



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:39 am BST

PDB ID : 1FZ6
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II SOAKED IN
1 M METHANOL
Authors : Whittington, D.A.; Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

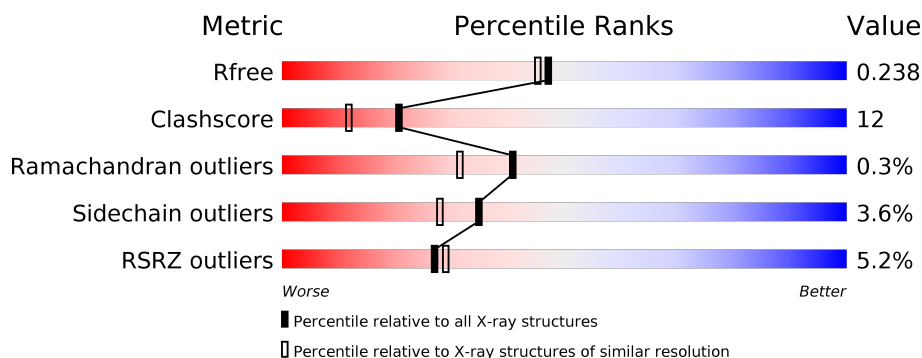
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	527	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
2	C	389	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>
2	D	389	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>•</div> </div> </div>
3	E	170	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• • •</div> </div> </div>
3	F	170	<div> <div>21%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18586 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	40	0	0
			4177	2673	719	767	18			
1	B	510	Total	C	N	O	S	36	0	0
			4173	2671	718	766	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	30	0	0
			3193	2054	551	580	8			
2	D	388	Total	C	N	O	S	42	0	0
			3193	2054	551	580	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	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	4	0	0
			1368	867	246	250	5			
3	F	166	Total	C	N	O	S	8	0	0
			1366	866	245	250	5			

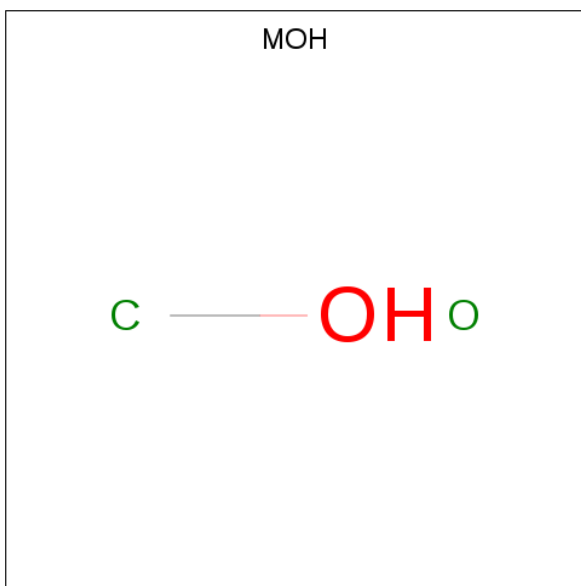
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is METHANOL (three-letter code: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		

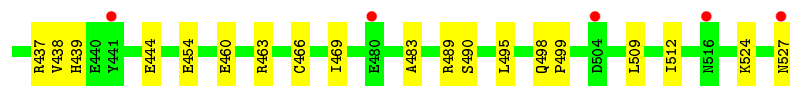
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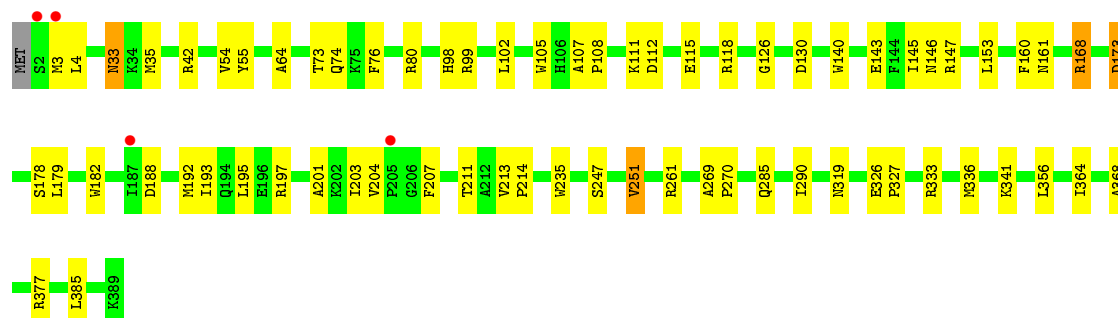
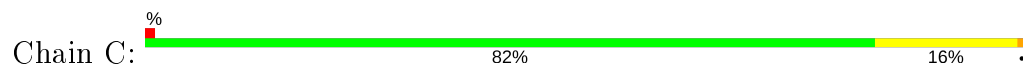
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	239	Total 239	O 239	0	0
7	C	286	Total 286	O 286	0	0
7	D	144	Total 144	O 144	0	0
7	E	125	Total 125	O 125	0	0
7	F	54	Total 54	O 54	0	0

• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

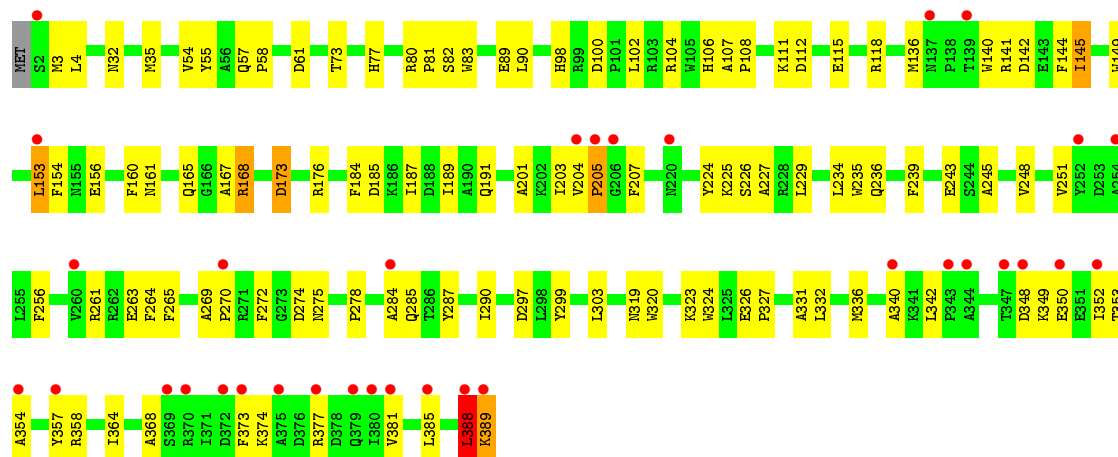




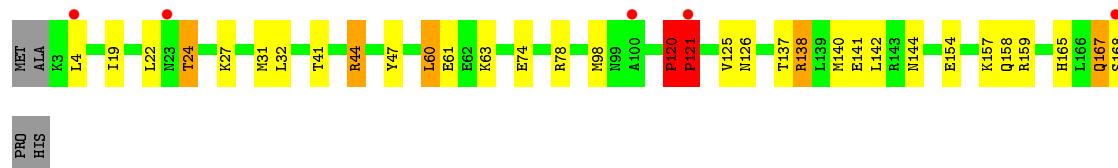
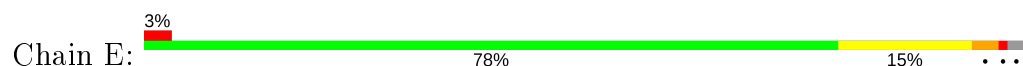
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

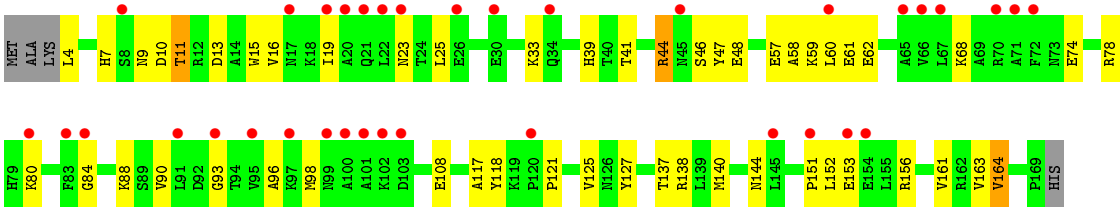


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• 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	70.67Å 171.29Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.05 29.87 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.90-2.05) 89.1 (29.87-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.244 0.211 , 0.238	Depositor DCC
R_{free} test set	5330 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	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	18586	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: CA, MOH, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	1/4302 (0.0%)	0.61	1/5842 (0.0%)
1	B	0.40	0/4298	0.60	0/5837
2	C	0.40	0/3289	0.60	0/4464
2	D	1.03	9/3289 (0.3%)	0.85	11/4464 (0.2%)
3	E	0.82	7/1396 (0.5%)	1.08	7/1880 (0.4%)
3	F	0.34	0/1395	0.57	1/1881 (0.1%)
All	All	0.60	17/17969 (0.1%)	0.70	20/24368 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	LYS	CB-CG	35.74	2.49	1.52
2	D	389	LYS	CA-C	32.22	2.36	1.52
3	E	167	GLN	C-N	-18.30	0.92	1.34
2	D	389	LYS	CA-CB	14.82	1.86	1.53
2	D	388	LEU	CA-C	13.22	1.87	1.52
3	E	167	GLN	CA-C	10.67	1.80	1.52
3	E	167	GLN	C-O	-10.08	1.04	1.23
2	D	389	LYS	N-CA	7.73	1.61	1.46
3	E	121	PRO	CG-CD	6.68	1.72	1.50
2	D	389	LYS	CG-CD	6.66	1.75	1.52
2	D	388	LEU	C-N	6.45	1.48	1.34
1	A	317	TRP	CB-CG	-6.25	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	121	PRO	N-CD	6.11	1.56	1.47
2	D	388	LEU	N-CA	5.86	1.58	1.46
2	D	388	LEU	C-O	-5.40	1.13	1.23
3	E	120	PRO	C-N	5.07	1.43	1.34
3	E	121	PRO	CA-C	5.04	1.62	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	120	PRO	C-N-CD	-27.86	59.30	120.60
2	D	389	LYS	N-CA-CB	-20.98	72.84	110.60
2	D	389	LYS	N-CA-C	16.70	156.10	111.00
2	D	389	LYS	CA-C-O	15.21	152.04	120.10
3	E	121	PRO	CA-N-CD	-14.31	91.47	111.50
2	D	389	LYS	CA-CB-CG	13.78	143.71	113.40
3	E	167	GLN	O-C-N	12.73	143.07	122.70
2	D	388	LEU	CA-C-N	12.16	143.95	117.20
2	D	388	LEU	CA-C-O	-9.59	99.96	120.10
3	E	121	PRO	N-CA-C	-9.39	87.69	112.10
3	E	167	GLN	CA-C-O	-9.09	101.00	120.10
2	D	389	LYS	CB-CA-C	7.87	126.14	110.40
2	D	389	LYS	CB-CG-CD	7.45	130.97	111.60
2	D	373	PHE	N-CA-C	-6.86	92.48	111.00
3	E	120	PRO	C-N-CA	6.39	148.83	122.00
1	A	317	TRP	N-CA-CB	-6.22	99.40	110.60
2	D	374	LYS	N-CA-C	-5.60	95.87	111.00
2	D	388	LEU	C-N-CA	5.37	135.13	121.70
3	E	121	PRO	CA-CB-CG	-5.25	94.02	104.00
3	F	39	HIS	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	120	PRO	Mainchain

