0.40
1:D:223:CYS:HB3	1:D:260:LEU:HD21	2.03	0.40
1:E:160:GLU:OE2	1:E:161:ASP:N	2.49	0.40
1:E:213:ASP:HB3	1:E:496:LEU:HD11	2.02	0.40
1:G:304:THR:CG2	1:G:329:ILE:HG22	2.48	0.40
1:H:27:LYS:HB3	1:H:27:LYS:HZ3	1.86	0.40
1:H:352:TYR:O	1:H:356:LYS:HG2	2.20	0.40
1:A:223:CYS:HB3	1:A:260:LEU:HD21	2.02	0.40
1:B:290:MET:SD	1:B:342:ALA:HB1	2.62	0.40
1:D:214:LEU:HA	1:D:217:MET:HE3	2.03	0.40
1:D:265:LEU:HA	1:D:272:ARG:NH1	2.36	0.40
1:D:497:ASN:O	1:D:498:ILE:HG22	2.21	0.40
1:E:302:LEU:HD23	1:E:305:MET:HE3	2.02	0.40
1:F:169:MET:CE	1:F:173:LYS:CB	3.00	0.40
1:F:211:ILE:O	1:F:215:VAL:HG23	2.21	0.40
1:F:237:ARG:O	1:F:241:ASN:ND2	2.34	0.40
1:F:430:ASP:HA	1:F:433:ARG:HH11	1.87	0.40
1:H:188:LYS:O	1:H:192:SER:HB2	2.21	0.40
1:A:27:LYS:HA	1:A:27:LYS:HD2	1.93	0.40
1:A:105:LEU:HB2	1:A:123:TYR:HB3	2.04	0.40
1:B:40:ARG:CZ	1:B:116:SER:HB3	2.52	0.40
1:F:135:ILE:HD11	1:F:152:ILE:CD1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/497 (100%)	477 (96%)	14 (3%)	4 (1%)	16	37
1	B	495/497 (100%)	481 (97%)	12 (2%)	2 (0%)	30	54
1	C	495/497 (100%)	481 (97%)	13 (3%)	1 (0%)	43	68
1	D	495/497 (100%)	478 (97%)	14 (3%)	3 (1%)	21	44
1	E	495/497 (100%)	480 (97%)	13 (3%)	2 (0%)	30	54
1	F	495/497 (100%)	480 (97%)	11 (2%)	4 (1%)	16	37
1	G	495/497 (100%)	479 (97%)	13 (3%)	3 (1%)	21	44
1	H	495/497 (100%)	479 (97%)	14 (3%)	2 (0%)	30	54
All	All	3960/3976 (100%)	3835 (97%)	104 (3%)	21 (0%)	24	48

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	LYS
1	B	165	ASN
1	D	139	SER
1	E	165	ASN
1	F	139	SER
1	F	165	ASN
1	F	493	LYS
1	G	165	ASN
1	H	165	ASN
1	A	139	SER
1	B	139	SER
1	C	139	SER
1	D	493	LYS
1	D	496	LEU
1	E	139	SER
1	G	139	SER
1	H	139	SER
1	F	497	ASN
1	A	497	ASN
1	G	374	VAL
1	A	165	ASN

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	427/427 (100%)	413 (97%)	14 (3%)	33	63
1	B	427/427 (100%)	414 (97%)	13 (3%)	36	66
1	C	427/427 (100%)	417 (98%)	10 (2%)	44	73
1	D	427/427 (100%)	416 (97%)	11 (3%)	40	70
1	E	427/427 (100%)	415 (97%)	12 (3%)	38	68
1	F	427/427 (100%)	411 (96%)	16 (4%)	30	59
1	G	427/427 (100%)	409 (96%)	18 (4%)	26	55
1	H	427/427 (100%)	415 (97%)	12 (3%)	38	68
All	All	3416/3416 (100%)	3310 (97%)	106 (3%)	35	65

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	27	LYS
1	A	34	GLU
1	A	43	LEU
1	A	97	VAL
1	A	162	VAL
1	A	173	LYS
1	A	235	SER
1	A	294	MET
1	A	370	THR
1	A	374	VAL
1	A	387	THR
1	A	485	THR
1	A	498	ILE
1	B	53	VAL
1	B	75	THR
1	B	154	LEU
1	B	162	VAL
1	B	238	GLU

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Mol	Chain	Res	Type
1	B	281	ARG
1	B	294	MET
1	B	299	GLU
1	B	303	THR
1	B	370	THR
1	B	453	LYS
1	B	491	LYS
1	B	498	ILE
1	C	26	VAL
1	C	36	VAL
1	C	60	VAL
1	C	97	VAL
1	C	135	ILE
1	C	281	ARG
1	C	307	THR
1	C	363	THR
1	C	370	THR
1	C	485	THR
1	D	53	VAL
1	D	75	THR
1	D	86	LEU
1	D	147	THR
1	D	240	VAL
1	D	294	MET
1	D	303	THR
1	D	363	THR
1	D	370	THR
1	D	477	ARG
1	D	497	ASN
1	E	26	VAL
1	E	36	VAL
1	E	53	VAL
1	E	75	THR
1	E	147	THR
1	E	162	VAL
1	E	191	LEU
1	E	281	ARG
1	E	303	THR
1	E	363	THR
1	E	485	THR
1	E	498	ILE
1	F	36	VAL

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Mol	Chain	Res	Type
1	F	60	VAL
1	F	75	THR
1	F	97	VAL
1	F	105	LEU
1	F	147	THR
1	F	192	SER
1	F	258	GLU
1	F	294	MET
1	F	302	LEU
1	F	303	THR
1	F	307	THR
1	F	363	THR
1	F	370	THR
1	F	387	THR
1	F	498	ILE
1	G	26	VAL
1	G	36	VAL
1	G	53	VAL
1	G	75	THR
1	G	97	VAL
1	G	110	THR
1	G	147	THR
1	G	162	VAL
1	G	195	SER
1	G	294	MET
1	G	303	THR
1	G	329	ILE
1	G	365	LEU
1	G	376	THR
1	G	387	THR
1	G	485	THR
1	G	497	ASN
1	G	498	ILE
1	H	26	VAL
1	H	36	VAL
1	H	56	LEU
1	H	147	THR
1	H	162	VAL
1	H	220	LEU
1	H	363	THR
1	H	387	THR
1	H	447	ILE

