



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1FYZ  
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II REDUCED  
BY SOAKING  
Authors : Whittington, D.A.; Lippard, S.J.  
Deposited on : 2000-10-03  
Resolution : 2.15 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

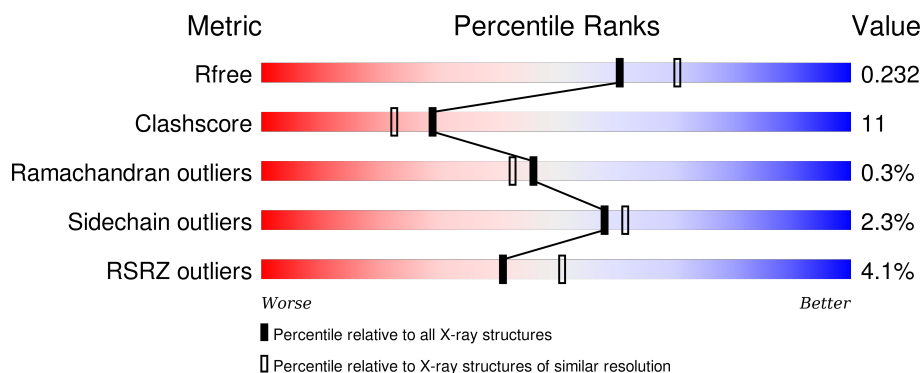
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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>74%</div> <div>22%</div> <div>• •</div> </div>
1	B	527	<div> <div>3%</div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
2	C	389	<div> <div>2%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>
2	D	389	<div> <div>8%</div> <div>69%</div> <div>30%</div> <div>• •</div> </div>
3	E	170	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	170	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment at the beginning labeled '12%', a green segment labeled '67%', a yellow segment labeled '30%', and a small grey segment at the end labeled '..'.

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18742 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	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	18			
1	B	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	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
			3193	2054	551	580	8			
2	D	387	Total	C	N	O	S	0	0	0
			3183	2048	549	578	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	167	Total	C	N	O	S	0	0	0
			1375	872	247	251	5			
3	F	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	C	2	Total 2	Ca 2	0	0

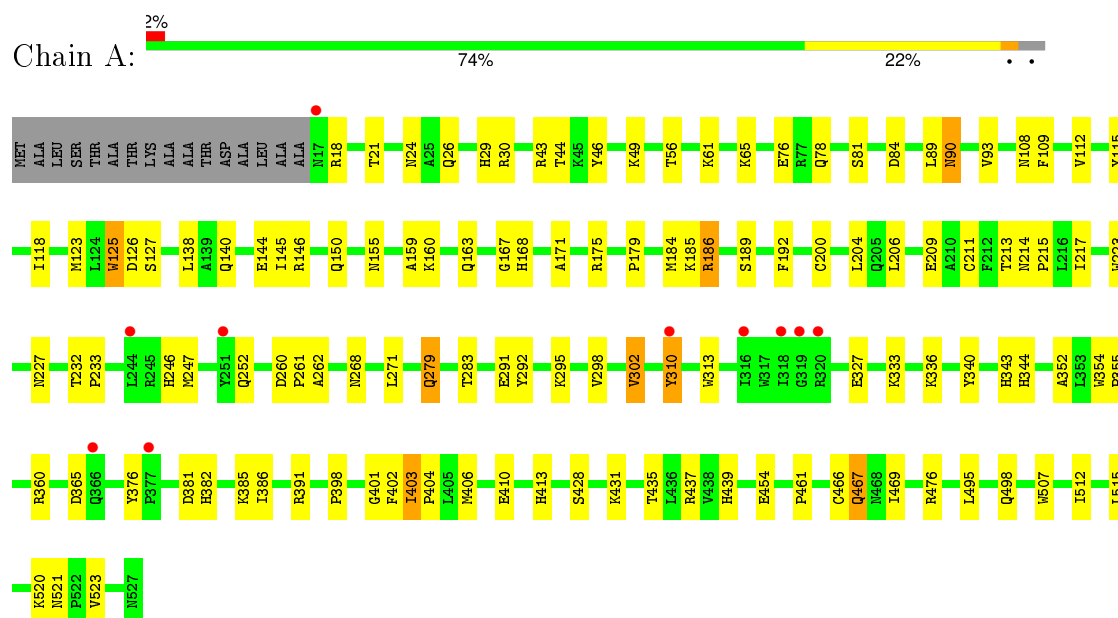
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total 281	O 281	0	0
6	B	263	Total 263	O 263	0	0
6	C	298	Total 298	O 298	0	0
6	D	171	Total 171	O 171	0	0
6	E	166	Total 166	O 166	0	0
6	F	49	Total 49	O 49	0	0

