



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:03 pm BST

PDB ID : 1XMH  
Title : Structure of Co(II) reconstituted methane monooxygenase hydroxylase 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](mailto: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.

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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	:	2.11
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



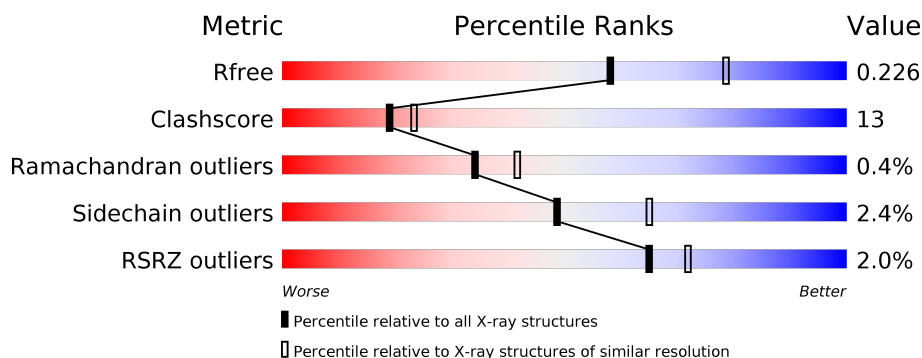
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	527	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
2	C	388	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>•</div> </div> </div>
2	D	388	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>32%</div> <div>•</div> </div> </div>
3	E	169	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>• •</div> </div> </div>
3	F	169	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>• •</div> </div> </div>



## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18154 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	511	Total	C	N	O	S	0	0	0
			4141	2648	712	763	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	167	Total	C	N	O	S	0	0	0
			1368	866	246	251	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).



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

- Molecule 5 is water.

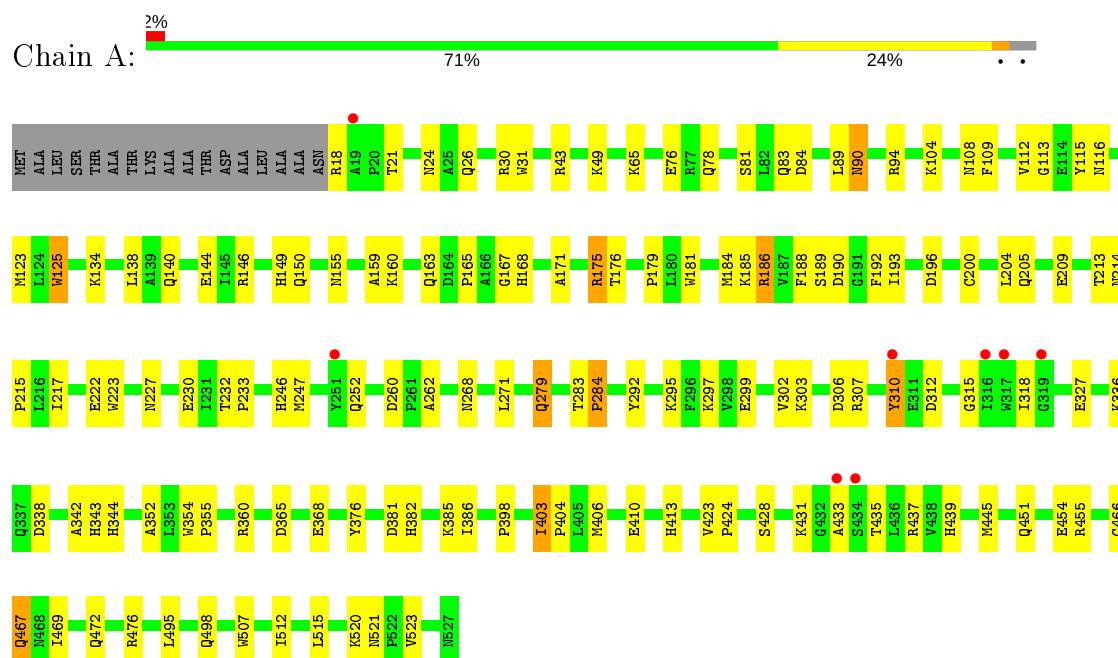
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		
5	B	189	Total	O	0	0
			189	189		
5	C	225	Total	O	0	0
			225	225		
5	D	97	Total	O	0	0
			97	97		
5	E	90	Total	O	0	0
			90	90		
5	F	39	Total	O	0	0
			39	39		



