Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 02:51 PM EDT

PDB ID	:	1XMG
Title	:	Crystal structure of apo methane monooxygenase hydroxylase from M. capsulatus (Bath)
Authors	:	Sazinsky, M.H.; Merkx, M.; Cadieux, E.; Tang, S.; Lippard, S.J.
Deposited on	:	2004-10-02
Resolution	:	2.10 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:

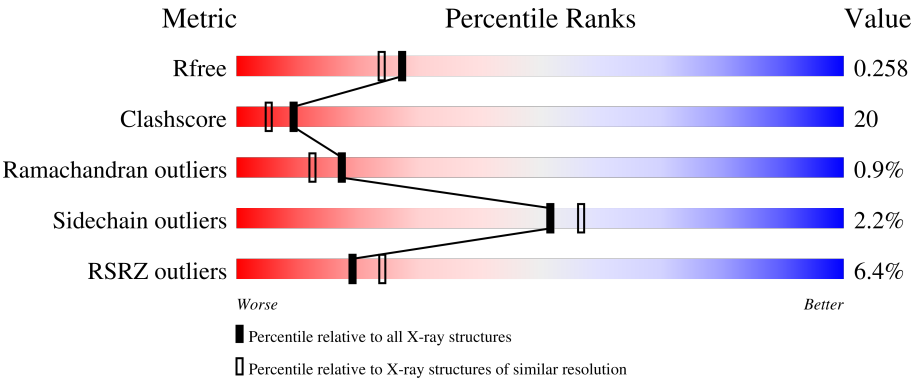
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	527	8% 63% 31%
1	B	527	6% 59% 35%
2	C	388	% 75% 24%
2	D	388	10% 54% 45%
3	E	169	% 78% 20%

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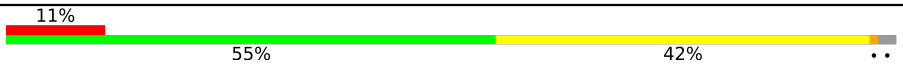
Mol	Chain	Length	Quality of chain
3	F	169	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18102 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3167	2038	545	576	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLU	ALA	conflict	UNP P18798
C	370	ARG	ALA	conflict	UNP P18798
D	18	GLU	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

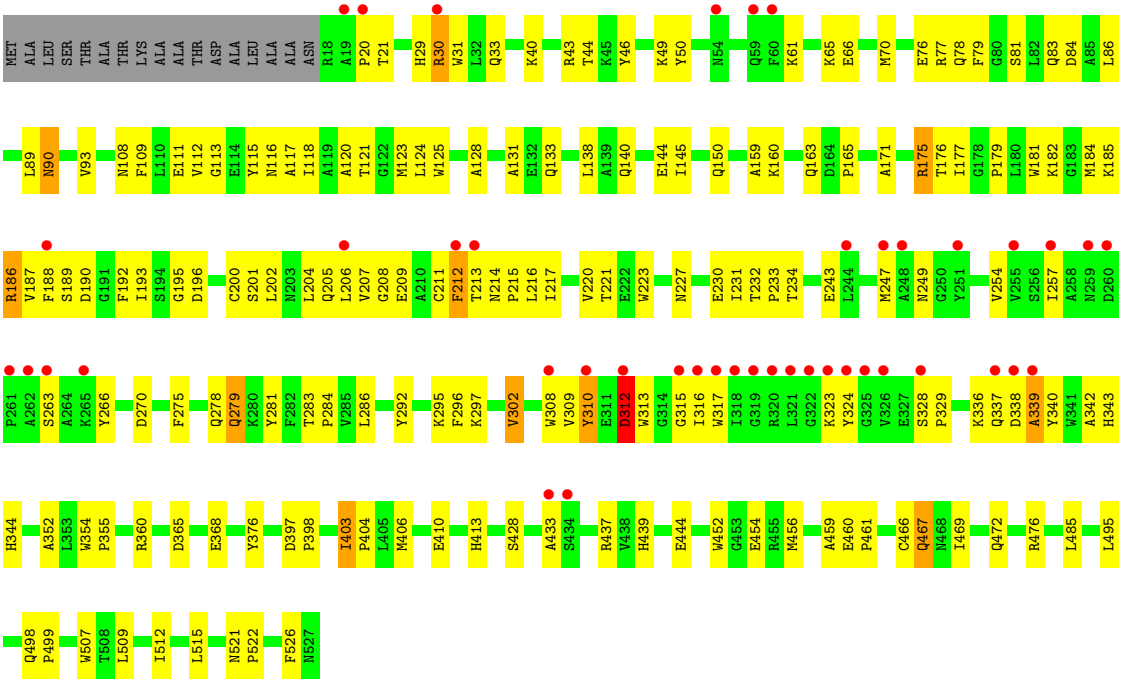
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	156	Total O 156 156	0	0
5	B	170	Total O 170 170	0	0
5	C	249	Total O 249 249	0	0
5	D	86	Total O 86 86	0	0
5	E	106	Total O 106 106	0	0
5	F	18	Total O 18 18	0	0

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.

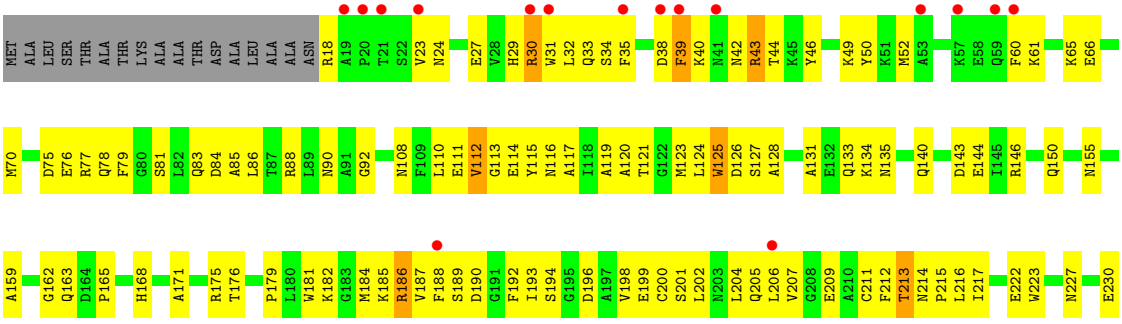
• Molecule 1: Methane monooxygenase component A alpha chain

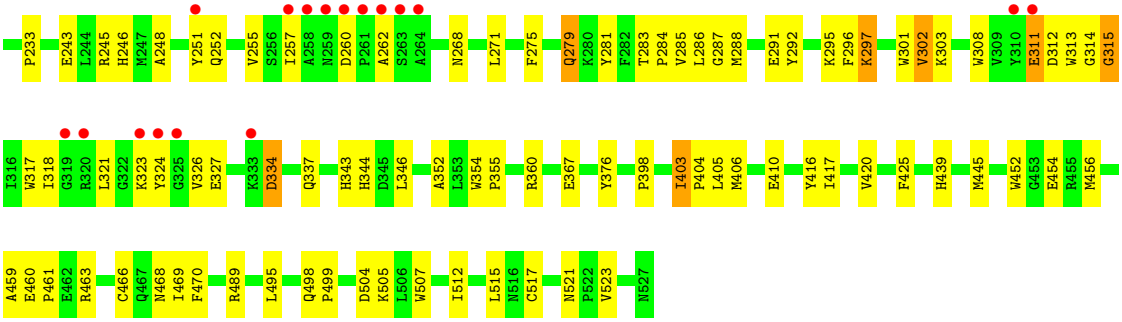
Chain A:



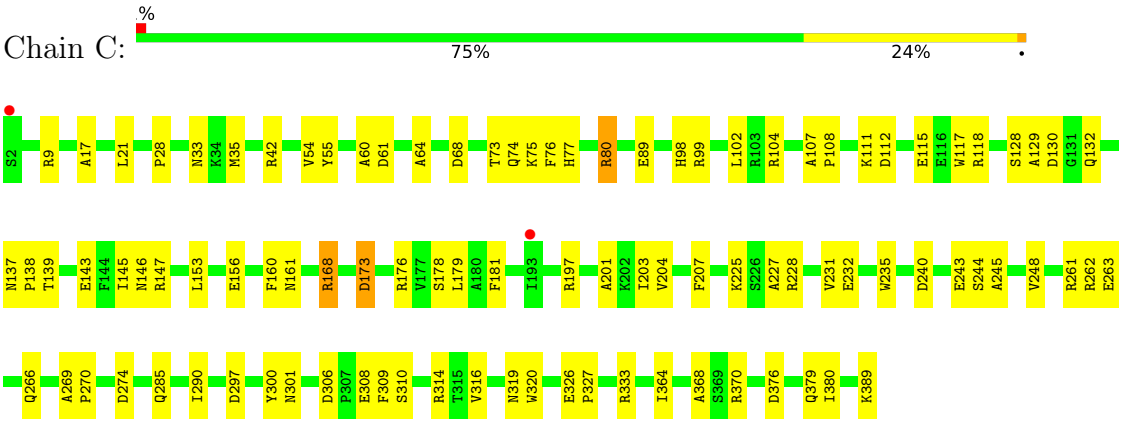
• Molecule 1: Methane monooxygenase component A alpha chain

Chain B:

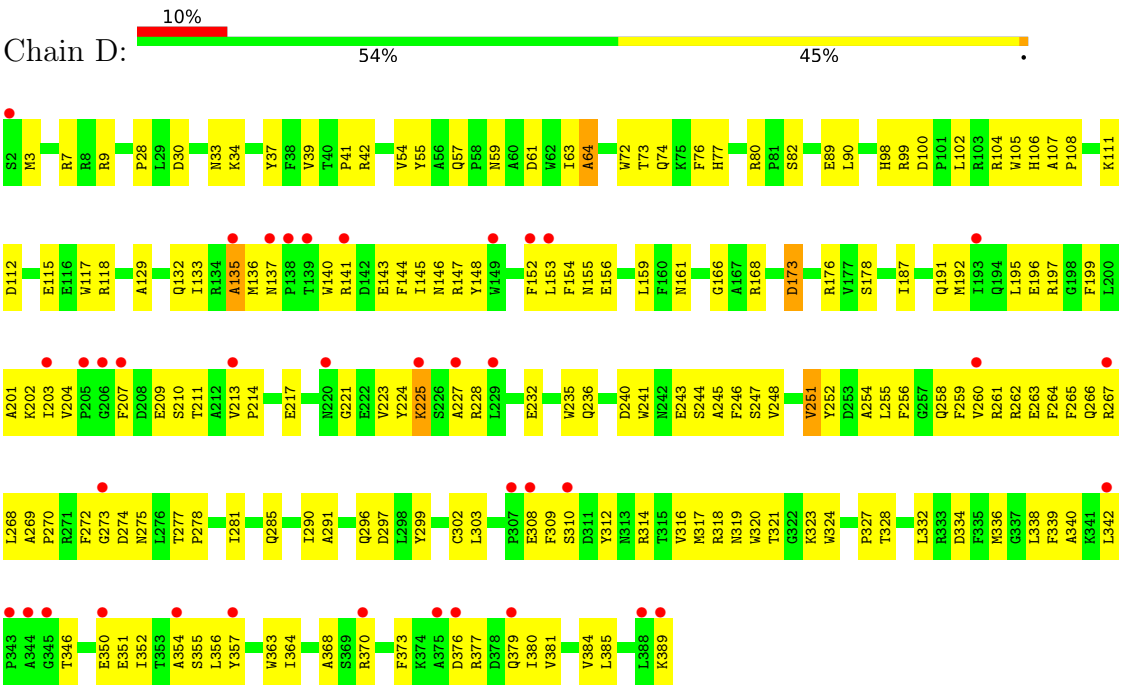




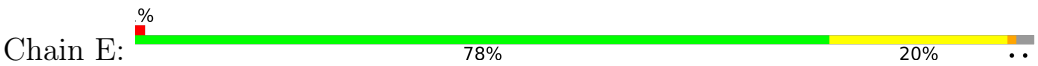
• Molecule 2: Methane monooxygenase component A beta chain

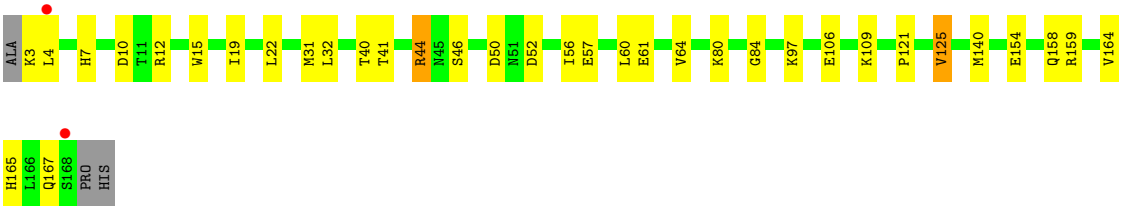


• Molecule 2: Methane monooxygenase component A beta chain

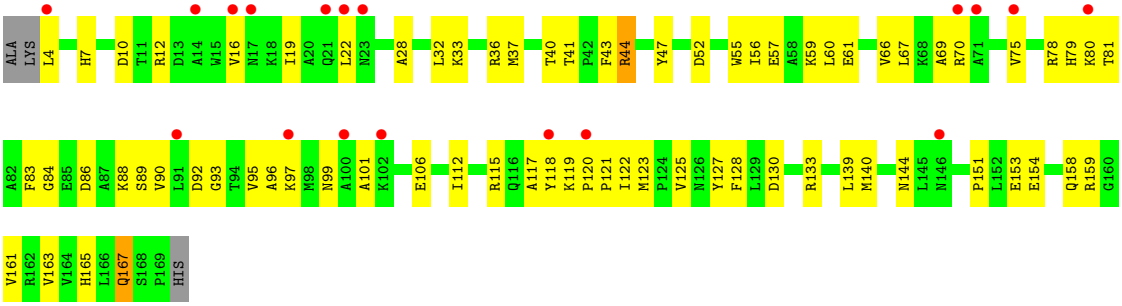


• Molecule 3: Methane monooxygenase component A gamma chain





• Molecule 3: Methane monooxygenase component A gamma chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.35Å 171.63Å 220.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.77 – 2.10 24.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.7 (24.77-2.10) 83.8 (24.79-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.261 0.218 , 0.258	Depositor DCC
R_{free} test set	4360 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18102	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA

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	0.35	0/4263	0.59	1/5797 (0.0%)
1	B	0.35	0/4262	0.56	0/5796
2	C	0.39	0/3263	0.58	0/4435
2	D	0.34	0/3247	0.54	0/4417
3	E	0.37	0/1392	0.60	0/1876
3	F	0.31	0/1387	0.53	0/1873
All	All	0.35	0/17814	0.57	1/24194 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	PHE	CB-CG-CD2	5.61	124.73	120.80