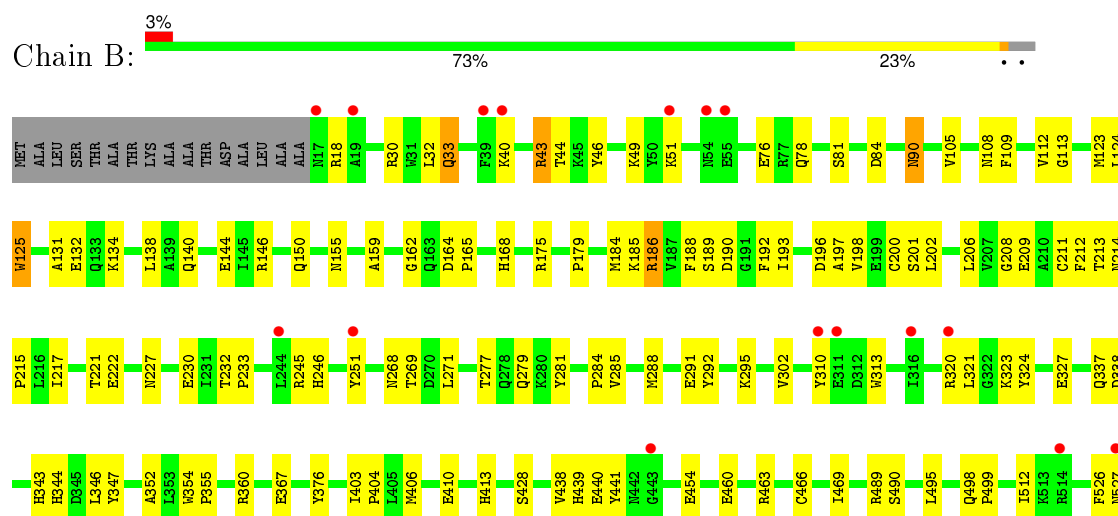
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

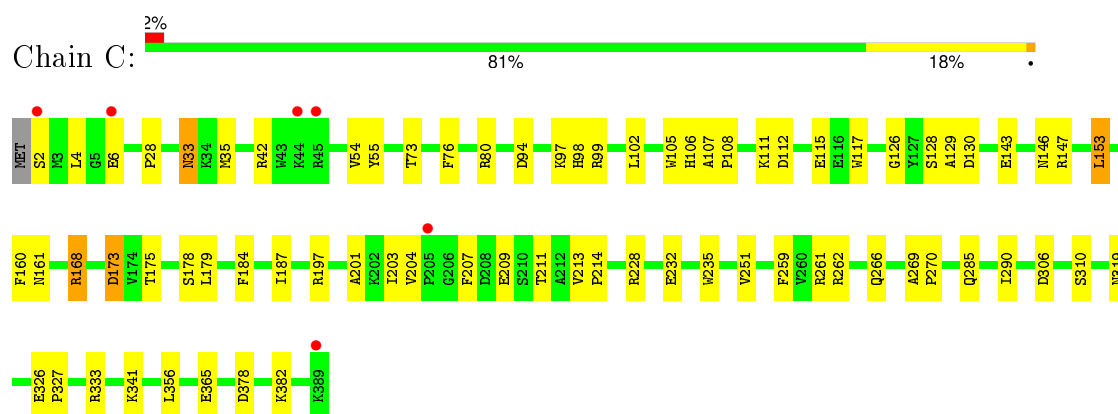
#### • Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



