



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:52 AM UTC

PDB ID : 1XMF / pdb_00001xmf
Title : Structure of Mn(II)-Soaked Apo Methane Monooxygenase Hydroxylase Crystals from *M. capsulatus* (Bath)
Authors : Sazinsky, M.H.; Merckx, M.; Cadieux, E.; Tang, S.; Lippard, S.J.
Deposited on : 2004-10-02
Resolution : 2.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

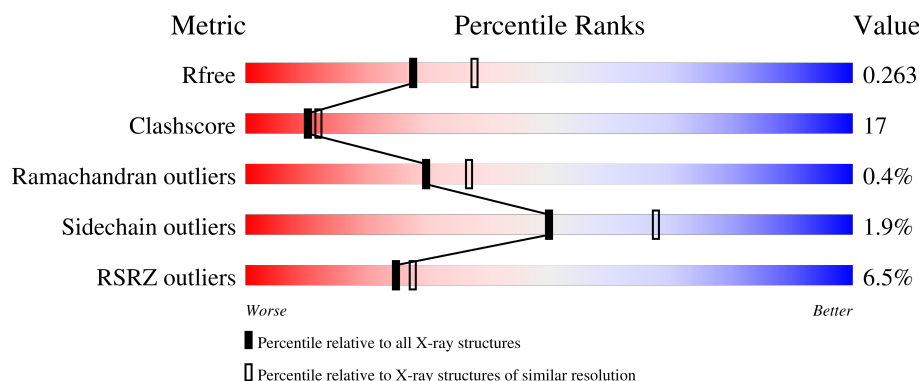
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	527	12% 60% 35% ..
1	B	527	8% 61% 34% ..
2	C	388	0% 73% 25% .
2	D	388	6% 69% 29% .
3	E	169	4% 75% 21% ..

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Mol	Chain	Length	Quality of chain
3	F	169	2% 74% 22% ••

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18436 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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0
4	B	2	Total Mn 2 2	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	3	Total Ca 3 3	0	0

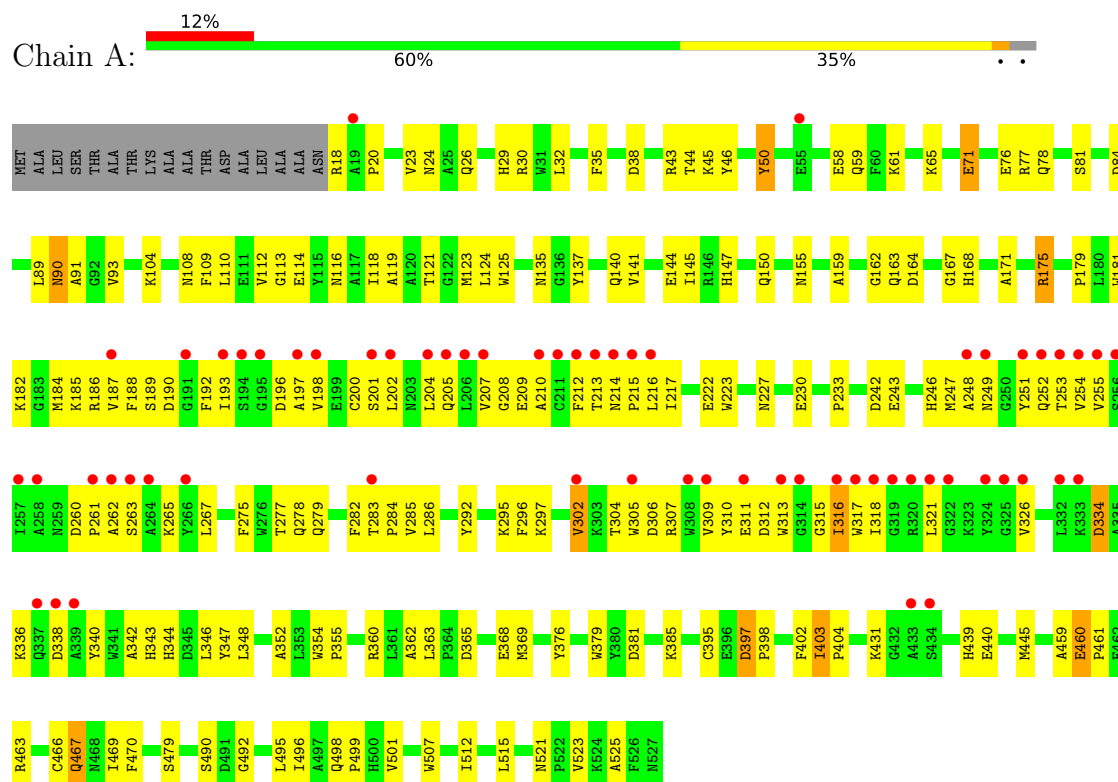
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	235	Total O 235 235	0	0
6	B	212	Total O 212 212	0	0
6	C	290	Total O 290 290	0	0
6	D	150	Total O 150 150	0	0
6	E	156	Total O 156 156	0	0
6	F	70	Total O 70 70	0	0

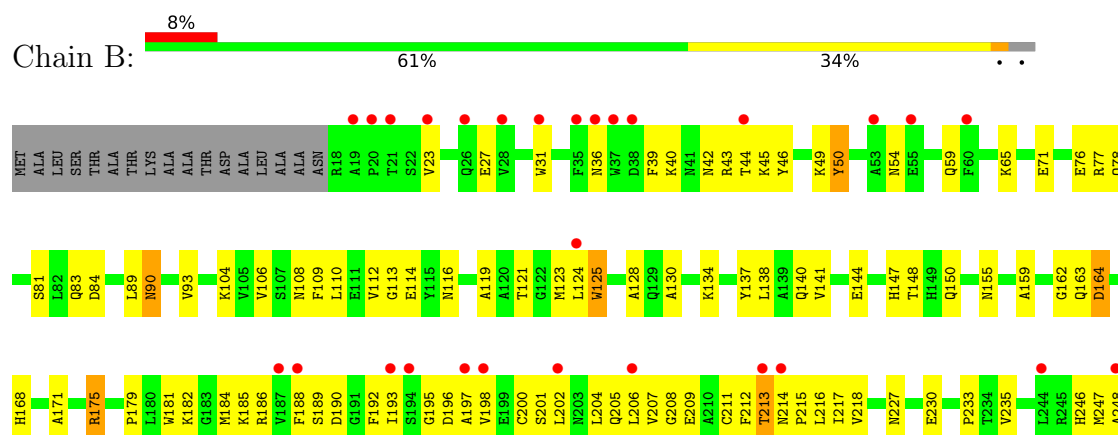
3 Residue-property plots

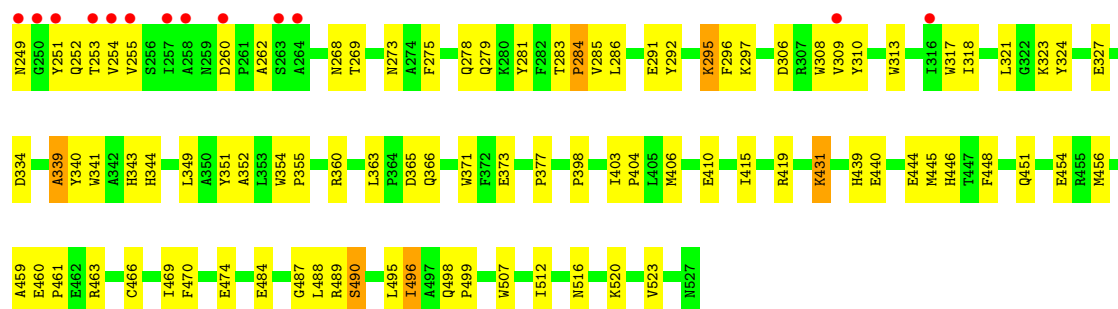
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Methane monooxygenase component A alpha chain