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Mol	Chain	Res	Type
1	H	477	ARG
1	H	485	THR
1	H	498	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	106	ASN
1	A	275	GLN
1	A	287	ASN
1	B	22	ASN
1	B	106	ASN
1	B	311	ASN
1	C	23	ASN
1	C	106	ASN
1	C	132	HIS
1	C	165	ASN
1	D	63	ASN
1	D	106	ASN
1	E	63	ASN
1	E	287	ASN
1	F	23	ASN
1	F	132	HIS
1	F	497	ASN
1	G	106	ASN
1	G	287	ASN
1	H	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KZ5	C	502	-	16,17,17	1.99	1 (6%)	16,25,25	1.20	3 (18%)
2	KZ5	G	501	-	16,17,17	1.63	1 (6%)	16,25,25	0.98	2 (12%)
2	KZ5	E	501	-	16,17,17	1.47	1 (6%)	16,25,25	1.04	2 (12%)
2	KZ5	H	501	-	16,17,17	1.63	1 (6%)	16,25,25	1.02	2 (12%)
2	KZ5	D	501	-	16,17,17	1.54	1 (6%)	16,25,25	1.12	3 (18%)
2	KZ5	F	501	-	16,17,17	2.02	1 (6%)	16,25,25	0.96	2 (12%)
2	KZ5	C	501	-	16,17,17	1.70	1 (6%)	16,25,25	0.99	2 (12%)
2	KZ5	A	501	-	16,17,17	1.90	1 (6%)	16,25,25	1.20	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KZ5	C	502	-	-	7/12/18/18	0/1/1/1
2	KZ5	G	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	E	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	H	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	D	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	F	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	C	501	-	-	7/12/18/18	0/1/1/1
2	KZ5	A	501	-	-	3/12/18/18	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	KZ5	C5-S14	-7.97	1.70	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	KZ5	C5-S14	-7.87	1.70	1.78
2	A	501	KZ5	C5-S14	-7.51	1.70	1.78
2	C	501	KZ5	C5-S14	-6.74	1.71	1.78
2	G	501	KZ5	C5-S14	-6.40	1.71	1.78
2	H	501	KZ5	C5-S14	-6.35	1.71	1.78
2	D	501	KZ5	C5-S14	-6.04	1.72	1.78
2	E	501	KZ5	C5-S14	-5.71	1.72	1.78

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	KZ5	C3-N4-C5	-2.75	107.73	114.87
2	C	502	KZ5	C13-N8-C7	2.73	119.85	112.22
2	F	501	KZ5	C3-N4-C5	-2.72	107.83	114.87
2	C	501	KZ5	C3-N4-C5	-2.71	107.83	114.87
2	C	502	KZ5	C3-N4-C5	-2.68	107.91	114.87
2	E	501	KZ5	C3-N4-C5	-2.64	108.03	114.87
2	D	501	KZ5	C3-N4-C5	-2.62	108.07	114.87
2	H	501	KZ5	C3-N4-C5	-2.62	108.08	114.87
2	G	501	KZ5	C3-N4-C5	-2.60	108.11	114.87
2	A	501	KZ5	C9-C7-N8	2.52	116.93	111.20
2	D	501	KZ5	N4-C5-N1	-2.39	111.02	115.25
2	E	501	KZ5	N4-C5-N1	-2.32	111.16	115.25
2	G	501	KZ5	N4-C5-N1	-2.31	111.17	115.25
2	C	501	KZ5	N4-C5-N1	-2.26	111.25	115.25
2	A	501	KZ5	N4-C5-N1	-2.26	111.26	115.25
2	H	501	KZ5	N4-C5-N1	-2.24	111.29	115.25
2	D	501	KZ5	C13-N8-C7	2.17	118.28	112.22
2	C	502	KZ5	N4-C5-N1	-2.14	111.46	115.25
2	F	501	KZ5	N4-C5-N1	-2.14	111.46	115.25

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	KZ5	C2-C6-C7-C9
2	A	501	KZ5	C2-C6-C7-N8
2	C	501	KZ5	C2-C6-C7-C9
2	C	501	KZ5	C2-C6-C7-N8
2	C	502	KZ5	C2-C6-C7-C9
2	C	502	KZ5	C2-C6-C7-N8
2	D	501	KZ5	C2-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
2	D	501	KZ5	C2-C6-C7-N8
2	F	501	KZ5	C2-C6-C7-C9
2	F	501	KZ5	C2-C6-C7-N8
2	G	501	KZ5	C2-C6-C7-C9
2	G	501	KZ5	C2-C6-C7-N8
2	E	501	KZ5	C3-C2-C6-C7
2	H	501	KZ5	C3-C2-C6-C7
2	C	502	KZ5	N1-C2-C6-C7
2	E	501	KZ5	N1-C2-C6-C7
2	F	501	KZ5	N1-C2-C6-C7
2	G	501	KZ5	N1-C2-C6-C7
2	H	501	KZ5	N1-C2-C6-C7
2	D	501	KZ5	N8-C7-C9-O10
2	F	501	KZ5	C3-C2-C6-C7
2	D	501	KZ5	C6-C7-C9-O10
2	C	501	KZ5	N1-C2-C6-C7
2	D	501	KZ5	C6-C7-N8-C12
2	G	501	KZ5	C6-C7-N8-C12
2	C	501	KZ5	C3-C2-C6-C7
2	C	502	KZ5	C3-C2-C6-C7
2	G	501	KZ5	C3-C2-C6-C7
2	E	501	KZ5	C6-C7-N8-C12
2	A	501	KZ5	C6-C7-N8-C13
2	C	501	KZ5	C6-C7-N8-C12
2	C	502	KZ5	C6-C7-N8-C12
2	F	501	KZ5	C6-C7-N8-C12
2	H	501	KZ5	C6-C7-N8-C12
2	C	501	KZ5	N8-C7-C9-O11
2	D	501	KZ5	N8-C7-C9-O11
2	E	501	KZ5	N8-C7-C9-O11
2	G	501	KZ5	N8-C7-C9-O11
2	H	501	KZ5	N8-C7-C9-O11
2	D	501	KZ5	C6-C7-C9-O11
2	E	501	KZ5	C2-C6-C7-C9
2	H	501	KZ5	C2-C6-C7-C9
2	E	501	KZ5	C2-C6-C7-N8
2	H	501	KZ5	C2-C6-C7-N8
2	C	501	KZ5	N8-C7-C9-O10
2	C	502	KZ5	N8-C7-C9-O10
2	C	502	KZ5	N8-C7-C9-O11
2	E	501	KZ5	N8-C7-C9-O10
2	F	501	KZ5	N8-C7-C9-O10

