



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 7XCL / pdb_00007xcl
Title : Crystal structure of trimethylamine methyltransferase MttB from Methanosarcina barkeri at 2.5 Å resolution
Authors : Li, J.; Chan, M.K.
Deposited on : 2022-03-24
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

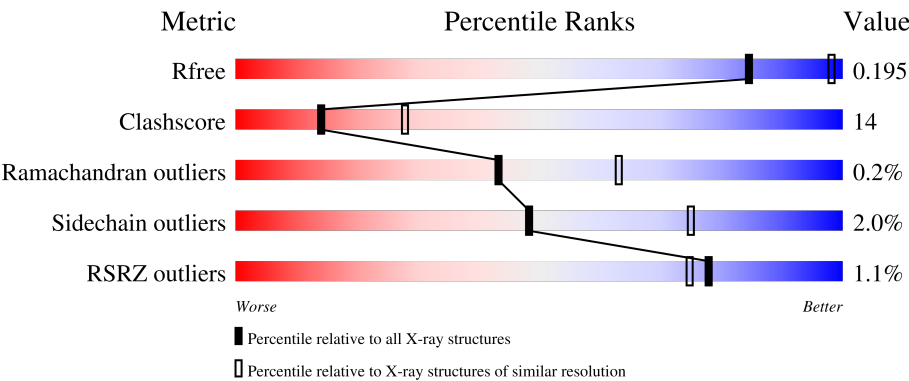
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	503	% 69%27%..
1	B	503	% 71%25%..
1	C	503	% 67%29%..
1	D	503	% 70%27%..
1	E	503	% 69%28%..

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Mol	Chain	Length	Quality of chain
1	F	503	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	602	-	-	X	-
2	GOL	F	601	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23762 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Trimethylamine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	9	0
			3854	2452	645	735	22			
1	B	494	Total	C	N	O	S	0	9	0
			3854	2452	645	735	22			
1	C	493	Total	C	N	O	S	0	9	0
			3846	2447	644	734	21			
1	D	494	Total	C	N	O	S	0	9	0
			3854	2452	645	735	22			
1	E	494	Total	C	N	O	S	0	9	0
			3854	2452	645	735	22			
1	F	494	Total	C	N	O	S	0	9	0
			3854	2452	645	735	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	GLY	-	expression tag	UNP A0A0E3QRM4
A	497	GLY	-	expression tag	UNP A0A0E3QRM4
A	498	HIS	-	expression tag	UNP A0A0E3QRM4
A	499	HIS	-	expression tag	UNP A0A0E3QRM4
A	500	HIS	-	expression tag	UNP A0A0E3QRM4
A	501	HIS	-	expression tag	UNP A0A0E3QRM4
A	502	HIS	-	expression tag	UNP A0A0E3QRM4
A	503	HIS	-	expression tag	UNP A0A0E3QRM4
B	496	GLY	-	expression tag	UNP A0A0E3QRM4
B	497	GLY	-	expression tag	UNP A0A0E3QRM4
B	498	HIS	-	expression tag	UNP A0A0E3QRM4
B	499	HIS	-	expression tag	UNP A0A0E3QRM4
B	500	HIS	-	expression tag	UNP A0A0E3QRM4
B	501	HIS	-	expression tag	UNP A0A0E3QRM4
B	502	HIS	-	expression tag	UNP A0A0E3QRM4
B	503	HIS	-	expression tag	UNP A0A0E3QRM4
C	496	GLY	-	expression tag	UNP A0A0E3QRM4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	497	GLY	-	expression tag	UNP A0A0E3QRM4
C	498	HIS	-	expression tag	UNP A0A0E3QRM4
C	499	HIS	-	expression tag	UNP A0A0E3QRM4
C	500	HIS	-	expression tag	UNP A0A0E3QRM4
C	501	HIS	-	expression tag	UNP A0A0E3QRM4
C	502	HIS	-	expression tag	UNP A0A0E3QRM4
C	503	HIS	-	expression tag	UNP A0A0E3QRM4
D	496	GLY	-	expression tag	UNP A0A0E3QRM4
D	497	GLY	-	expression tag	UNP A0A0E3QRM4
D	498	HIS	-	expression tag	UNP A0A0E3QRM4
D	499	HIS	-	expression tag	UNP A0A0E3QRM4
D	500	HIS	-	expression tag	UNP A0A0E3QRM4
D	501	HIS	-	expression tag	UNP A0A0E3QRM4
D	502	HIS	-	expression tag	UNP A0A0E3QRM4
D	503	HIS	-	expression tag	UNP A0A0E3QRM4
E	496	GLY	-	expression tag	UNP A0A0E3QRM4
E	497	GLY	-	expression tag	UNP A0A0E3QRM4
E	498	HIS	-	expression tag	UNP A0A0E3QRM4
E	499	HIS	-	expression tag	UNP A0A0E3QRM4
E	500	HIS	-	expression tag	UNP A0A0E3QRM4
E	501	HIS	-	expression tag	UNP A0A0E3QRM4
E	502	HIS	-	expression tag	UNP A0A0E3QRM4
E	503	HIS	-	expression tag	UNP A0A0E3QRM4
F	496	GLY	-	expression tag	UNP A0A0E3QRM4
F	497	GLY	-	expression tag	UNP A0A0E3QRM4
F	498	HIS	-	expression tag	UNP A0A0E3QRM4
F	499	HIS	-	expression tag	UNP A0A0E3QRM4
F	500	HIS	-	expression tag	UNP A0A0E3QRM4
F	501	HIS	-	expression tag	UNP A0A0E3QRM4
F	502	HIS	-	expression tag	UNP A0A0E3QRM4
F	503	HIS	-	expression tag	UNP A0A0E3QRM4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total 100	O 100	0	0
4	B	116	Total 116	O 116	0	0
4	C	69	Total 69	O 69	0	0
4	D	87	Total 87	O 87	0	0
4	E	97	Total 97	O 97	0	0
4	F	105	Total 105	O 105	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.49Å 175.49Å 301.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.5 (20.00-2.50) 93.3 (20.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.218 0.193 , 0.195	Depositor DCC
R_{free} test set	8522 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23762	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: GOL, NA, PYL

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	0.39	0/3913	0.91	8/5305 (0.2%)
1	B	0.42	0/3913	0.92	14/5305 (0.3%)
1	C	0.38	0/3905	0.90	12/5295 (0.2%)
1	D	0.40	0/3913	0.92	12/5305 (0.2%)
1	E	0.39	0/3913	0.92	11/5305 (0.2%)
1	F	0.39	0/3913	0.91	11/5305 (0.2%)
All	All	0.40	0/23470	0.92	68/31820 (0.2%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	ILE	N-CA-C	8.37	115.18	107.56
1	C	69	ILE	N-CA-C	8.28	115.75	107.55
1	B	22	THR	N-CA-C	-7.83	98.87	110.46
1	A	90	ARG	N-CA-C	-7.41	103.70	112.89
1	E	69	ILE	N-CA-C	7.26	115.10	107.76
1	B	224	LEU	N-CA-C	7.18	121.43	111.74
1	D	69	ILE	N-CA-C	7.16	114.08	107.56
1	A	224	LEU	N-CA-C	7.14	121.51	111.52
1	F	22	THR	N-CA-C	-7.07	100.00	110.46
1	D	90	ARG	N-CA-C	-7.05	103.64	111.82
1	E	22	THR	N-CA-C	-6.89	100.26	110.46
1	A	22	THR	N-CA-C	-6.87	100.05	110.14
1	B	220	PRO	N-CA-C	-6.82	101.68	111.22
1	F	213	ILE	N-CA-C	-6.76	106.41	112.90
1	A	220	PRO	N-CA-C	-6.74	101.30	111.41
1	D	224	LEU	N-CA-C	6.68	120.61	111.39
1	A	292	SER	N-CA-C	-6.64	102.30	112.99
1	A	167	HIS	N-CA-C	-6.60	104.17	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ARG	N-CA-C	-6.51	104.59	112.54
1	E	292	SER	N-CA-C	-6.45	102.60	112.99
1	C	224	LEU	N-CA-C	6.42	120.41	111.74
1	D	292	SER	N-CA-C	-6.41	102.86	112.54
1	A	289	TYR	N-CA-C	-6.38	96.69	107.99
1	D	22	THR	N-CA-C	-6.15	100.61	110.14
1	E	290	GLY	N-CA-C	6.14	123.28	112.10
1	E	220	PRO	N-CA-C	-6.14	102.20	111.41
1	C	292	SER	N-CA-C	-6.05	103.24	112.99
1	B	292	SER	N-CA-C	-6.00	103.33	112.99
1	E	224	LEU	N-CA-C	5.98	119.65	111.39
1	C	213	ILE	N-CA-C	-5.98	106.91	112.83
1	E	291	SER	N-CA-C	5.93	118.13	108.76
1	C	175	ASN	N-CA-C	5.88	120.15	113.15
1	B	167	HIS	N-CA-C	-5.88	104.95	111.36
1	C	22	THR	N-CA-C	-5.82	101.40	110.42
1	D	41	GLY	N-CA-C	-5.75	104.64	112.52
1	E	216	MET	N-CA-C	5.66	117.87	108.99
1	F	86	VAL	N-CA-C	5.65	116.44	108.36
1	B	213	ILE	N-CA-C	-5.64	107.24	112.83
1	F	395	GLN	N-CA-C	-5.64	105.89	112.89
1	B	128	SER	N-CA-C	5.64	118.16	110.55
1	B	289	TYR	N-CA-C	-5.63	97.28	107.75
1	D	167	HIS	N-CA-C	-5.63	105.23	111.36
1	F	167	HIS	N-CA-C	-5.61	105.25	111.36
1	D	467	ASN	N-CA-C	5.57	120.80	112.94
1	B	467	ASN	N-CA-C	5.55	120.94	113.72
1	F	292	SER	N-CA-C	-5.42	104.27	112.99
1	D	220	PRO	N-CA-C	-5.39	102.81	111.38
1	D	290	GLY	N-CA-C	5.36	120.89	111.57
1	B	371	LEU	N-CA-C	5.35	118.96	111.90
1	C	89	GLY	N-CA-C	-5.33	103.37	112.64
1	C	90	ARG	N-CA-C	-5.30	105.67	111.82
1	F	90	ARG	N-CA-C	-5.26	105.67	111.71
1	B	69	ILE	N-CA-C	5.25	113.07	107.76
1	C	86	VAL	N-CA-C	5.25	115.87	108.36
1	E	89	GLY	N-CA-C	-5.17	102.69	112.10
1	C	144	GLU	N-CA-C	5.15	116.89	111.28
1	E	86	VAL	N-CA-C	5.14	115.36	108.17
1	F	224	LEU	N-CA-C	5.13	118.47	111.39
1	A	89	GLY	N-CA-C	-5.10	103.76	112.64
1	F	144	GLU	N-CA-C	5.09	116.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	HIS	N-CA-C	-5.09	105.81	111.36
1	E	374	THR	N-CA-C	5.08	117.85	109.72
1	B	374	THR	N-CA-C	5.04	117.82	109.85
1	D	21	PHE	N-CA-C	5.02	116.83	109.24
1	C	414	ILE	N-CA-C	5.01	115.57	109.30
1	D	175	ASN	N-CA-C	5.01	119.04	113.02
1	B	330	VAL	N-CA-C	5.01	117.22	108.95
1	F	220	PRO	N-CA-C	-5.00	103.25	111.21

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	3854	0	3848	115	0
1	B	3854	0	3848	109	0
1	C	3846	0	3839	120	0
1	D	3854	0	3848	117	0
1	E	3854	0	3848	120	0
1	F	3854	0	3848	130	0
2	A	12	0	16	4	0
2	B	12	0	16	1	0
2	C	6	0	8	0	0
2	D	18	0	24	0	0
2	E	12	0	16	2	0
2	F	6	0	8	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	100	0	0	2	0
4	B	116	0	0	4	0
4	C	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	87	0	0	3	0
4	E	97	0	0	3	0
4	F	105	0	0	2	0
All	All	23762	0	23167	664	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 14.