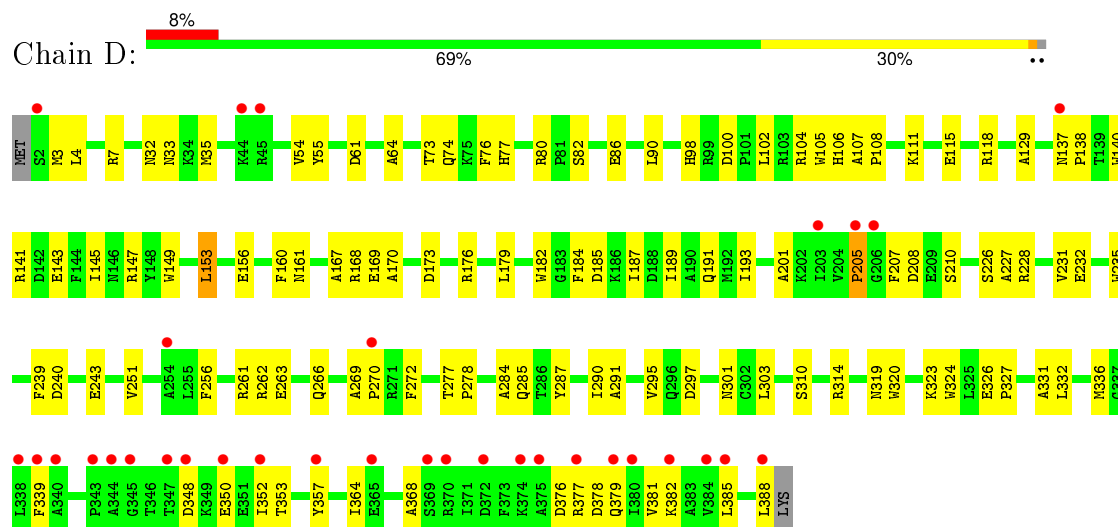
#### • Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



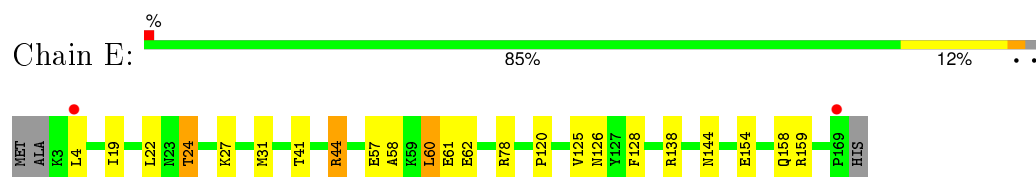
#### • Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



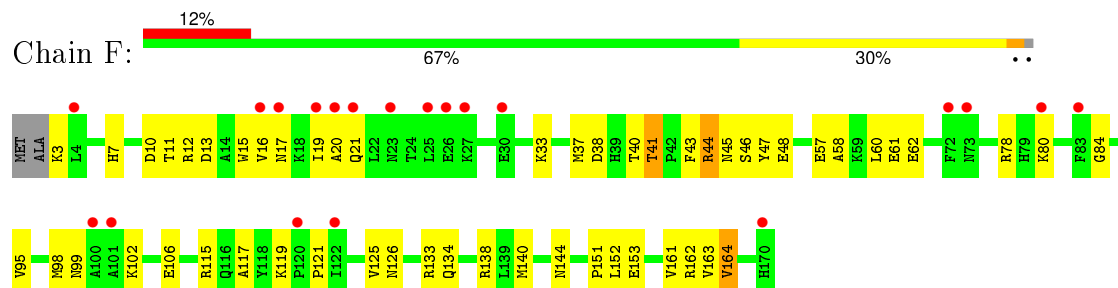
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• 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, $\alpha$ , $\beta$ , $\gamma$	71.27Å 171.66Å 221.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.15 29.79 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.79-2.15) 93.6 (29.79-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.189 , 0.230 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	4903 reflections (3.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 145230 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE2

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	0/4310	0.55	0/5853
1	B	0.32	0/4310	0.55	0/5853
2	C	0.36	0/3289	0.56	0/4464
2	D	0.32	0/3279	0.52	0/4453
3	E	0.33	0/1404	0.58	0/1892
3	F	0.29	0/1416	0.49	0/1907
All	All	0.33	0/18008	0.55	0/24422

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4185	0	3981	104	0
1	B	4185	0	3981	124	0
2	C	3193	0	3042	63	0
2	D	3183	0	3029	88	0
3	E	1375	0	1370	17	0
3	F	1386	0	1377	50	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	281	0	0	5	0
6	B	263	0	0	6	0
6	C	298	0	0	9	0
6	D	171	0	0	2	0
6	E	166	0	0	0	0
6	F	49	0	0	1	0
All	All	18742	0	16780	391	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 11.