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Mol	Chain	Res	Type	Atoms
2	F	501	KZ5	N8-C7-C9-O11
2	G	501	KZ5	N8-C7-C9-O10
2	H	501	KZ5	N8-C7-C9-O10

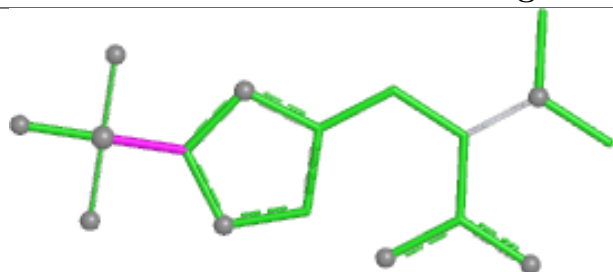
There are no ring outliers.

8 monomers are involved in 21 short contacts:

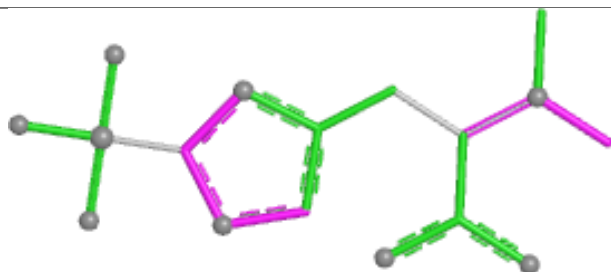
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	KZ5	3	0
2	G	501	KZ5	4	0
2	E	501	KZ5	2	0
2	H	501	KZ5	2	0
2	D	501	KZ5	4	0
2	F	501	KZ5	3	0
2	C	501	KZ5	2	0
2	A	501	KZ5	1	0

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.