All (664) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ILE:HG22	1:B:481:MET:HE2	1.29	1.14
1:B:473:ILE:HG21	1:B:481:MET:HE1	1.45	0.98
1:C:111:THR:HG22	1:C:151:LEU:O	1.66	0.96
1:A:371:LEU:HD22	1:F:441:MET:HE1	1.48	0.95
1:F:417:ASN:HD21	1:F:419:LEU:HB2	1.31	0.95
1:E:473:ILE:HD13	1:E:481:MET:HE1	1.48	0.95
1:D:477:ILE:HG22	1:D:481:MET:HE2	1.49	0.93
1:F:61:ASN:OD1	1:F:63:LYS:HG2	1.71	0.91
1:A:477:ILE:HG22	1:A:481:MET:HE2	1.56	0.88
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.37	0.88
1:A:473:ILE:HD13	1:A:481:MET:HE1	1.56	0.87
1:E:473:ILE:HG21	1:E:481:MET:HE1	1.57	0.86
1:B:194:ARG:HG2	1:B:194:ARG:HH11	1.42	0.83
1:B:371:LEU:HD22	1:E:441:MET:HE1	1.61	0.83
1:C:61:ASN:OD1	1:C:63:LYS:HG2	1.79	0.82
1:C:477:ILE:HG22	1:C:481:MET:HE2	1.64	0.80
1:E:122[A]:LYS:H	1:E:122[A]:LYS:HD3	1.46	0.80
1:D:61:ASN:OD1	1:D:63:LYS:HG2	1.82	0.79
1:F:477:ILE:HG22	1:F:481:MET:HE2	1.64	0.78
1:B:478:PHE:HA	1:B:481:MET:HE3	1.63	0.78
1:C:281:THR:HG22	1:C:282:VAL:HG23	1.66	0.78
1:A:493:ARG:C	1:A:495:MET:H	1.91	0.77
1:F:47:PRO:HA	1:F:50:ARG:NH1	2.00	0.77
1:D:251:MET:HG2	1:D:296:PHE:HB2	1.67	0.76
1:B:61:ASN:OD1	1:B:63:LYS:HG2	1.86	0.76
1:E:473:ILE:HG21	1:E:481:MET:CE	2.15	0.76
1:C:305:VAL:HG22	1:C:310:LEU:HD22	1.67	0.76
1:A:437:LEU:HD22	1:F:343:GLN:HG3	1.68	0.76
1:A:473:ILE:HG21	1:A:481:MET:HE1	1.68	0.76
1:C:47:PRO:HA	1:C:50:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ILE:HD12	1:D:273:SER:HB3	1.67	0.75
1:A:117[A]:LYS:HB2	2:A:602:GOL:H12	1.67	0.74
1:C:51:GLN:O	1:C:55:GLU:HG3	1.88	0.74
1:A:111:THR:HB	1:A:151:LEU:O	1.88	0.73
1:A:473:ILE:HG21	1:A:481:MET:CE	2.19	0.73
1:F:192:TYR:O	1:F:196:ILE:HG12	1.89	0.73
1:E:110:GLY:HA3	1:E:183:ILE:HD12	1.71	0.72
1:E:47:PRO:HA	1:E:50:ARG:NH1	2.04	0.72
1:B:441:MET:HE1	1:E:371:LEU:HD22	1.71	0.72
1:C:342:ASP:HB3	1:D:453:LEU:HD23	1.72	0.72
1:F:217:LEU:HD23	1:F:218:LEU:N	2.04	0.71
1:F:50:ARG:HH21	1:F:65:ASN:ND2	1.87	0.71
1:C:217:LEU:HD23	1:C:218:LEU:N	2.06	0.71
1:B:111:THR:HG22	1:B:183:ILE:HB	1.71	0.71
1:F:171:THR:HB	1:F:172:PRO:HD3	1.74	0.70
1:C:145:ASN:H	1:C:384:ASN:HD21	1.38	0.70
1:C:473:ILE:HG21	1:C:481:MET:HE1	1.74	0.70
1:D:305:VAL:HG23	1:D:310:LEU:HD13	1.73	0.70
1:E:190:VAL:HA	1:E:193:TYR:CD2	2.27	0.70
1:B:145:ASN:H	1:B:384:ASN:HD21	1.40	0.69
1:B:182:HIS:HD2	1:B:184:ASP:H	1.41	0.69
1:B:122[A]:LYS:HD3	1:B:122[A]:LYS:N	2.08	0.68
1:C:171:THR:HB	1:C:172:PRO:HD3	1.75	0.68
1:E:61:ASN:OD1	1:E:63:LYS:HG2	1.93	0.68
1:B:493:ARG:C	1:B:495:MET:H	2.02	0.68
1:D:473:ILE:HG21	1:D:481:MET:HE1	1.75	0.68
1:B:473:ILE:HG21	1:B:481:MET:CE	2.22	0.68
1:A:145:ASN:H	1:A:384:ASN:HD21	1.42	0.68
1:E:350:MET:HE2	1:E:354:LEU:HD11	1.76	0.68
1:E:113:VAL:HG23	1:E:114:LYS:HG3	1.75	0.67
1:F:113:VAL:HG23	1:F:114:LYS:HG3	1.76	0.67
1:C:42:ILE:HD12	1:C:273:SER:HB3	1.76	0.67
1:F:354:LEU:HB2	1:F:355:PRO:HD3	1.77	0.67
1:C:373:MET:HE3	1:C:373:MET:HA	1.75	0.67
1:C:192:TYR:O	1:C:196:ILE:HG12	1.94	0.67
1:C:217:LEU:HD23	1:C:217:LEU:C	2.20	0.67
1:C:453:LEU:HD23	1:D:342:ASP:HB3	1.76	0.67
1:C:42:ILE:HD12	1:C:273:SER:CB	2.25	0.66
1:C:437:LEU:HD22	1:D:343:GLN:HG3	1.74	0.66
1:F:84[B]:ARG:HD3	1:F:84[B]:ARG:N	2.10	0.66
1:A:354:LEU:HB2	1:A:355:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ASN:HD21	1:F:63:LYS:HE2	1.59	0.66
1:C:229:ASN:O	1:C:233:VAL:HG23	1.96	0.66
1:D:145:ASN:H	1:D:384:ASN:HD21	1.42	0.66
1:E:182:HIS:HD2	1:E:184:ASP:H	1.43	0.65
1:C:50:ARG:HH21	1:C:65:ASN:ND2	1.95	0.65
1:E:142:TRP:HE1	2:E:601:GOL:H32	1.62	0.65
1:D:217:LEU:HD23	1:D:218:LEU:N	2.11	0.65
1:F:373:MET:HE3	1:F:373:MET:HA	1.79	0.65
1:B:305:VAL:HG23	1:B:310:LEU:HD13	1.78	0.65
1:E:145:ASN:H	1:E:384:ASN:HD21	1.45	0.64
1:D:51:GLN:HE21	1:D:55:GLU:HG3	1.62	0.64
1:F:42:ILE:CD1	1:F:273:SER:HB3	2.27	0.64
1:D:452:ASP:OD1	1:D:455:THR:HG22	1.97	0.64
1:A:348:LYS:O	1:A:352:THR:HG22	1.97	0.64
1:B:217:LEU:HD23	1:B:218:LEU:N	2.12	0.64
1:D:354:LEU:HB2	1:D:355:PRO:HD3	1.80	0.64
1:F:118[B]:TYR:H	2:F:601:GOL:H31	1.63	0.64
1:A:192:TYR:O	1:A:196:ILE:HG12	1.98	0.63
1:C:139:LEU:HD22	1:C:377:MET:HE2	1.80	0.63
1:A:145:ASN:HB2	1:A:384:ASN:ND2	2.13	0.63
1:E:216:MET:HE3	1:E:233:VAL:HG13	1.81	0.63
1:D:473:ILE:HG21	1:D:481:MET:CE	2.29	0.63
1:B:42:ILE:HD12	1:B:273:SER:HB3	1.80	0.63
1:A:272:LEU:O	1:A:276:VAL:HG23	1.99	0.63
1:B:119[A]:GLN:HG3	1:B:120[A]:ASP:N	2.12	0.63
1:B:166:VAL:HG12	1:B:485:VAL:HG22	1.80	0.62
1:F:371:LEU:N	1:F:371:LEU:HD12	2.14	0.62
1:C:218:LEU:HD13	1:C:230:ALA:HB1	1.81	0.62
1:D:139:LEU:HD22	1:D:377:MET:HE2	1.81	0.62
1:F:217:LEU:HD23	1:F:217:LEU:C	2.24	0.62
1:B:342:ASP:HB3	1:E:453:LEU:HD23	1.81	0.62
4:A:706:HOH:O	1:F:300:LYS:HE2	1.98	0.62
1:D:113:VAL:HG22	1:D:373:MET:HE2	1.81	0.62
1:F:84[B]:ARG:HB3	1:F:99:GLU:HG3	1.81	0.62
1:A:422:LYS:O	1:A:426:GLN:HG3	2.00	0.62
1:A:353:LEU:HD23	1:F:353:LEU:HD23	1.81	0.62
1:D:111:THR:HB	1:D:151:LEU:O	2.00	0.62
1:B:194:ARG:HG2	1:B:194:ARG:NH1	2.13	0.61
1:C:353:LEU:HD21	1:D:350:MET:HE3	1.83	0.61
1:D:452:ASP:O	1:D:456:VAL:HG23	2.01	0.61
1:E:108:CYS:HA	1:E:366:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:LEU:HD22	1:F:377:MET:HE2	1.82	0.61
1:F:145:ASN:H	1:F:384:ASN:HD21	1.48	0.61