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	4177	0	3975	99	0
1	B	4173	0	3969	125	0
2	C	3193	0	3042	56	0
2	D	3193	0	3042	107	0
3	E	1368	0	1362	33	0
3	F	1366	0	1357	44	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	2	0	0	0	0
7	A	259	0	0	6	0
7	B	239	0	0	6	0
7	C	286	0	0	3	0
7	D	144	0	0	0	0
7	E	125	0	0	2	0
7	F	54	0	0	0	0
All	All	18586	0	16747	415	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 12.

All (415) 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:389:LYS:CD	2:D:389:LYS:CG	1.75	1.59
2:D:389:LYS:CA	2:D:389:LYS:CB	1.86	1.50
3:E:167:GLN:C	3:E:167:GLN:CA	1.80	1.49
2:D:388:LEU:C	2:D:388:LEU:CA	1.87	1.42
2:D:389:LYS:N	2:D:389:LYS:CB	2.07	1.17
3:E:165:HIS:CE1	3:E:167:GLN:HE21	1.66	1.13
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.48	1.12
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.49	0.94
2:D:389:LYS:C	2:D:389:LYS:HA	1.87	0.93
2:D:389:LYS:CA	2:D:389:LYS:C	2.36	0.93
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.17	0.92
2:D:389:LYS:CB	2:D:389:LYS:CG	2.49	0.91
1:A:44:THR:HG22	1:A:46:TYR:H	1.35	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.16	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:167:GLN:CA	3:E:168:SER:N	2.32	0.88
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.19	0.88
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.58	0.86
3:F:41:THR:O	3:F:44:ARG:HD2	1.76	0.85
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.85
3:E:22:LEU:HD11	3:E:31:MET:SD	2.18	0.84
3:E:167:GLN:O	3:E:167:GLN:CA	2.24	0.83
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.28	0.81
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.63	0.81
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
3:F:4:LEU:HD21	3:F:10:ASP:H	1.47	0.80
3:E:165:HIS:HE1	3:E:167:GLN:HE21	0.79	0.79
3:E:165:HIS:CE1	3:E:167:GLN:NE2	2.38	0.79
3:F:58:ALA:O	3:F:62:GLU:HG3	1.83	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.78
2:D:389:LYS:H	2:D:389:LYS:CB	1.95	0.78
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.84	0.77
1:A:313:TRP:CD1	1:A:317:TRP:CD1	2.72	0.77
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.83	0.75
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.75
1:A:268:ASN:HD21	1:A:327:GLU:H	1.34	0.75
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.69	0.75
1:B:33:GLN:HE22	1:B:132:GLU:H	1.34	0.74
3:F:153:GLU:CD	3:F:153:GLU:H	1.90	0.74
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.53	0.74
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.88	0.73
3:F:13:ASP:O	3:F:16:VAL:HG22	1.86	0.73
1:A:213:THR:O	1:A:217:ILE:HG12	1.88	0.73
3:E:24:THR:HG22	3:E:27:LYS:H	1.51	0.73
1:A:467:GLN:HG3	7:A:5223:HOH:O	1.89	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.36	0.72
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.70	0.72
2:D:388:LEU:O	2:D:388:LEU:CA	2.34	0.72
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.20	0.71
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
3:E:41:THR:O	3:E:44:ARG:HD2	1.91	0.70
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.76	0.69
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.40	0.69
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.72	0.69
3:F:151:PRO:HB2	3:F:153:GLU:OE1	1.93	0.69
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.07	0.69
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.94	0.68
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.91	0.68
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.23	0.68
1:A:435:THR:HG21	1:A:437:ARG:HE	1.60	0.67
1:A:243:GLU:O	1:A:247:MET:HG2	1.95	0.67
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.30	0.66
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.76	0.66
1:B:213:THR:O	1:B:217:ILE:HG12	1.95	0.66
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.78	0.66
2:C:105:TRP:O	2:C:108:PRO:HD2	1.96	0.66
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.78	0.65
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.45	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.65
1:B:422:GLN:O	1:B:424:PRO:HD3	1.96	0.65
1:B:33:GLN:NE2	1:B:132:GLU:H	1.93	0.65
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.63	0.64
1:A:429:LEU:O	1:A:429:LEU:HG	1.96	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.46	0.64
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.79	0.64
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.80	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.62	0.63