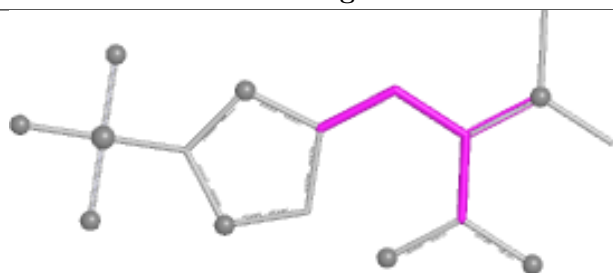
Ligand KZ5 C 502



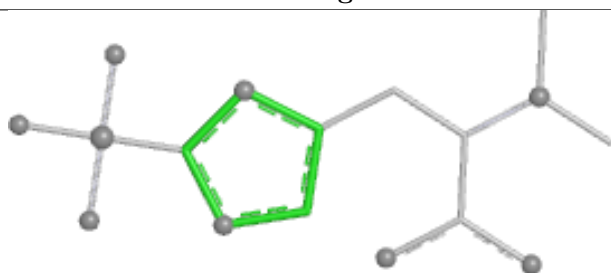
Bond lengths



Bond angles

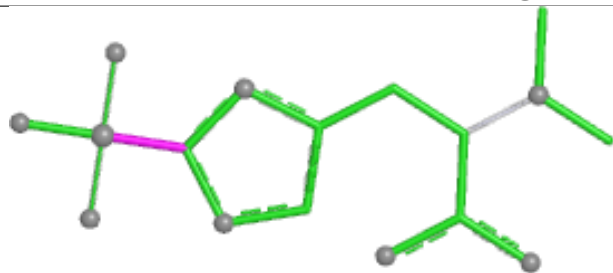


Torsions

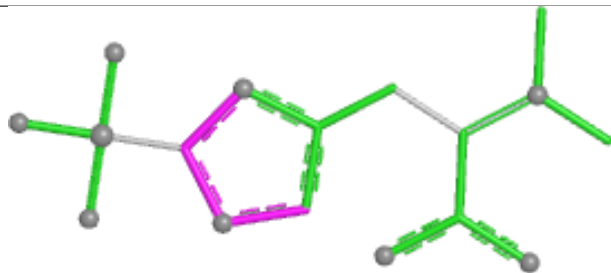


Rings

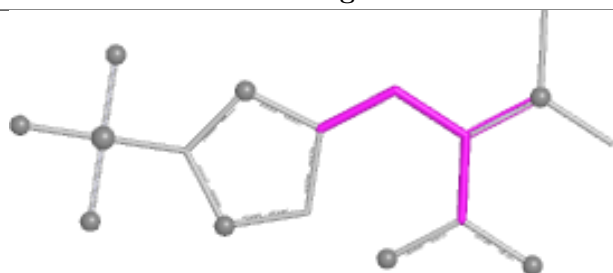
Ligand KZ5 G 501



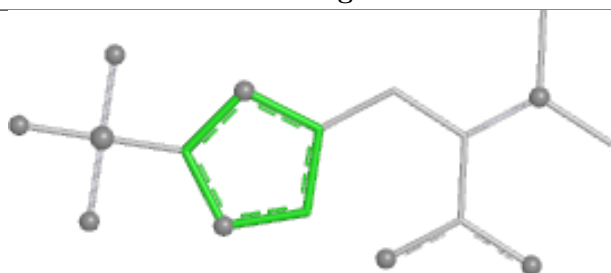
Bond lengths



Bond angles

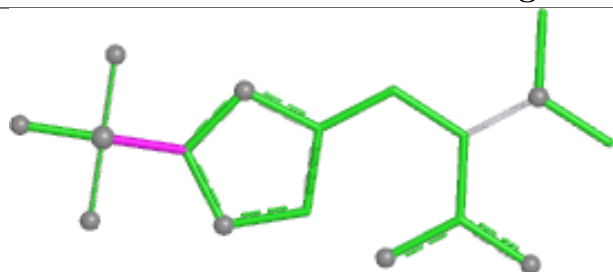


Torsions

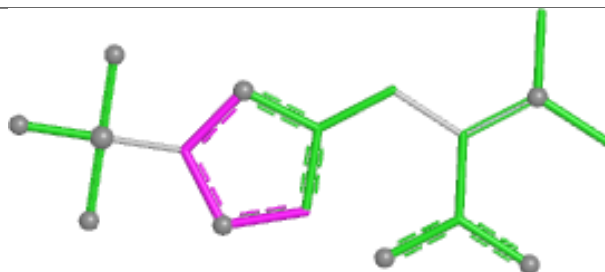


Rings

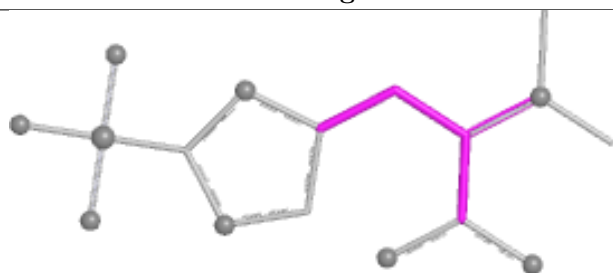
Ligand KZ5 E 501



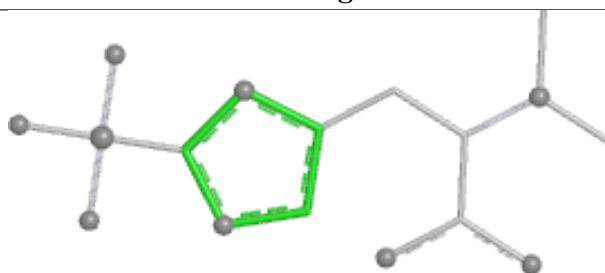
Bond lengths



Bond angles

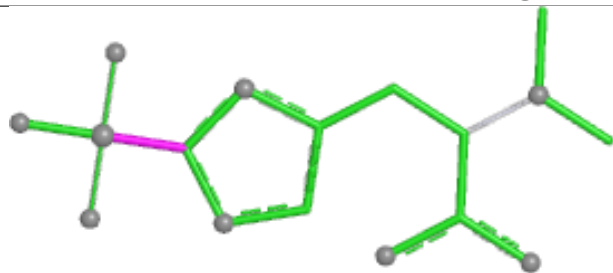


Torsions

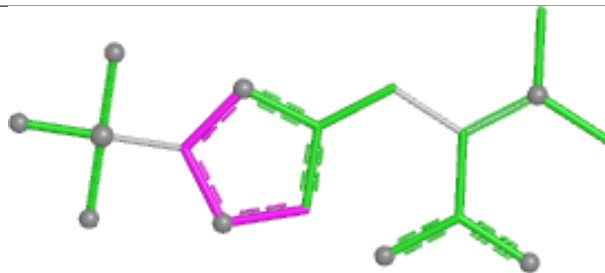


Rings