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.66	0.60
1:D:441:MET:HA	1:D:441:MET:HE2	1.82	0.60
1:A:171:THR:HB	1:A:172:PRO:HD3	1.83	0.60
1:B:122[A]:LYS:HD3	1:B:122[A]:LYS:H	1.65	0.60
1:F:218:LEU:HD13	1:F:230:ALA:HB1	1.83	0.60
1:D:218:LEU:HD22	1:D:234:ILE:HG13	1.83	0.60
1:F:190:VAL:HA	1:F:193:TYR:CD2	2.37	0.60
1:F:111:THR:CG2	1:F:183:ILE:HB	2.31	0.60
1:A:455:THR:HG21	4:A:792:HOH:O	2.02	0.60
1:E:171:THR:HB	1:E:172:PRO:HD3	1.84	0.60
1:B:113:VAL:HG23	1:B:114:LYS:HG3	1.81	0.59
1:A:117[B]:LYS:HB3	2:A:602:GOL:H12	1.84	0.59
1:F:460:LYS:O	1:F:464:VAL:HG23	2.02	0.59
1:A:441:MET:HE2	1:A:441:MET:HA	1.85	0.59
1:B:354:LEU:HB2	1:B:355:PRO:HD3	1.83	0.59
1:E:281:THR:HG22	1:E:282:VAL:HG23	1.83	0.59
1:E:430:TYR:HB3	1:E:431:PRO:HD3	1.84	0.59
1:C:109:PHE:CG	1:C:110:GLY:N	2.71	0.59
1:B:111:THR:CG2	1:B:183:ILE:HB	2.32	0.59
1:C:48:GLU:O	1:C:52:ILE:HG12	2.03	0.59
1:A:493:ARG:C	1:A:495:MET:N	2.59	0.59
1:F:218:LEU:HD22	1:F:234:ILE:HG13	1.83	0.59
1:C:354:LEU:HB2	1:C:355:PRO:HD3	1.84	0.58
1:C:380:LEU:HD13	1:C:380:LEU:C	2.28	0.58
1:A:194:ARG:HG2	1:A:194:ARG:NH1	2.10	0.58
1:F:305:VAL:O	1:F:310:LEU:HD22	2.03	0.58
1:F:84[A]:ARG:HB3	1:F:99:GLU:HG3	1.85	0.58
1:F:473:ILE:HG21	1:F:481:MET:CE	2.33	0.58
1:A:478:PHE:HA	1:A:481:MET:HE3	1.86	0.57
1:C:84[A]:ARG:NH1	1:E:35:GLU:HG3	2.19	0.57
1:C:473:ILE:HG21	1:C:481:MET:CE	2.33	0.57
1:A:110:GLY:HA3	1:A:183:ILE:HD12	1.86	0.57
1:A:281:THR:HG22	1:A:282:VAL:HG23	1.87	0.57
1:B:245:ASN:HA	1:B:288:TRP:HB2	1.85	0.57
1:E:63:LYS:HG3	1:E:64:THR:HG23	1.87	0.57
1:B:353:LEU:HD23	1:E:353:LEU:HD23	1.86	0.57
1:B:171:THR:HB	1:B:172:PRO:HD3	1.87	0.57
1:C:430:TYR:HB3	1:C:431:PRO:HD3	1.86	0.57
1:E:473:ILE:CD1	1:E:481:MET:HE1	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HG21	1:C:167:HIS:CD2	2.39	0.57
1:D:422:LYS:O	1:D:426:GLN:HG3	2.04	0.57
1:D:171:THR:HB	1:D:172:PRO:HD3	1.87	0.57
1:A:35:GLU:OE2	1:E:84[A]:ARG:NH2	2.37	0.56
1:F:60:VAL:HG22	1:F:67:VAL:HG22	1.86	0.56
1:F:477:ILE:HG22	1:F:481:MET:CE	2.32	0.56
1:E:194:ARG:HH11	1:E:194:ARG:HG2	1.69	0.56
1:B:477:ILE:CG2	1:B:481:MET:HE2	2.20	0.56
1:C:109:PHE:CB	1:C:368:MET:HB2	2.35	0.56
1:B:118[B]:TYR:H	2:B:601:GOL:C1	2.19	0.56
1:E:139:LEU:HD22	1:E:377:MET:HE2	1.86	0.56
1:C:251:MET:HG2	1:C:296:PHE:HB2	1.87	0.56
1:E:111:THR:HG22	1:E:183:ILE:HB	1.88	0.56
1:A:217:LEU:C	1:A:217:LEU:HD23	2.31	0.56
1:A:119[B]:GLN:HB2	1:A:122[B]:LYS:CD	2.36	0.56
1:E:109:PHE:CG	1:E:110:GLY:N	2.73	0.56
1:A:108:CYS:HA	1:A:366:ALA:HB3	1.88	0.56
1:B:281:THR:HG22	1:B:282:VAL:HG23	1.87	0.55
1:C:349:THR:HA	1:C:352:THR:HG22	1.88	0.55
1:D:192:TYR:O	1:D:196:ILE:HG12	2.07	0.55
1:E:51:GLN:O	1:E:55:GLU:HG3	2.06	0.55
1:C:397:ILE:N	1:C:397:ILE:HD12	2.20	0.55
1:F:377:MET:HE1	1:F:465:LEU:HD11	1.89	0.55
1:D:109:PHE:CB	1:D:368:MET:HB2	2.36	0.55
1:F:377:MET:HE1	1:F:465:LEU:HD21	1.88	0.55
1:B:109:PHE:CG	1:B:368:MET:HB2	2.42	0.55
1:D:109:PHE:HB2	1:D:368:MET:HB2	1.88	0.55
1:F:492:PHE:O	1:F:495:MET:HG2	2.07	0.55
1:A:251:MET:HG2	1:A:296:PHE:HB2	1.88	0.55
1:A:113:VAL:HG23	1:A:114:LYS:HG3	1.88	0.55
1:E:109:PHE:CG	1:E:368:MET:HB2	2.41	0.55
1:F:209:ARG:NH2	1:F:239:ARG:O	2.40	0.55
1:D:109:PHE:CG	1:D:110:GLY:N	2.75	0.54
1:F:380:LEU:HD13	1:F:380:LEU:C	2.32	0.54
1:E:478:PHE:HA	1:E:481:MET:HE3	1.89	0.54
1:E:354:LEU:HB2	1:E:355:PRO:HD3	1.89	0.54
1:C:183:ILE:HD12	1:C:217:LEU:HD13	1.90	0.54
1:D:334:PYL:HG3	1:D:368:MET:HE3	1.89	0.54
1:E:350:MET:HE2	1:E:354:LEU:CD1	2.37	0.54
1:F:94:PHE:CG	1:F:178:LYS:HG2	2.42	0.54
1:F:305:VAL:HG13	1:F:334:PYL:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD12	1:F:428:VAL:HA	1.90	0.54
1:B:217:LEU:HD23	1:B:217:LEU:C	2.33	0.54
1:B:453:LEU:HD23	1:E:342:ASP:HB3	1.90	0.54
1:C:129:VAL:HG23	1:C:131:LYS:H	1.71	0.54
1:C:346:HIS:CE1	1:D:386:ILE:HG23	2.42	0.54
1:F:229:ASN:O	1:F:233:VAL:HG23	2.07	0.54
1:E:305:VAL:CG1	1:E:368:MET:HE1	2.37	0.54
1:B:302:THR:CG2	1:E:441:MET:HE3	2.38	0.54
1:C:296:PHE:CD2	1:C:298:LEU:HD23	2.43	0.54
1:E:63:LYS:HG3	1:E:64:THR:N	2.23	0.54
1:C:118[B]:TYR:HB3	1:C:458:HIS:CE1	2.43	0.54
1:F:473:ILE:HG21	1:F:481:MET:HE1	1.90	0.54
1:D:281:THR:HG22	1:D:282:VAL:HG23	1.89	0.54
1:E:252:SER:HB2	1:E:295:THR:HA	1.90	0.54
1:B:109:PHE:CB	1:B:368:MET:HB2	2.38	0.53
1:C:477:ILE:HG22	1:C:481:MET:CE	2.36	0.53
1:D:51:GLN:HE21	1:D:55:GLU:CG	2.20	0.53
1:D:218:LEU:HD13	1:D:230:ALA:HB1	1.89	0.53
1:B:373:MET:HE3	1:B:373:MET:HA	1.90	0.53
1:C:332:GLY:O	1:C:333:SER:HB3	2.07	0.53
1:B:100:CYS:SG	1:B:325:GLY:HA2	2.49	0.53
1:D:114:LYS:HD2	1:D:125:THR:HG22	1.90	0.53
1:D:305:VAL:HG22	1:D:310:LEU:HD22	1.89	0.53
1:E:478:PHE:HA	1:E:481:MET:CE	2.37	0.53
1:B:437:LEU:HD22	1:E:343:GLN:HG3	1.90	0.53
1:C:109:PHE:CG	1:C:368:MET:HB2	2.44	0.53
1:A:218:LEU:HD21	1:A:234:ILE:HG12	1.90	0.53
1:A:47:PRO:HA	1:A:50:ARG:NH1	2.24	0.53
1:B:84[A]:ARG:NH2	1:D:35:GLU:OE2	2.42	0.53
1:C:111:THR:CG2	1:C:183:ILE:HB	2.39	0.53
1:D:245:ASN:HA	1:D:288:TRP:HB2	1.91	0.53
1:E:51:GLN:HG3	1:E:55:GLU:OE1	2.09	0.53
1:C:111:THR:HG21	1:C:151:LEU:HD23	1.91	0.53
1:B:109:PHE:CG	1:B:110:GLY:N	2.77	0.52
1:F:64:THR:O	1:F:65:ASN:HB2	2.09	0.52
1:A:217:LEU:HD23	1:A:218:LEU:N	2.24	0.52
1:F:332:GLY:O	1:F:333:SER:HB3	2.09	0.52