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	4138	0	3897	176	0
1	B	4137	0	3888	212	0
2	C	3167	0	2987	96	0
2	D	3151	0	2957	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1364	0	1352	34	0
3	F	1358	0	1335	63	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	156	0	0	16	0
5	B	170	0	0	13	0
5	C	249	0	0	15	0
5	D	86	0	0	3	0
5	E	106	0	0	1	0
5	F	18	0	0	0	0
All	All	18102	0	16416	663	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 (663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.18	1.11
1:B:44:THR:HG22	1:B:46:TYR:H	1.14	1.05
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.41	1.01
1:A:243:GLU:OE1	5:A:1135:HOH:O	1.79	0.99
2:C:376:ASP:HB3	2:C:379:GLN:NE2	1.79	0.97
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.13	0.96
3:F:41:THR:O	3:F:44:ARG:HD2	1.69	0.92
1:A:171:ALA:O	1:A:175:ARG:HG2	1.68	0.92
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.33	0.91
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.94	0.91
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.51	0.91
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.72	0.88
3:E:80:LYS:HD3	3:E:84:GLY:HA2	1.55	0.88
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.18	0.88
1:B:209:GLU:HA	1:B:213:THR:OG1	1.75	0.86
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.58	0.86
1:B:18:ARG:O	2:D:129:ALA:HA	1.76	0.86
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.41	0.86
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.58	0.85
1:A:433:ALA:HB2	5:A:1152:HOH:O	1.79	0.83
1:A:243:GLU:OE2	5:A:1135:HOH:O	1.97	0.82
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.61	0.82
1:A:216:LEU:HD13	1:A:286:LEU:HD13	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD22	1:B:206:LEU:HD22	1.62	0.81
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.45	0.81
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.80	0.80
1:B:288:MET:HE1	1:B:346:LEU:HG	1.63	0.79
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.12	0.79
1:A:243:GLU:CD	5:A:1135:HOH:O	2.12	0.79
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.78	0.79
1:A:175:ARG:HD3	1:A:181:TRP:CE2	2.19	0.78
1:B:175:ARG:HD3	1:B:181:TRP:CE2	2.18	0.78
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.06	0.78
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.78
1:A:44:THR:HG22	1:A:46:TYR:H	1.50	0.77
1:A:467:GLN:HG3	5:A:1086:HOH:O	1.84	0.77
2:C:333:ARG:NH1	5:C:1245:HOH:O	2.16	0.77
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.77	0.77
2:C:379:GLN:NE2	2:C:379:GLN:H	1.80	0.77
2:D:352:ILE:O	2:D:356:LEU:HD23	1.85	0.76
3:F:153:GLU:H	3:F:153:GLU:CD	1.87	0.76
2:C:376:ASP:HB2	2:C:379:GLN:HB2	1.68	0.75
3:F:101:ALA:HA	3:F:106:GLU:OE2	1.85	0.75
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.69	0.75
1:A:188:PHE:HZ	1:A:213:THR:HG1	1.34	0.75
1:A:202:LEU:HD23	1:A:206:LEU:HD12	1.69	0.74
2:D:187:ILE:O	2:D:191:GLN:HG3	1.86	0.74
1:B:283:THR:HB	1:B:284:PRO:HD3	1.69	0.74
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.68	0.74
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.33	0.74
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.70	0.74
3:F:80:LYS:HD3	3:F:84:GLY:HA2	1.70	0.73
1:A:342:ALA:HB3	5:A:1147:HOH:O	1.87	0.73
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.86	0.73
2:D:135:ALA:O	2:D:273:GLY:HA3	1.88	0.73
3:E:97:LYS:NZ	3:E:97:LYS:HB3	2.04	0.72
1:A:338:ASP:OD1	1:A:342:ALA:HB2	1.89	0.72
2:D:153:LEU:HD12	2:D:154:PHE:N	2.04	0.71
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.20	0.71
2:C:376:ASP:CB	2:C:379:GLN:NE2	2.54	0.71
2:D:77:HIS:HB3	3:F:139:LEU:HD23	1.72	0.70
2:C:333:ARG:NH2	5:C:1243:HOH:O	2.24	0.70
3:F:151:PRO:HB2	3:F:153:GLU:OE1	1.91	0.70
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:LYS:O	2:C:115:GLU:HG3	1.92	0.70
1:B:268:ASN:HD21	1:B:327:GLU:H	1.37	0.70
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.56	0.69
2:D:377:ARG:O	2:D:381:VAL:HG23	1.91	0.69
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.73	0.69
2:D:342:LEU:HD22	2:D:346:THR:HG21	1.73	0.69
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.75	0.69
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.73	0.69
1:B:198:VAL:O	1:B:202:LEU:HG	1.92	0.69
1:B:227:ASN:HD21	1:B:295:LYS:H	1.41	0.69
1:A:86:LEU:HD22	5:A:1140:HOH:O	1.92	0.68
1:B:406:MET:O	1:B:410:GLU:HG3	1.93	0.68
1:A:190:ASP:HB3	2:C:74:GLN:O	1.94	0.68
1:A:206:LEU:HD11	1:A:254:VAL:CG2	2.24	0.68
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.23	0.68
2:C:379:GLN:H	2:C:379:GLN:HE21	1.38	0.68
1:B:88:ARG:NH1	5:B:656:HOH:O	2.26	0.68
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.91	0.68
1:A:209:GLU:HA	1:A:213:THR:HB	1.76	0.68
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.23	0.68
1:B:44:THR:HG22	1:B:46:TYR:N	1.99	0.67
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.74	0.67
1:B:281:TYR:O	1:B:284:PRO:HD2	1.93	0.67
1:A:206:LEU:HD11	1:A:254:VAL:HG22	1.76	0.67
1:B:85:ALA:HA	1:B:88:ARG:NH1	2.10	0.67
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.77	0.67
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.77	0.66
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.60	0.66
2:C:333:ARG:CZ	5:C:1243:HOH:O	2.42	0.66
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.76	0.66
3:F:119:LYS:HA	3:F:128:PHE:CE1	2.31	0.66
2:D:259:PHE:CE1	2:D:356:LEU:HD22	2.32	0.65
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.31	0.65
1:A:476:ARG:NH1	5:A:1150:HOH:O	2.17	0.65
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.78	0.65
1:A:336:LYS:C	1:A:338:ASP:H	1.99	0.65
1:B:52:MET:HG3	5:B:693:HOH:O	1.97	0.65
3:F:165:HIS:HE1	3:F:167:GLN:HE21	1.44	0.65
1:A:231:ILE:HD13	5:A:1140:HOH:O	1.96	0.65
1:A:188:PHE:HZ	1:A:213:THR:OG1	1.80	0.64
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:ASP:CB	2:C:379:GLN:HE21	2.11	0.64
2:C:179:LEU:HD21	2:C:245:ALA:HB2	1.78	0.64
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.80	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.43	0.64
2:D:269:ALA:HB1	2:D:274:ASP:OD2	1.98	0.64
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.78	0.63
2:C:376:ASP:HB3	2:C:379:GLN:HE21	1.63	0.63
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.25	0.63
2:D:376:ASP:CG	2:D:379:GLN:HG2	2.19	0.63
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.80	0.63
1:B:88:ARG:NE	5:B:657:HOH:O	2.31	0.63
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.92	0.63
1:B:185:LYS:O	1:B:189:SER:HB2	1.99	0.63
3:E:3:LYS:O	3:E:4:LEU:HD12	1.99	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HE	1.45	0.63
1:B:171:ALA:O	1:B:175:ARG:HG2	1.98	0.63