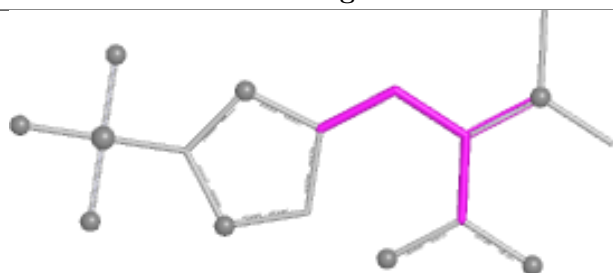
Ligand KZ5 H 501



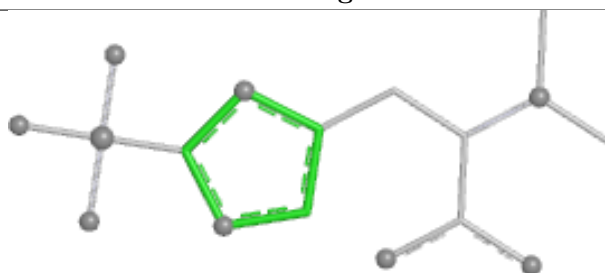
Bond lengths



Bond angles

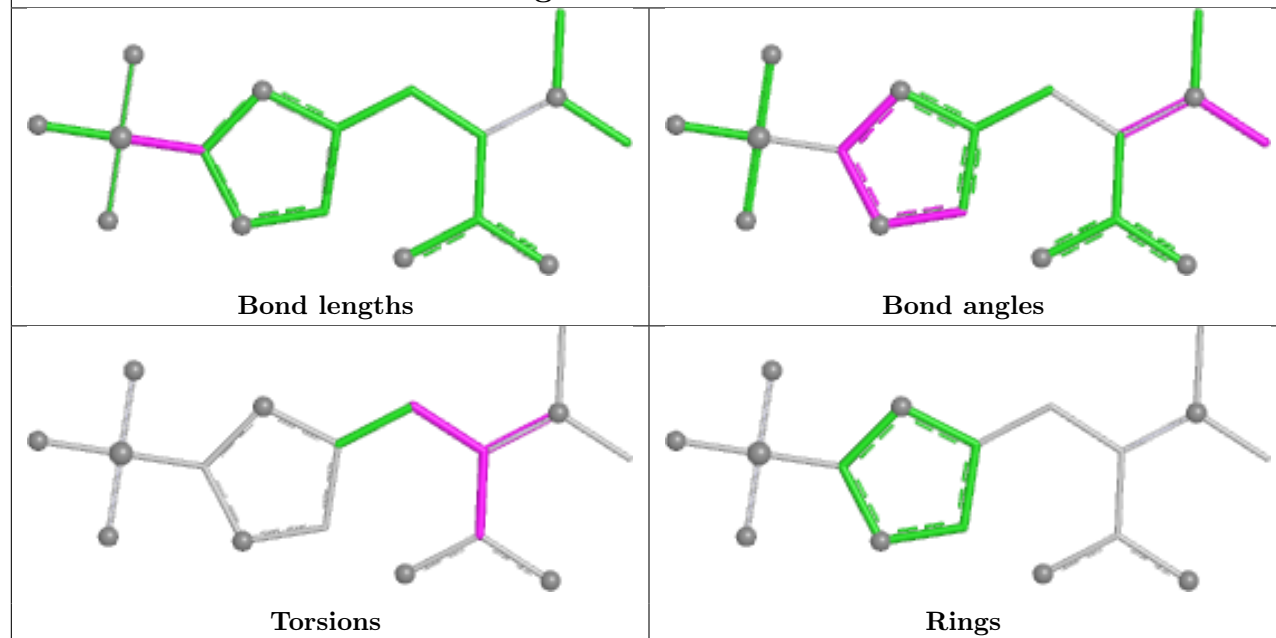


Torsions

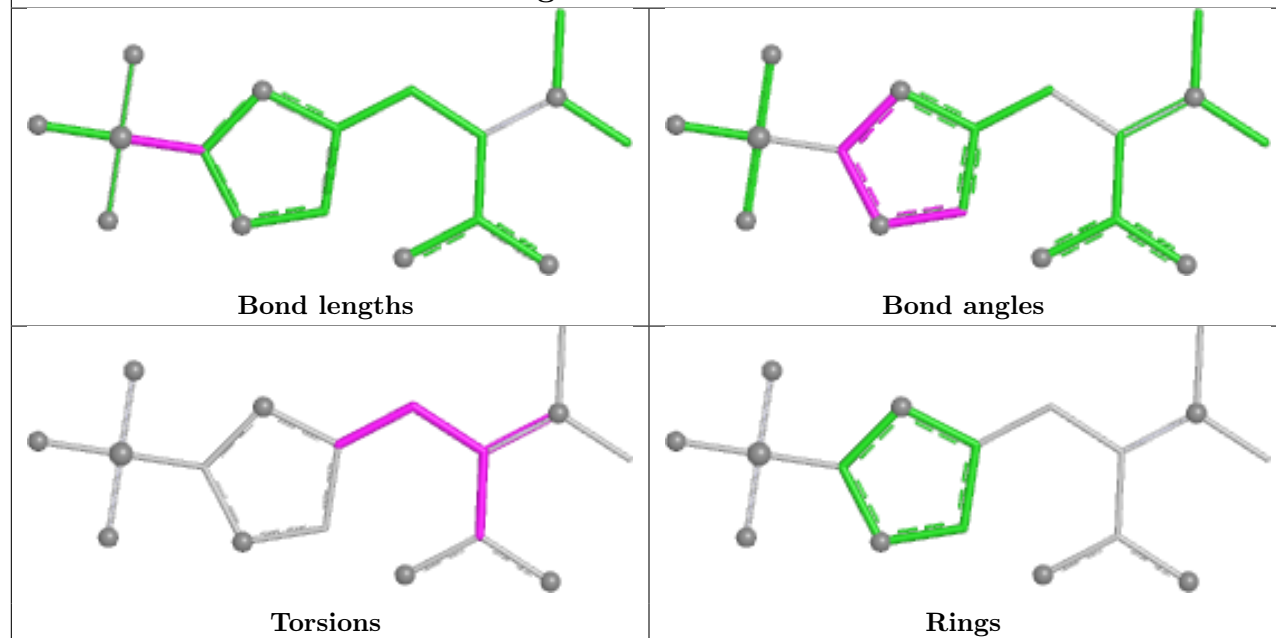


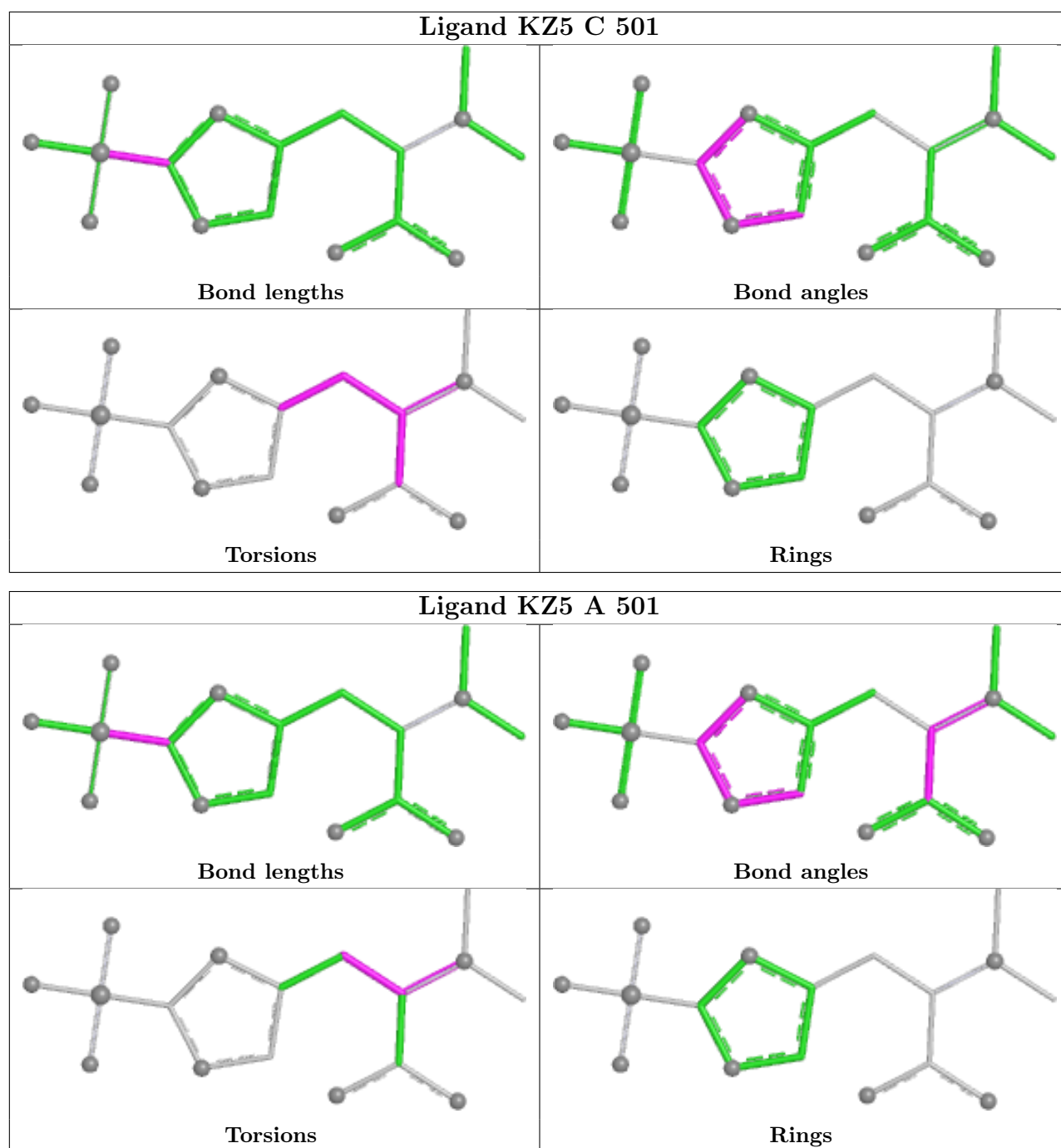
Rings

Ligand KZ5 D 501



Ligand KZ5 F 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/497 (100%)	-1.62	0 100 100	12, 21, 34, 52	0
1	B	497/497 (100%)	-1.63	0 100 100	12, 22, 36, 46	0
1	C	497/497 (100%)	-1.61	0 100 100	11, 24, 36, 44	0
1	D	497/497 (100%)	-1.64	0 100 100	11, 23, 36, 47	0
1	E	497/497 (100%)	-1.58	0 100 100	14, 26, 38, 53	0
1	F	497/497 (100%)	-1.59	0 100 100	14, 25, 38, 49	0
1	G	497/497 (100%)	-1.57	0 100 100	12, 27, 39, 51	0