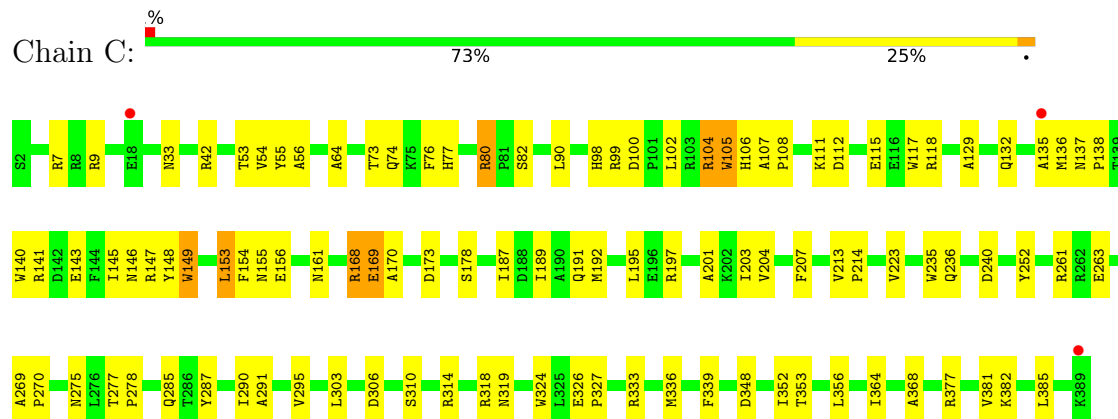


- Molecule 1: Methane monooxygenase component A alpha chain





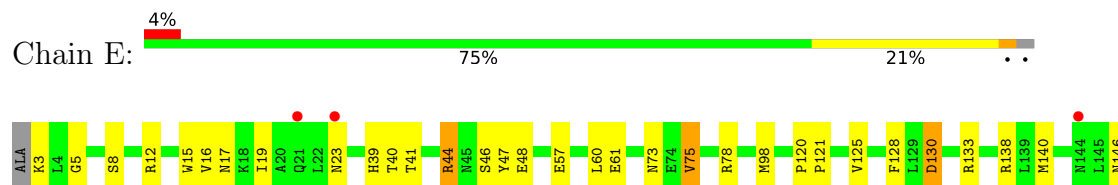
• Molecule 2: Methane monooxygenase component A beta chain



• 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.82Å 171.68Å 220.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 2.32 28.76 – 2.32	Depositor EDS
% Data completeness (in resolution range)	84.3 (28.76-2.32) 84.2 (28.76-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.263 0.218 , 0.263	Depositor DCC
R_{free} test set	3543 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18436	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: MN, 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	0.40	0/4263	0.92	17/5797 (0.3%)
1	B	0.40	0/4262	0.91	14/5796 (0.2%)
2	C	0.43	0/3263	0.87	8/4435 (0.2%)
2	D	0.38	0/3247	0.88	9/4417 (0.2%)
3	E	0.41	0/1392	0.86	4/1876 (0.2%)
3	F	0.37	0/1387	0.87	5/1873 (0.3%)
All	All	0.40	0/17814	0.89	57/24194 (0.2%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NE-CZ-NH2	7.84	126.26	119.20
3	F	130	ASP	N-CA-C	-7.44	103.25	111.36
1	A	77	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	164	ASP	CA-C-N	7.11	126.94	119.05
1	A	164	ASP	C-N-CA	7.11	126.94	119.05
1	B	164	ASP	CA-C-N	7.04	126.87	119.05
1	B	164	ASP	C-N-CA	7.04	126.87	119.05
3	E	130	ASP	N-CA-C	-6.98	103.76	111.36
1	B	496	ILE	N-CA-C	-6.79	104.15	110.53
1	B	431	LYS	N-CA-C	-6.55	105.11	113.23
1	A	285	VAL	N-CA-C	6.48	118.07	111.00
3	F	6	ILE	N-CA-C	6.31	116.46	110.53
1	B	77	ARG	NE-CZ-NH2	-6.19	113.62	119.20
2	C	106	HIS	N-CA-C	6.16	118.50	111.11
2	D	105	TRP	N-CA-C	-6.01	101.09	110.17
1	A	496	ILE	N-CA-C	-5.99	104.90	110.53
2	D	169	GLU	N-CA-C	5.98	120.64	113.23
1	B	77	ARG	CD-NE-CZ	5.98	132.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	106	HIS	N-CA-C	5.95	118.25	111.11
2	C	105	TRP	N-CA-C	-5.88	101.29	110.17
2	C	169	GLU	N-CA-C	5.87	120.51	113.23
1	A	397	ASP	CA-C-N	5.87	125.56	119.05
1	A	397	ASP	C-N-CA	5.87	125.56	119.05
2	D	236	GLN	N-CA-C	5.86	120.59	113.38
2	C	56	ALA	N-CA-C	-5.82	105.07	111.82
1	A	93	VAL	N-CA-C	5.82	116.81	111.81
1	A	460	GLU	CA-C-N	5.73	125.20	119.24
1	A	460	GLU	C-N-CA	5.73	125.20	119.24
2	D	149	TRP	N-CA-C	-5.67	105.18	111.36
2	C	236	GLN	N-CA-C	5.64	120.32	113.38
2	D	56	ALA	N-CA-C	-5.61	105.25	111.71
2	C	104	ARG	N-CA-C	5.60	117.42	108.41
1	B	339	ALA	N-CA-C	5.59	120.11	112.68
2	D	252	TYR	N-CA-C	5.57	117.03	111.07
2	C	149	TRP	N-CA-C	-5.51	105.35	111.36
1	B	295	LYS	N-CA-C	-5.50	104.60	112.13
1	A	77	ARG	CD-NE-CZ	5.49	132.08	124.40
2	D	104	ARG	N-CA-C	5.45	117.18	108.41
3	E	39	HIS	N-CA-C	5.33	121.61	113.61
3	F	73	ASN	N-CA-C	-5.33	102.64	110.52
1	B	77	ARG	NE-CZ-NH1	5.32	126.82	121.50
3	F	39	HIS	N-CA-C	5.28	121.53	113.61
1	A	346	LEU	N-CA-C	5.22	118.11	111.69
1	A	304	THR	N-CA-C	-5.17	105.72	111.36
1	B	148	THR	N-CA-C	-5.13	105.58	111.07
3	E	73	ASN	N-CA-C	-5.11	102.96	110.52
1	B	93	VAL	N-CA-C	5.10	116.51	111.67
2	D	318	ARG	N-CA-C	-5.10	105.72	111.28
3	E	5	GLY	N-CA-C	5.10	120.29	111.98
1	A	205	GLN	N-CA-C	5.09	119.35	111.56
3	F	118	TYR	N-CA-C	5.06	120.08	113.30
1	B	490	SER	N-CA-C	5.04	118.20	111.75
2	C	53	THR	N-CA-C	5.04	119.63	112.93
1	A	431	LYS	N-CA-C	-5.03	105.94	113.89
1	B	205	GLN	N-CA-C	5.02	119.24	111.56
1	A	38	ASP	N-CA-C	5.02	117.99	109.76
1	B	162	GLY	N-CA-C	5.01	120.78	112.66

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	185	0
1	B	4137	0	3888	178	0
2	C	3167	0	2987	105	0
2	D	3151	0	2957	113	0
3	E	1364	0	1352	36	0
3	F	1358	0	1335	40	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	0	0
6	A	235	0	0	9	0
6	B	212	0	0	11	0
6	C	290	0	0	14	0
6	D	150	0	0	8	0
6	E	156	0	0	6	0
6	F	70	0	0	2	0
All	All	18436	0	16416	578	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 17.