1:B:216:LEU:HD13	1:B:286:LEU:HD13	1.80	0.63
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.80	0.63
1:A:213:THR:O	1:A:217:ILE:HG12	1.99	0.62
1:B:337:GLN:C	5:B:692:HOH:O	2.37	0.62
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.34	0.62
2:D:336:MET:HE3	2:D:385:LEU:HA	1.81	0.62
3:F:97:LYS:NZ	3:F:97:LYS:HB3	2.14	0.62
2:D:136:MET:HE3	2:D:141:ARG:HB2	1.81	0.62
1:A:202:LEU:CD2	1:A:206:LEU:HD12	2.28	0.62
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.81	0.62
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.80	0.62
1:B:128:ALA:HB1	1:B:133:GLN:HB3	1.79	0.62
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.35	0.62
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.81	0.62
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.80	0.62
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.82	0.62
2:D:275:ASN:C	2:D:278:PRO:HD2	2.20	0.62
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.30	0.62
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.81	0.62
1:B:134:LYS:HD3	2:D:161:ASN:ND2	2.14	0.61
1:A:120:ALA:HA	1:A:193:ILE:HG22	1.83	0.61
1:A:185:LYS:O	1:A:189:SER:HB2	1.99	0.61
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.81	0.61
1:B:110:LEU:O	1:B:114:GLU:HG2	2.00	0.61
1:A:113:GLY:HA2	1:A:188:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.61
1:A:140:GLN:OE1	1:A:249:ASN:OD1	2.17	0.61
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.83	0.61
2:D:9:ARG:NH2	5:D:447:HOH:O	2.34	0.61
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.82	0.61
2:C:333:ARG:NE	5:C:1243:HOH:O	2.32	0.61
1:B:44:THR:HG21	5:B:653:HOH:O	1.99	0.61
1:A:185:LYS:HA	1:A:189:SER:HB2	1.82	0.60
1:B:186:ARG:HB3	5:B:685:HOH:O	2.00	0.60
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.98	0.60
3:E:22:LEU:HD11	3:E:31:MET:SD	2.41	0.60
2:C:61:ASP:OD1	3:E:7:HIS:HD2	1.83	0.60
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.84	0.60
1:B:23:VAL:HG13	1:B:27:GLU:OE2	2.02	0.60
1:B:190:ASP:HB3	2:D:74:GLN:O	2.01	0.60
3:E:57:GLU:O	3:E:61:GLU:HG3	2.02	0.60
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.36	0.60
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.37	0.60
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.84	0.60
1:B:209:GLU:HG2	5:B:682:HOH:O	2.02	0.59
1:A:140:GLN:O	1:A:144:GLU:HG2	2.02	0.59
1:B:185:LYS:HA	1:B:189:SER:HB2	1.83	0.59
3:F:12:ARG:O	3:F:16:VAL:HG23	2.03	0.59
2:D:228:ARG:O	2:D:232:GLU:HG3	2.02	0.59
1:B:209:GLU:OE2	1:B:246:HIS:HB3	2.02	0.59
2:D:310:SER:O	2:D:314:ARG:HG3	2.03	0.59
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.36	0.59
2:C:379:GLN:NE2	2:C:379:GLN:N	2.49	0.59
2:C:98:HIS:HE1	2:C:178:SER:OG	1.86	0.58
2:D:340:ALA:HA	2:D:389:LYS:NZ	2.18	0.58
3:E:15:TRP:HB2	3:E:56:ILE:HD12	1.85	0.58
1:A:312:ASP:O	1:A:316:ILE:HB	2.03	0.58
1:B:179:PRO:HD3	5:B:608:HOH:O	2.04	0.58
1:A:186:ARG:HA	2:C:73:THR:OG1	2.04	0.58
1:B:186:ARG:HD3	1:B:186:ARG:C	2.23	0.58
1:A:216:LEU:O	1:A:220:VAL:HG23	2.04	0.58
1:A:444:GLU:HB3	5:A:1148:HOH:O	2.03	0.58
1:B:24:ASN:OD1	1:B:27:GLU:HG3	2.04	0.58
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.85	0.58
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.86	0.57
3:E:167:GLN:NE2	5:E:221:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:O	1:A:338:ASP:N	2.36	0.57
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.86	0.57
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.84	0.57
1:A:227:ASN:HD21	1:A:295:LYS:H	1.52	0.57
2:C:225:LYS:HE2	5:C:1251:HOH:O	2.04	0.57
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.34	0.57
1:A:339:ALA:HA	5:A:1147:HOH:O	2.04	0.57
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.40	0.57
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.39	0.57
1:A:323:LYS:HE2	1:A:324:TYR:CE1	2.40	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.05	0.57
1:B:175:ARG:HG3	1:B:176:THR:N	2.20	0.57
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.40	0.57
1:B:202:LEU:HA	1:B:206:LEU:HB3	1.86	0.56
1:A:66:GLU:O	1:A:70:MET:HG2	2.04	0.56
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.27	0.56
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.35	0.56
1:B:209:GLU:HA	1:B:213:THR:CB	2.35	0.56
3:F:57:GLU:O	3:F:61:GLU:HG3	2.04	0.56
1:B:321:LEU:HB3	1:B:326:VAL:HG21	1.87	0.56
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.41	0.56
1:B:469:ILE:HG21	5:B:608:HOH:O	2.04	0.56
2:C:310:SER:O	2:C:314:ARG:HG3	2.05	0.56
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.88	0.56
3:E:41:THR:O	3:E:44:ARG:HD2	2.05	0.56
3:F:4:LEU:HD22	3:F:10:ASP:H	1.70	0.56
1:A:175:ARG:HD3	1:A:181:TRP:CZ2	2.40	0.56
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.88	0.56
2:D:351:GLU:O	2:D:354:ALA:N	2.39	0.56
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.87	0.56
2:D:376:ASP:O	2:D:380:ILE:HG12	2.06	0.56
1:B:213:THR:O	1:B:217:ILE:HG12	2.05	0.56
2:C:266:GLN:NE2	2:D:132:GLN:OE1	2.39	0.56
1:B:288:MET:HE1	1:B:346:LEU:CG	2.33	0.56
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.36	0.56
2:C:261:ARG:NE	2:C:285:GLN:HE22	1.93	0.56
1:B:123:MET:HE1	2:D:76:PHE:CE2	2.41	0.56
1:B:214:ASN:OD1	1:B:243:GLU:HG2	2.06	0.56
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.71	0.56
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.05	0.56
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:C	1:A:340:TYR:H	2.08	0.56
2:D:143:GLU:O	2:D:147:ARG:HB3	2.06	0.56
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.55
3:E:41:THR:O	3:E:44:ARG:CD	2.54	0.55
1:B:403:ILE:HG21	1:B:515:LEU:HD13	1.88	0.55
2:D:197:ARG:HH12	2:D:209:GLU:C	2.09	0.55
1:A:84:ASP:HB3	1:B:81:SER:OG	2.07	0.55
1:B:288:MET:CE	1:B:346:LEU:HB3	2.37	0.55
1:B:466:CYS:HB2	2:D:73:THR:HA	1.88	0.55
3:E:80:LYS:CD	3:E:84:GLY:HA2	2.34	0.55
2:D:296:GLN:NE2	2:D:370:ARG:HH12	2.05	0.55
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.40	0.55
2:D:269:ALA:O	2:D:274:ASP:HB3	2.07	0.55
1:A:227:ASN:ND2	1:A:295:LYS:H	2.05	0.55
1:A:338:ASP:O	1:A:340:TYR:N	2.40	0.55
1:B:32:LEU:HD12	1:B:35:PHE:CD2	2.42	0.55
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.04	0.55
2:D:224:TYR:O	2:D:227:ALA:HB3	2.07	0.55
1:A:184:MET:CE	1:A:188:PHE:HB2	2.38	0.54
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.88	0.54
3:E:12:ARG:HA	3:E:56:ILE:HD11	1.89	0.54
1:A:81:SER:OG	1:B:84:ASP:HB3	2.06	0.54
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.90	0.54
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.42	0.54
2:C:244:SER:O	2:C:248:VAL:HG23	2.08	0.54
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.90	0.54
2:D:277:THR:HG22	2:D:281:ILE:HD11	1.89	0.54
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.38	0.54