1	H	497/497 (100%)	-1.57	0 100 100	14, 27, 46, 62	0
All	All	3976/3976 (100%)	-1.60	0 100 100	11, 24, 39, 62	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

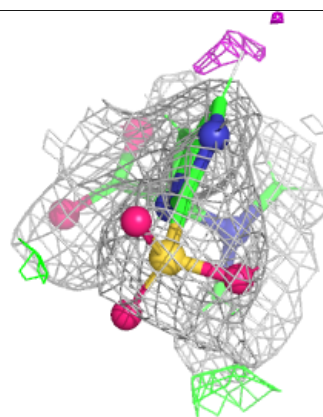
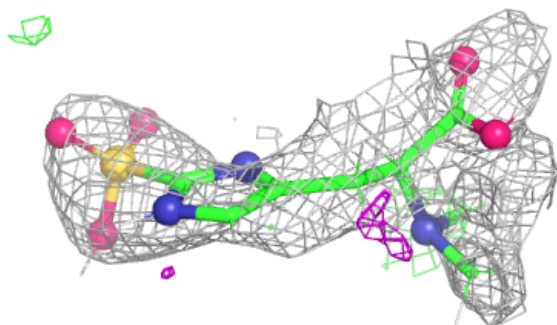
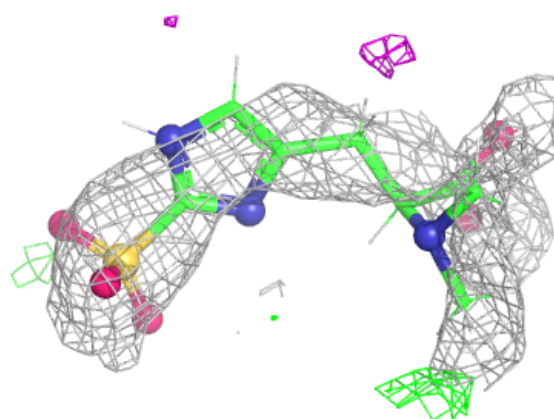
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KZ5	F	501	17/17	0.98	0.07	28,34,39,42	30
2	KZ5	C	501	17/17	0.99	0.05	21,27,32,36	30
2	KZ5	C	502	17/17	0.99	0.05	21,26,30,33	30
2	KZ5	D	501	17/17	0.99	0.04	23,28,33,34	30
2	KZ5	E	501	17/17	0.99	0.05	31,36,43,44	30
2	KZ5	A	501	17/17	0.99	0.05	17,22,31,31	30
2	KZ5	G	501	17/17	0.99	0.05	21,26,31,33	30
2	KZ5	H	501	17/17	0.99	0.04	20,27,35,35	30

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.