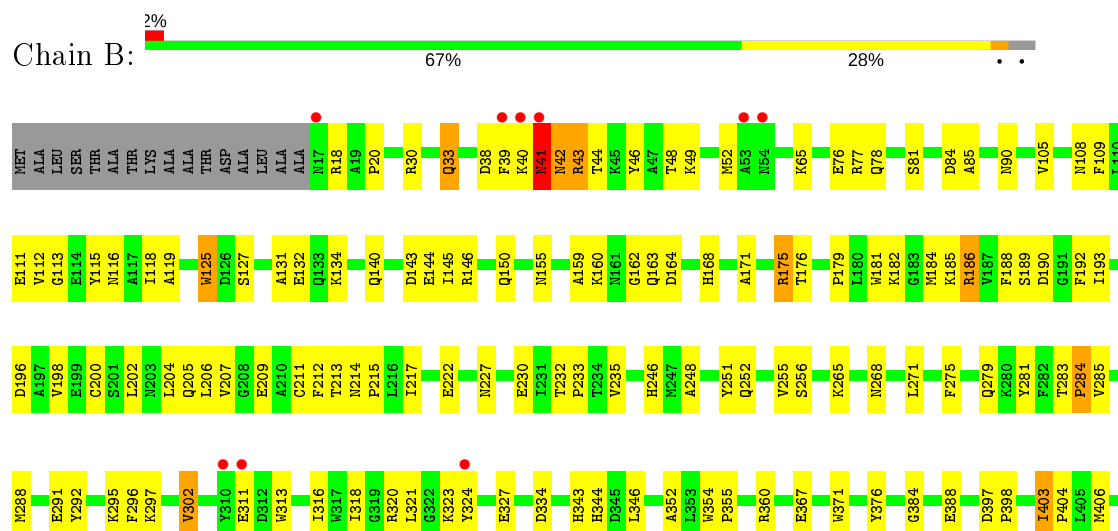
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



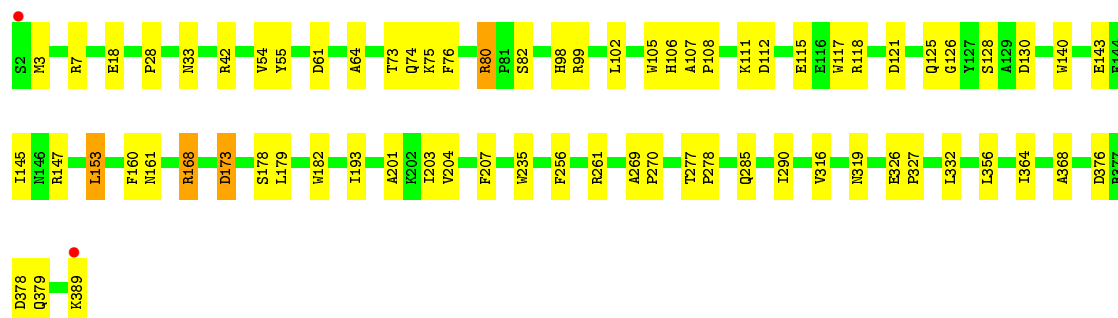
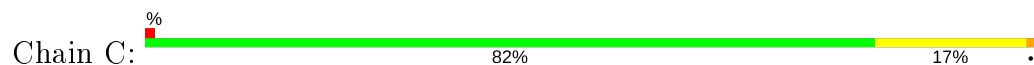
- Molecule 1: Methane monooxygenase component A alpha chain



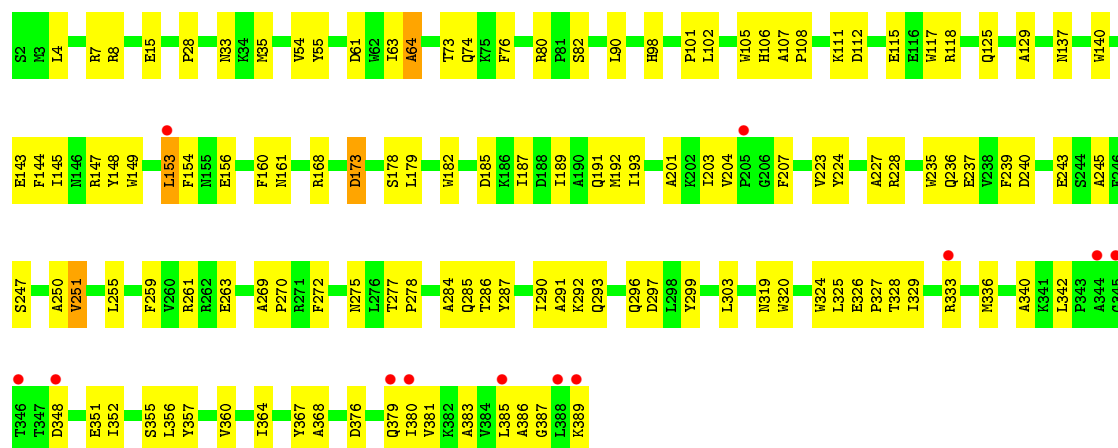




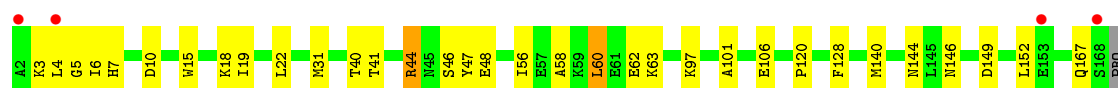
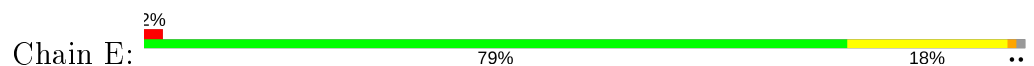
- Molecule 2: Methane monooxygenase component A beta chain



- Molecule 2: Methane monooxygenase component A beta chain



- Molecule 3: Methane monooxygenase component A gamma chain



HIS

- 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, $\alpha$ , $\beta$ , $\gamma$	71.44Å 171.84Å 220.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.32 29.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.55-2.32) 90.9 (29.55-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.194 , 0.225 0.194 , 0.226	Depositor DCC
$R_{free}$ test set	3972 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CO