1:A:243:GLU:O	1:A:247:MET:HG2	2.08	0.54
1:B:186:ARG:HA	2:D:73:THR:OG1	2.08	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.56	0.53
3:F:81:THR:C	3:F:83:PHE:H	2.10	0.53
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.42	0.53
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.09	0.53
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.43	0.53
3:E:154:GLU:O	3:E:158:GLN:HG3	2.07	0.53
1:B:85:ALA:HA	1:B:88:ARG:HH12	1.72	0.53
1:B:196:ASP:HB2	3:F:140:MET:SD	2.49	0.53
2:C:80:ARG:CZ	5:C:1249:HOH:O	2.56	0.53
1:B:113:GLY:CA	1:B:188:PHE:HB3	2.38	0.53
2:D:195:LEU:O	2:D:195:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:ASP:OD1	3:F:125:VAL:HG21	2.09	0.53
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.38	0.53
1:A:113:GLY:CA	1:A:188:PHE:HB3	2.38	0.53
2:D:312:TYR:O	2:D:316:VAL:HG23	2.09	0.53
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.23	0.53
1:B:360:ARG:HD2	1:B:489:ARG:NH2	2.24	0.53
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.91	0.53
2:D:147:ARG:NH1	2:D:217:GLU:OE1	2.42	0.52
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.09	0.52
2:C:54:VAL:O	2:C:55:TYR:HB2	2.08	0.52
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.91	0.52
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.10	0.52
1:B:23:VAL:HB	2:D:195:LEU:CD2	2.40	0.52
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.52
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.91	0.52
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.38	0.52
1:A:406:MET:O	1:A:410:GLU:HG3	2.09	0.52
1:A:109:PHE:O	1:A:112:VAL:HG12	2.10	0.52
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.92	0.52
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.91	0.52
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.74	0.52
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.90	0.52
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.30	0.52
2:C:225:LYS:CE	5:C:1251:HOH:O	2.58	0.52
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.75	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.93	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.45	0.51
2:C:306:ASP:O	2:C:310:SER:HB2	2.10	0.51
2:D:291:ALA:HB2	5:D:473:HOH:O	2.09	0.51
1:A:40:LYS:HB3	5:A:1049:HOH:O	2.10	0.51
2:D:136:MET:HE3	2:D:141:ARG:CG	2.40	0.51
1:A:121:THR:HG21	1:A:140:GLN:CG	2.40	0.51
3:E:106:GLU:HA	3:E:109:LYS:HD2	1.93	0.51
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.46	0.51
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.46	0.51
2:C:266:GLN:HE21	2:D:132:GLN:CD	2.14	0.51
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.94	0.51
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.76	0.50
1:B:367:GLU:HG3	5:B:638:HOH:O	2.10	0.50
1:A:175:ARG:HG3	1:A:176:THR:N	2.27	0.50
2:D:153:LEU:HD12	2:D:153:LEU:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.93	0.50
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.94	0.50
1:A:175:ARG:HD2	5:C:1159:HOH:O	2.12	0.50
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.11	0.50
1:B:66:GLU:O	1:B:70:MET:HG2	2.12	0.50
1:B:186:ARG:HD3	1:B:186:ARG:O	2.12	0.50
2:D:321:THR:HG21	2:D:373:PHE:CD2	2.47	0.50
1:B:185:LYS:CA	1:B:189:SER:HB2	2.41	0.50
2:D:39:VAL:O	2:D:41:PRO:HD3	2.12	0.50
2:D:340:ALA:HA	2:D:389:LYS:HZ3	1.75	0.50
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.47	0.50
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.58	0.50
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.93	0.50
1:A:79:PHE:O	1:A:83:GLN:HG3	2.12	0.50
1:A:283:THR:HB	1:A:284:PRO:CD	2.41	0.50
1:A:413:HIS:HD2	1:A:428:SER:OG	1.95	0.50
1:B:88:ARG:NH2	5:B:657:HOH:O	2.45	0.50
3:F:86:ASP:O	3:F:89:SER:HB2	2.12	0.50
1:B:251:TYR:O	1:B:255:VAL:HG23	2.12	0.50
1:B:337:GLN:O	5:B:692:HOH:O	2.20	0.50
2:D:111:LYS:O	2:D:115:GLU:HG3	2.11	0.50
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.12	0.49
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:B:44:THR:OG1	1:B:127:SER:HA	2.12	0.49
1:B:115:TYR:OH	2:D:173:ASP:HA	2.12	0.49
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.12	0.49
2:C:263:GLU:OE2	2:C:263:GLU:HA	2.12	0.49
1:A:208:GLY:HA2	1:A:278:GLN:HE21	1.76	0.49
1:B:439:HIS:CD2	3:F:163:VAL:HA	2.32	0.49
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.45	0.49
3:E:165:HIS:HE1	3:E:167:GLN:HB2	1.77	0.49
3:F:19:ILE:HG12	3:F:60:LEU:HD13	1.94	0.49
1:B:38:ASP:O	1:B:39:PHE:HB3	2.11	0.49
2:D:133:ILE:HD11	2:D:136:MET:HE1	1.94	0.49
2:C:308:GLU:HB3	2:C:309:PHE:CD1	2.48	0.49
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.47	0.49
2:D:350:GLU:HG3	5:D:425:HOH:O	2.12	0.49
1:A:185:LYS:CA	1:A:189:SER:HB2	2.43	0.49
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.48	0.49
2:D:159:LEU:HD22	2:D:248:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:75:VAL:O	3:F:79:HIS:HD2	1.96	0.49
1:A:499:PRO:HG3	1:A:507:TRP:NE1	2.28	0.49
1:B:113:GLY:HA2	1:B:188:PHE:O	2.12	0.49
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.45	0.49
1:B:42:ASN:HA	2:D:236:GLN:HG3	1.95	0.48
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.94	0.48
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.94	0.48
2:C:297:ASP:O	2:C:301:ASN:HB3	2.12	0.48
1:A:108:ASN:O	1:A:111:GLU:HB3	2.13	0.48
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.49	0.48
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.13	0.48
2:D:105:TRP:O	2:D:108:PRO:HD2	2.12	0.48
3:E:3:LYS:HB3	3:E:10:ASP:OD1	2.13	0.48
3:F:33:LYS:O	3:F:37:MET:HG2	2.13	0.48
1:B:212:PHE:O	1:B:215:PRO:HD2	2.13	0.48
1:A:93:VAL:HG11	2:D:3:MET:HG2	1.95	0.48
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.46	0.48
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.44	0.48
3:F:61:GLU:O	3:F:121:PRO:HG3	2.13	0.48
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.48
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.48
1:A:343:HIS:CD2	1:A:343:HIS:H	2.31	0.48
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.49	0.48
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.78	0.48
2:D:370:ARG:HH11	2:D:370:ARG:HG3	1.79	0.48
1:A:182:LYS:O	2:C:73:THR:HG21	2.14	0.48
1:A:77:ARG:HH22	1:B:83:GLN:HB3	1.79	0.48
1:B:44:THR:HG23	1:B:126:ASP:OD1	2.14	0.48
1:B:123:MET:HE1	2:D:76:PHE:HE2	1.78	0.48
1:A:202:LEU:HD12	1:A:270:ASP:HB3	1.95	0.47
1:A:323:LYS:HG3	1:A:324:TYR:CE1	2.49	0.47
1:A:338:ASP:HB2	5:A:1152:HOH:O	2.14	0.47
1:B:186:ARG:NH1	1:B:420:VAL:HG12	2.29	0.47
2:C:181:PHE:HD1	5:C:1180:HOH:O	1.97	0.47
1:B:31:TRP:CH2	2:D:210:SER:HA	2.49	0.47
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.47
2:D:266:GLN:HG3	2:D:266:GLN:O	2.13	0.47
2:D:264:PHE:O	2:D:268:LEU:HB2	2.14	0.47