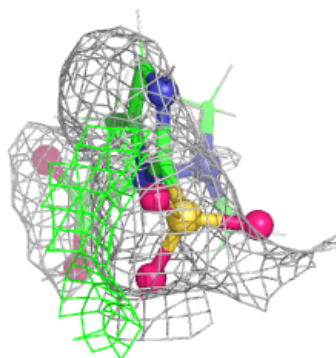
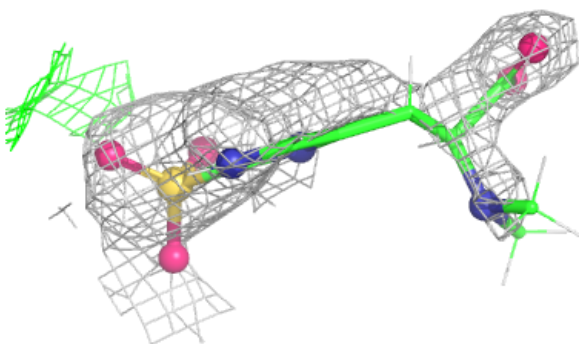
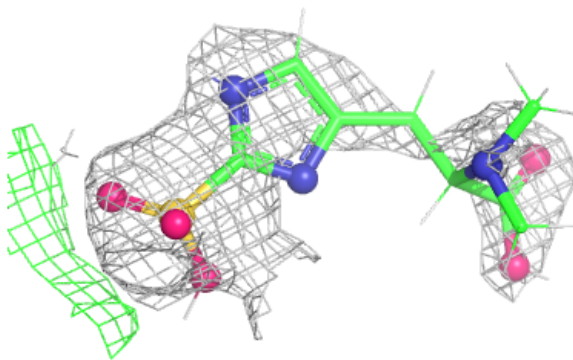
Electron density around KZ5 F 501:

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

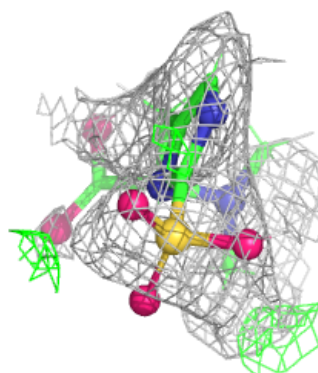
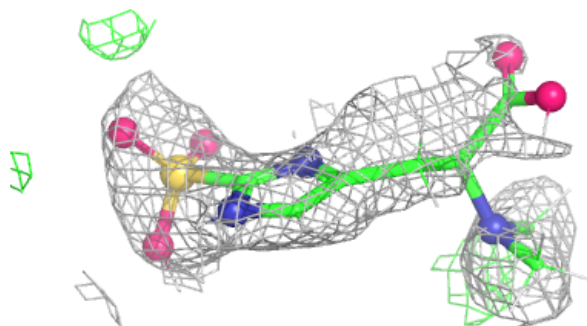
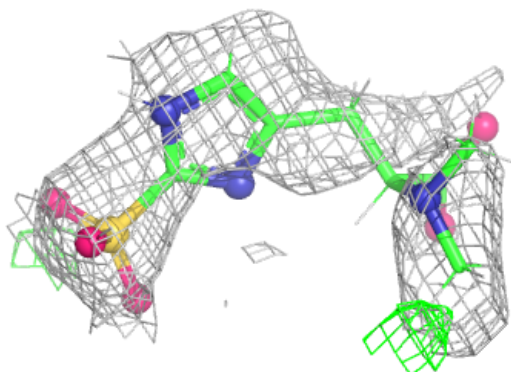


Electron density around KZ5 C 501:

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

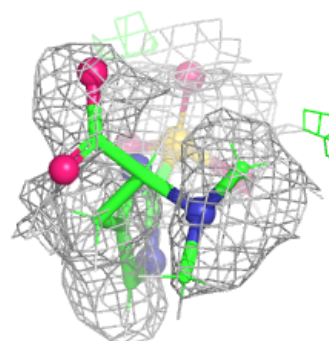
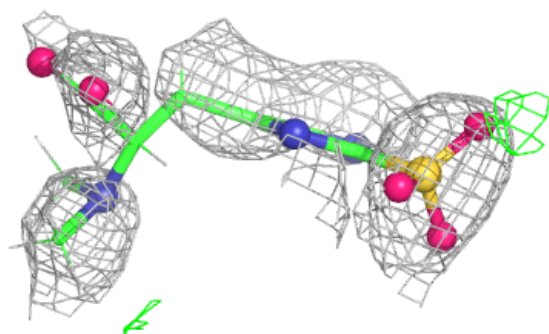
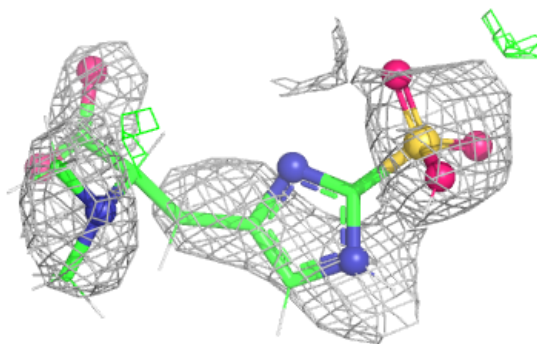
**Electron density around KZ5 C 502:**

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

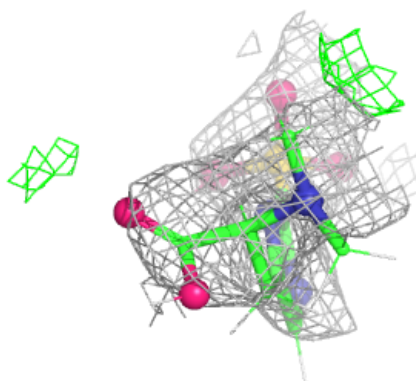
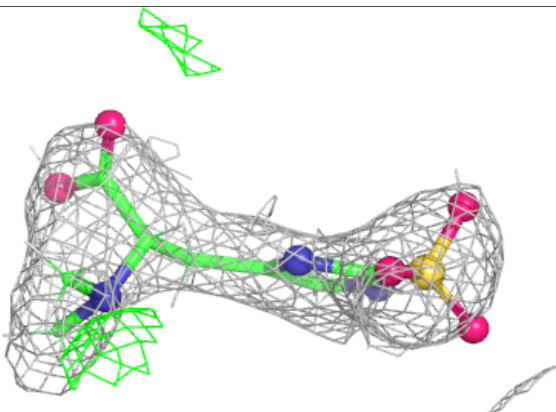
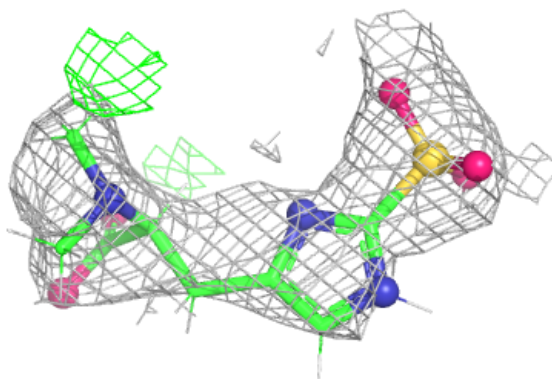