3:E:61:GLU:HB3	3:E:121:PRO:HG2	1.81	0.63
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.62	0.63
2:D:153:LEU:HD12	2:D:153:LEU:C	2.20	0.62
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.00	0.62
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.62
2:D:275:ASN:C	2:D:278:PRO:HD2	2.20	0.62
2:D:385:LEU:HD12	2:D:388:LEU:CD1	2.30	0.62
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.33	0.61
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.36	0.61
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.94	0.61
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	0.61
1:B:268:ASN:HD21	1:B:327:GLU:H	1.47	0.60
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.83	0.60
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.83	0.60
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.60
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.01	0.60
1:B:227:ASN:HD21	1:B:295:LYS:H	1.49	0.60
3:E:167:GLN:C	3:E:167:GLN:CB	2.68	0.60
1:A:227:ASN:ND2	1:A:295:LYS:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.84	0.59
2:D:389:LYS:CE	2:D:389:LYS:CG	2.77	0.59
1:B:198:VAL:O	1:B:202:LEU:HG	2.02	0.59
1:B:288:MET:CE	1:B:346:LEU:HB3	2.31	0.59
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.36	0.59
1:A:104:LYS:HG2	1:A:168:HIS:CD2	2.37	0.59
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.18	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.04	0.58
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.84	0.58
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.03	0.58
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.86	0.58
2:D:389:LYS:OXT	2:D:389:LYS:HA	2.03	0.58
1:A:222:GLU:HA	1:A:222:GLU:OE1	2.04	0.58
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.39	0.57
2:C:3:MET:HG3	2:C:4:LEU:N	2.18	0.57
1:A:435:THR:CG2	1:A:437:ARG:HE	2.17	0.57
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.86	0.57
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.68	0.57
2:D:340:ALA:CB	2:D:389:LYS:HD3	2.35	0.57
1:A:268:ASN:ND2	1:A:327:GLU:H	2.02	0.57
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.57
2:C:111:LYS:O	2:C:115:GLU:HG3	2.05	0.56
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.87	0.56
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.95	0.56
1:A:209:GLU:HA	1:A:213:THR:HB	1.87	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.56
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.56
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.40	0.56
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.87	0.56
1:A:44:THR:OG1	1:A:127:SER:HA	2.06	0.56
1:B:43:ARG:HD2	1:B:43:ARG:O	2.06	0.56
2:D:82:SER:O	2:D:168:ARG:NH2	2.34	0.56
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.36	0.56
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.88	0.55
1:A:207:VAL:O	1:A:211:CYS:HB3	2.06	0.55
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.42	0.55
1:A:313:TRP:CD1	1:A:317:TRP:HD1	2.25	0.55
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.06	0.55
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.88	0.55
3:E:167:GLN:O	3:E:167:GLN:N	2.39	0.55
2:D:224:TYR:O	2:D:227:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ILE:O	2:D:168:ARG:NH1	2.40	0.55
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.39	0.55
1:A:382:HIS:O	1:A:386:ILE:HG13	2.07	0.55
1:B:175:ARG:CZ	1:B:181:TRP:CH2	2.90	0.54
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.59	0.54
3:F:15:TRP:O	3:F:19:ILE:HG23	2.08	0.54
1:A:84:ASP:HB3	1:B:81:SER:OG	2.08	0.54
3:F:74:GLU:O	3:F:78:ARG:HG3	2.08	0.54
3:E:167:GLN:C	3:E:167:GLN:N	2.57	0.53
1:A:140:GLN:O	1:A:144:GLU:HG2	2.08	0.53
1:B:355:PRO:HG2	1:B:403:ILE:HD12	1.91	0.53
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.43	0.53
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.91	0.53
3:E:22:LEU:O	3:E:63:LYS:HE2	2.09	0.53
3:F:25:LEU:HD22	3:F:68:LYS:HA	1.91	0.53
1:B:283:THR:HB	1:B:284:PRO:HD3	1.91	0.53
2:C:333:ARG:HD2	7:C:5166:HOH:O	2.09	0.53
2:D:336:MET:HE3	2:D:388:LEU:HD11	1.90	0.53
1:B:288:MET:HE1	1:B:346:LEU:C	2.29	0.52
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.45	0.52
2:D:385:LEU:HD12	2:D:388:LEU:HD11	1.92	0.52
1:B:44:THR:HG21	7:B:9009:HOH:O	2.09	0.52
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.93	0.52
1:B:246:HIS:N	1:B:246:HIS:CD2	2.76	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.91	0.52