3:E:97:LYS:HB3	3:E:97:LYS:HZ2	1.77	0.47
3:F:120:PRO:HD3	3:F:128:PHE:CD1	2.49	0.47
1:B:469:ILE:HG13	1:B:470:PHE:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:GLU:O	3:F:158:GLN:HG3	2.14	0.47
1:A:336:LYS:C	1:A:338:ASP:N	2.66	0.47
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.95	0.47
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.47
3:F:66:VAL:O	3:F:69:ALA:HB3	2.14	0.47
2:D:260:VAL:O	2:D:265:PHE:HD1	1.97	0.47
1:A:116:ASN:CB	1:A:189:SER:HA	2.44	0.47
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.45	0.47
1:B:405:LEU:HD23	1:B:517:CYS:SG	2.54	0.47
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.49	0.47
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.49	0.47
1:A:187:VAL:HG11	1:A:281:TYR:HB3	1.97	0.47
1:B:88:ARG:CZ	5:B:657:HOH:O	2.62	0.47
1:B:184:MET:HE1	1:B:188:PHE:CD2	2.50	0.47
2:D:197:ARG:HB3	2:D:197:ARG:NH1	2.29	0.47
2:D:259:PHE:CD1	2:D:263:GLU:HB2	2.49	0.47
1:B:452:TRP:O	1:B:456:MET:HG3	2.16	0.46
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.97	0.46
2:D:166:GLY:HA2	2:D:241:TRP:HB2	1.96	0.46
3:E:165:HIS:CE1	3:E:167:GLN:HB2	2.51	0.46
1:B:248:ALA:O	1:B:252:GLN:HG2	2.14	0.46
1:A:313:TRP:HA	1:A:317:TRP:HB3	1.97	0.46
1:B:175:ARG:HD3	1:B:181:TRP:CZ2	2.50	0.46
1:B:313:TRP:HA	1:B:317:TRP:HB3	1.98	0.46
1:B:34:SER:O	2:D:154:PHE:HE2	1.98	0.46
1:B:207:VAL:O	1:B:211:CYS:HB3	2.15	0.46
2:D:144:PHE:HA	2:D:148:TYR:HD1	1.81	0.46
3:F:88:LYS:HB2	3:F:127:TYR:HE2	1.81	0.46
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.96	0.46
1:A:230:GLU:C	1:A:233:PRO:HD2	2.36	0.46
2:C:76:PHE:CE2	5:C:1249:HOH:O	2.67	0.46
2:D:136:MET:HE3	2:D:141:ARG:CB	2.44	0.46
1:A:128:ALA:CB	1:A:133:GLN:HG2	2.45	0.46
1:A:205:GLN:NE2	1:A:249:ASN:HB3	2.31	0.46
1:A:338:ASP:C	1:A:340:TYR:N	2.70	0.46
1:A:472:GLN:NE2	5:A:1086:HOH:O	2.48	0.46
1:B:60:PHE:N	1:B:60:PHE:CD1	2.84	0.46
1:B:287:GLY:HA3	1:B:301:TRP:CD1	2.51	0.46
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.50	0.46
1:B:504:ASP:OD2	1:B:505:LYS:HG3	2.15	0.46
2:C:139:THR:O	2:C:143:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:97:LYS:HB3	3:E:97:LYS:HZ3	1.76	0.46
3:F:4:LEU:CD2	3:F:10:ASP:H	2.29	0.46
1:A:163:GLN:HG2	5:A:1033:HOH:O	2.15	0.46
1:B:125:TRP:O	1:B:134:LYS:HG2	2.16	0.46
2:C:99:ARG:NH2	5:C:1170:HOH:O	2.23	0.45
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.45
2:D:376:ASP:OD1	2:D:379:GLN:HG2	2.14	0.45
1:A:83:GLN:HB3	1:B:77:ARG:NH2	2.31	0.45
2:D:98:HIS:HE1	2:D:178:SER:OG	1.99	0.45
1:B:268:ASN:ND2	1:B:327:GLU:H	2.09	0.45
2:D:98:HIS:HA	2:D:302:CYS:SG	2.55	0.45
2:D:316:VAL:HG12	2:D:320:TRP:CE2	2.52	0.45
1:B:222:GLU:OE2	2:D:7:ARG:NH1	2.50	0.45
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.52	0.45
3:F:159:ARG:HG3	3:F:161:VAL:HG13	1.99	0.45
1:B:92:GLY:O	1:B:162:GLY:HA2	2.16	0.45
1:A:50:TYR:CD2	1:A:257:ILE:HD12	2.52	0.45
1:A:192:PHE:O	1:A:200:CYS:HB3	2.17	0.45
2:D:148:TYR:CE2	2:D:338:LEU:HD13	2.51	0.45
2:D:255:LEU:HB2	2:D:328:THR:HG21	1.98	0.45
1:A:116:ASN:CG	1:A:189:SER:HA	2.37	0.45
1:A:184:MET:HE1	1:A:188:PHE:HB2	1.98	0.45
1:A:257:ILE:O	1:A:263:SER:HB2	2.17	0.45
1:B:29:HIS:CD2	1:B:61:LYS:HA	2.52	0.45
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.52	0.45
2:C:168:ARG:HH11	2:C:168:ARG:CG	2.30	0.45
3:F:52:ASP:O	3:F:56:ILE:HG12	2.17	0.45
1:A:212:PHE:O	1:A:216:LEU:CB	2.65	0.45
1:B:27:GLU:CD	2:D:202:LYS:HZ1	2.20	0.45
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.52	0.45
2:D:57:GLN:NE2	2:D:59:ASN:HD21	2.15	0.45
1:B:216:LEU:HD11	1:B:286:LEU:HD22	1.99	0.45
3:E:40:THR:C	3:E:41:THR:HG23	2.37	0.45
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.45
2:D:140:TRP:CE2	2:D:269:ALA:HA	2.53	0.45
1:B:190:ASP:OD1	2:D:72:TRP:HB3	2.17	0.44
2:D:357:TYR:CE2	2:D:377:ARG:NH1	2.85	0.44
2:D:203:ILE:HG13	2:D:204:VAL:HG23	1.99	0.44
3:F:75:VAL:O	3:F:79:HIS:CD2	2.71	0.44
1:A:77:ARG:NH2	1:B:83:GLN:HB3	2.33	0.44
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ALA:C	1:B:461:PRO:HD3	2.38	0.44
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.47	0.44
1:A:207:VAL:HG22	1:A:313:TRP:HZ2	1.82	0.44
2:D:204:VAL:HG12	2:D:204:VAL:O	2.16	0.44
2:D:211:THR:HA	2:D:214:PRO:HG2	1.99	0.44
1:A:234:THR:HG23	1:B:84:ASP:OD1	2.18	0.44
2:D:176:ARG:NH1	2:D:176:ARG:HB2	2.32	0.44
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.80	0.44
1:A:439:HIS:HE1	1:A:454:GLU:OE1	2.01	0.44
1:B:403:ILE:CG2	1:B:515:LEU:HD13	2.47	0.44
3:F:115:ARG:O	3:F:119:LYS:HB2	2.17	0.44
1:A:159:ALA:O	2:C:33:ASN:HB2	2.17	0.44
1:B:114:GLU:O	1:B:117:ALA:HB3	2.18	0.44
2:D:34:LYS:O	2:D:37:TYR:HB3	2.18	0.44
1:B:116:ASN:CG	1:B:189:SER:HA	2.39	0.43
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.18	0.43
1:B:163:GLN:O	2:D:28:PRO:HA	2.18	0.43
1:B:209:GLU:CA	1:B:213:THR:OG1	2.58	0.43
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.52	0.43
2:D:54:VAL:O	2:D:55:TYR:HB2	2.18	0.43
2:D:240:ASP:HB3	2:D:243:GLU:HB3	2.00	0.43
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.53	0.43
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.43
1:A:196:ASP:HB2	3:E:140:MET:SD	2.58	0.43
1:B:146:ARG:HB2	2:D:106:HIS:CD2	2.54	0.43
2:C:153:LEU:C	2:C:153:LEU:HD12	2.38	0.43
2:D:37:TYR:CD1	2:D:37:TYR:C	2.92	0.43
2:D:318:ARG:O	2:D:321:THR:HB	2.18	0.43
1:A:109:PHE:O	1:A:184:MET:HE2	2.18	0.43
1:B:120:ALA:O	1:B:124:LEU:HG	2.19	0.43
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.54	0.43
3:F:165:HIS:CE1	3:F:167:GLN:HE21	2.31	0.43
1:A:221:THR:HG22	1:A:233:PRO:HA	2.00	0.43
1:B:108:ASN:O	1:B:111:GLU:HB3	2.18	0.43
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.00	0.43
1:A:120:ALA:CA	1:A:193:ILE:HG22	2.48	0.43
1:B:112:VAL:HG21	1:B:181:TRP:HH2	1.83	0.43
1:B:460:GLU:HB3	1:B:463:ARG:HG3	2.01	0.43
1:A:30:ARG:HD3	1:A:31:TRP:CD1	2.53	0.43
1:A:163:GLN:O	2:C:28:PRO:HA	2.18	0.43
2:C:376:ASP:OD2	2:C:376:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:SER:O	2:D:248:VAL:HG23	2.18	0.43
2:D:270:PRO:O	2:D:273:GLY:N	2.50	0.43
1:B:65:LYS:HE2	2:D:192:MET:HE2	2.00	0.43
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.37	0.43
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.43
2:D:82:SER:O	2:D:168:ARG:NH2	2.48	0.43
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.19	0.43
2:D:102:LEU:HB2	2:D:104:ARG:HD2	2.01	0.43
2:D:197:ARG:NH1	2:D:209:GLU:O	2.48	0.43
1:A:21:THR:HG22	2:C:128:SER:CB	2.49	0.43
1:A:211:CYS:SG	1:A:309:VAL:HG22	2.58	0.43
5:C:1040:HOH:O	3:E:121:PRO:HB3	2.19	0.43
2:D:246:PHE:CZ	2:D:317:MET:HB3	2.53	0.43
3:F:153:GLU:CD	3:F:153:GLU:N	2.63	0.43
1:B:32:LEU:HD21	1:B:135:ASN:CB	2.49	0.43
1:B:206:LEU:HD11	1:B:321:LEU:HD11	2.00	0.43
1:B:460:GLU:N	1:B:461:PRO:HD3	2.34	0.43