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	0.33	0/4263	0.56	0/5797
1	B	0.36	1/4266 (0.0%)	0.61	3/5801 (0.1%)
2	C	0.37	0/3263	0.58	0/4435
2	D	0.33	0/3247	0.54	0/4417
3	E	0.35	0/1396	0.60	0/1881
3	F	0.29	0/1387	0.53	0/1873
All	All	0.35	1/17822 (0.0%)	0.57	3/24204 (0.0%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	ASN	C-N	6.34	1.48	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASN	O-C-N	-10.78	105.46	122.70
1	B	41	ASN	CA-C-N	5.72	129.78	117.20
1	B	41	ASN	OD1-CG-ND2	-5.40	109.48	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	41	ASN	Sidechain

## 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	123	0
1	B	4141	0	3889	154	0
2	C	3167	0	2987	63	0
2	D	3151	0	2957	113	0
3	E	1368	0	1353	24	0
3	F	1358	0	1335	38	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	187	0	0	8	0
5	B	189	0	0	6	0
5	C	225	0	0	1	0
5	D	97	0	0	2	0
5	E	90	0	0	1	0
5	F	39	0	0	3	0
All	All	18154	0	16418	439	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 13.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.39	1.00
1:A:435:THR:CG2	1:A:437:ARG:HE	1.80	0.94
1:B:155:ASN:HD22	1:B:168:HIS:HD2	1.12	0.94
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.08	0.92
2:C:3:MET:HE3	2:D:28:PRO:HG3	1.55	0.89
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.18	0.88
1:A:209:GLU:HA	1:A:213:THR:HB	1.55	0.85
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.24	0.85
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.21	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.61	0.81
1:A:467:GLN:HG3	5:A:5315:HOH:O	1.80	0.80
1:A:435:THR:HG21	1:A:437:ARG:HE	1.43	0.80
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.63	0.80
1:B:268:ASN:HD21	1:B:327:GLU:H	1.25	0.79
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.29	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.78
1:B:288:MET:HE1	1:B:346:LEU:HG	1.67	0.76
3:E:4:LEU:HD12	3:E:5:GLY:H	1.52	0.74
1:B:33:GLN:HE22	1:B:132:GLU:H	1.37	0.73
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.53	0.73
3:F:41:THR:O	3:F:44:ARG:HD2	1.88	0.73
3:E:22:LEU:O	3:E:63:LYS:HD3	1.89	0.72
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.35	0.72
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.20	0.72
2:D:340:ALA:HB2	2:D:389:LYS:HB2	1.72	0.71
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.73	0.71
1:B:163:GLN:HA	2:C:3:MET:HE2	1.72	0.70
2:D:286:THR:O	2:D:290:ILE:HG12	1.89	0.70
3:F:58:ALA:O	3:F:62:GLU:HG3	1.91	0.70
1:A:24:ASN:OD1	1:A:26:GLN:HG3	1.92	0.70
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.74	0.69
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.55	0.69
3:E:41:THR:O	3:E:44:ARG:HD2	1.91	0.69
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.75	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.23	0.69
1:B:38:ASP:O	1:B:39:PHE:HB3	1.92	0.69
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.75	0.68
1:A:268:ASN:HD21	1:A:327:GLU:H	1.42	0.68
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.74	0.68
1:A:406:MET:O	1:A:410:GLU:HG3	1.94	0.68
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.75	0.68
1:B:163:GLN:HA	2:C:3:MET:CE	2.24	0.67
1:B:406:MET:O	1:B:410:GLU:HG3	1.94	0.67
2:C:3:MET:CE	2:D:28:PRO:HG3	2.24	0.67
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.93	0.67
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.77	0.67
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.67
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.75	0.67
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.76	0.67
1:B:18:ARG:O	2:D:129:ALA:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.77	0.66
1:B:175:ARG:HG3	1:B:181:TRP:CD2	2.30	0.66
1:B:283:THR:HB	1:B:284:PRO:HD3	1.76	0.66
3:F:57:GLU:O	3:F:61:GLU:HG3	1.94	0.66
1:B:268:ASN:ND2	1:B:327:GLU:H	1.93	0.66
1:A:435:THR:HG22	1:A:437:ARG:HE	1.58	0.66
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.96	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.95	0.65
1:B:44:THR:HG22	1:B:46:TYR:H	1.62	0.65
1:A:204:LEU:O	1:A:209:GLU:HG3	1.97	0.65
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.78	0.65
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.80	0.64
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.79	0.64
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.79	0.64
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.32	0.64
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.90	0.64
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.80	0.63
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.63	0.63
1:B:209:GLU:HA	1:B:213:THR:HB	1.79	0.63
1:B:213:THR:O	1:B:217:ILE:HG12	1.98	0.63
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.79	0.62
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.82	0.62
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.35	0.62