All (578) 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:D:340:ALA:HB2	2:D:389:LYS:HB2	1.31	1.06
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.46	0.95
1:B:44:THR:HG22	1:B:46:TYR:H	1.33	0.93
1:B:209:GLU:HA	1:B:213:THR:HB	1.51	0.93
1:A:44:THR:HG22	1:A:46:TYR:H	1.34	0.92
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.12	0.91
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.51	0.90
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.55	0.88
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.54	0.88
1:A:209:GLU:HA	1:A:213:THR:HB	1.55	0.88
1:A:210:ALA:HA	1:A:247:MET:HE1	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.56	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.87
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.21	0.86
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.57	0.84
1:B:283:THR:HB	1:B:284:PRO:HD3	1.59	0.84
1:B:59:GLN:NE2	1:B:248:ALA:HB1	1.92	0.83
2:C:136:MET:HE2	2:C:141:ARG:HB2	1.61	0.82
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.26	0.82
1:A:185:LYS:O	1:A:189:SER:HB2	1.80	0.81
1:A:216:LEU:HD13	1:A:286:LEU:HD13	1.63	0.80
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.24	0.80
1:A:76:GLU:HG2	1:B:76:GLU:HG2	1.64	0.80
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.62	0.80
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.65	0.79
1:B:268:ASN:HD21	1:B:327:GLU:H	1.28	0.79
1:B:185:LYS:O	1:B:189:SER:HB2	1.83	0.79
3:E:48:GLU:HB3	6:E:229:HOH:O	1.81	0.78
1:A:227:ASN:HD21	1:A:295:LYS:H	1.31	0.78
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.13	0.78
2:D:136:MET:HE2	2:D:141:ARG:HB2	1.66	0.77
1:A:59:GLN:NE2	1:A:248:ALA:HB1	1.99	0.77
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.16	0.76
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.35	0.74
1:B:227:ASN:HD21	1:B:295:LYS:H	1.35	0.74
1:A:190:ASP:HB3	2:C:74:GLN:O	1.88	0.74
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.36	0.74
3:F:41:THR:O	3:F:44:ARG:HD2	1.88	0.72
1:A:196:ASP:HB2	3:E:140:MET:SD	2.30	0.72
2:D:385:LEU:O	2:D:388:LEU:HB2	1.89	0.72
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.72	0.71
3:E:41:THR:O	3:E:44:ARG:HD2	1.90	0.71
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.37	0.71
1:A:198:VAL:O	1:A:202:LEU:HG	1.90	0.71
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.72	0.71
1:B:198:VAL:O	1:B:202:LEU:HG	1.90	0.71
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.55	0.70
2:D:389:LYS:OXT	2:D:389:LYS:HD2	1.91	0.70
2:D:388:LEU:HD23	2:D:389:LYS:HG3	1.75	0.69
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.74	0.69
1:B:108:ASN:HD21	1:B:175:ARG:HE	1.40	0.69
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:HIS:HB3	3:E:161:VAL:HG21	1.75	0.69
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.74	0.69
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.75	0.69
1:A:192:PHE:O	1:A:200:CYS:HB3	1.92	0.69
1:B:192:PHE:O	1:B:200:CYS:HB3	1.94	0.68
1:B:175:ARG:HG3	1:B:181:TRP:CD2	2.28	0.68
3:F:4:LEU:HB3	6:F:226:HOH:O	1.92	0.68
1:B:190:ASP:HB3	2:D:74:GLN:O	1.94	0.67
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.76	0.67
1:A:116:ASN:CG	1:A:189:SER:HA	2.19	0.67
1:B:213:THR:O	1:B:217:ILE:HG12	1.94	0.67
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.77	0.66
3:E:98:MET:HG3	3:E:138:ARG:HG2	1.77	0.66
1:B:45:LYS:HE3	6:D:497:HOH:O	1.94	0.66
1:B:281:TYR:O	1:B:284:PRO:HD2	1.95	0.66
1:B:309:VAL:HG12	1:B:309:VAL:O	1.95	0.66
1:A:24:ASN:OD1	1:A:26:GLN:HG2	1.96	0.66
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.78	0.66
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.89	0.66
3:F:4:LEU:HD21	3:F:10:ASP:CG	2.21	0.66
1:A:227:ASN:ND2	1:A:295:LYS:H	1.93	0.65
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.79	0.65
1:B:406:MET:O	1:B:410:GLU:HG3	1.97	0.65
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.79	0.65
1:B:306:ASP:O	1:B:310:TYR:HB2	1.97	0.65
2:C:333:ARG:HD3	6:C:5134:HOH:O	1.97	0.65
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.80	0.64
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.78	0.64
1:A:213:THR:O	1:A:217:ILE:HG12	1.96	0.64
3:F:57:GLU:O	3:F:61:GLU:HG3	1.98	0.64
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.27	0.64
2:C:333:ARG:HD2	6:C:5040:HOH:O	1.98	0.64
2:C:80:ARG:HB2	6:E:174:HOH:O	1.99	0.63
1:A:18:ARG:O	2:C:129:ALA:HA	1.99	0.62
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.81	0.62
1:A:467:GLN:HG3	6:A:5123:HOH:O	1.98	0.62
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.80	0.62
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.80	0.62
3:E:12:ARG:O	3:E:16:VAL:HG23	1.99	0.62
1:B:23:VAL:HG13	1:B:27:GLU:OE2	2.00	0.62
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:O	1:A:209:GLU:HG3	1.99	0.62
3:F:12:ARG:O	3:F:16:VAL:HG23	2.00	0.62
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.63	0.61
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.36	0.61
1:B:254:VAL:HG11	1:B:321:LEU:HD22	1.83	0.61
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.82	0.61
2:C:100:ASP:OD1	2:C:104:ARG:NH1	2.34	0.61
1:B:196:ASP:HB2	3:F:140:MET:SD	2.41	0.60
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.37	0.60
1:B:50:TYR:CG	1:B:198:VAL:HG21	2.35	0.60
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.60
1:B:489:ARG:NH1	1:B:496:ILE:HA	2.16	0.60
2:D:153:LEU:C	2:D:153:LEU:HD12	2.26	0.60
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.66	0.60
1:B:121:THR:HG21	1:B:140:GLN:HG2	1.82	0.60
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.83	0.60
2:C:348:ASP:O	2:C:352:ILE:HG12	2.02	0.60
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.83	0.60
2:D:213:VAL:HG23	6:D:397:HOH:O	2.01	0.60
1:A:23:VAL:HB	2:C:195:LEU:CD1	2.32	0.60
1:B:140:GLN:O	1:B:144:GLU:HG2	2.01	0.60
2:D:350:GLU:HG2	6:D:432:HOH:O	2.01	0.60