All (391) 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)
3:F:41:THR:HG23	3:F:43:PHE:H	1.27	0.99
1:A:44:THR:HG22	1:A:46:TYR:H	1.32	0.95
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.02	0.94
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.50	0.93
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.01	0.91
1:A:435:THR:HG21	1:A:437:ARG:HE	1.36	0.91
1:B:268:ASN:HD21	1:B:327:GLU:H	1.20	0.90
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.51	0.90
1:A:467:GLN:HG3	6:A:5252:HOH:O	1.69	0.90
1:A:435:THR:CG2	1:A:437:ARG:HE	1.88	0.86
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.21	0.85
1:A:209:GLU:HA	1:A:213:THR:HB	1.59	0.84
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.59	0.84
3:F:41:THR:O	3:F:44:ARG:HD2	1.80	0.82
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.59	0.81
1:B:406:MET:O	1:B:410:GLU:HG3	1.81	0.80
1:A:268:ASN:HD21	1:A:327:GLU:H	1.31	0.79
1:B:44:THR:HG22	1:B:46:TYR:H	1.47	0.79
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.48	0.79
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.29	0.78
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.33	0.77
1:B:208:GLY:O	1:B:213:THR:HG23	1.85	0.76
1:A:406:MET:O	1:A:410:GLU:HG3	1.86	0.76
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.81	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLU:HA	1:B:213:THR:OG1	1.87	0.75
1:A:109:PHE:HB3	1:A:184:MET:HE3	1.67	0.74
3:F:40:THR:O	3:F:41:THR:HG22	1.89	0.72
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.88	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.83	0.72
3:F:13:ASP:O	3:F:16:VAL:HG22	1.90	0.72
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.20	0.72
2:D:167:ALA:O	2:D:176:ARG:NH1	2.23	0.72
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.56	0.71
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.36	0.71
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.37	0.71
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.82	0.71
1:B:33:GLN:HE22	1:B:132:GLU:H	1.40	0.70
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.74	0.70
3:F:3:LYS:HG3	3:F:10:ASP:OD2	1.91	0.70
1:B:18:ARG:O	2:D:129:ALA:HA	1.92	0.69
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.75	0.69
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.56	0.69
3:E:41:THR:O	3:E:44:ARG:HD2	1.92	0.68
1:B:489:ARG:HD2	1:B:495:LEU:O	1.93	0.68
2:D:228:ARG:O	2:D:232:GLU:HG3	1.93	0.68
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.76	0.67
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.59	0.67
1:B:30:ARG:O	1:B:30:ARG:HD3	1.95	0.67
3:F:58:ALA:O	3:F:62:GLU:HG3	1.95	0.67
3:F:57:GLU:O	3:F:61:GLU:HG3	1.95	0.66
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.66
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.77	0.66
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.26	0.66
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.44	0.65
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.42	0.65
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.77	0.65
2:C:97:LYS:HD2	6:C:5058:HOH:O	1.97	0.65
3:E:24:THR:HG22	3:E:27:LYS:H	1.63	0.64
2:D:111:LYS:O	2:D:115:GLU:HG3	1.96	0.64
1:A:268:ASN:ND2	1:A:327:GLU:H	1.95	0.64
3:F:15:TRP:O	3:F:19:ILE:HG23	1.97	0.64
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.79	0.64
1:B:227:ASN:HD21	1:B:295:LYS:H	1.44	0.64
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.80	0.63
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:ILE:O	2:D:191:GLN:HG3	1.98	0.63
2:C:333:ARG:HD3	6:C:5162:HOH:O	1.98	0.62
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.48	0.62
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.64	0.62
1:B:268:ASN:ND2	1:B:327:GLU:H	1.95	0.62
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.34	0.62
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.35	0.62
1:B:367:GLU:HG3	6:B:5014:HOH:O	2.00	0.62
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.62
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.81	0.62
1:B:44:THR:HG21	6:B:5215:HOH:O	2.00	0.62
2:C:365:GLU:HG3	6:C:5182:HOH:O	2.00	0.61
2:C:333:ARG:HD2	6:C:5161:HOH:O	2.00	0.61
1:B:288:MET:HE1	1:B:346:LEU:HG	1.82	0.61
1:A:108:ASN:ND2	1:A:175:ARG:HH11	1.98	0.61
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.66	0.61
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.83	0.60
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.60
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.83	0.60