2:D:153:LEU:C	2:D:153:LEU:HD12	2.20	0.62
3:E:58:ALA:O	3:E:62:GLU:HG3	2.00	0.62
2:C:61:ASP:OD1	3:E:7:HIS:HD2	1.83	0.61
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.35	0.61
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.34	0.61
1:B:288:MET:HE1	1:B:346:LEU:CG	2.29	0.61
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.00	0.61
2:D:329:ILE:HD11	2:D:380:ILE:HD12	1.83	0.61
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.83	0.60
3:F:12:ARG:O	3:F:16:VAL:HG23	2.01	0.60
1:B:171:ALA:O	1:B:175:ARG:HB3	2.01	0.60
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.01	0.60
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.60
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.36	0.60
2:D:111:LYS:O	2:D:115:GLU:HG3	2.00	0.60
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.60
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.84	0.60
2:D:145:ILE:O	2:D:149:TRP:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.37	0.59
1:B:175:ARG:HG2	1:B:176:THR:N	2.17	0.59
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.84	0.59
1:A:175:ARG:HG2	1:A:176:THR:N	2.17	0.59
1:B:367:GLU:HG3	5:B:5184:HOH:O	2.02	0.59
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.37	0.58
1:B:227:ASN:HD21	1:B:295:LYS:H	1.50	0.58
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.35	0.58
1:B:108:ASN:HD21	1:B:175:ARG:HE	1.49	0.58
1:A:227:ASN:HD21	1:A:295:LYS:H	1.50	0.58
1:B:281:TYR:O	1:B:284:PRO:HD2	2.02	0.58
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.94	0.58
1:B:155:ASN:HD22	1:B:168:HIS:CD2	2.05	0.58
1:B:185:LYS:O	1:B:189:SER:HB2	2.03	0.58
2:C:179:LEU:HD23	2:C:182:TRP:CE3	2.38	0.58
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.04	0.58
1:A:451:GLN:HB2	3:E:152:LEU:HD11	1.86	0.57
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.05	0.57
1:A:171:ALA:O	1:A:175:ARG:HB3	2.04	0.57
1:A:21:THR:HG22	2:C:128:SER:CB	2.35	0.57
1:B:33:GLN:NE2	1:B:132:GLU:H	2.02	0.57
1:B:41:ASN:HD22	2:D:237:GLU:HG3	1.70	0.57
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.01	0.57
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.87	0.57
1:A:185:LYS:O	1:A:189:SER:HB2	2.05	0.57
2:D:187:ILE:O	2:D:191:GLN:HG3	2.05	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.87	0.56
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.23	0.56
1:A:204:LEU:HG	1:A:205:GLN:HG3	1.87	0.56
3:E:46:SER:OG	3:E:48:GLU:HG2	2.06	0.56
1:B:265:LYS:CB	5:B:5311:HOH:O	2.54	0.56
1:A:109:PHE:O	1:A:112:VAL:HG12	2.05	0.56
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.71	0.56
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.52	0.56
2:D:381:VAL:O	2:D:385:LEU:HD13	2.06	0.56
2:D:376:ASP:CG	2:D:379:GLN:HG2	2.27	0.56
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.26	0.55
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.36	0.55
1:B:41:ASN:HD22	2:D:237:GLU:CG	2.18	0.55
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.88	0.55
2:D:352:ILE:O	2:D:356:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:ILE:HG13	2:D:204:VAL:HG23	1.87	0.55
1:B:384:GLY:O	1:B:388:GLU:HG3	2.06	0.55
1:A:83:GLN:HB3	1:B:77:ARG:HH21	1.72	0.55
1:B:41:ASN:ND2	2:D:237:GLU:CG	2.69	0.55
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.88	0.55
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.53	0.55
5:D:465:HOH:O	3:F:125:VAL:HG22	2.07	0.54
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.25	0.54
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.42	0.54
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.42	0.54
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.89	0.54
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.99	0.54
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.40	0.54
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.61	0.54
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.22	0.54
2:D:259:PHE:CE1	2:D:356:LEU:HD22	2.42	0.54
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.73	0.54
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.43	0.54
1:B:227:ASN:HD21	1:B:296:PHE:H	1.56	0.54
1:B:30:ARG:NH1	1:B:30:ARG:HG2	2.22	0.54
3:F:4:LEU:CD1	3:F:9:ASN:HA	2.38	0.54
1:B:354:TRP:CZ2	1:B:403:ILE:HD11	2.43	0.53
1:A:140:GLN:O	1:A:144:GLU:HG2	2.09	0.53
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.39	0.53
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.44	0.53
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.43	0.53
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.53
1:B:472:GLN:NE2	5:B:5316:HOH:O	2.41	0.53
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.43	0.53
3:F:33:LYS:O	3:F:37:MET:HG2	2.09	0.53
1:A:190:ASP:HB3	2:C:74:GLN:O	2.08	0.53
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.92	0.53
1:A:213:THR:O	1:A:217:ILE:HG12	2.09	0.53
2:C:3:MET:HE3	2:D:28:PRO:CG	2.36	0.53