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.31	0.52
1:A:406:MET:O	1:A:410:GLU:HG3	2.10	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.51
1:B:212:PHE:O	1:B:215:PRO:HD2	2.10	0.51
1:B:43:ARG:HD2	1:B:43:ARG:C	2.30	0.51
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.92	0.51
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.14	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.09	0.51
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.08	0.51
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.40	0.51
1:B:269:THR:HG23	7:B:9185:HOH:O	2.10	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
1:A:413:HIS:HD2	1:A:428:SER:OG	1.94	0.51
2:D:167:ALA:O	2:D:176:ARG:NH1	2.43	0.51
1:A:314:GLY:C	1:A:318:ILE:HG21	2.30	0.51
1:A:354:TRP:CZ2	1:A:403:ILE:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:PRO:HD2	2:D:83:TRP:HZ3	1.75	0.51
1:A:314:GLY:O	1:A:318:ILE:HG21	2.10	0.51
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.46	0.51
2:C:188:ASP:O	2:C:192:MET:HG2	2.11	0.51
1:B:123:MET:HE3	1:B:197:ALA:HA	1.93	0.51
1:A:413:HIS:CD2	1:A:429:LEU:HB2	2.47	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.11	0.50
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.46	0.50
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.12	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.12	0.50
2:C:211:THR:O	2:C:214:PRO:HD2	2.11	0.50
2:D:269:ALA:HB1	2:D:274:ASP:OD2	2.10	0.50
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.46	0.50
1:B:119:ALA:HA	2:D:167:ALA:O	2.11	0.50
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.43	0.50
1:B:70:MET:HE3	7:B:9140:HOH:O	2.11	0.50
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.93	0.50
1:A:159:ALA:O	2:C:33:ASN:HB2	2.12	0.50
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.50
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.50
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.94	0.50
1:B:106:VAL:O	1:B:110:LEU:HB2	2.12	0.50
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.12	0.49
2:C:3:MET:CG	2:C:4:LEU:H	2.24	0.49
1:A:520:LYS:HZ2	1:A:520:LYS:HB3	1.75	0.49
2:C:235:TRP:CD1	2:C:235:TRP:C	2.86	0.49
2:D:389:LYS:HG3	2:D:389:LYS:CD	2.20	0.49
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.95	0.49
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.49
1:B:227:ASN:HD21	1:B:296:PHE:H	1.60	0.49
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.48	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.94	0.49
1:B:41:ASN:O	2:D:236:GLN:HB3	2.12	0.49
1:A:421:SER:O	1:A:422:GLN:HB2	2.13	0.49
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.95	0.49
2:C:341:LYS:HE3	7:C:5020:HOH:O	2.12	0.49
3:F:80:LYS:HE3	3:F:84:GLY:O	2.12	0.49
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.49
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.24	0.49
3:E:157:LYS:HD2	7:E:295:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASP:HB2	3:E:140:MET:SD	2.53	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.12	0.48
2:D:377:ARG:O	2:D:381:VAL:HG23	2.13	0.48
1:B:112:VAL:CG2	2:D:58:PRO:HG3	2.43	0.48
2:C:3:MET:CE	2:C:4:LEU:HD13	2.43	0.48
1:A:403:ILE:HD12	7:A:5094:HOH:O	2.12	0.48
1:B:112:VAL:HG21	1:B:181:TRP:HH2	1.78	0.48
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.95	0.48
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.78	0.48
2:D:111:LYS:O	2:D:115:GLU:HG3	2.13	0.48
2:C:3:MET:HE2	2:C:4:LEU:HD13	1.96	0.48
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.49	0.48
1:B:146:ARG:HG2	1:B:150:GLN:OE1	2.14	0.48
1:B:406:MET:O	1:B:410:GLU:HG3	2.13	0.48
1:A:110:LEU:O	1:A:114:GLU:HG2	2.14	0.48
1:B:367:GLU:HG3	7:B:9131:HOH:O	2.13	0.48
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.79	0.48
3:F:46:SER:OG	3:F:48:GLU:HG2	2.14	0.48
1:A:219:ALA:O	1:A:223:TRP:HD1	1.97	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
1:B:466:CYS:HB2	2:D:73:THR:HA	1.95	0.47
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.96	0.47
1:B:78:GLN:NE2	1:B:150:GLN:HE21	2.05	0.47
2:D:234:LEU:HD13	2:D:248:VAL:HG22	1.95	0.47
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.49	0.47
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.80	0.47
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.47
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.95	0.47
2:D:226:SER:HB2	2:D:331:ALA:HA	1.96	0.47
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.30	0.47
1:B:414:PRO:O	1:B:426:CYS:SG	2.70	0.47