1:C:113:VAL:HG22	1:C:373:MET:HE2	1.90	0.52
1:A:109:PHE:CG	1:A:368:MET:HB2	2.45	0.52
1:F:118[B]:TYR:H	2:F:601:GOL:C3	2.21	0.52
1:C:172:PRO:O	1:C:176:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:VAL:HA	1:D:193:TYR:CD2	2.43	0.52
1:E:42:ILE:CD1	1:E:273:SER:HB3	2.39	0.52
1:B:118[B]:TYR:HB3	1:B:458:HIS:ND1	2.24	0.52
1:C:47:PRO:HA	1:C:50:ARG:HH12	1.73	0.52
1:E:332:GLY:O	1:E:333:SER:HB3	2.10	0.52
1:B:380:LEU:C	1:B:380:LEU:HD13	2.35	0.52
1:F:182:HIS:HD2	1:F:184:ASP:H	1.58	0.52
1:B:119[A]:GLN:HG3	1:B:120[A]:ASP:H	1.75	0.52
1:C:377:MET:HE1	1:C:465:LEU:HD21	1.92	0.52
1:E:122[B]:LYS:H	1:E:122[B]:LYS:HD3	1.74	0.52
1:E:217:LEU:HD23	1:E:218:LEU:N	2.25	0.52
1:F:245:ASN:HA	1:F:288:TRP:HB2	1.91	0.52
1:A:245:ASN:HA	1:A:288:TRP:HB2	1.92	0.52
1:D:42:ILE:HD12	1:D:273:SER:CB	2.37	0.52
1:F:117[B]:LYS:HA	2:F:601:GOL:H31	1.92	0.52
1:D:111:THR:HG21	1:D:184:ASP:OD2	2.10	0.52
1:C:122[A]:LYS:HD3	1:C:122[A]:LYS:N	2.25	0.51
1:C:245:ASN:HA	1:C:288:TRP:HB2	1.92	0.51
1:E:122[A]:LYS:HD3	1:E:122[A]:LYS:N	2.21	0.51
1:F:118[B]:TYR:HB3	1:F:458:HIS:ND1	2.25	0.51
1:B:119[B]:GLN:HB2	1:B:122[B]:LYS:CD	2.40	0.51
1:C:343:GLN:HG3	1:D:437:LEU:HD22	1.91	0.51
1:C:422:LYS:O	1:C:426:GLN:HG3	2.11	0.51
1:A:430:TYR:HB3	1:A:431:PRO:HD3	1.92	0.51
1:C:189:ASN:HB3	1:C:192:TYR:HD2	1.75	0.51
1:C:190:VAL:HA	1:C:193:TYR:CD2	2.45	0.51
1:D:217:LEU:HD23	1:D:217:LEU:C	2.35	0.51
1:A:8:ALA:O	1:A:9:GLY:C	2.53	0.51
1:B:111:THR:HB	1:B:151:LEU:O	2.10	0.51
1:D:412:VAL:HG13	1:D:416:ASN:HB2	1.93	0.51
1:E:109:PHE:CB	1:E:368:MET:HB2	2.41	0.51
1:D:84[A]:ARG:NH2	1:F:35:GLU:OE2	2.44	0.51
1:E:305:VAL:HG22	1:E:310:LEU:HD22	1.92	0.51
1:A:119[B]:GLN:HB2	1:A:122[B]:LYS:HD3	1.92	0.51
1:A:380:LEU:HD13	1:A:380:LEU:C	2.35	0.51
1:A:42:ILE:HD12	1:A:273:SER:HB3	1.93	0.51
1:C:86:VAL:HG22	1:C:97:VAL:HG22	1.93	0.51
1:D:162:GLY:HA2	1:D:492:PHE:CD2	2.46	0.51
1:E:42:ILE:HD12	1:E:273:SER:HB3	1.92	0.51
1:E:221:THR:HB	1:E:225:GLU:HB2	1.93	0.51
1:F:42:ILE:HD13	1:F:273:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:HA	1:A:425:ARG:NH1	2.25	0.50
1:C:371:LEU:N	1:C:371:LEU:HD12	2.26	0.50
1:F:374:THR:HG22	1:F:375:PHE:N	2.25	0.50
1:A:84[B]:ARG:HB3	1:A:99:GLU:HG3	1.93	0.50
1:C:111:THR:HG23	1:C:183:ILE:HB	1.94	0.50
1:D:51:GLN:NE2	1:D:55:GLU:HG3	2.26	0.50
1:E:188:GLU:HG3	4:E:742:HOH:O	2.10	0.50
1:A:99:GLU:OE2	1:C:31:TYR:HB3	2.12	0.50
1:B:118[B]:TYR:HB3	1:B:458:HIS:CE1	2.46	0.50
1:A:105:HIS:NE2	1:D:4:ASN:HB2	2.27	0.50
1:B:302:THR:HG21	1:E:441:MET:HE3	1.93	0.50
1:C:259:TYR:CD2	1:D:403:THR:HA	2.46	0.50
1:F:109:PHE:CG	1:F:110:GLY:N	2.79	0.50
1:A:182:HIS:CD2	1:A:184:ASP:H	2.30	0.50
1:A:190:VAL:HA	1:A:193:TYR:CD2	2.47	0.50
1:B:332:GLY:O	1:B:333:SER:HB3	2.12	0.50
1:B:422:LYS:HA	1:B:425:ARG:NH1	2.27	0.50
1:D:48:GLU:O	1:D:52:ILE:HG12	2.12	0.50
1:D:313:ILE:O	1:D:317:VAL:HG23	2.11	0.50
1:F:194:ARG:HG2	1:F:194:ARG:HH11	1.77	0.50
1:B:35:GLU:HB2	1:F:84[A]:ARG:NH2	2.25	0.50
1:C:107:THR:HG23	1:C:364:TYR:HB2	1.92	0.50
1:D:63:LYS:HG3	1:D:64:THR:HG23	1.93	0.50
1:E:322:GLN:NE2	4:E:703:HOH:O	2.45	0.50
1:B:64:THR:O	1:B:65:ASN:HB2	2.11	0.50
1:B:455:THR:HG21	4:B:803:HOH:O	2.11	0.50
1:C:183:ILE:CD1	1:C:217:LEU:HD13	2.41	0.50
1:C:307:SER:HB2	1:C:308:PRO:HD2	1.93	0.50
1:C:474:ASP:OD2	1:C:477:ILE:HG12	2.12	0.50
1:E:396:GLY:C	1:E:397:ILE:HD12	2.36	0.50
1:A:252:SER:HB2	1:A:295:THR:HA	1.94	0.50
1:E:124[B]:VAL:HG12	1:E:126:VAL:HG13	1.94	0.50
1:A:64:THR:O	1:A:65:ASN:HB2	2.12	0.49
1:D:397:ILE:HD12	1:D:397:ILE:N	2.27	0.49
1:B:392:LYS:O	1:B:395:GLN:HB3	2.13	0.49
1:D:380:LEU:C	1:D:380:LEU:HD13	2.37	0.49
1:D:430:TYR:N	1:D:431:PRO:CD	2.76	0.49
1:F:158:ILE:HG21	1:F:167:HIS:CD2	2.47	0.49
1:A:370:GLU:C	1:A:371:LEU:HD12	2.37	0.49
1:F:295:THR:HG22	1:F:296:PHE:N	2.26	0.49
1:A:42:ILE:CD1	1:A:273:SER:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:O	1:B:426:GLN:HG3	2.12	0.49
1:A:109:PHE:CG	1:A:110:GLY:N	2.80	0.49
1:A:122[A]:LYS:HD3	1:A:122[A]:LYS:N	2.28	0.49
1:A:221:THR:HB	1:A:225:GLU:HB2	1.95	0.49
1:B:374:THR:HG22	1:B:375:PHE:N	2.28	0.49
1:D:296:PHE:CD2	1:D:298:LEU:HD23	2.47	0.49
1:B:349:THR:HA	1:B:352:THR:HG22	1.95	0.49
1:F:150:SER:O	1:F:151:LEU:C	2.56	0.49
1:A:48:GLU:O	1:A:52:ILE:HG12	2.13	0.49
1:B:477:ILE:HG22	1:B:481:MET:CE	2.21	0.49
1:A:109:PHE:CB	1:A:368:MET:HB2	2.42	0.49
1:C:108:CYS:HA	1:C:366:ALA:HB3	1.95	0.49
1:C:296:PHE:HD2	1:C:298:LEU:HD23	1.78	0.49
1:E:119[A]:GLN:HG3	1:E:120[A]:ASP:OD1	2.13	0.49
1:E:158:ILE:HG22	1:E:158:ILE:O	2.13	0.49
1:D:334:PYL:CG	1:D:368:MET:HE3	2.44	0.48
1:A:196:ILE:HD13	1:A:484:ILE:HB	1.94	0.48
1:A:229:ASN:O	1:A:233:VAL:HG23	2.14	0.48
1:B:24:ASP:HB3	1:E:10:PHE:CE1	2.47	0.48
1:D:196:ILE:HD13	1:D:484:ILE:HB	1.95	0.48
1:E:111:THR:HB	1:E:151:LEU:O	2.13	0.48
1:D:373:MET:HE3	1:D:373:MET:HA	1.95	0.48
1:E:332:GLY:HA3	1:E:363:ILE:HG23	1.96	0.48
1:E:451:LYS:HB3	1:E:455:THR:OG1	2.13	0.48
1:A:251:MET:HA	1:A:294:THR:O	2.13	0.48
1:C:396:GLY:C	1:C:397:ILE:HD12	2.38	0.48
1:E:371:LEU:HD12	1:E:371:LEU:N	2.28	0.48
1:A:24:ASP:HB3	1:F:10:PHE:CE1	2.48	0.48
1:E:245:ASN:HA	1:E:288:TRP:HB2	1.95	0.48
1:F:296:PHE:CD2	1:F:298:LEU:HD23	2.48	0.48
1:D:305:VAL:O	1:D:310:LEU:HD22	2.13	0.48