1:B:212:PHE:O	1:B:215:PRO:HD2	2.09	0.52
2:D:385:LEU:C	2:D:387:GLY:H	2.13	0.52
1:B:196:ASP:HB2	3:F:140:MET:SD	2.49	0.52
3:F:74:GLU:O	3:F:78:ARG:HG3	2.08	0.52
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.09	0.52
2:D:360:VAL:O	2:D:364:ILE:HG13	2.09	0.52
2:D:153:LEU:HD12	2:D:154:PHE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:SER:O	2:D:168:ARG:NH2	2.42	0.52
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.10	0.52
2:C:143:GLU:O	2:C:147:ARG:HB3	2.09	0.52
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.91	0.52
1:B:288:MET:CE	1:B:346:LEU:HB3	2.38	0.52
1:A:184:MET:CE	1:A:188:PHE:HB2	2.39	0.52
1:B:48:THR:O	3:F:137:THR:HG23	2.10	0.52
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.40	0.51
1:A:186:ARG:HA	2:C:73:THR:OG1	2.11	0.51
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.75	0.51
1:B:186:ARG:HA	2:D:73:THR:OG1	2.10	0.51
3:F:4:LEU:HD12	3:F:9:ASN:HA	1.92	0.51
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.93	0.51
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.41	0.51
1:B:155:ASN:ND2	1:B:168:HIS:HD2	1.95	0.51
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.46	0.51
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.92	0.51
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.45	0.51
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.92	0.51
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.93	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
2:D:54:VAL:O	2:D:55:TYR:HB2	2.11	0.51
2:C:98:HIS:HE1	2:C:178:SER:OG	1.93	0.50
1:B:190:ASP:HB3	2:D:74:GLN:O	2.11	0.50
1:A:271:LEU:HD21	1:A:318:ILE:HD11	1.92	0.50
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.09	0.50
3:F:153:GLU:CD	3:F:153:GLU:H	2.13	0.50
2:C:121:ASP:O	2:C:125:GLN:HG3	2.11	0.50
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.47	0.50
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.47	0.50
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.58	0.50
1:A:382:HIS:O	1:A:386:ILE:HG13	2.12	0.50
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.47	0.50
1:A:268:ASN:ND2	1:A:327:GLU:H	2.09	0.49
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.94	0.49
1:A:163:GLN:HG2	5:A:5205:HOH:O	2.11	0.49
1:B:33:GLN:NE2	1:B:33:GLN:HA	2.24	0.49
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.47	0.49
1:B:108:ASN:HD21	1:B:175:ARG:NE	2.11	0.49
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.60	0.49
1:B:466:CYS:HB2	2:D:73:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG2	1:B:76:GLU:HG2	1.95	0.49
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.60	0.49
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.95	0.49
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.94	0.49
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.28	0.49
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.77	0.48
1:B:43:ARG:HD2	1:B:43:ARG:C	2.32	0.48
1:A:116:ASN:CG	1:A:189:SER:HA	2.34	0.48
1:A:466:CYS:HB2	2:C:73:THR:HA	1.94	0.48
1:A:445:MET:HB3	1:A:523:VAL:HG21	1.95	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.10	0.48
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.96	0.48
2:D:101:PRO:HG2	2:D:293:GLN:HB3	1.94	0.48
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.96	0.48
1:B:160:LYS:HA	2:D:33:ASN:HB2	1.94	0.48
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.78	0.48
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.46	0.48
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.48	0.48
1:A:160:LYS:HE3	5:A:5240:HOH:O	2.14	0.48
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.44	0.48
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.95	0.47
1:A:193:ILE:HD11	2:C:82:SER:HB3	1.95	0.47
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.15	0.47
2:D:275:ASN:C	2:D:278:PRO:HD2	2.34	0.47
1:B:488:LEU:HB2	5:B:5344:HOH:O	2.13	0.47
3:E:4:LEU:HD12	3:E:5:GLY:N	2.26	0.47
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.50	0.47
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.96	0.47
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.14	0.47
1:B:140:GLN:O	1:B:144:GLU:HG2	2.15	0.47
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.11	0.47
1:A:306:ASP:OD2	1:A:336:LYS:NZ	2.46	0.47
1:B:288:MET:HE3	1:B:346:LEU:HD23	1.97	0.47
2:D:292:LYS:O	2:D:296:GLN:HG3	2.15	0.47
1:B:316:ILE:O	1:B:320:ARG:HG3	2.15	0.47
3:E:41:THR:O	3:E:44:ARG:CD	2.60	0.47
1:B:248:ALA:O	1:B:252:GLN:HG3	2.15	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.47
2:C:105:TRP:O	2:C:108:PRO:HD2	2.15	0.47
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.49	0.47
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:HIS:HE1	2:D:178:SER:OG	1.98	0.47
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.98	0.47
1:B:288:MET:HE1	1:B:346:LEU:CB	2.45	0.47
1:A:343:HIS:H	1:A:343:HIS:CD2	2.34	0.46
1:A:472:GLN:NE2	5:A:5315:HOH:O	2.48	0.46