1:B:288:MET:HE1	1:B:346:LEU:C	2.22	0.60
1:B:526:PHE:O	1:B:527:ASN:HB2	2.02	0.60
2:D:153:LEU:HD12	2:D:153:LEU:C	2.22	0.60
2:C:6:GLU:HG3	6:C:5133:HOH:O	2.02	0.59
2:D:145:ILE:O	2:D:149:TRP:HB3	2.02	0.59
3:E:22:LEU:HD11	3:E:31:MET:SD	2.42	0.59
3:F:41:THR:HG23	3:F:43:PHE:N	2.10	0.59
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.59
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.02	0.59
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.96	0.59
3:F:153:GLU:CD	3:F:153:GLU:H	2.05	0.59
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.01	0.59
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.84	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.02	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.03	0.58
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.01	0.58
1:A:44:THR:OG1	1:A:127:SER:HA	2.04	0.58
1:A:109:PHE:HD2	1:A:184:MET:HE2	1.67	0.58
1:A:204:LEU:O	1:A:209:GLU:HG3	2.03	0.57
2:C:211:THR:O	2:C:214:PRO:HD2	2.04	0.57
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.85	0.57
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:HD21	1:A:295:LYS:H	1.52	0.57
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.87	0.57
1:A:140:GLN:O	1:A:144:GLU:HG2	2.04	0.57
2:D:378:ASP:O	2:D:382:LYS:HG3	2.04	0.57
1:A:333:LYS:HG2	6:A:5248:HOH:O	2.05	0.57
1:B:33:GLN:NE2	1:B:132:GLU:H	2.02	0.56
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.33	0.56
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.87	0.56
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.06	0.56
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.87	0.56
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.87	0.56
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.71	0.56
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.88	0.56
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.36	0.56
1:B:188:PHE:CZ	1:B:213:THR:HG22	2.36	0.55
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.54	0.55
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.54
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.88	0.54
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.72	0.54
1:A:109:PHE:O	1:A:112:VAL:HG12	2.07	0.54
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.90	0.54
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.37	0.54
2:D:105:TRP:O	2:D:108:PRO:HD2	2.07	0.54
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.41	0.54
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.31	0.54
1:B:213:THR:O	1:B:217:ILE:HG12	2.07	0.54
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.89	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.54
1:B:123:MET:HE3	1:B:197:ALA:HA	1.90	0.54
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.43	0.54
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.08	0.54
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.90	0.54
2:D:82:SER:O	2:D:168:ARG:NH2	2.40	0.54
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.90	0.54
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.26	0.53
1:A:213:THR:O	1:A:217:ILE:HG12	2.08	0.53
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.90	0.53
2:D:324:TRP:O	2:D:327:PRO:HD2	2.09	0.53
3:E:4:LEU:HG	3:E:4:LEU:O	2.09	0.53
1:A:160:LYS:HD2	6:A:5238:HOH:O	2.08	0.53
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.90	0.53
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.09	0.53
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.74	0.53
6:C:5117:HOH:O	3:E:125:VAL:HG22	2.08	0.53
1:B:403:ILE:HG22	1:B:406:MET:SD	2.49	0.53
2:D:381:VAL:O	2:D:385:LEU:HB2	2.08	0.53
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.24	0.52
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.44	0.52
1:B:186:ARG:HD3	1:B:186:ARG:O	2.09	0.52
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.45	0.52
1:B:269:THR:HG23	6:B:5097:HOH:O	2.09	0.52
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.91	0.52
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.52
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.86	0.52
2:D:352:ILE:HG13	2:D:353:THR:N	2.24	0.52
2:D:310:SER:O	2:D:314:ARG:HG3	2.09	0.52
2:C:175:THR:O	2:C:179:LEU:HD13	2.10	0.52
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.44	0.52
2:D:277:THR:HB	2:D:278:PRO:HD3	1.92	0.52
2:C:2:SER:HB2	6:C:5232:HOH:O	2.09	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.04	0.51
1:B:288:MET:CE	1:B:346:LEU:HB3	2.40	0.51
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.45	0.51