2:C:333:ARG:HD3	7:C:5024:HOH:O	2.13	0.47
1:B:48:THR:O	3:F:137:THR:HG23	2.14	0.47
2:C:146:ASN:O	2:C:214:PRO:HG3	2.15	0.47
1:A:520:LYS:NZ	1:A:520:LYS:HB3	2.30	0.47
1:B:140:GLN:O	1:B:144:GLU:HG2	2.15	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.49	0.47
1:B:355:PRO:CG	1:B:403:ILE:HD11	2.44	0.47
2:D:349:LYS:HE2	2:D:385:LEU:HD21	1.96	0.47
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.96	0.47
2:C:336:MET:CE	2:C:385:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.45	0.47
1:B:288:MET:HE1	1:B:346:LEU:HG	1.97	0.46
1:A:171:ALA:O	1:A:175:ARG:HD2	2.15	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
1:B:444:GLU:HA	1:B:444:GLU:OE2	2.15	0.46
2:C:146:ASN:HB2	2:C:207:PHE:CZ	2.51	0.46
1:B:192:PHE:O	1:B:200:CYS:HB3	2.16	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.16	0.46
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.98	0.46
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.50	0.46
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.46
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.16	0.46
3:E:125:VAL:HG23	3:E:126:ASN:N	2.31	0.46
1:A:227:ASN:HD21	1:A:296:PHE:H	1.63	0.46
1:B:288:MET:HE1	1:B:346:LEU:CB	2.46	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.46
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.51	0.46
1:A:321:LEU:O	1:A:326:VAL:HB	2.16	0.45
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.79	0.45
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.16	0.45
1:B:175:ARG:CZ	1:B:181:TRP:CZ2	2.99	0.45
1:B:227:ASN:ND2	1:B:295:LYS:H	2.14	0.45
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.98	0.45
2:C:269:ALA:N	2:C:270:PRO:CD	2.80	0.45
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.97	0.45
1:B:334:ASP:HB2	7:B:9103:HOH:O	2.16	0.45
1:A:109:PHE:O	1:A:112:VAL:HG12	2.17	0.45
2:C:247:SER:O	2:C:251:VAL:HB	2.17	0.45
3:E:154:GLU:O	3:E:158:GLN:HG3	2.17	0.45
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.99	0.45
2:D:189:ILE:HD11	2:D:284:ALA:HA	1.99	0.45
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.52	0.45
3:F:152:LEU:O	3:F:156:ARG:HG3	2.16	0.45
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.83	0.44
1:A:435:THR:HG22	1:A:436:LEU:N	2.32	0.44
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.52	0.44
2:C:98:HIS:HE1	2:C:178:SER:OG	1.99	0.44
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.53	0.44
1:B:524:LYS:O	1:B:527:ASN:HB2	2.18	0.44
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.99	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:LEU:C	2:D:388:LEU:CB	2.78	0.44
3:F:4:LEU:HD11	3:F:10:ASP:OD2	2.17	0.44
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.52	0.44
2:D:352:ILE:HD12	2:D:388:LEU:HD11	1.99	0.44
1:A:512:ILE:O	1:A:515:LEU:HB2	2.17	0.44
1:B:317:TRP:CE3	1:B:320:ARG:NH2	2.85	0.44
2:D:235:TRP:CD1	2:D:235:TRP:C	2.90	0.44
3:F:88:LYS:HB2	3:F:127:TYR:CE2	2.53	0.44
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.99	0.44
2:D:225:LYS:O	2:D:229:LEU:HG	2.18	0.44
2:D:80:ARG:HD2	2:D:81:PRO:O	2.18	0.44
1:A:472:GLN:NE2	7:A:5223:HOH:O	2.51	0.44
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.47	0.44
3:F:61:GLU:O	3:F:121:PRO:HG2	2.17	0.44
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.53	0.43
1:B:196:ASP:HB2	3:F:140:MET:SD	2.58	0.43
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.18	0.43
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.43
1:A:184:MET:HE2	1:A:188:PHE:HB2	2.01	0.43
2:D:141:ARG:HG2	2:D:142:ASP:N	2.33	0.43
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.33	0.43
2:D:189:ILE:HD12	2:D:284:ALA:HB2	2.00	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.43
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.43
1:B:54:ASN:HB3	1:B:129:GLN:HB2	2.00	0.43
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.54	0.43
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.01	0.43
1:A:372:PHE:O	1:A:376:TYR:N	2.45	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.00	0.43
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.02	0.43
1:B:123:MET:CE	1:B:197:ALA:HA	2.49	0.43
1:B:292:TYR:OH	1:B:344:HIS:HD2	2.02	0.43
1:B:483:ALA:HB2	1:B:509:LEU:HD21	2.00	0.43
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.52	0.43
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.01	0.43
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.54	0.43
1:A:312:ASP:O	1:A:316:ILE:HB	2.19	0.42
2:D:57:GLN:HA	2:D:58:PRO:HD3	1.89	0.42