1:D:392:LYS:O	1:D:395:GLN:HB3	2.14	0.48
1:F:477:ILE:CG2	1:F:481:MET:HE2	2.39	0.48
1:A:84[A]:ARG:NH2	1:C:35:GLU:OE2	2.46	0.48
1:A:110:GLY:HA2	1:A:111:THR:HA	1.59	0.48
1:B:107:THR:HG23	1:B:364:TYR:HB2	1.96	0.48
1:E:88:TRP:O	1:E:213:ILE:HA	2.13	0.48
1:A:222:SER:HA	1:A:223:PRO:HA	1.59	0.48
1:C:218:LEU:HD22	1:C:234:ILE:HG13	1.94	0.48
1:E:142:TRP:NE1	2:E:601:GOL:H32	2.27	0.48
1:E:250:ALA:HB3	1:E:293:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:O	1:A:381:VAL:HG22	2.14	0.48
1:C:88:TRP:O	1:C:213:ILE:HA	2.13	0.48
1:C:289:TYR:CE1	1:C:317:VAL:HG13	2.49	0.48
1:F:109:PHE:CB	1:F:368:MET:HB2	2.43	0.48
1:A:305:VAL:O	1:A:310:LEU:HD22	2.14	0.47
1:D:119[B]:GLN:HB2	1:D:122[B]:LYS:HE2	1.96	0.47
1:F:417:ASN:HD21	1:F:419:LEU:CB	2.13	0.47
1:B:218:LEU:HD23	1:B:244:VAL:CG1	2.44	0.47
1:F:245:ASN:HB2	1:F:288:TRP:CE3	2.49	0.47
1:A:334:PYL:HG3	1:A:368:MET:HE3	1.96	0.47
1:C:91:ASP:HB2	1:C:177:ALA:HB1	1.96	0.47
1:E:119[B]:GLN:HB2	1:E:122[B]:LYS:HE2	1.96	0.47
1:A:332:GLY:O	1:A:333:SER:HB3	2.15	0.47
4:B:763:HOH:O	1:E:298:LEU:HB2	2.13	0.47
1:F:118[B]:TYR:HB3	1:F:458:HIS:CE1	2.50	0.47
1:F:218:LEU:CD2	1:F:234:ILE:HG13	2.43	0.47
1:C:448:ALA:O	1:C:451:LYS:HE3	2.15	0.47
1:E:84[A]:ARG:HB3	1:E:99:GLU:HG3	1.97	0.47
1:F:452:ASP:OD1	1:F:455:THR:HG22	2.15	0.47
1:D:245:ASN:C	1:D:245:ASN:ND2	2.72	0.47
1:A:268:ASN:ND2	1:A:289:TYR:OH	2.47	0.47
1:A:334:PYL:O2	1:A:368:MET:HE2	2.15	0.47
1:A:453:LEU:HD23	1:F:342:ASP:HB3	1.95	0.47
1:E:397:ILE:HD12	1:E:397:ILE:N	2.30	0.47
1:B:50:ARG:NH1	1:B:62:GLU:OE2	2.48	0.47
1:B:300:LYS:HE2	4:E:760:HOH:O	2.14	0.47
1:D:158:ILE:O	1:D:158:ILE:HG22	2.14	0.47
1:E:222:SER:HA	1:E:223:PRO:HA	1.58	0.47
1:A:259:TYR:CD2	1:F:403:THR:HA	2.50	0.47
1:B:42:ILE:CD1	1:B:273:SER:HB3	2.43	0.47
1:B:441:MET:HE3	1:E:302:THR:CG2	2.45	0.47
1:D:87:LEU:HD21	1:D:288:TRP:CH2	2.50	0.47
1:E:245:ASN:C	1:E:245:ASN:ND2	2.73	0.47
1:D:493:ARG:C	1:D:495:MET:H	2.23	0.47
1:F:223:PRO:HB3	1:F:255:SER:O	2.15	0.46
1:C:13:LEU:HD23	1:D:20:LEU:C	2.41	0.46
1:B:222:SER:HA	1:B:223:PRO:HA	1.63	0.46
1:B:430:TYR:HB3	1:B:431:PRO:HD3	1.96	0.46
1:B:84[A]:ARG:HB3	1:B:99:GLU:HG3	1.98	0.46
1:D:56:ASN:CG	1:D:280:LEU:HD22	2.40	0.46
1:D:455:THR:O	1:D:459:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ASP:HB2	1:F:228:VAL:HA	1.97	0.46
1:F:110:GLY:HA3	1:F:183:ILE:HG13	1.98	0.46
1:B:94:PHE:CG	1:B:178:LYS:HG2	2.50	0.46
1:B:305:VAL:O	1:B:310:LEU:HD22	2.14	0.46
1:B:389:MET:HA	1:B:389:MET:HE2	1.96	0.46
1:E:18:LEU:HD23	1:E:18:LEU:C	2.40	0.46
1:F:318:ALA:O	1:F:322:GLN:HG3	2.16	0.46
1:D:122[A]:LYS:N	1:D:122[A]:LYS:HD3	2.31	0.46
1:F:158:ILE:HG22	1:F:158:ILE:O	2.15	0.46
1:F:251:MET:HG2	1:F:296:PHE:HB2	1.97	0.46
1:F:430:TYR:HB3	1:F:431:PRO:HD3	1.97	0.46
1:C:158:ILE:HG22	1:C:158:ILE:O	2.16	0.46
1:C:452:ASP:O	1:C:456:VAL:HG23	2.16	0.46
1:E:159:ALA:O	1:E:161:GLN:HG2	2.16	0.46
1:B:50:ARG:HG2	1:B:60:VAL:HG11	1.97	0.46
1:B:343:GLN:HG3	1:E:437:LEU:HD22	1.97	0.46
1:D:422:LYS:HA	1:D:425:ARG:NH1	2.31	0.46
1:E:217:LEU:HD23	1:E:217:LEU:C	2.40	0.46
1:E:380:LEU:HD13	1:E:380:LEU:C	2.40	0.46
1:A:343:GLN:HG3	1:F:437:LEU:HD22	1.98	0.46
1:C:64:THR:O	1:C:65:ASN:HB2	2.16	0.46
1:D:286:LYS:NZ	4:D:704:HOH:O	2.49	0.46
1:E:109:PHE:HB2	1:E:368:MET:HB2	1.98	0.46
1:F:117[A]:LYS:HA	2:F:601:GOL:H31	1.98	0.46
1:F:349:THR:HA	1:F:352:THR:HG22	1.97	0.46
1:A:100:CYS:SG	1:A:325:GLY:HA2	2.56	0.46
1:B:63:LYS:HG3	1:B:64:THR:HG23	1.97	0.46
1:B:452:ASP:OD1	1:B:455:THR:HG23	2.16	0.46
1:C:332:GLY:HA3	1:C:363:ILE:HG23	1.99	0.46
1:A:302:THR:CG2	1:F:441:MET:HE3	2.46	0.45
1:A:332:GLY:HA3	1:A:363:ILE:HG23	1.97	0.45
1:B:111:THR:HG22	1:B:183:ILE:CB	2.44	0.45
1:B:435:MET:HG2	1:B:436:LEU:CD1	2.46	0.45
1:F:42:ILE:HD13	1:F:273:SER:CB	2.46	0.45
1:F:61:ASN:ND2	1:F:63:LYS:HE2	2.27	0.45
1:F:452:ASP:OD1	1:F:452:ASP:C	2.59	0.45
1:A:196:ILE:CD1	1:A:484:ILE:HB	2.46	0.45
1:E:305:VAL:HG11	1:E:368:MET:HE1	1.97	0.45
1:F:422:LYS:O	1:F:426:GLN:HG3	2.15	0.45
1:D:110:GLY:HA2	1:D:111:THR:HA	1.70	0.45
1:D:451:LYS:HB3	1:D:455:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:ASN:C	1:E:245:ASN:HD22	2.23	0.45
1:F:475:ALA:O	1:F:479:LYS:HG3	2.16	0.45
1:C:104:VAL:HG22	1:C:360:ALA:O	2.17	0.45
1:D:307:SER:HB2	1:D:308:PRO:HD2	1.99	0.45
1:C:158:ILE:HG21	1:C:167:HIS:HD2	1.80	0.45
1:D:185:PRO:HG3	1:D:216:MET:HB2	1.98	0.45
1:D:196:ILE:CD1	1:D:484:ILE:HB	2.46	0.45
1:F:51:GLN:O	1:F:55:GLU:HG3	2.16	0.45
1:F:473:ILE:HG21	1:F:481:MET:HE3	1.98	0.45
1:A:369:LEU:HD12	1:A:376:SER:HB2	1.99	0.45
1:E:378:GLU:O	1:E:381:VAL:HG22	2.17	0.45
1:C:217:LEU:C	1:C:217:LEU:CD2	2.89	0.45
1:D:113:VAL:CG2	1:D:373:MET:HE2	2.45	0.45
1:A:139:LEU:HD22	1:A:377:MET:HE2	1.98	0.45
1:C:221:THR:O	1:C:225:GLU:HB2	2.16	0.45
1:F:122[B]:LYS:HE2	4:F:716:HOH:O	2.15	0.45
1:C:54:LYS:HB2	1:C:60:VAL:HG21	1.99	0.45
1:C:84[A]:ARG:HB3	1:C:99:GLU:HG3	1.98	0.45
1:A:111:THR:HA	1:A:152:PRO:O	2.17	0.45
1:B:145:ASN:HB2	1:B:384:ASN:ND2	2.31	0.45
1:B:412:VAL:O	1:B:416:ASN:HB2	2.16	0.45
1:E:370:GLU:C	1:E:371:LEU:HD12	2.41	0.45
1:E:452:ASP:OD1	1:E:452:ASP:C	2.60	0.45
1:B:332:GLY:HA3	1:B:363:ILE:HG23	1.99	0.44
1:E:192:TYR:O	1:E:196:ILE:HG12	2.17	0.44
1:D:109:PHE:CG	1:D:368:MET:HB2	2.51	0.44