Electron density around KZ5 D 501:

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

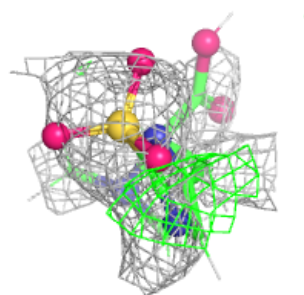
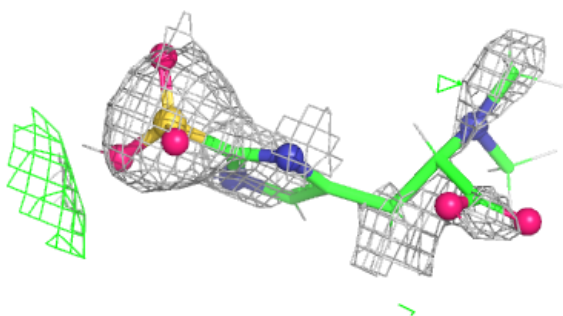
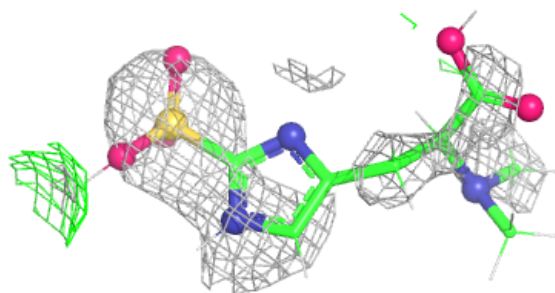
**Electron density around KZ5 E 501:**

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

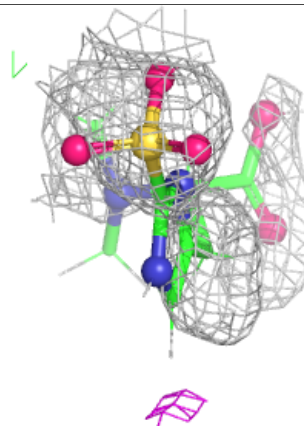
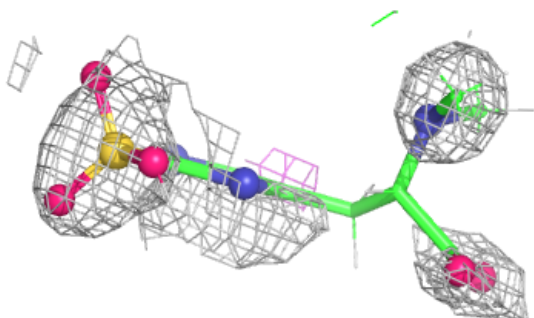
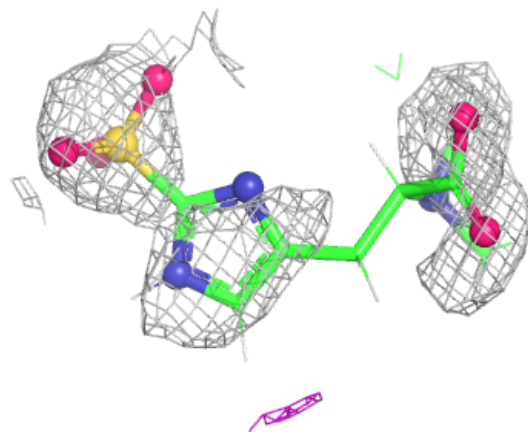


Electron density around KZ5 A 501:

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

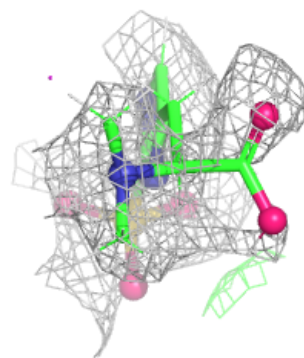
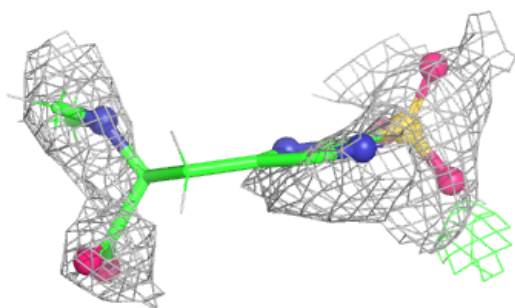
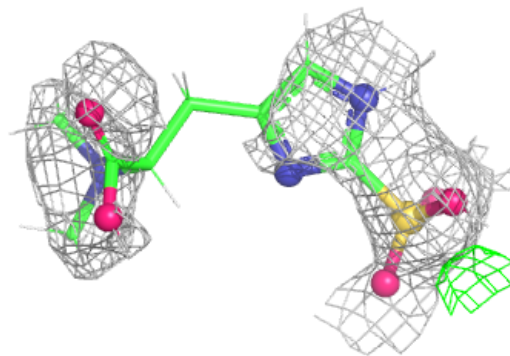
**Electron density around KZ5 G 501:**

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



Electron density around KZ5 H 501:

$2mF_o-DF_c$ (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.