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.67	0.42
2:C:211:THR:C	2:C:214:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.20	0.42
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.42
1:B:56:THR:HG21	1:B:256:SER:OG	2.18	0.42
1:B:30:ARG:HD3	1:B:31:TRP:CD1	2.55	0.42
1:A:318:ILE:HG23	1:A:319:GLY:N	2.35	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.01	0.42
2:D:145:ILE:O	2:D:149:TRP:HB3	2.20	0.42
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.54	0.42
2:C:143:GLU:O	2:C:147:ARG:HB3	2.20	0.42
2:D:58:PRO:HD2	2:D:83:TRP:CZ3	2.54	0.42
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.20	0.42
1:A:190:ASP:HB3	2:C:74:GLN:O	2.20	0.42
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.01	0.42
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.17	0.42
1:B:288:MET:HE3	1:B:346:LEU:HB3	2.01	0.42
1:B:437:ARG:NH1	1:B:454:GLU:OE2	2.52	0.42
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.02	0.42
1:B:244:LEU:HB2	7:B:9224:HOH:O	2.19	0.42
1:B:283:THR:HB	1:B:284:PRO:CD	2.49	0.42
1:A:109:PHE:HB3	1:A:184:MET:SD	2.60	0.42
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.42
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.20	0.42
3:F:41:THR:O	3:F:44:ARG:CD	2.59	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
1:B:317:TRP:HE3	1:B:320:ARG:NH2	2.17	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.55	0.42
2:D:184:PHE:O	2:D:187:ILE:HG22	2.20	0.42
2:C:33:ASN:HD22	2:C:33:ASN:N	2.17	0.41
3:E:4:LEU:O	3:E:4:LEU:CG	2.68	0.41
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.35	0.41
2:D:77:HIS:CG	3:F:140:MET:HG2	2.55	0.41
3:F:93:GLY:O	3:F:96:ALA:HB3	2.20	0.41
1:A:40:LYS:HD2	7:A:5122:HOH:O	2.20	0.41
1:B:210:ALA:HA	1:B:247:MET:CE	2.50	0.41
2:D:354:ALA:O	2:D:358:ARG:HG3	2.20	0.41
3:F:59:LYS:HA	3:F:59:LYS:HD3	1.86	0.41
1:A:266:TYR:HB3	7:A:5058:HOH:O	2.19	0.41
3:E:137:THR:O	3:E:141:GLU:HG3	2.21	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.03	0.41
2:C:193:ILE:O	2:C:197:ARG:HG3	2.20	0.41
2:D:349:LYS:CE	2:D:385:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LEU:HD13	3:E:60:LEU:HB3	2.03	0.41
3:E:74:GLU:O	3:E:78:ARG:HG3	2.21	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.21	0.41
2:D:264:PHE:HD2	2:D:265:PHE:CD1	2.39	0.41
2:D:389:LYS:HG2	2:D:389:LYS:CD	2.20	0.41
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.51	0.41
1:B:116:ASN:CG	1:B:189:SER:HA	2.41	0.41
2:D:389:LYS:CA	2:D:389:LYS:HB2	2.25	0.41
3:E:4:LEU:O	3:E:4:LEU:HD12	2.20	0.41
1:B:217:ILE:O	1:B:221:THR:HG23	2.21	0.41
1:B:288:MET:HE1	1:B:346:LEU:CG	2.50	0.41
1:B:30:ARG:HD3	1:B:31:TRP:NE1	2.36	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.56	0.41
2:D:385:LEU:CD1	2:D:388:LEU:CD1	2.97	0.41
1:A:23:VAL:HA	1:A:27:GLU:OE2	2.20	0.41
1:A:381:ASP:HA	1:A:385:LYS:HE2	2.03	0.41
2:D:136:MET:HE2	2:D:274:ASP:HA	2.02	0.41
2:D:144:PHE:CD1	2:D:144:PHE:N	2.89	0.41
2:D:153:LEU:HG	2:D:154:PHE:CD1	2.56	0.41
3:F:153:GLU:CD	3:F:153:GLU:N	2.67	0.41
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.40
1:B:243:GLU:O	1:B:247:MET:HG2	2.21	0.40
1:B:355:PRO:CD	1:B:403:ILE:HD11	2.51	0.40
1:A:147:HIS:CE1	7:A:5219:HOH:O	2.74	0.40
1:A:204:LEU:O	1:A:209:GLU:HG3	2.21	0.40
1:B:185:LYS:O	1:B:189:SER:HB2	2.22	0.40
1:A:183:GLY:HA2	1:A:422:GLN:HB2	2.03	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.21	0.40
3:F:98:MET:HG3	3:F:138:ARG:CG	2.51	0.40
2:D:352:ILE:HG13	2:D:353:THR:N	2.35	0.40
2:D:340:ALA:HA	2:D:389:LYS:HD3	2.03	0.40
3:E:24:THR:HG23	7:E:183:HOH:O	2.22	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%)	487 (96%)	21 (4%)	0	100	100
1	B	508/527 (96%)	479 (94%)	28 (6%)	1 (0%)	47	39
2	C	386/389 (99%)	372 (96%)	12 (3%)	2 (0%)	29	18
2	D	386/389 (99%)	362 (94%)	21 (5%)	3 (1%)	19	10
3	E	164/170 (96%)	159 (97%)	4 (2%)	1 (1%)	25	15
3	F	164/170 (96%)	153 (93%)	11 (7%)	0	100	100
All	All	2116/2172 (97%)	2012 (95%)	97 (5%)	7 (0%)	41	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	121	PRO
1	B	40	LYS
2	D	388	LEU
2	C	64	ALA
2	D	251	VAL
2	C	251	VAL
2	D	205	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/442 (98%)	416 (96%)	16 (4%)	34	27
1	B	431/442 (98%)	412 (96%)	19 (4%)	28	21
2	C	322/323 (100%)	312 (97%)	10 (3%)	40	33
2	D	322/323 (100%)	314 (98%)	8 (2%)	47	40
3	E	144/147 (98%)	138 (96%)	6 (4%)	30	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	144/147 (98%)	139 (96%)	5 (4%)	36	29
All	All	1795/1824 (98%)	1731 (96%)	64 (4%)	35	28