1:B:232:THR:HB	1:B:233:PRO:HD3	1.96	0.46
2:C:235:TRP:CD1	2:C:235:TRP:C	2.89	0.46
1:B:445:MET:HB3	1:B:523:VAL:HG21	1.98	0.46
3:E:22:LEU:HD11	3:E:31:MET:SD	2.55	0.46
3:F:102:LYS:HD3	3:F:102:LYS:N	2.31	0.46
1:A:435:THR:HG21	1:A:437:ARG:NE	2.22	0.46
2:C:316:VAL:O	2:C:319:ASN:HB3	2.16	0.46
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.98	0.46
1:B:186:ARG:HD3	1:B:186:ARG:C	2.36	0.46
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.98	0.46
2:D:348:ASP:OD2	2:D:351:GLU:HG3	2.16	0.46
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.64	0.46
1:A:227:ASN:ND2	1:A:295:LYS:H	2.12	0.46
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.81	0.46
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.46	0.46
3:F:15:TRP:O	3:F:19:ILE:HG13	2.16	0.46
1:A:163:GLN:O	2:C:28:PRO:HA	2.16	0.46
1:A:196:ASP:HB2	3:E:140:MET:SD	2.55	0.45
1:A:209:GLU:HA	1:A:213:THR:CB	2.39	0.45
2:C:111:LYS:O	2:C:115:GLU:HG3	2.15	0.45
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.16	0.45
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.98	0.45
2:C:75:LYS:HB3	2:C:80:ARG:O	2.15	0.45
2:D:105:TRP:O	2:D:108:PRO:HD2	2.15	0.45
3:F:146:ASN:HB3	3:F:149:ASP:CG	2.36	0.45
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.45
3:F:63:LYS:O	3:F:67:LEU:HG	2.16	0.45
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.49	0.45
2:D:235:TRP:CD1	2:D:235:TRP:C	2.89	0.45
2:D:8:ARG:NH2	2:D:15:GLU:HB3	2.30	0.45
1:B:44:THR:HG23	1:B:127:SER:HA	1.97	0.45
1:B:43:ARG:HD2	1:B:43:ARG:O	2.16	0.45
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.34	0.45
2:C:7:ARG:HH11	2:C:7:ARG:HG3	1.81	0.45
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.98	0.45
2:D:243:GLU:HB2	2:D:320:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ARG:HG3	2:D:7:ARG:HH11	1.81	0.45
3:E:3:LYS:HB3	3:E:10:ASP:OD1	2.17	0.45
1:B:288:MET:HE1	1:B:346:LEU:C	2.36	0.45
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.50	0.45
1:A:159:ALA:O	2:C:33:ASN:HB2	2.17	0.45
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.81	0.45
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.52	0.44
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.98	0.44
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.81	0.44
1:A:84:ASP:HB3	1:B:81:SER:OG	2.17	0.44
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.52	0.44
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.17	0.44
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.44
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.18	0.44
1:B:192:PHE:O	1:B:200:CYS:HB3	2.18	0.44
2:D:63:ILE:O	2:D:64:ALA:C	2.55	0.44
3:F:120:PRO:HA	3:F:122:ILE:N	2.33	0.44
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.47	0.44
1:A:175:ARG:HG3	1:A:181:TRP:CG	2.52	0.44
1:A:18:ARG:N	5:A:5258:HOH:O	2.51	0.44
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.64	0.44
1:B:230:GLU:C	1:B:233:PRO:HD2	2.38	0.44
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.33	0.44
1:A:90:ASN:HA	1:A:90:ASN:HD22	1.59	0.44
1:B:476:ARG:HH11	1:B:476:ARG:HG3	1.82	0.44
1:A:222:GLU:OE1	2:C:7:ARG:NH1	2.51	0.44
1:A:214:ASN:ND2	1:A:247:MET:SD	2.90	0.44
1:B:222:GLU:OE1	2:D:7:ARG:NH1	2.51	0.44
1:B:439:HIS:CE1	1:B:454:GLU:OE1	2.68	0.44
2:D:324:TRP:HA	2:D:327:PRO:HD2	2.00	0.44
1:B:198:VAL:O	1:B:202:LEU:HG	2.18	0.43
2:C:256:PHE:HA	2:C:332:LEU:HD21	2.00	0.43
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.43
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.54	0.43
2:D:153:LEU:HA	2:D:193:ILE:HD12	2.00	0.43
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.53	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.43
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.84	0.43
1:B:460:GLU:HB3	1:B:463:ARG:HG3	2.01	0.43
1:B:488:LEU:HD13	1:B:492:GLY:C	2.39	0.43
2:D:179:LEU:HD23	2:D:182:TRP:CZ3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:ILE:HD11	2:D:284:ALA:HA	1.99	0.43
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.18	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.63	0.43
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.53	0.43
2:C:389:LYS:HD2	5:C:448:HOH:O	2.18	0.43
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.99	0.43
2:C:376:ASP:CG	2:C:379:GLN:HG2	2.39	0.43
2:D:143:GLU:O	2:D:147:ARG:HB3	2.18	0.43
1:B:116:ASN:CG	1:B:189:SER:HA	2.38	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
2:D:376:ASP:HB3	2:D:379:GLN:HB2	2.01	0.43
1:A:382:HIS:CB	1:A:431:LYS:HD2	2.49	0.43
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.70	0.43
2:D:277:THR:HB	2:D:278:PRO:HD3	2.00	0.43
1:B:125:TRP:C	1:B:125:TRP:CD1	2.92	0.42
2:D:255:LEU:HB2	2:D:328:THR:HG21	2.01	0.42
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.33	0.42
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.53	0.42
1:A:413:HIS:HD2	1:A:428:SER:OG	2.01	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.19	0.42