1:F:86:VAL:HG22	1:F:97:VAL:HG22	1.98	0.44
1:A:218:LEU:HD22	1:A:234:ILE:HG13	1.98	0.44
1:C:122[A]:LYS:HD3	1:C:122[A]:LYS:H	1.83	0.44
1:D:172:PRO:O	1:D:176:THR:HG22	2.17	0.44
1:D:374:THR:HG22	1:D:375:PHE:N	2.32	0.44
1:F:422:LYS:HA	1:F:425:ARG:NH1	2.32	0.44
1:A:327:PRO:HA	1:A:361:ASN:OD1	2.18	0.44
1:B:84[B]:ARG:HB3	1:B:99:GLU:HG3	1.98	0.44
1:C:72:TYR:CE1	1:C:73:LEU:HG	2.52	0.44
1:D:51:GLN:O	1:D:55:GLU:HG3	2.17	0.44
1:D:245:ASN:C	1:D:245:ASN:HD22	2.24	0.44
1:F:368:MET:SD	1:F:369:LEU:N	2.90	0.44
1:A:84[A]:ARG:NH2	1:C:35:GLU:CD	2.76	0.44
1:C:458:HIS:O	1:C:462:GLU:HG2	2.17	0.44
1:D:369:LEU:HD12	1:D:376:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119[B]:GLN:HB2	1:C:122[B]:LYS:HE2	1.98	0.44
1:C:305:VAL:CG1	1:C:368:MET:HE1	2.48	0.44
1:D:194:ARG:HG2	1:D:194:ARG:NH1	2.29	0.44
1:D:296:PHE:CE2	1:D:298:LEU:HD23	2.52	0.44
1:E:333:SER:C	1:E:348:LYS:HD3	2.43	0.44
1:A:169:THR:O	1:A:172:PRO:HD2	2.17	0.44
1:D:305:VAL:CG1	1:D:368:MET:HE1	2.48	0.44
1:F:119[A]:GLN:HB3	1:F:120[A]:ASP:H	1.61	0.44
1:A:194:ARG:NH1	1:A:194:ARG:CG	2.80	0.44
1:B:132:ASP:O	1:B:136:ILE:HG13	2.17	0.44
1:B:371:LEU:HD22	1:E:441:MET:CE	2.42	0.44
1:B:4:ASN:HD22	1:C:105:HIS:CE1	2.36	0.44
1:E:168:GLU:O	1:E:172:PRO:HG2	2.18	0.44
1:F:268:ASN:ND2	1:F:289:TYR:OH	2.51	0.44
1:B:124[A]:VAL:HG12	1:B:126:VAL:HG13	1.99	0.43
1:D:119[A]:GLN:HB3	1:D:120[A]:ASP:H	1.55	0.43
1:D:322:GLN:NE2	4:D:702:HOH:O	2.49	0.43
1:C:160:GLY:O	1:C:161:GLN:NE2	2.51	0.43
1:D:452:ASP:OD1	1:D:452:ASP:C	2.60	0.43
1:E:332:GLY:HA3	1:E:363:ILE:CG2	2.48	0.43
1:F:217:LEU:C	1:F:217:LEU:CD2	2.91	0.43
1:F:348:LYS:O	1:F:352:THR:HG22	2.17	0.43
1:A:4:ASN:HD22	1:D:105:HIS:CE1	2.37	0.43
1:D:139:LEU:CD2	1:D:377:MET:HE2	2.47	0.43
1:D:182:HIS:HD2	1:D:184:ASP:H	1.65	0.43
1:F:119[A]:GLN:HB3	4:F:716:HOH:O	2.19	0.43
1:F:295:THR:CG2	1:F:296:PHE:N	2.82	0.43
1:A:117[A]:LYS:HB2	2:A:602:GOL:C1	2.41	0.43
1:A:132:ASP:O	1:A:136:ILE:HG13	2.18	0.43
1:A:332:GLY:HA3	1:A:363:ILE:CG2	2.47	0.43
1:C:38:MET:O	1:C:68:LYS:HD3	2.19	0.43
1:C:145:ASN:H	1:C:384:ASN:ND2	2.12	0.43
1:E:493:ARG:C	1:E:495:MET:H	2.26	0.43
1:F:370:GLU:C	1:F:371:LEU:HD12	2.44	0.43
1:A:149:PHE:CZ	1:A:152:PRO:HD3	2.54	0.43
1:A:374:THR:HG22	1:A:375:PHE:N	2.33	0.43
1:A:392:LYS:HG2	1:A:432:SER:HB3	2.01	0.43
1:B:123[B]:TYR:OH	1:B:454:ALA:HB1	2.19	0.43
1:B:221:THR:HB	1:B:225:GLU:HB2	2.00	0.43
1:B:305:VAL:CG2	1:B:310:LEU:HD13	2.46	0.43
1:D:332:GLY:O	1:D:333:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:SER:CB	1:E:317:VAL:HG21	2.48	0.43
1:B:232:GLN:HE21	1:B:236:LYS:HE3	1.84	0.43
1:A:118[B]:TYR:H	2:A:602:GOL:H12	1.83	0.43
1:B:251:MET:HG2	1:B:296:PHE:HB2	2.00	0.43
1:E:368:MET:SD	1:E:369:LEU:N	2.91	0.43
1:F:118[B]:TYR:N	2:F:601:GOL:H31	2.32	0.43
1:F:145:ASN:HB2	1:F:384:ASN:ND2	2.34	0.43
1:F:222:SER:HA	1:F:223:PRO:HA	1.65	0.43
1:A:389:MET:HE2	1:A:389:MET:HA	2.01	0.43
1:A:495:MET:HE2	1:A:495:MET:HA	2.01	0.43
1:B:88:TRP:O	1:B:213:ILE:HA	2.19	0.43
1:B:119[A]:GLN:CG	1:B:120[A]:ASP:N	2.81	0.43
1:B:190:VAL:HA	1:B:193:TYR:CD2	2.53	0.43
1:C:8:ALA:O	1:C:9:GLY:C	2.61	0.43
1:D:222:SER:HA	1:D:223:PRO:HA	1.71	0.43
1:D:378:GLU:O	1:D:382:ILE:HG13	2.19	0.43
1:F:110:GLY:HA2	1:F:111:THR:HA	1.64	0.43
1:A:442:PHE:CD1	1:A:442:PHE:C	2.96	0.42
1:D:477:ILE:CG2	1:D:481:MET:HE2	2.33	0.42
1:E:182:HIS:CD2	1:E:184:ASP:H	2.29	0.42
1:A:475:ALA:O	1:A:479:LYS:HG3	2.19	0.42
1:B:38:MET:HG2	4:B:720:HOH:O	2.19	0.42
1:F:109:PHE:CG	1:F:368:MET:HB2	2.54	0.42
1:F:334:PYL:HG3	1:F:368:MET:HE3	2.01	0.42
1:E:217:LEU:HD11	1:E:247:LEU:HD13	2.00	0.42
1:F:236:LYS:HB3	1:F:240:PHE:CE2	2.55	0.42
1:F:251:MET:HA	1:F:294:THR:O	2.18	0.42
1:F:350:MET:HE2	1:F:354:LEU:HD11	2.02	0.42
1:B:493:ARG:C	1:B:495:MET:N	2.68	0.42
1:C:113:VAL:HG23	1:C:114:LYS:HG3	2.02	0.42
1:C:148:TYR:OH	1:C:362:THR:HG21	2.19	0.42
1:D:120[A]:ASP:H	1:D:122[A]:LYS:HE2	1.84	0.42
1:E:232:GLN:HE21	1:E:236:LYS:HE3	1.83	0.42
1:C:119[B]:GLN:HB2	1:C:122[B]:LYS:CD	2.49	0.42
1:D:216:MET:HE3	1:D:233:VAL:HG13	2.00	0.42
1:F:448:ALA:O	1:F:451:LYS:HE3	2.19	0.42
1:A:93:LYS:HE3	1:A:94:PHE:CZ	2.54	0.42
1:B:299:LYS:HE3	1:E:428:VAL:O	2.19	0.42
1:B:322:GLN:NE2	4:B:703:HOH:O	2.51	0.42
1:B:403:THR:HA	1:E:259:TYR:CD2	2.54	0.42
1:C:182:HIS:HD2	1:C:184:ASP:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ASN:HB2	1:C:288:TRP:CE3	2.55	0.42
1:D:119[A]:GLN:HB3	1:D:122[A]:LYS:HE3	1.99	0.42
1:E:107:THR:HG23	1:E:364:TYR:HB2	2.01	0.42
1:A:346:HIS:CE1	1:F:386:ILE:HG23	2.55	0.42
1:D:291:SER:HB3	1:D:317:VAL:HG11	2.01	0.42
1:F:117[A]:LYS:HE2	2:F:601:GOL:O1	2.20	0.42
1:E:392:LYS:NZ	1:E:395:GLN:HE22	2.17	0.42
1:C:110:GLY:HA2	1:C:111:THR:HA	1.63	0.42
1:E:374:THR:HG22	1:E:375:PHE:N	2.35	0.42
1:A:309:GLU:O	1:A:313:ILE:HG13	2.20	0.42
1:C:194:ARG:HH11	1:C:194:ARG:HG2	1.82	0.42
1:C:452:ASP:OD1	1:C:452:ASP:C	2.62	0.42
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.92	0.42
1:A:392:LYS:O	1:A:395:GLN:HB3	2.19	0.41
1:B:8:ALA:O	1:B:9:GLY:C	2.61	0.41
1:D:451:LYS:HB3	1:D:455:THR:CG2	2.50	0.41
1:E:169:THR:C	1:E:172:PRO:HD2	2.44	0.41
1:E:209:ARG:O	1:E:212:PRO:HD3	2.20	0.41
1:F:480:ASP:O	1:F:483:ALA:HB3	2.20	0.41
1:B:334:PYL:HG3	1:B:368:MET:HE3	2.01	0.41