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.82	0.60
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.99	0.60
1:B:193:ILE:HD12	2:D:168:ARG:HH21	1.67	0.59
2:D:340:ALA:HB2	2:D:389:LYS:CB	2.20	0.59
2:D:348:ASP:O	2:D:352:ILE:HG12	2.02	0.59
1:A:140:GLN:O	1:A:144:GLU:HG2	2.03	0.59
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.37	0.59
2:D:100:ASP:OD1	2:D:104:ARG:NH1	2.35	0.59
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.86	0.59
2:D:111:LYS:O	2:D:115:GLU:HG3	2.02	0.59
1:B:39:PHE:CE2	2:D:232:GLU:HG2	2.38	0.59
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.84	0.59
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.84	0.58
1:A:123:MET:HE2	1:A:197:ALA:HA	1.85	0.58
2:C:213:VAL:HG23	6:C:5035:HOH:O	2.03	0.58
1:A:171:ALA:O	1:A:175:ARG:HB3	2.03	0.58
1:B:171:ALA:O	1:B:175:ARG:HB3	2.04	0.58
1:A:186:ARG:O	1:A:186:ARG:HD3	2.03	0.58
1:A:313:TRP:HA	1:A:317:TRP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:HG2	6:B:5034:HOH:O	2.01	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.04	0.58
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.86	0.58
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.58
2:C:111:LYS:O	2:C:115:GLU:HG3	2.03	0.58
1:A:23:VAL:HB	2:C:195:LEU:HD11	1.85	0.58
2:C:136:MET:HE2	2:C:141:ARG:CB	2.33	0.58
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.57
1:B:255:VAL:HG22	1:B:324:TYR:CE2	2.39	0.57
2:D:9:ARG:NH2	6:D:487:HOH:O	2.37	0.57
1:B:186:ARG:HD3	1:B:186:ARG:O	2.04	0.57
2:D:143:GLU:O	2:D:147:ARG:HB3	2.05	0.57
1:A:439:HIS:HB3	3:E:161:VAL:CG2	2.34	0.57
1:B:186:ARG:HD3	1:B:186:ARG:C	2.30	0.57
3:E:57:GLU:O	3:E:61:GLU:HG3	2.04	0.57
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.87	0.57
3:F:165:HIS:CE1	3:F:167:GLN:HE21	2.23	0.57
1:A:262:ALA:HA	1:A:265:LYS:NZ	2.20	0.57
2:C:135:ALA:HB3	6:C:5268:HOH:O	2.05	0.57
2:C:153:LEU:C	2:C:153:LEU:HD12	2.30	0.57
1:A:186:ARG:HD3	1:A:186:ARG:C	2.29	0.56
1:B:459:ALA:C	1:B:461:PRO:HD3	2.30	0.56
2:C:104:ARG:NE	6:C:5234:HOH:O	2.38	0.56
1:A:305:TRP:CH2	1:A:336:LYS:HA	2.40	0.56
1:A:460:GLU:HB3	1:A:463:ARG:HG3	1.87	0.56
3:E:17:ASN:HB3	6:E:194:HOH:O	2.04	0.56
1:A:230:GLU:HG3	1:B:89:LEU:HD21	1.86	0.56
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.41	0.56
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.88	0.56
1:A:113:GLY:CA	1:A:188:PHE:HB3	2.36	0.56
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.98	0.56
1:B:201:SER:OG	1:B:253:THR:HG21	2.05	0.56
1:B:269:THR:HB	6:B:5192:HOH:O	2.05	0.56
2:C:143:GLU:O	2:C:147:ARG:HB3	2.06	0.56
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.00	0.56
1:A:50:TYR:CG	1:A:198:VAL:HG21	2.41	0.56
3:F:19:ILE:HG12	3:F:60:LEU:HD13	1.87	0.56
1:A:182:LYS:O	2:C:73:THR:HG21	2.06	0.55
1:A:208:GLY:HA2	1:A:278:GLN:HE21	1.70	0.55
1:A:76:GLU:OE2	1:B:76:GLU:HG2	2.06	0.55
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HG2	2:C:129:ALA:O	2.06	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.07	0.55
1:A:227:ASN:HD21	1:A:295:LYS:N	2.04	0.55
2:D:102:LEU:HD11	2:D:290:ILE:HG12	1.89	0.55
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.37	0.55
3:E:19:ILE:HG12	3:E:60:LEU:CD1	2.37	0.55
3:F:165:HIS:HE1	3:F:167:GLN:HG3	1.71	0.55
1:B:466:CYS:HB2	2:D:73:THR:HA	1.89	0.54
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.30	0.54
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.25	0.54
1:A:306:ASP:O	1:A:310:TYR:HB2	2.08	0.54
1:B:520:LYS:HD2	6:B:5190:HOH:O	2.07	0.54
1:A:18:ARG:N	6:A:5188:HOH:O	2.39	0.54
1:A:193:ILE:HB	2:C:168:ARG:CZ	2.37	0.54
1:B:247:MET:HE2	1:B:247:MET:HA	1.89	0.54
2:C:318:ARG:HD2	6:C:5165:HOH:O	2.07	0.54
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.32	0.54
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.89	0.54
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.43	0.54
3:E:3:LYS:N	6:E:300:HOH:O	2.40	0.54
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.89	0.54
1:B:31:TRP:CH2	2:D:210:SER:HA	2.42	0.54
1:B:489:ARG:NH1	1:B:496:ILE:O	2.41	0.53
3:E:165:HIS:HE1	3:E:167:GLN:HG3	1.73	0.53
1:A:302:VAL:CG1	1:A:340:TYR:HA	2.39	0.53
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.43	0.53
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.43	0.53
2:C:306:ASP:O	2:C:310:SER:HB2	2.08	0.53
2:C:324:TRP:C	2:C:327:PRO:HD2	2.33	0.53
2:D:291:ALA:O	2:D:295:VAL:HG23	2.09	0.53
3:F:165:HIS:CE1	3:F:167:GLN:HG3	2.44	0.53
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.43	0.53
1:A:84:ASP:HB3	1:B:81:SER:OG	2.08	0.53
1:B:488:LEU:HB2	6:B:5167:HOH:O	2.08	0.53
1:A:110:LEU:O	1:A:114:GLU:HG2	2.08	0.53
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.43	0.53
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.90	0.53
1:B:268:ASN:ND2	1:B:327:GLU:H	2.01	0.53
6:B:5208:HOH:O	3:F:143:ARG:HG2	2.07	0.53
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.90	0.53
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:ARG:NH2	6:C:5234:HOH:O	2.39	0.53
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.44	0.53
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.53
2:C:192:MET:HE2	2:C:192:MET:HA	1.90	0.53
2:D:192:MET:HA	2:D:192:MET:HE2	1.91	0.53
1:B:208:GLY:HA2	1:B:278:GLN:HE21	1.73	0.53
2:C:54:VAL:O	2:C:55:TYR:HB2	2.09	0.53
1:A:302:VAL:HG11	1:A:340:TYR:CD1	2.44	0.52
1:A:466:CYS:HB2	2:C:73:THR:HA	1.91	0.52
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.90	0.52
1:B:460:GLU:N	1:B:461:PRO:HD3	2.25	0.52
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.44	0.52
2:C:275:ASN:C	2:C:278:PRO:HD2	2.34	0.52
2:D:153:LEU:HD12	2:D:154:PHE:N	2.23	0.52
1:A:251:TYR:O	1:A:255:VAL:HG23	2.10	0.52
1:A:312:ASP:HA	1:A:316:ILE:CG2	2.40	0.52
1:B:251:TYR:O	1:B:255:VAL:HG23	2.08	0.52
2:D:310:SER:O	2:D:314:ARG:HG3	2.10	0.52
1:A:81:SER:OG	1:B:84:ASP:HB3	2.08	0.52
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.10	0.52