2:C:104:ARG:NH1	5:C:1180:HOH:O	2.52	0.43
2:C:227:ALA:O	2:C:231:VAL:HG23	2.18	0.43
2:C:228:ARG:O	2:C:232:GLU:HG3	2.19	0.43
2:D:146:ASN:OD1	2:D:146:ASN:O	2.37	0.43
2:D:255:LEU:HD21	2:D:363:TRP:CD2	2.54	0.43
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.43
1:B:417:ILE:HG13	1:B:468:ASN:HB2	2.00	0.43
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.48	0.43
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.54	0.43
2:D:277:THR:N	2:D:278:PRO:CD	2.82	0.43
2:D:336:MET:C	2:D:338:LEU:H	2.22	0.43
1:B:202:LEU:HA	1:B:206:LEU:CB	2.49	0.42
1:B:227:ASN:HD21	1:B:296:PHE:H	1.67	0.42
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.53	0.42
2:D:140:TRP:HE1	2:D:145:ILE:HD11	1.83	0.42
1:A:117:ALA:HA	1:A:120:ALA:HB3	2.00	0.42
1:B:79:PHE:O	1:B:83:GLN:HG3	2.19	0.42
1:B:108:ASN:HD21	1:B:175:ARG:NE	2.15	0.42
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.83	0.42
2:C:77:HIS:CG	3:E:140:MET:HG2	2.53	0.42
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.01	0.42
1:A:459:ALA:C	1:A:461:PRO:HD3	2.40	0.42
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.42
1:B:445:MET:HB3	1:B:523:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:HG3	5:A:1155:HOH:O	2.19	0.42
1:A:495:LEU:HD21	1:A:509:LEU:HA	2.00	0.42
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.54	0.42
1:B:186:ARG:HH12	1:B:420:VAL:HG12	1.83	0.42
2:C:130:ASP:HB3	2:C:132:GLN:HG3	2.01	0.42
2:C:376:ASP:O	2:C:380:ILE:HG12	2.18	0.42
2:D:90:LEU:HD13	2:D:303:LEU:HD13	2.01	0.42
2:D:213:VAL:N	2:D:214:PRO:HD2	2.34	0.42
3:F:86:ASP:HB3	3:F:89:SER:OG	2.19	0.42
1:A:279:GLN:HE21	1:A:279:GLN:HB3	1.67	0.42
1:B:302:VAL:HG23	1:B:303:LYS:H	1.85	0.42
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.42
2:C:389:LYS:HB3	5:C:1123:HOH:O	2.20	0.42
2:D:224:TYR:O	2:D:225:LYS:C	2.58	0.42
2:C:61:ASP:OD1	3:E:7:HIS:CD2	2.69	0.42
1:B:121:THR:HA	1:B:124:LEU:HD12	2.02	0.42
3:F:40:THR:C	3:F:41:THR:HG23	2.39	0.42
1:A:466:CYS:HB2	2:C:73:THR:HA	2.01	0.42
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.91	0.42
1:B:230:GLU:C	1:B:233:PRO:HD2	2.40	0.42
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.71	0.42
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.42
2:C:145:ILE:HD11	2:C:274:ASP:OD2	2.20	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.42
1:A:115:TYR:OH	2:C:173:ASP:HA	2.20	0.42
1:A:186:ARG:HD3	1:A:186:ARG:O	2.20	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42
1:B:187:VAL:HG23	1:B:188:PHE:N	2.34	0.42
1:B:196:ASP:HB3	1:B:199:GLU:HB2	2.02	0.42
2:C:143:GLU:O	2:C:147:ARG:HB3	2.19	0.42
2:D:196:GLU:O	2:D:199:PHE:HB3	2.20	0.42
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.84	0.42
1:A:227:ASN:HD21	1:A:296:PHE:H	1.68	0.42
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.55	0.42
2:C:168:ARG:HH11	2:C:168:ARG:HG2	1.85	0.42
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.20	0.42
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.35	0.42
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.18	0.41
1:A:188:PHE:CD1	1:A:192:PHE:CZ	3.08	0.41
1:B:140:GLN:HA	1:B:143:ASP:HB2	2.02	0.41
3:E:32:LEU:HA	3:E:60:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:32:LEU:HD21	3:F:36:ARG:NH2	2.35	0.41
1:A:328:SER:HA	1:A:329:PRO:HD3	1.87	0.41
1:B:193:ILE:O	2:D:76:PHE:CZ	2.73	0.41
1:B:313:TRP:C	1:B:315:GLY:H	2.23	0.41
1:B:416:TYR:HB2	1:B:425:PHE:CE1	2.54	0.41
3:F:43:PHE:CE2	3:F:112:ILE:HD12	2.55	0.41
1:A:121:THR:HA	1:A:124:LEU:HD12	2.02	0.41
1:A:302:VAL:HG11	1:A:340:TYR:CD1	2.55	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.55	0.41
1:B:334:ASP:CG	1:B:452:TRP:HE1	2.24	0.41
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.67	0.41
3:F:81:THR:C	3:F:83:PHE:N	2.73	0.41
1:A:20:PRO:HG3	2:C:129:ALA:HB2	2.03	0.41
1:B:123:MET:CE	2:D:168:ARG:NH1	2.84	0.41
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.54	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.66	0.41
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.41
3:F:4:LEU:HD21	3:F:10:ASP:CG	2.41	0.41
1:A:207:VAL:HG22	1:A:313:TRP:CZ2	2.55	0.41
2:C:17:ALA:O	2:C:21:LEU:HG	2.20	0.41
2:C:75:LYS:HB3	2:C:80:ARG:O	2.20	0.41
2:C:176:ARG:NH1	2:C:176:ARG:HB2	2.36	0.41
2:D:254:ALA:O	2:D:258:GLN:HB2	2.20	0.41
3:F:93:GLY:O	3:F:96:ALA:HB3	2.21	0.41
1:A:83:GLN:HB3	1:B:77:ARG:HH22	1.85	0.41
1:A:128:ALA:HB2	1:A:133:GLN:HG2	2.01	0.41
1:A:521:ASN:HA	1:A:522:PRO:HD2	1.94	0.41
2:C:60:ALA:HA	2:C:68:ASP:HB3	2.02	0.41
1:A:193:ILE:HB	2:C:168:ARG:NE	2.36	0.41
1:A:195:GLY:HA2	5:C:1217:HOH:O	2.20	0.41
1:B:155:ASN:OD1	1:B:168:HIS:HD2	2.04	0.41
1:B:460:GLU:HG2	2:D:77:HIS:CE1	2.56	0.41
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.95	0.41
2:D:308:GLU:HB3	2:D:309:PHE:CD1	2.56	0.41
1:A:212:PHE:O	1:A:216:LEU:HB2	2.20	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.35	0.41
1:A:526:PHE:HB3	3:E:164:VAL:HG11	2.02	0.41
1:B:194:SER:HA	2:D:76:PHE:CE1	2.55	0.41
1:B:216:LEU:CD1	1:B:286:LEU:HD22	2.51	0.41
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.69	0.41
2:D:213:VAL:HB	2:D:214:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.48	0.41
2:D:339:PHE:O	2:D:342:LEU:HB2	2.21	0.41
3:E:64:VAL:CG1	3:E:121:PRO:HG2	2.51	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
1:B:182:LYS:O	2:D:73:THR:HG21	2.21	0.41
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.03	0.41
2:D:267:ARG:HG2	2:D:267:ARG:HH11	1.85	0.41
1:A:230:GLU:OE2	2:C:9:ARG:NH1	2.54	0.40
2:C:243:GLU:HA	2:C:320:TRP:CZ3	2.57	0.40
2:D:168:ARG:HD2	2:D:168:ARG:HA	1.95	0.40
1:A:49:LYS:HE3	1:A:266:TYR:HB3	2.04	0.40
1:A:232:THR:HB	1:A:233:PRO:HD3	2.03	0.40
2:C:316:VAL:O	2:C:319:ASN:HB3	2.21	0.40
2:D:63:ILE:O	2:D:64:ALA:C	2.59	0.40
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.56	0.40
1:B:288:MET:CE	1:B:346:LEU:CB	2.99	0.40
2:C:300:TYR:CD1	2:C:370:ARG:HG3	2.57	0.40
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.04	0.40
2:D:243:GLU:HB2	2:D:320:TRP:CE2	2.56	0.40
3:E:52:ASP:O	3:E:56:ILE:HG12	2.21	0.40
3:F:97:LYS:HB3	3:F:97:LYS:HZ3	1.85	0.40
1:A:118:ILE:CG2	2:C:176:ARG:HD3	2.52	0.40
1:A:452:TRP:O	1:A:456:MET:HG3	2.22	0.40
1:B:165:PRO:HD2	2:D:30:ASP:HB3	2.03	0.40
2:D:152:PHE:O	2:D:155:ASN:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	508/527 (96%)	476 (94%)	27 (5%)	5 (1%)	15 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	508/527 (96%)	478 (94%)	24 (5%)	6 (1%)	13 8
2	C	386/388 (100%)	371 (96%)	14 (4%)	1 (0%)	41 41
2	D	386/388 (100%)	344 (89%)	37 (10%)	5 (1%)	12 7
3	E	164/169 (97%)	161 (98%)	3 (2%)	0	100 100
3	F	164/169 (97%)	148 (90%)	15 (9%)	1 (1%)	25 21
All	All	2116/2168 (98%)	1978 (94%)	120 (6%)	18 (1%)	17 12