1:C:109:PHE:HB2	1:C:365:GLY:HA2	2.02	0.41
1:D:387:PHE:O	1:D:391:LYS:HG3	2.20	0.41
1:D:412:VAL:CG1	1:D:416:ASN:HB2	2.49	0.41
1:F:196:ILE:HD13	1:F:484:ILE:HB	2.02	0.41
1:A:397:ILE:N	1:A:397:ILE:HD12	2.36	0.41
1:D:123[B]:TYR:OH	1:D:454:ALA:HB1	2.21	0.41
1:E:8:ALA:O	1:E:9:GLY:C	2.63	0.41
1:E:110:GLY:HA2	1:E:111:THR:HA	1.62	0.41
1:E:305:VAL:O	1:E:310:LEU:HD22	2.21	0.41
1:A:145:ASN:HB2	1:A:384:ASN:HD22	1.85	0.41
1:A:158:ILE:O	1:A:158:ILE:HG22	2.20	0.41
1:B:84[A]:ARG:HH11	1:B:84[A]:ARG:HG3	1.85	0.41
1:C:295:THR:HG22	1:C:296:PHE:N	2.35	0.41
1:B:35:GLU:OE2	1:F:84[A]:ARG:NH1	2.53	0.41
1:B:473:ILE:O	1:B:474:ASP:C	2.64	0.41
1:C:460:LYS:O	1:C:464:VAL:HG23	2.20	0.41
1:D:305:VAL:HG22	1:D:305:VAL:O	2.21	0.41
1:E:204:ASP:OD1	1:E:206:GLU:HB2	2.21	0.41
1:F:96:THR:HG23	1:F:105:HIS:CD2	2.56	0.41
1:A:20:LEU:C	1:F:13:LEU:HD23	2.46	0.41
1:A:107:THR:HG23	1:A:364:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:OE2	1:D:442:PHE:HB2	2.19	0.41
1:C:421:LEU:HD12	1:C:421:LEU:HA	1.91	0.41
1:D:332:GLY:HA3	1:D:363:ILE:HG23	2.02	0.41
1:F:196:ILE:O	1:F:199:ALA:HB3	2.21	0.41
1:F:369:LEU:HD12	1:F:376:SER:HB2	2.03	0.41
1:A:119[B]:GLN:HB2	1:A:122[B]:LYS:HE2	2.02	0.41
1:E:473:ILE:HG21	1:E:481:MET:HE2	2.00	0.41
1:B:16:VAL:HG22	1:E:20:LEU:CD2	2.50	0.41
1:B:217:LEU:HA	1:B:245:ASN:HB3	2.02	0.41
1:C:480:ASP:O	1:C:483:ALA:HB3	2.21	0.41
1:D:104:VAL:HG22	1:D:360:ALA:O	2.21	0.41
1:E:216:MET:HE3	1:E:233:VAL:CG1	2.49	0.41
1:F:63:LYS:HG3	1:F:64:THR:HG23	2.02	0.41
1:F:221:THR:O	1:F:225:GLU:HB2	2.20	0.41
1:F:435:MET:HG2	1:F:436:LEU:HD12	2.02	0.41
1:F:442:PHE:CD1	1:F:442:PHE:C	2.98	0.41
1:A:209:ARG:NH2	1:A:239:ARG:O	2.54	0.41
1:A:349:THR:HA	1:A:352:THR:HG22	2.03	0.41
1:A:493:ARG:O	1:A:495:MET:N	2.53	0.41
1:B:194:ARG:NH1	1:B:194:ARG:CG	2.79	0.41
1:C:100:CYS:SG	1:C:325:GLY:HA2	2.61	0.41
1:C:223:PRO:HB3	1:C:255:SER:O	2.21	0.41
1:C:289:TYR:HE1	1:C:317:VAL:HG13	1.84	0.41
1:D:182:HIS:CD2	1:D:184:ASP:H	2.38	0.41
1:D:371:LEU:HD12	1:D:371:LEU:N	2.35	0.41
1:E:137:ALA:HA	1:E:149:PHE:CE1	2.56	0.41
1:E:194:ARG:NH1	1:E:195:ASP:OD1	2.54	0.41
1:F:142:TRP:HZ3	1:F:381:VAL:HG12	1.85	0.41
1:B:109:PHE:HB2	1:B:365:GLY:HA2	2.03	0.41
1:B:165:ASP:O	1:B:182:HIS:HE1	2.04	0.41
1:D:107:THR:HG23	1:D:364:TYR:HB2	2.02	0.41
1:D:477:ILE:HG22	1:D:481:MET:CE	2.35	0.41
1:E:145:ASN:H	1:E:384:ASN:ND2	2.13	0.41
1:E:165:ASP:O	1:E:182:HIS:HE1	2.03	0.41
1:F:100:CYS:SG	1:F:325:GLY:HA2	2.61	0.41
1:F:139:LEU:HD22	1:F:377:MET:CE	2.50	0.41
1:C:232:GLN:HE21	1:C:236:LYS:HE3	1.85	0.40
1:C:473:ILE:CG2	1:C:481:MET:HE1	2.47	0.40
1:D:200:TYR:HA	1:D:477:ILE:CG2	2.50	0.40
1:D:430:TYR:N	1:D:431:PRO:HD3	2.36	0.40
1:D:448:ALA:O	1:D:451:LYS:HE3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:TYR:O	1:E:197:VAL:HG23	2.21	0.40
1:A:84[A]:ARG:HB3	1:A:99:GLU:HG3	2.02	0.40
1:A:245:ASN:C	1:A:245:ASN:ND2	2.79	0.40
1:B:182:HIS:CD2	1:B:184:ASP:H	2.28	0.40
1:B:448:ALA:O	1:B:451:LYS:HE3	2.22	0.40
1:C:84[A]:ARG:HH11	1:C:84[A]:ARG:HG3	1.85	0.40
1:E:268:ASN:ND2	1:E:289:TYR:OH	2.55	0.40
1:E:420:ALA:O	1:E:425:ARG:NH1	2.54	0.40
1:C:218:LEU:HD23	1:C:244:VAL:CG1	2.52	0.40
1:F:305:VAL:O	1:F:305:VAL:HG13	2.20	0.40
1:A:305:VAL:CG1	1:A:368:MET:HE1	2.51	0.40
1:C:119[B]:GLN:HB2	1:C:122[B]:LYS:HD3	2.02	0.40
1:C:218:LEU:CD2	1:C:234:ILE:HG13	2.51	0.40
1:F:455:THR:O	1:F:459:GLU:HG3	2.21	0.40
1:C:420:ALA:O	1:C:425:ARG:NH1	2.55	0.40
1:D:38:MET:HG2	4:D:748:HOH:O	2.22	0.40
1:E:100:CYS:SG	1:E:325:GLY:HA2	2.61	0.40
1:E:119[B]:GLN:HG3	1:E:124[B]:VAL:CG2	2.52	0.40
1:F:327:PRO:HA	1:F:361:ASN:OD1	2.21	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	500/503 (99%)	480 (96%)	17 (3%)	3 (1%)	21	38
1	B	500/503 (99%)	477 (95%)	21 (4%)	2 (0%)	30	49
1	C	499/503 (99%)	474 (95%)	24 (5%)	1 (0%)	43	63
1	D	500/503 (99%)	482 (96%)	18 (4%)	0	100	100
1	E	500/503 (99%)	474 (95%)	26 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	500/503 (99%)	475 (95%)	23 (5%)	2 (0%)	30	49
All	All	2999/3018 (99%)	2862 (95%)	129 (4%)	8 (0%)	43	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119[A]	GLN
1	A	119[B]	GLN
1	F	119[A]	GLN
1	F	119[B]	GLN
1	A	9	GLY
1	B	119[A]	GLN
1	B	119[B]	GLN
1	C	371	LEU

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	412/411 (100%)	402 (98%)	10 (2%)	43	70
1	B	412/411 (100%)	401 (97%)	11 (3%)	39	67
1	C	411/411 (100%)	405 (98%)	6 (2%)	57	80
1	D	412/411 (100%)	403 (98%)	9 (2%)	45	73
1	E	412/411 (100%)	402 (98%)	10 (2%)	43	70
1	F	412/411 (100%)	402 (98%)	10 (2%)	43	70
All	All	2471/2466 (100%)	2415 (98%)	56 (2%)	48	72

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	111	THR
1	A	122[A]	LYS

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Mol	Chain	Res	Type
1	A	122[B]	LYS
1	A	194	ARG
1	A	217	LEU
1	A	249	MET
1	A	277	LEU
1	A	373	MET
1	A	455	THR
1	B	111	THR
1	B	122[A]	LYS
1	B	122[B]	LYS
1	B	217	LEU
1	B	218	LEU
1	B	249	MET
1	B	268	ASN
1	B	277	LEU
1	B	373	MET
1	B	436	LEU
1	B	455	THR
1	C	50	ARG
1	C	91	ASP
1	C	122[A]	LYS
1	C	122[B]	LYS
1	C	218	LEU
1	C	277	LEU
1	D	91	ASP
1	D	111	THR
1	D	119[A]	GLN
1	D	119[B]	GLN
1	D	122[A]	LYS
1	D	122[B]	LYS
1	D	217	LEU
1	D	277	LEU
1	D	350	MET