1:B:159:ALA:O	2:D:33:ASN:HB2	2.10	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.51
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.75	0.51
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.58	0.51
2:D:105:TRP:O	2:D:108:PRO:HD2	2.10	0.51
1:B:123:MET:HE2	1:B:197:ALA:HA	1.93	0.51
2:D:306:ASP:O	2:D:310:SER:HB2	2.10	0.51
1:A:243:GLU:O	1:A:247:MET:HG2	2.10	0.51
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.55	0.51
1:B:349:LEU:HD22	1:B:415:ILE:HD13	1.91	0.51
2:D:136:MET:HE2	2:D:141:ARG:CB	2.37	0.51
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.92	0.51
2:D:54:VAL:O	2:D:55:TYR:HB2	2.10	0.51
2:C:104:ARG:CZ	6:C:5234:HOH:O	2.57	0.51
2:C:104:ARG:HG3	2:C:104:ARG:HH11	1.75	0.51
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.45	0.51
1:B:36:ASN:HD21	1:B:42:ASN:HD21	1.58	0.51
1:B:43:ARG:HD2	1:B:43:ARG:C	2.36	0.51
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.45	0.51
2:D:82:SER:O	2:D:168:ARG:NH2	2.43	0.51
2:D:104:ARG:HG3	2:D:104:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MET:HE2	1:A:197:ALA:CA	2.41	0.51
1:A:163:GLN:HG2	6:A:5011:HOH:O	2.11	0.51
3:F:4:LEU:CD2	3:F:10:ASP:H	2.24	0.51
1:B:209:GLU:HA	1:B:213:THR:CB	2.34	0.51
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.45	0.51
2:D:235:TRP:CD1	2:D:235:TRP:C	2.89	0.51
3:E:3:LYS:HE2	3:E:8:SER:OG	2.11	0.51
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.93	0.50
1:A:184:MET:HE3	1:A:188:PHE:CB	2.35	0.50
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.09	0.50
3:E:23:ASN:HB2	6:E:216:HOH:O	2.12	0.50
1:B:50:TYR:CD1	1:B:50:TYR:N	2.79	0.50
2:D:339:PHE:CE2	2:D:352:ILE:HD12	2.46	0.50
1:A:76:GLU:HG2	1:B:76:GLU:CG	2.39	0.50
1:A:137:TYR:O	1:A:141:VAL:HG23	2.12	0.50
2:C:187:ILE:O	2:C:191:GLN:HG3	2.11	0.50
2:D:379:GLN:HB3	6:D:528:HOH:O	2.11	0.50
3:F:153:GLU:H	3:F:153:GLU:CD	2.19	0.50
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.58	0.50
1:A:222:GLU:OE1	2:C:7:ARG:HD3	2.11	0.50
1:B:184:MET:HE3	1:B:188:PHE:CB	2.36	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.11	0.50
3:F:46:SER:OG	3:F:48:GLU:HG2	2.10	0.50
1:A:43:ARG:C	1:A:43:ARG:HD2	2.36	0.50
2:D:336:MET:HE3	2:D:388:LEU:HG	1.94	0.50
1:A:50:TYR:CD1	1:A:50:TYR:N	2.79	0.50
1:A:76:GLU:CG	1:B:76:GLU:HG2	2.37	0.50
1:B:351:TYR:CE2	1:B:363:LEU:HD21	2.47	0.50
3:E:46:SER:OG	3:E:48:GLU:HG2	2.12	0.50
3:E:61:GLU:HB3	3:E:121:PRO:HD3	1.94	0.50
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.09	0.50
1:A:297:LYS:N	1:A:297:LYS:HD2	2.27	0.50
1:A:365:ASP:OD2	1:A:365:ASP:C	2.55	0.50
1:A:310:TYR:OH	1:A:336:LYS:HD2	2.10	0.49
1:A:116:ASN:CB	1:A:189:SER:HA	2.42	0.49
2:C:82:SER:O	2:C:168:ARG:NH2	2.44	0.49
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.13	0.49
1:B:137:TYR:O	1:B:141:VAL:HG23	2.13	0.49
1:B:218:VAL:HG12	6:B:5171:HOH:O	2.13	0.49
2:D:336:MET:HB3	2:D:388:LEU:HA	1.93	0.49
1:A:159:ALA:O	2:C:33:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.93	0.49
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.49
2:C:153:LEU:HD12	2:C:154:PHE:N	2.28	0.49
1:A:230:GLU:C	1:A:233:PRO:HD2	2.38	0.49
2:D:388:LEU:HD23	2:D:389:LYS:N	2.27	0.49
1:A:334:ASP:N	1:A:334:ASP:OD2	2.46	0.49
1:A:440:GLU:HG3	1:A:445:MET:SD	2.53	0.49
1:B:175:ARG:HG3	1:B:181:TRP:CE2	2.48	0.49
2:C:270:PRO:CB	2:D:270:PRO:HB3	2.33	0.49
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.95	0.49
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.38	0.48
1:A:369:MET:HG2	1:A:379:TRP:CH2	2.49	0.48
1:A:109:PHE:O	1:A:112:VAL:HG12	2.13	0.48
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.48	0.48
2:C:105:TRP:O	2:C:108:PRO:HD2	2.13	0.48
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.13	0.48
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.48
3:F:165:HIS:HE1	3:F:167:GLN:HE21	1.61	0.48
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.49	0.48
1:A:216:LEU:HD11	1:A:286:LEU:HD22	1.95	0.48
1:A:354:TRP:CZ3	1:A:499:PRO:HD3	2.48	0.48
2:D:146:ASN:HD21	2:D:197:ARG:HH21	1.60	0.48
1:B:65:LYS:HB3	2:D:117:TRP:CD2	2.48	0.48
1:B:186:ARG:HA	2:D:73:THR:OG1	2.13	0.48
1:B:189:SER:O	1:B:193:ILE:HG12	2.14	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.13	0.48
1:B:213:THR:O	1:B:216:LEU:HB3	2.12	0.48
2:D:388:LEU:CD2	2:D:389:LYS:HG3	2.42	0.48
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.48	0.48
2:D:339:PHE:HB2	2:D:389:LYS:HG2	1.95	0.48
1:B:113:GLY:CA	1:B:188:PHE:HB3	2.44	0.48
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.48
2:D:213:VAL:HB	2:D:214:PRO:CD	2.44	0.48
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.47
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.49	0.47
3:E:153:GLU:CD	3:E:153:GLU:H	2.22	0.47
2:C:336:MET:HE1	2:C:352:ILE:CG2	2.44	0.47
1:B:487:GLY:C	1:B:488:LEU:HD12	2.38	0.47
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.50	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.15	0.47
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.15	0.47
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.79	0.47
1:A:189:SER:O	1:A:193:ILE:HG12	2.14	0.47
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.50	0.47
1:B:216:LEU:HD13	1:B:286:LEU:HD13	1.96	0.47
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.63	0.47
1:A:282:PHE:O	1:A:283:THR:C	2.58	0.46
1:B:155:ASN:HD22	1:B:168:HIS:HD2	1.61	0.46
1:B:419:ARG:HA	6:B:5157:HOH:O	2.14	0.46
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.50	0.46
1:A:104:LYS:HG2	1:A:168:HIS:CD2	2.50	0.46
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.96	0.46
2:C:310:SER:O	2:C:314:ARG:HG3	2.15	0.46
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.49	0.46
1:B:365:ASP:OD2	1:B:365:ASP:C	2.57	0.46
1:B:470:PHE:O	1:B:474:GLU:HB2	2.16	0.46
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.96	0.46
1:B:185:LYS:HA	1:B:189:SER:HB2	1.98	0.46