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	38	ASP
1	A	43	ARG
1	A	90	ASN
1	A	112	VAL
1	A	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	338	ASP
1	A	403	ILE
1	A	437	ARG
1	A	467	GLN
1	A	516	ASN
1	A	520	LYS
1	B	30	ARG
1	B	33	GLN
1	B	43	ARG
1	B	88	ARG
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	222	GLU
1	B	279	GLN
1	B	310	TYR
1	B	311	GLU
1	B	377	PRO
1	B	395	CYS
1	B	398	PRO
1	B	404	PRO
1	B	427	PRO
2	C	33	ASN

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Mol	Chain	Res	Type
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	160	PHE
2	C	168	ARG
2	C	173	ASP
2	C	195	LEU
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	35	MET
2	D	145	ILE
2	D	153	LEU
2	D	168	ARG
2	D	173	ASP
2	D	205	PRO
2	D	388	LEU
3	E	24	THR
3	E	44	ARG
3	E	60	LEU
3	E	120	PRO
3	E	121	PRO
3	E	138	ARG
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	108	GLU
3	F	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) 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	155	ASN
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN

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Mol	Chain	Res	Type
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	411	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	516	ASN
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	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	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN

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Mol	Chain	Res	Type
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	45	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MOH	B	9001	4	1,1,1	0.46	0	-		

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	167:GLN	C	168:SER	N	0.92

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%)	0.16	13 (2%) 57 61	21, 32, 49, 63	10 (1%)
1	B	510/527 (96%)	0.15	19 (3%) 41 45	20, 33, 50, 62	9 (1%)
2	C	388/389 (99%)	-0.16	4 (1%) 82 84	18, 25, 39, 54	7 (1%)
2	D	388/389 (99%)	0.59	34 (8%) 10 10	21, 40, 61, 79	10 (2%)
3	E	166/170 (97%)	0.05	5 (3%) 50 54	21, 30, 44, 59	1 (0%)
3	F	166/170 (97%)	1.12	35 (21%) 1 0	37, 49, 67, 75	2 (1%)
All	All	2128/2172 (97%)	0.24	110 (5%) 27 29	18, 33, 55, 79	39 (1%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	9.2
2	D	205	PRO	5.9
3	F	100	ALA	5.4
2	C	2	SER	5.1
3	F	101	ALA	4.8
1	A	319	GLY	4.8
1	B	527	ASN	4.8
1	A	310	TYR	4.8
2	D	385	LEU	4.7
3	F	21	GLN	4.3
2	D	354	ALA	4.3
3	F	23	ASN	4.2
3	E	4	LEU	4.0
2	D	344	ALA	4.0
1	B	259	ASN	4.0
2	D	220	ASN	4.0
2	D	381	VAL	3.9
3	F	19	ILE	3.9
1	A	323	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
3	F	26	GLU	3.7
2	C	3	MET	3.7
3	F	84	GLY	3.6
2	D	380	ILE	3.6
2	D	350	GLU	3.6
2	D	388	LEU	3.6
1	B	264	ALA	3.6
3	F	22	LEU	3.5
3	F	102	LYS	3.3
2	D	352	ILE	3.3
2	D	2	SER	3.3
1	A	338	ASP	3.2
3	F	20	ALA	3.2
3	F	30	GLU	3.1
3	F	103	ASP	3.1
3	F	120	PRO	3.0
2	D	379	GLN	3.0
3	E	168	SER	3.0
3	F	93	GLY	3.0
2	D	137	ASN	3.0
2	D	343	PRO	3.0
1	B	289	LEU	2.9
2	D	270	PRO	2.9
3	F	72	PHE	2.8
2	D	348	ASP	2.8
1	A	317	TRP	2.8
1	B	325	GLY	2.8
2	D	372	ASP	2.8
3	E	100	ALA	2.8
1	B	258	ALA	2.7
1	B	54	ASN	2.7
3	F	17	ASN	2.7
1	A	316	ILE	2.7
3	E	121	PRO	2.6
3	F	71	ALA	2.6
3	F	80	LYS	2.6
1	B	39	PHE	2.6
2	D	357	TYR	2.6
2	D	375	ALA	2.6
2	D	284	ALA	2.5
1	A	366	GLN	2.5
3	F	83	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	139	THR	2.5
1	B	504	ASP	2.5
2	D	252	TYR	2.4
3	F	65	ALA	2.4
3	F	67	LEU	2.4
2	C	187	ILE	2.4
2	C	205	PRO	2.4
2	D	260	VAL	2.4
1	B	310	TYR	2.4
2	D	369	SER	2.4
1	B	19	ALA	2.4
1	A	318	ILE	2.4
1	A	324	TYR	2.4
3	F	66	VAL	2.3
2	D	254	ALA	2.3
3	F	34	GLN	2.3
1	A	259	ASN	2.3
3	F	95	VAL	2.3
1	B	306	ASP	2.3
1	B	441	TYR	2.2
1	A	60	PHE	2.2
2	D	153	LEU	2.2
1	B	38	ASP	2.2
3	F	99	ASN	2.2
1	A	325	GLY	2.2
2	D	206	GLY	2.2
1	B	320	ARG	2.2
2	D	340	ALA	2.2
1	B	349	LEU	2.1
2	D	373	PHE	2.1
2	D	370	ARG	2.1
3	F	151	PRO	2.1
3	F	8	SER	2.1
3	F	91	LEU	2.1
3	F	70	ARG	2.1
1	B	480	GLU	2.1
3	F	153	GLU	2.1
3	F	145	LEU	2.1
1	B	516	ASN	2.1
2	D	377	ARG	2.1
3	E	23	ASN	2.0
3	F	60	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	2.0
2	D	204	VAL	2.0
3	F	154	GLU	2.0
1	B	261	PRO	2.0
3	F	97	LYS	2.0
2	D	347	THR	2.0
3	F	45	ASN	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 carbohydrates 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(\AA^2)	Q<0.9
5	CA	C	5007	1/1	0.49	0.09	77,77,77,77	0
6	MOH	B	9001	2/2	0.90	0.20	43,43,43,45	0
5	CA	B	5005	1/1	0.94	0.10	68,68,68,68	0
5	CA	A	5006	1/1	0.97	0.13	45,45,45,45	0
4	FE	A	5002	1/1	0.98	0.03	42,42,42,42	0
4	FE	A	5001	1/1	0.99	0.02	30,30,30,30	0
4	FE	B	5004	1/1	0.99	0.02	41,41,41,41	0
4	FE	B	5003	1/1	0.99	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.