1	E	91	ASP
1	E	111	THR
1	E	122[A]	LYS
1	E	122[B]	LYS
1	E	184	ASP
1	E	249	MET
1	E	251	MET
1	E	277	LEU
1	E	373	MET

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Mol	Chain	Res	Type
1	E	436	LEU
1	F	111	THR
1	F	119[A]	GLN
1	F	119[B]	GLN
1	F	216	MET
1	F	217	LEU
1	F	249	MET
1	F	277	LEU
1	F	305	VAL
1	F	373	MET
1	F	455	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	182	HIS
1	A	232	GLN
1	A	245	ASN
1	A	268	ASN
1	A	322	GLN
1	A	379	GLN
1	A	384	ASN
1	A	395	GLN
1	A	410	GLN
1	A	426	GLN
1	A	440	HIS
1	A	482	GLN
1	B	43	GLN
1	B	51	GLN
1	B	182	HIS
1	B	232	GLN
1	B	245	ASN
1	B	268	ASN
1	B	322	GLN
1	B	379	GLN
1	B	384	ASN
1	B	395	GLN
1	B	410	GLN
1	B	440	HIS
1	C	51	GLN
1	C	65	ASN

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Mol	Chain	Res	Type
1	C	161	GLN
1	C	167	HIS
1	C	175	ASN
1	C	232	GLN
1	C	268	ASN
1	C	322	GLN
1	C	384	ASN
1	C	410	GLN
1	C	426	GLN
1	C	440	HIS
1	C	467	ASN
1	C	482	GLN
1	D	51	GLN
1	D	105	HIS
1	D	175	ASN
1	D	182	HIS
1	D	232	GLN
1	D	245	ASN
1	D	322	GLN
1	D	379	GLN
1	D	384	ASN
1	D	395	GLN
1	D	410	GLN
1	D	467	ASN
1	D	482	GLN
1	E	14	ASN
1	E	51	GLN
1	E	164	GLN
1	E	182	HIS
1	E	232	GLN
1	E	245	ASN
1	E	268	ASN
1	E	322	GLN
1	E	384	ASN
1	E	395	GLN
1	E	410	GLN
1	E	482	GLN
1	F	65	ASN
1	F	161	GLN
1	F	167	HIS
1	F	182	HIS
1	F	232	GLN

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Mol	Chain	Res	Type
1	F	245	ASN
1	F	268	ASN
1	F	322	GLN
1	F	384	ASN
1	F	395	GLN
1	F	410	GLN
1	F	417	ASN
1	F	469	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z > 2$
2	GOL	B	602	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	A	601	-	5,5,5	0.34	0	5,5,5	0.34	0
2	GOL	E	602	-	5,5,5	0.30	0	5,5,5	0.61	0
2	GOL	C	601	-	5,5,5	0.29	0	5,5,5	0.31	0
2	GOL	F	601	-	5,5,5	0.34	0	5,5,5	0.50	0
2	GOL	D	603	-	5,5,5	0.33	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	E	601	-	5,5,5	0.35	0	5,5,5	0.25	0
2	GOL	B	601	-	5,5,5	0.26	0	5,5,5	0.69	0
2	GOL	A	602	-	5,5,5	0.32	0	5,5,5	0.52	0
2	GOL	D	602	-	5,5,5	0.29	0	5,5,5	0.43	0
2	GOL	D	601	-	5,5,5	0.35	0	5,5,5	0.34	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
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	601	-	-	3/4/4/4	-
2	GOL	E	602	-	-	2/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	F	601	-	-	2/4/4/4	-
2	GOL	D	603	-	-	4/4/4/4	-
2	GOL	E	601	-	-	4/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	D	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O2-C2-C3-O3
2	D	602	GOL	C1-C2-C3-O3
2	D	603	GOL	C1-C2-C3-O3
2	D	603	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	E	601	GOL	O1-C1-C2-O2
2	E	601	GOL	O1-C1-C2-C3
2	E	601	GOL	C1-C2-C3-O3
2	F	601	GOL	O1-C1-C2-O2
2	F	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-C3
2	D	603	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-O2
2	B	602	GOL	O2-C2-C3-O3
2	D	602	GOL	O2-C2-C3-O3
2	D	603	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
2	E	601	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
2	E	602	GOL	C1-C2-C3-O3
2	E	602	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	GOL	6	0
2	E	601	GOL	2	0
2	B	601	GOL	1	0
2	A	602	GOL	4	0

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	493/503 (98%)	-0.48	5 (1%) 79 76	17, 42, 63, 78	9 (1%)
1	B	493/503 (98%)	-0.57	5 (1%) 79 76	17, 39, 60, 76	9 (1%)
1	C	492/503 (97%)	-0.12	5 (1%) 79 76	20, 52, 75, 92	9 (1%)
1	D	493/503 (98%)	-0.39	6 (1%) 76 73	19, 44, 67, 87	9 (1%)
1	E	493/503 (98%)	-0.39	5 (1%) 79 76	18, 43, 68, 119	9 (1%)
1	F	493/503 (98%)	-0.31	8 (1%) 70 67	20, 46, 72, 112	9 (1%)
All	All	2957/3018 (97%)	-0.38	34 (1%) 78 75	17, 44, 69, 119	54 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	494	GLY	6.0
1	C	120[A]	ASP	5.7
1	D	298	LEU	4.9
1	D	495	MET	4.6
1	E	120[A]	ASP	4.6
1	C	298	LEU	4.6
1	A	120[A]	ASP	4.5
1	D	120[A]	ASP	4.4
1	B	121[A]	GLY	4.4
1	D	119[A]	GLN	4.0
1	C	119[A]	GLN	3.9
1	E	119[A]	GLN	3.9
1	B	120[A]	ASP	3.8
1	F	119[A]	GLN	3.7
1	F	122[A]	LYS	3.7
1	F	298	LEU	3.6
1	E	495	MET	3.6
1	F	160	GLY	3.4
1	F	120[A]	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	495	MET	3.3
1	C	122[A]	LYS	3.2
1	F	495	MET	3.2
1	B	122[A]	LYS	2.9
1	A	122[A]	LYS	2.6
1	A	119[A]	GLN	2.5
1	E	122[A]	LYS	2.4
1	A	495	MET	2.4
1	D	122[A]	LYS	2.3
1	A	121[A]	GLY	2.3
1	F	121[A]	GLY	2.3
1	F	161	GLN	2.1
1	D	10	PHE	2.1
1	B	119[A]	GLN	2.0
1	E	118[A]	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	601	6/6	0.78	0.19	64,70,74,76	0
2	GOL	B	602	6/6	0.78	0.20	63,74,74,77	0
2	GOL	C	601	6/6	0.80	0.18	77,84,85,85	0
2	GOL	E	602	6/6	0.80	0.21	79,84,86,88	0
2	GOL	D	603	6/6	0.82	0.18	65,73,75,75	0
2	GOL	D	601	6/6	0.83	0.21	65,84,86,88	0
2	GOL	E	601	6/6	0.84	0.17	60,74,79,81	0
2	GOL	A	602	6/6	0.85	0.15	65,77,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	602	6/6	0.87	0.13	58,68,71,72	0
2	GOL	F	601	6/6	0.87	0.14	65,74,78,79	0
2	GOL	B	601	6/6	0.88	0.12	61,79,82,83	0
3	NA	A	603	1/1	0.95	0.09	42,42,42,42	0
3	NA	C	602	1/1	0.95	0.09	41,41,41,41	0
3	NA	E	603	1/1	0.95	0.08	39,39,39,39	0
3	NA	F	602	1/1	0.95	0.08	38,38,38,38	0
3	NA	D	604	1/1	0.96	0.12	49,49,49,49	0
3	NA	B	603	1/1	0.99	0.07	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.