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.48	0.46
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.50	0.46
2:D:381:VAL:O	2:D:385:LEU:HB2	2.16	0.46
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.51	0.46
1:A:185:LYS:HA	1:A:189:SER:HB2	1.98	0.46
1:A:459:ALA:C	1:A:461:PRO:HD3	2.41	0.46
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.49	0.46
1:A:262:ALA:HA	1:A:265:LYS:HZ3	1.80	0.46
1:B:23:VAL:HB	2:D:195:LEU:HD11	1.98	0.46
2:C:213:VAL:HB	2:C:214:PRO:CD	2.46	0.46
2:C:339:PHE:CZ	2:C:352:ILE:HD12	2.51	0.46
1:A:525:ALA:HA	6:A:5199:HOH:O	2.16	0.46
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.46
1:A:162:GLY:HA3	6:A:5007:HOH:O	2.15	0.46
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.51	0.46
2:D:145:ILE:O	2:D:149:TRP:HB3	2.16	0.46
1:B:484:GLU:OE1	3:F:6:ILE:N	2.49	0.46
2:D:146:ASN:ND2	2:D:197:ARG:HH21	2.13	0.46
1:A:188:PHE:CE1	1:A:282:PHE:CE2	3.05	0.45
1:A:227:ASN:HD21	1:A:296:PHE:H	1.63	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.50	0.45
2:D:240:ASP:OD1	3:F:125:VAL:HG21	2.17	0.45
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.50	0.45
3:F:40:THR:C	3:F:41:THR:HG23	2.41	0.45
1:B:50:TYR:CD1	1:B:198:VAL:HG21	2.51	0.45
1:A:125:TRP:CD1	1:A:125:TRP:C	2.95	0.45
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.29	0.45
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.45
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.50	0.45
1:A:316:ILE:HG12	1:A:316:ILE:O	2.16	0.45
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.99	0.45
1:B:185:LYS:C	1:B:189:SER:HB2	2.42	0.45
1:B:490:SER:OG	2:D:32:ASN:HB2	2.16	0.45
2:C:336:MET:HE1	2:C:352:ILE:HG22	1.99	0.45
1:A:186:ARG:HB3	6:A:5035:HOH:O	2.16	0.45
1:A:187:VAL:HG12	1:A:277:THR:HG22	1.98	0.45
1:A:310:TYR:C	1:A:312:ASP:H	2.25	0.45
1:A:445:MET:HE1	3:E:164:VAL:HG21	1.98	0.45
1:A:490:SER:C	1:A:492:GLY:H	2.25	0.45
1:B:65:LYS:HD2	2:D:117:TRP:HB2	1.99	0.45
3:F:120:PRO:HD3	3:F:128:PHE:CG	2.52	0.45
1:B:108:ASN:HD21	1:B:175:ARG:NE	2.09	0.45
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.52	0.45
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.17	0.45
1:A:306:ASP:OD2	1:A:336:LYS:NZ	2.50	0.45
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.47	0.45
1:A:32:LEU:HD12	1:A:35:PHE:CD2	2.53	0.44
1:A:119:ALA:O	2:C:168:ARG:HD2	2.17	0.44
2:C:102:LEU:HD13	6:C:5267:HOH:O	2.17	0.44
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.82	0.44
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.52	0.44
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.83	0.44
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.52	0.44
1:B:182:LYS:O	2:D:73:THR:HG21	2.17	0.44
1:B:460:GLU:HB3	1:B:463:ARG:HG3	1.99	0.44
1:B:489:ARG:HH11	1:B:496:ILE:HA	1.81	0.44
2:D:325:LEU:O	2:D:329:ILE:HG13	2.18	0.44
3:F:19:ILE:HG12	3:F:60:LEU:CD1	2.47	0.44
1:A:249:ASN:HA	1:A:252:GLN:HG2	2.00	0.44
1:B:23:VAL:HB	2:D:195:LEU:CD1	2.47	0.44
1:A:230:GLU:OE2	2:C:9:ARG:NH1	2.50	0.44
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.44
1:B:116:ASN:CG	1:B:189:SER:HA	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:ASN:HD21	2:D:270:PRO:HG2	1.82	0.44
1:A:20:PRO:HG3	2:C:129:ALA:HB2	2.00	0.44
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.42	0.44
1:B:119:ALA:O	2:D:168:ARG:HD2	2.17	0.44
1:B:104:LYS:HG2	1:B:168:HIS:CD2	2.53	0.44
2:C:318:ARG:NH2	6:C:5045:HOH:O	2.51	0.44
2:D:80:ARG:HB2	6:D:390:HOH:O	2.17	0.44
3:F:44:ARG:HG3	3:F:46:SER:O	2.18	0.44
1:A:292:TYR:CD2	1:A:347:TYR:CD2	3.06	0.44
1:A:469:ILE:HG13	1:A:470:PHE:N	2.32	0.44
3:E:40:THR:C	3:E:41:THR:HG23	2.43	0.44
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.44
1:A:185:LYS:C	1:A:189:SER:HB2	2.40	0.44
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.52	0.44
1:A:343:HIS:CD2	1:A:343:HIS:H	2.36	0.43
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.16	0.43
2:D:136:MET:HE3	2:D:140:TRP:HD1	1.83	0.43
1:B:444:GLU:OE2	1:B:444:GLU:HA	2.18	0.43
2:D:189:ILE:HD12	2:D:284:ALA:HB2	2.00	0.43
1:A:116:ASN:ND2	1:A:189:SER:HA	2.33	0.43
1:A:263:SER:O	1:A:267:LEU:HB2	2.18	0.43
1:A:283:THR:HB	1:A:284:PRO:CD	2.47	0.43
1:B:185:LYS:CA	1:B:189:SER:HB2	2.49	0.43
1:B:373:GLU:OE2	1:B:377:PRO:HA	2.18	0.43
1:A:58:GLU:OE2	1:A:135:ASN:HB3	2.19	0.43
1:B:249:ASN:HA	1:B:252:GLN:HG2	2.00	0.43
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.81	0.43
2:C:169:GLU:O	2:C:170:ALA:C	2.61	0.43
1:B:49:LYS:HD3	3:F:140:MET:HB3	2.01	0.43
1:B:106:VAL:O	1:B:110:LEU:HG	2.19	0.43
1:B:516:ASN:ND2	6:B:5139:HOH:O	2.51	0.43
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.53	0.43
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.19	0.43
3:F:15:TRP:O	3:F:19:ILE:HG13	2.19	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.64	0.43
3:F:73:ASN:OD1	3:F:75:VAL:HG13	2.18	0.43
1:A:45:LYS:HA	3:E:133:ARG:HD2	2.00	0.43
2:C:336:MET:HE2	2:C:385:LEU:HD23	2.00	0.43
1:B:116:ASN:CB	1:B:189:SER:HA	2.49	0.43
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.54	0.43
2:C:136:MET:HE3	2:C:140:TRP:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:O	2:C:149:TRP:HB3	2.19	0.43
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.49	0.43
1:A:185:LYS:CA	1:A:189:SER:HB2	2.48	0.43
2:C:277:THR:HB	2:C:278:PRO:HD3	1.99	0.43
2:C:353:THR:HG21	6:C:5233:HOH:O	2.17	0.43
2:D:152:PHE:O	2:D:155:ASN:HB3	2.19	0.43
2:C:314:ARG:O	2:C:318:ARG:HB2	2.19	0.43
2:C:333:ARG:NH1	6:C:5040:HOH:O	2.41	0.43
2:D:8:ARG:HH22	2:D:15:GLU:CD	2.27	0.43
1:A:321:LEU:O	1:A:326:VAL:HB	2.19	0.42
1:A:334:ASP:HB3	6:A:5181:HOH:O	2.19	0.42
1:B:212:PHE:O	1:B:215:PRO:HD2	2.19	0.42
1:B:339:ALA:O	1:B:340:TYR:C	2.62	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.01	0.42
2:D:292:LYS:NZ	6:D:522:HOH:O	2.51	0.42
2:D:377:ARG:O	2:D:381:VAL:HG23	2.19	0.42
1:A:362:ALA:HB2	1:A:501:VAL:HG13	2.00	0.42
1:B:121:THR:HG21	1:B:140:GLN:CG	2.48	0.42
1:B:489:ARG:HB3	2:D:30:ASP:OD2	2.19	0.42