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	B	40	LYS
1	B	311	GLU
1	A	339	ALA
1	B	312	ASP
1	B	315	GLY
2	D	251	VAL
1	A	308	TRP
1	A	315	GLY
2	D	64	ALA
2	D	135	ALA
1	A	312	ASP
1	B	39	PHE
2	C	64	ALA
2	D	225	LYS
2	D	221	GLY
3	F	122	ILE
1	B	314	GLY

5.3.2 Protein sidechains (i)

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	423/442 (96%)	410 (97%)	13 (3%)	40 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	422/442 (96%)	409 (97%)	13 (3%)	40	43
2	C	316/323 (98%)	312 (99%)	4 (1%)	69	75
2	D	312/323 (97%)	309 (99%)	3 (1%)	76	82
3	E	143/146 (98%)	140 (98%)	3 (2%)	53	59
3	F	142/146 (97%)	139 (98%)	3 (2%)	53	59
All	All	1758/1822 (96%)	1719 (98%)	39 (2%)	52	57

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

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	90	ASN
1	A	125	TRP
1	A	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	312	ASP
1	A	403	ILE
1	A	437	ARG
1	A	467	GLN
1	B	30	ARG
1	B	43	ARG
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	279	GLN
1	B	297	LYS
1	B	302	VAL
1	B	311	GLU
1	B	334	ASP
1	B	403	ILE
2	C	35	MET
2	C	80	ARG
2	C	168	ARG
2	C	173	ASP

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Mol	Chain	Res	Type
2	D	80	ARG
2	D	173	ASP
2	D	334	ASP
3	E	44	ARG
3	E	46	SER
3	E	125	VAL
3	F	44	ARG
3	F	92	ASP
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	133	GLN
1	A	147	HIS
1	A	155	ASN
1	A	168	HIS
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	259	ASN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	33	GLN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	116	ASN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	246	HIS
1	B	249	ASN
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	413	HIS
1	B	439	HIS
1	B	442	ASN
1	B	451	GLN
1	B	527	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	296	GLN
2	C	301	ASN
2	C	379	GLN
2	D	57	GLN
2	D	98	HIS
2	D	132	GLN
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
3	E	7	HIS
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	F	7	HIS
3	F	39	HIS
3	F	45	ASN

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Mol	Chain	Res	Type
3	F	99	ASN
3	F	144	ASN
3	F	165	HIS
3	F	167	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	510/527 (96%)	0.29	43 (8%) 11 14	18, 38, 74, 82	0
1	B	510/527 (96%)	0.18	33 (6%) 18 23	22, 37, 70, 77	0
2	C	388/388 (100%)	-0.36	2 (0%) 91 92	17, 26, 39, 50	0
2	D	388/388 (100%)	0.46	38 (9%) 7 10	23, 46, 64, 87	0
3	E	166/169 (98%)	-0.42	2 (1%) 79 82	20, 29, 48, 63	0
3	F	166/169 (98%)	0.81	18 (10%) 5 7	36, 54, 64, 70	0
All	All	2128/2168 (98%)	0.16	136 (6%) 19 24	17, 37, 67, 87	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	ILE	8.1
1	A	326	VAL	6.6
1	A	434	SER	6.5
1	A	262	ALA	6.0
1	B	39	PHE	5.6
2	D	389	LYS	5.1
1	B	261	PRO	4.9
1	B	258	ALA	4.8
1	B	310	TYR	4.7
1	B	259	ASN	4.6
2	D	139	THR	4.6
1	A	19	ALA	4.6
3	E	4	LEU	4.4
1	A	260	ASP	4.2
1	A	339	ALA	4.1
2	D	375	ALA	4.0
1	A	60	PHE	3.9
1	A	323	LYS	3.9
1	A	206	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	259	ASN	3.8
1	B	325	GLY	3.8
1	B	264	ALA	3.8
1	B	53	ALA	3.7
2	D	220	ASN	3.7
1	A	315	GLY	3.7
1	A	319	GLY	3.7
2	D	206	GLY	3.7
1	A	251	TYR	3.7
1	A	312	ASP	3.6
1	B	324	TYR	3.6
1	A	325	GLY	3.6
1	B	251	TYR	3.5
1	A	261	PRO	3.5
1	B	41	ASN	3.5
3	F	102	LYS	3.5
2	D	137	ASN	3.5
1	B	263	SER	3.4
1	A	310	TYR	3.4
3	F	16	VAL	3.4
1	A	324	TYR	3.3
1	B	59	GLN	3.3
2	D	205	PRO	3.3
2	D	343	PRO	3.3
3	F	80	LYS	3.3
3	F	4	LEU	3.3
2	D	229	LEU	3.2
1	A	213	THR	3.2
3	F	14	ALA	3.2
1	A	265	LYS	3.2
2	D	260	VAL	3.2
2	D	379	GLN	3.1
2	D	227	ALA	3.1
1	A	255	VAL	3.1
2	D	344	ALA	3.0
1	B	60	PHE	3.0
2	C	2	SER	3.0
1	A	308	TRP	3.0
1	A	20	PRO	3.0
3	F	23	ASN	2.9
3	F	118	TYR	2.8
1	A	248	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	310	SER	2.8
1	A	59	GLN	2.8
1	A	338	ASP	2.8
1	A	318	ILE	2.8
2	D	149	TRP	2.8
3	E	168	SER	2.8
2	D	203	ILE	2.8
1	B	21	THR	2.7
1	B	262	ALA	2.7
2	D	388	LEU	2.7
1	A	328	SER	2.7
1	B	31	TRP	2.7
1	A	247	MET	2.7
3	F	70	ARG	2.7
3	F	97	LYS	2.6
2	D	307	PRO	2.6
3	F	17	ASN	2.6
3	F	22	LEU	2.6
3	F	91	LEU	2.6
1	A	257	ILE	2.6
1	B	19	ALA	2.6
1	B	206	LEU	2.6
1	B	333	LYS	2.6
1	A	54	ASN	2.6
3	F	21	GLN	2.6
2	D	135	ALA	2.5
1	B	311	GLU	2.5
1	B	35	PHE	2.5
1	B	320	ARG	2.5
2	D	207	PHE	2.5
2	D	357	TYR	2.5
2	D	345	GLY	2.5
2	D	2	SER	2.4
2	D	153	LEU	2.4
1	B	20	PRO	2.4
1	B	257	ILE	2.4
2	D	138	PRO	2.4
3	F	120	PRO	2.4
1	A	322	GLY	2.4
1	B	188	PHE	2.4
2	D	152	PHE	2.4
2	D	225	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	193	ILE	2.3
1	B	38	ASP	2.3
1	A	188	PHE	2.3
1	B	57	LYS	2.3
1	B	260	ASP	2.3
2	D	273	GLY	2.2
1	A	244	LEU	2.2
1	B	30	ARG	2.2
3	F	146	ASN	2.2
1	A	263	SER	2.2
1	B	23	VAL	2.2
1	A	337	GLN	2.2
2	D	342	LEU	2.2
2	D	354	ALA	2.2
2	D	308	GLU	2.2
2	D	350	GLU	2.2
1	A	212	PHE	2.2
1	B	323	LYS	2.1
1	B	319	GLY	2.1
3	F	100	ALA	2.1
1	A	321	LEU	2.1
3	F	75	VAL	2.1
2	D	141	ARG	2.1
2	C	193	ILE	2.1
2	D	213	VAL	2.1
1	A	433	ALA	2.1
3	F	71	ALA	2.1
1	A	317	TRP	2.1
2	D	267	ARG	2.1
1	A	320	ARG	2.1
2	D	376	ASP	2.0
1	A	30	ARG	2.0
2	D	370	ARG	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 monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
4	CA	A	1001	1/1	0.92	0.06	50,50,50,50	0
4	CA	C	1002	1/1	0.97	0.03	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.