1:B:451:GLN:HG2	5:B:5271:HOH:O	2.18	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.54	0.42
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.54	0.42
1:A:252:GLN:NE2	1:A:252:GLN:HA	2.33	0.42
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.18	0.42
1:B:251:TYR:O	1:B:255:VAL:HG23	2.19	0.42
2:D:185:ASP:O	2:D:189:ILE:HG12	2.18	0.42
3:F:61:GLU:O	3:F:121:PRO:HG3	2.18	0.42
2:D:325:LEU:O	2:D:329:ILE:HG13	2.19	0.42
3:F:154:GLU:HG2	5:F:326:HOH:O	2.20	0.42
1:B:108:ASN:O	1:B:111:GLU:HB3	2.19	0.42
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.54	0.42
1:B:39:PHE:CD2	1:B:42:ASN:HB2	2.54	0.42
2:D:333:ARG:HG3	2:D:387:GLY:HA3	2.01	0.42
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.42
1:A:382:HIS:CG	1:A:431:LYS:HD2	2.54	0.42
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.55	0.42
3:F:97:LYS:HE3	3:F:97:LYS:HB2	1.79	0.42
2:C:153:LEU:C	2:C:153:LEU:HD12	2.40	0.42
1:B:41:ASN:ND2	2:D:237:GLU:HG2	2.35	0.42
2:D:102:LEU:HD13	2:D:290:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:HB2	2:D:125:GLN:HE21	1.85	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.83	0.42
1:A:167:GLY:O	1:A:171:ALA:HB2	2.20	0.41
1:A:283:THR:HB	1:A:284:PRO:HD3	2.02	0.41
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.50	0.41
1:B:52:MET:HA	1:B:256:SER:O	2.21	0.41
2:D:340:ALA:CB	2:D:389:LYS:HD2	2.50	0.41
3:E:97:LYS:HE3	3:E:97:LYS:HB2	1.79	0.41
1:A:232:THR:HB	1:A:233:PRO:HD3	2.01	0.41
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.56	0.41
1:B:105:VAL:O	1:B:109:PHE:HB2	2.20	0.41
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.85	0.41
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.33	0.41
1:B:39:PHE:HZ	2:D:236:GLN:HG3	1.84	0.41
2:D:291:ALA:HB2	5:D:410:HOH:O	2.19	0.41
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.41
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.21	0.41
1:A:230:GLU:C	1:A:233:PRO:HD2	2.41	0.41
1:B:39:PHE:CZ	2:D:236:GLN:HG3	2.55	0.41
2:D:250:ALA:HA	2:D:367:TYR:CD2	2.56	0.41
2:D:364:ILE:HA	2:D:368:ALA:HB3	2.02	0.41
3:F:73:ASN:ND2	3:F:76:ASP:OD2	2.54	0.41
1:A:113:GLY:HA2	1:A:188:PHE:O	2.21	0.41
1:B:162:GLY:HA3	5:B:5179:HOH:O	2.20	0.41
1:B:313:TRP:O	1:B:318:ILE:HG12	2.20	0.41
1:B:39:PHE:CE2	1:B:42:ASN:HB2	2.56	0.41
3:F:145:LEU:HD12	5:F:626:HOH:O	2.20	0.41
2:D:324:TRP:C	2:D:327:PRO:HD2	2.41	0.41
1:B:182:LYS:O	2:D:73:THR:HG21	2.21	0.41
1:A:165:PRO:HG3	5:A:5325:HOH:O	2.20	0.41
1:B:108:ASN:HD21	1:B:175:ARG:NH2	2.19	0.41
1:B:44:THR:CG2	1:B:127:SER:HA	2.51	0.41
2:C:80:ARG:HB2	5:E:232:HOH:O	2.21	0.41
1:A:192:PHE:O	1:A:200:CYS:HB3	2.21	0.41
1:A:21:THR:HG21	2:C:203:ILE:HG22	2.03	0.41
1:A:104:LYS:HG2	1:A:168:HIS:CG	2.57	0.40
1:A:268:ASN:HA	1:A:268:ASN:HD22	1.76	0.40
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.55	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.21	0.40
2:C:54:VAL:O	2:C:55:TYR:HB2	2.21	0.40
1:B:115:TYR:OH	2:D:173:ASP:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:MET:HE1	2:D:352:ILE:HG21	2.04	0.40
1:A:299:GLU:OE1	1:A:303:LYS:HE2	2.20	0.40
1:A:31:TRP:HA	5:A:5189:HOH:O	2.21	0.40
2:C:270:PRO:HB3	2:D:270:PRO:HB3	2.04	0.40
5:A:5316:HOH:O	3:E:6:ILE:HD13	2.21	0.40
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.02	0.40
1:B:206:LEU:HD23	1:B:271:LEU:HD13	2.04	0.40
1:B:143:ASP:CB	1:B:246:HIS:HE2	2.33	0.40
2:D:224:TYR:O	2:D:227:ALA:HB3	2.21	0.40
2:D:247:SER:O	2:D:251:VAL:HB	2.21	0.40
2:D:333:ARG:NH2	2:D:383:ALA:O	2.54	0.40
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.57	0.40
3:F:121:PRO:HA	5:F:677:HOH:O	2.20	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.93	0.40
1:A:81:SER:HB3	1:B:85:ALA:HB2	2.04	0.40
2:C:153:LEU:HA	2:C:193:ILE:HD12	2.04	0.40
2:C:277:THR:HB	2:C:278:PRO:HD3	2.02	0.40
2:D:137:ASN:CB	2:D:272:PHE:HB3	2.48	0.40
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.86	0.40
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.56	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%)	484 (95%)	21 (4%)	3 (1%)	25	30
1	B	509/527 (97%)	476 (94%)	31 (6%)	2 (0%)	34	41
2	C	386/388 (100%)	376 (97%)	9 (2%)	1 (0%)	41	50
2	D	386/388 (100%)	365 (95%)	18 (5%)	3 (1%)	19	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	165/169 (98%)	163 (99%)	2 (1%)	0	100	100
3	F	164/169 (97%)	158 (96%)	6 (4%)	0	100	100
All	All	2118/2168 (98%)	2022 (96%)	87 (4%)	9 (0%)	34	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	386	ALA
2	C	64	ALA
1	A	94	ARG
1	A	284	PRO
1	A	315	GLY
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/442 (96%)	411 (97%)	12 (3%)	43	59
1	B	422/442 (96%)	409 (97%)	13 (3%)	40	55
2	C	316/323 (98%)	309 (98%)	7 (2%)	52	68
2	D	312/323 (97%)	306 (98%)	6 (2%)	57	73
3	E	143/146 (98%)	140 (98%)	3 (2%)	53	70
3	F	142/146 (97%)	140 (99%)	2 (1%)	67	80
All	All	1758/1822 (96%)	1715 (98%)	43 (2%)	49	65