2:C:189:ILE:HD11	2:C:287:TYR:CD1	2.54	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.61	0.42
2:C:291:ALA:O	2:C:295:VAL:HG23	2.19	0.42
3:E:41:THR:O	3:E:44:ARG:CD	2.64	0.42
1:A:315:GLY:N	1:A:318:ILE:HG22	2.35	0.42
1:B:207:VAL:O	1:B:211:CYS:HB3	2.19	0.42
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.42
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.50	0.42
2:C:102:LEU:HD11	2:C:290:ILE:HG12	2.02	0.42
2:C:263:GLU:OE2	2:C:263:GLU:HA	2.19	0.42
1:A:71:GLU:OE2	1:A:242:ASP:OD2	2.38	0.42
1:A:363:LEU:HD11	1:A:395:CYS:SG	2.59	0.42
1:B:44:THR:HG21	6:B:5175:HOH:O	2.19	0.42
1:B:313:TRP:HA	1:B:317:TRP:HB3	2.01	0.42
2:C:240:ASP:OD1	3:E:125:VAL:HG21	2.19	0.42
1:B:403:ILE:HG13	1:B:403:ILE:O	2.18	0.42
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.05	0.42
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.52	0.42
3:E:44:ARG:HG3	3:E:46:SER:O	2.20	0.42
1:B:249:ASN:HA	1:B:252:GLN:CG	2.49	0.42
1:B:323:LYS:HG3	1:B:324:TYR:CE1	2.55	0.42
3:F:69:ALA:HA	6:F:225:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.91	0.42
2:D:146:ASN:HD21	2:D:197:ARG:NH2	2.17	0.42
1:A:91:ALA:HB1	6:A:5010:HOH:O	2.19	0.42
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.01	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42
1:A:249:ASN:HA	1:A:252:GLN:CG	2.49	0.42
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.85	0.42
1:A:302:VAL:HG12	1:A:340:TYR:HA	2.02	0.41
2:C:98:HIS:HE1	2:C:178:SER:OG	2.04	0.41
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.19	0.41
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.41
1:A:116:ASN:HB2	1:A:188:PHE:O	2.20	0.41
2:D:184:PHE:O	2:D:187:ILE:HG22	2.20	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.01	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.36	0.41
1:B:193:ILE:HB	2:D:168:ARG:NH2	2.35	0.41
2:C:324:TRP:O	2:C:327:PRO:HD2	2.20	0.41
3:E:15:TRP:O	3:E:19:ILE:HG13	2.21	0.41
3:E:75:VAL:HG12	6:E:190:HOH:O	2.19	0.41
1:A:50:TYR:CD1	1:A:198:VAL:HG21	2.56	0.41
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.41
2:C:377:ARG:O	2:C:381:VAL:HG23	2.21	0.41
2:D:299:TYR:O	2:D:317:MET:HE1	2.21	0.41
1:A:336:LYS:C	1:A:338:ASP:H	2.28	0.41
1:A:402:PHE:O	1:A:403:ILE:HD12	2.19	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.59	0.41
1:A:201:SER:OG	1:A:253:THR:HG21	2.20	0.41
1:A:338:ASP:O	1:A:342:ALA:CB	2.69	0.41
1:B:212:PHE:O	1:B:213:THR:C	2.63	0.41
1:B:439:HIS:HB3	3:F:161:VAL:HG22	2.01	0.41
2:C:155:ASN:ND2	2:C:252:TYR:OH	2.52	0.41
2:C:223:VAL:HG23	6:C:5021:HOH:O	2.19	0.41
1:A:23:VAL:HB	2:C:195:LEU:HD12	2.03	0.41
1:A:167:GLY:O	1:A:171:ALA:HB2	2.21	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.59	0.41
1:B:113:GLY:HA3	1:B:188:PHE:HD2	1.86	0.41
1:B:273:ASN:CB	1:B:456:MET:HE2	2.51	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.20	0.41
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.02	0.41
2:D:314:ARG:O	2:D:318:ARG:HB2	2.21	0.41
1:A:283:THR:HB	1:A:284:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.41
2:D:102:LEU:CD1	2:D:290:ILE:HG12	2.51	0.41
1:A:193:ILE:HB	2:C:168:ARG:NH2	2.36	0.41
1:B:268:ASN:HD22	1:B:268:ASN:HA	1.69	0.41
1:B:446:HIS:HB3	1:B:448:PHE:CZ	2.56	0.41
2:D:98:HIS:HE1	2:D:178:SER:OG	2.04	0.41
3:F:165:HIS:HE1	3:F:167:GLN:NE2	2.19	0.41
1:B:128:ALA:O	1:B:134:LYS:HE2	2.21	0.41
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.55	0.41
3:E:130:ASP:OD1	3:E:133:ARG:NH1	2.54	0.41
1:A:260:ASP:HA	1:A:261:PRO:HD3	1.96	0.40
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.20	0.40
1:B:195:GLY:HA2	6:D:516:HOH:O	2.21	0.40
1:B:227:ASN:HD21	1:B:296:PHE:H	1.68	0.40
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.56	0.40
1:A:212:PHE:O	1:A:216:LEU:CB	2.68	0.40
1:A:315:GLY:C	1:A:317:TRP:H	2.28	0.40
1:B:39:PHE:CD2	2:D:232:GLU:HG2	2.56	0.40
1:B:83:GLN:HG2	6:B:5128:HOH:O	2.20	0.40
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.40
1:A:254:VAL:O	1:A:254:VAL:HG12	2.20	0.40
2:C:147:ARG:HD2	2:C:148:TYR:CE1	2.57	0.40
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.21	0.40
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.03	0.40
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.57	0.40
1:A:460:GLU:HB3	1:A:463:ARG:CG	2.50	0.40
1:B:110:LEU:O	1:B:114:GLU:HG2	2.21	0.40
1:B:254:VAL:O	1:B:254:VAL:HG12	2.22	0.40
1:B:366:GLN:HG3	6:B:5123:HOH:O	2.22	0.40
2:C:132:GLN:HB3	6:C:5188:HOH:O	2.21	0.40
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.03	0.40
6:A:5161:HOH:O	1:B:76:GLU:HB3	2.21	0.40
1:B:50:TYR:HB2	1:B:198:VAL:HG21	2.02	0.40
1:B:54:ASN:C	1:B:130:ALA:HB2	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/527 (96%)	466 (92%)	40 (8%)	2 (0%)	30	37
1	B	508/527 (96%)	470 (92%)	35 (7%)	3 (1%)	21	25
2	C	386/388 (100%)	369 (96%)	16 (4%)	1 (0%)	36	45
2	D	386/388 (100%)	372 (96%)	12 (3%)	2 (0%)	24	30
3	E	164/169 (97%)	161 (98%)	3 (2%)	0	100	100
3	F	164/169 (97%)	161 (98%)	3 (2%)	0	100	100
All	All	2116/2168 (98%)	1999 (94%)	109 (5%)	8 (0%)	30	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	A	311	GLU
2	C	64	ALA
2	D	64	ALA
1	B	213	THR
1	A	316	ILE
1	B	284	PRO
2	D	251	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/442 (96%)	412 (97%)	11 (3%)	40	57
1	B	422/442 (96%)	413 (98%)	9 (2%)	47	65
2	C	316/323 (98%)	310 (98%)	6 (2%)	50	67
2	D	312/323 (97%)	307 (98%)	5 (2%)	55	72
3	E	143/146 (98%)	141 (99%)	2 (1%)	59	75
3	F	142/146 (97%)	141 (99%)	1 (1%)	76	86
All	All	1758/1822 (96%)	1724 (98%)	34 (2%)	50	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	50	TYR
1	A	71	GLU
1	A	90	ASN
1	A	175	ARG
1	A	302	VAL
1	A	334	ASP
1	A	348	LEU
1	A	403	ILE
1	A	467	GLN
1	A	479	SER
1	B	50	TYR
1	B	71	GLU
1	B	90	ASN
1	B	125	TRP
1	B	175	ARG
1	B	279	GLN
1	B	334	ASP
1	B	440	GLU
1	B	451	GLN
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	356	LEU
2	C	382	LYS
2	D	80	ARG

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Mol	Chain	Res	Type
2	D	153	LEU
2	D	168	ARG
2	D	173	ASP
2	D	356	LEU
3	E	44	ARG
3	E	75	VAL
3	F	44	ARG

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	59	GLN
1	A	78	GLN
1	A	83	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	155	ASN
1	A	161	ASN
1	A	205	GLN
1	A	227	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	382	HIS
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	42	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	155	ASN
1	B	161	ASN
1	B	168	HIS
1	B	203	ASN

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Mol	Chain	Res	Type
1	B	205	GLN
1	B	227	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	411	ASN
1	B	413	HIS
1	B	422	GLN
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	220	ASN
2	C	266	GLN
2	C	275	ASN
2	C	285	GLN
2	C	296	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	146	ASN
2	D	161	ASN
2	D	220	ASN
2	D	266	GLN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	134	GLN
3	E	158	GLN
3	E	165	HIS
3	F	39	HIS
3	F	45	ASN
3	F	134	GLN

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Mol	Chain	Res	Type
3	F	158	GLN
3	F	165	HIS

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 8 ligands modelled in this entry, 8 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 [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	510/527 (96%)	0.60	62 (12%) 8 9	23, 41, 98, 114	0
1	B	510/527 (96%)	0.46	41 (8%) 18 20	23, 39, 82, 104	0
2	C	388/388 (100%)	0.13	3 (0%) 82 84	22, 33, 52, 61	0
2	D	388/388 (100%)	0.61	22 (5%) 29 32	26, 41, 60, 98	0
3	E	166/169 (98%)	0.46	6 (3%) 46 49	26, 40, 57, 65	0
3	F	166/169 (98%)	0.81	4 (2%) 59 62	32, 47, 60, 68	0
All	All	2128/2168 (98%)	0.49	138 (6%) 25 27	22, 40, 78, 114	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	5.5
1	A	194	SER	4.4
1	B	188	PHE	4.3
1	A	253	THR	4.3
1	A	317	TRP	4.3
1	A	213	THR	4.2
1	A	195	GLY	4.1
1	A	316	ILE	4.1
1	A	212	PHE	4.0
3	E	23	ASN	4.0
1	B	23	VAL	3.9
1	A	252	GLN	3.8
1	A	201	SER	3.8
1	A	197	ALA	3.7
1	A	249	ASN	3.7
1	A	214	ASN	3.7
1	A	321	LEU	3.6
1	B	21	THR	3.6
3	F	4	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	3.5
1	A	254	VAL	3.4
1	A	255	VAL	3.4
1	A	248	ALA	3.4
1	A	337	GLN	3.4
2	D	375	ALA	3.4
3	F	69	ALA	3.4
1	A	308	TRP	3.3
1	B	20	PRO	3.3
1	A	258	ALA	3.2
1	B	248	ALA	3.2
1	A	205	GLN	3.2
1	A	318	ILE	3.2
1	B	257	ILE	3.1
2	D	384	VAL	3.1
1	A	257	ILE	3.1
1	A	251	TYR	3.0
1	A	322	GLY	3.0
1	A	324	TYR	3.0
1	B	251	TYR	3.0
3	E	168	SER	3.0
1	A	55	GLU	2.9
1	A	210	ALA	2.9
1	B	19	ALA	2.9
1	B	53	ALA	2.9
1	A	320	ARG	2.9
1	B	263	SER	2.8
1	A	204	LEU	2.8
1	A	191	GLY	2.8
2	D	136	MET	2.8
1	B	253	THR	2.8
1	A	256	SER	2.8
1	B	206	LEU	2.8
1	B	55	GLU	2.8
1	A	264	ALA	2.8
2	D	227	ALA	2.8
1	B	35	PHE	2.8
2	D	388	LEU	2.7
1	B	249	ASN	2.7
1	B	197	ALA	2.7
3	E	167	GLN	2.7
1	A	262	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	213	THR	2.7
2	D	338	LEU	2.7
1	A	305	TRP	2.6
1	B	264	ALA	2.6
1	A	309	VAL	2.6
2	D	223	VAL	2.6
1	A	263	SER	2.6
1	B	258	ALA	2.5
3	E	144	ASN	2.5
1	A	325	GLY	2.5
1	B	31	TRP	2.5
1	B	28	VAL	2.5
1	B	198	VAL	2.5
1	B	254	VAL	2.5
1	B	202	LEU	2.5
1	B	255	VAL	2.4
2	D	148	TYR	2.4
1	B	38	ASP	2.4
2	C	135	ALA	2.4
2	D	389	LYS	2.4
3	E	21	GLN	2.4
2	D	328	THR	2.4
1	A	198	VAL	2.4
3	F	72	PHE	2.4
1	B	44	THR	2.3
2	D	264	PHE	2.3
1	A	216	LEU	2.3
1	A	338	ASP	2.3
1	A	339	ALA	2.3
1	B	193	ILE	2.3
1	B	316	ILE	2.3
1	A	311	GLU	2.3
1	B	187	VAL	2.3
1	A	319	GLY	2.3
2	D	335	PHE	2.3
1	B	124	LEU	2.3
3	E	147	TYR	2.3
1	B	37	TRP	2.3
1	A	434	SER	2.3
3	F	21	GLN	2.3
1	A	187	VAL	2.3
2	D	270	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	2.2
1	A	283	THR	2.2
2	D	357	TYR	2.2
1	A	193	ILE	2.2
2	D	380	ILE	2.2
1	A	302	VAL	2.2
2	D	137	ASN	2.2
2	D	141	ARG	2.2
1	A	211	CYS	2.2
2	C	18	GLU	2.2
1	A	207	VAL	2.2
1	A	313	TRP	2.1
1	A	332	LEU	2.1
1	B	309	VAL	2.1
1	A	261	PRO	2.1
1	B	250	GLY	2.1
1	A	19	ALA	2.1
2	D	135	ALA	2.1
1	B	260	ASP	2.1
1	A	215	PRO	2.1
1	B	26	GLN	2.1
1	B	194	SER	2.1
2	D	383	ALA	2.1
1	A	333	LYS	2.1
1	B	214	ASN	2.1
1	A	326	VAL	2.1
2	D	322	GLY	2.1
2	D	138	PRO	2.1
1	B	60	PHE	2.1
1	B	36	ASN	2.0
1	A	266	TYR	2.0
1	A	314	GLY	2.0
2	C	389	LYS	2.0
1	B	244	LEU	2.0
2	D	352	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	C	5007	1/1	0.95	0.05	57,57,57,57	0
5	CA	C	5005	1/1	0.97	0.06	37,37,37,37	0
5	CA	A	5006	1/1	0.97	0.05	47,47,47,47	0
5	CA	C	5008	1/1	0.97	0.05	56,56,56,56	0
4	MN	B	5003	1/1	0.98	0.03	35,35,35,35	0
4	MN	B	5004	1/1	0.98	0.03	48,48,48,48	0
4	MN	A	5002	1/1	0.98	0.03	39,39,39,39	0
4	MN	A	5001	1/1	0.99	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.