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG

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Mol	Chain	Res	Type
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	310	TYR
1	A	403	ILE
1	A	455	ARG
1	A	467	GLN
1	A	520	LYS
1	B	33	GLN
1	B	43	ARG
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP
1	B	175	ARG
1	B	186	ARG
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	334	ASP
1	B	403	ILE
1	B	440	GLU
2	C	18	GLU
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	356	LEU
2	C	378	ASP
2	D	4	LEU
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	160	PHE
2	D	173	ASP
3	E	44	ARG
3	E	60	LEU
3	E	167	GLN
3	F	4	LEU
3	F	44	ARG



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	116	ASN
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
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	411	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	516	ASN
1	B	33	GLN
1	B	36	ASN
1	B	41	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	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	366	GLN
1	B	411	ASN
1	B	413	HIS

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Mol	Chain	Res	Type
1	B	439	HIS
1	B	451	GLN
1	B	527	ASN
2	C	98	HIS
2	C	125	GLN
2	C	155	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	301	ASN
3	E	7	HIS
3	E	45	ASN
3	E	144	ASN
3	E	146	ASN
3	E	167	GLN
3	F	7	HIS
3	F	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
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 carbohydrates in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	510/527 (96%)	-0.32	8 (1%) 72 78	22, 34, 56, 69	0
1	B	511/527 (96%)	-0.42	10 (1%) 65 72	15, 35, 53, 66	0
2	C	388/388 (100%)	-0.65	2 (0%) 91 94	18, 25, 41, 53	0
2	D	388/388 (100%)	-0.08	12 (3%) 49 56	25, 42, 58, 86	0
3	E	167/169 (98%)	-0.59	4 (2%) 59 66	19, 29, 42, 65	0
3	F	166/169 (98%)	0.31	7 (4%) 36 43	36, 51, 64, 70	0
All	All	2130/2168 (98%)	-0.33	43 (2%) 65 72	15, 35, 57, 86	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	2	ALA	6.7
2	D	389	LYS	6.3
3	F	100	ALA	4.4
1	B	40	LYS	4.2
3	E	168	SER	3.9
3	F	23	ASN	3.5
3	F	20	ALA	3.4
1	B	39	PHE	3.4
1	B	41	ASN	3.3
1	B	527	ASN	3.1
3	F	69	ALA	3.1
2	D	205	PRO	3.0
1	A	310	TYR	2.9
1	A	434	SER	2.9
2	C	2	SER	2.9
1	B	17	ASN	2.8
1	B	310	TYR	2.7
3	F	22	LEU	2.7
2	D	344	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	2.6
1	A	316	ILE	2.6
2	D	333	ARG	2.5
1	B	54	ASN	2.5
2	D	388	LEU	2.4
2	D	345	GLY	2.4
1	A	251	TYR	2.4
2	D	385	LEU	2.4
3	E	4	LEU	2.4
1	A	317	TRP	2.3
2	D	380	ILE	2.3
3	F	70	ARG	2.3
2	C	389	LYS	2.3
3	F	21	GLN	2.3
2	D	346	THR	2.2
2	D	379	GLN	2.2
1	A	19	ALA	2.2
2	D	153	LEU	2.2
1	A	319	GLY	2.2
1	B	311	GLU	2.2
2	D	348	ASP	2.1
1	B	53	ALA	2.1
3	E	153	GLU	2.1
1	B	324	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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
4	CO	B	5173	1/1	0.98	0.04	50,50,50,50	0
4	CO	A	5170	1/1	0.99	0.02	42,42,42,42	0
4	CO	A	5171	1/1	0.99	0.04	30,30,30,30	0
4	CO	B	5172	1/1	1.00	0.06	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.