3:E:41:THR:O	3:E:44:ARG:CD	2.56	0.51
3:E:57:GLU:O	3:E:61:GLU:HG3	2.10	0.51
1:B:212:PHE:O	1:B:215:PRO:HD2	2.11	0.51
1:B:51:LYS:HG3	6:B:5190:HOH:O	2.10	0.51
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.29	0.51
3:F:19:ILE:C	3:F:19:ILE:HD12	2.31	0.51
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.51
1:A:21:THR:HG22	2:C:128:SER:CB	2.41	0.51
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.92	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.11	0.50
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.46	0.50
1:A:18:ARG:O	2:C:129:ALA:HA	2.12	0.50
1:B:466:CYS:HB2	2:D:73:THR:HA	1.94	0.50
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.94	0.50
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.12	0.50
2:C:211:THR:C	2:C:214:PRO:HD2	2.32	0.50
1:B:186:ARG:HD3	1:B:186:ARG:C	2.32	0.50
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:HB3	1:B:81:SER:OG	2.11	0.50
1:A:81:SER:OG	1:B:84:ASP:HB3	2.11	0.50
1:A:109:PHE:HD2	1:A:184:MET:CE	2.25	0.50
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.94	0.50
1:A:206:LEU:HD23	1:A:271:LEU:HD13	1.93	0.50
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.50
2:D:377:ARG:O	2:D:381:VAL:HG23	2.11	0.50
1:B:454:GLU:OE2	3:F:152:LEU:HD13	2.12	0.50
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.94	0.50
2:C:111:LYS:O	2:C:115:GLU:HG3	2.11	0.49
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.45	0.49
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.94	0.49
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.94	0.49
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.95	0.49
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.09	0.49
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.93	0.49
2:C:54:VAL:O	2:C:55:TYR:HB2	2.13	0.49
1:A:186:ARG:HA	2:C:73:THR:OG1	2.13	0.49
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.49
1:B:32:LEU:C	1:B:32:LEU:HD23	2.33	0.49
1:B:251:TYR:HE2	1:B:320:ARG:HH12	1.61	0.49
1:A:401:GLY:HA2	1:A:515:LEU:CD2	2.43	0.49
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.78	0.49
1:B:162:GLY:HA3	6:B:5119:HOH:O	2.13	0.48
1:B:413:HIS:HD2	1:B:428:SER:OG	1.96	0.48
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.26	0.48
2:D:226:SER:HB2	2:D:331:ALA:HA	1.95	0.48
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.48
1:A:163:GLN:O	2:C:28:PRO:HA	2.14	0.48
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.48	0.48
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.94	0.48
1:B:526:PHE:O	1:B:527:ASN:CB	2.61	0.48
2:C:126:GLY:O	2:C:130:ASP:HB2	2.13	0.48
2:D:324:TRP:C	2:D:327:PRO:HD2	2.34	0.48
1:A:56:THR:CG2	1:A:252:GLN:HE21	2.26	0.48
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.48	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.14	0.48
1:A:115:TYR:OH	2:C:173:ASP:HA	2.14	0.48
1:A:227:ASN:ND2	1:A:295:LYS:H	2.12	0.48
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.49	0.47
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
3:F:38:ASP:HA	3:F:45:ASN:HB2	1.96	0.47
3:E:154:GLU:O	3:E:158:GLN:HG3	2.12	0.47
3:F:19:ILE:HD12	3:F:20:ALA:N	2.29	0.47
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.80	0.47
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.49	0.47
2:C:143:GLU:O	2:C:147:ARG:HB3	2.14	0.47
1:B:232:THR:HB	1:B:233:PRO:HD3	1.96	0.47
2:D:184:PHE:O	2:D:187:ILE:HG22	2.15	0.47
2:C:228:ARG:O	2:C:232:GLU:HG3	2.15	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.50	0.47
3:F:33:LYS:O	3:F:37:MET:HG2	2.13	0.47
2:D:143:GLU:O	2:D:147:ARG:HB3	2.15	0.47
1:B:198:VAL:O	1:B:202:LEU:HG	2.14	0.47
1:B:440:GLU:OE1	3:F:162:ARG:HD3	2.15	0.47
1:A:26:GLN:HG2	6:A:5123:HOH:O	2.15	0.47
1:B:288:MET:HE1	1:B:346:LEU:CG	2.45	0.47
1:B:32:LEU:O	1:B:32:LEU:HD23	2.15	0.47
2:C:341:LYS:HE3	6:C:5159:HOH:O	2.14	0.47
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.15	0.47
1:A:232:THR:HB	1:A:233:PRO:HD3	1.96	0.47
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.50	0.47
3:E:58:ALA:O	3:E:62:GLU:HG3	2.15	0.46
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.14	0.46
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.30	0.46
1:B:159:ALA:O	2:D:33:ASN:HB2	2.15	0.46
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.97	0.46
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.02	0.46
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.51	0.46
2:C:105:TRP:O	2:C:108:PRO:HD2	2.15	0.46
1:B:186:ARG:HA	2:D:73:THR:OG1	2.15	0.46
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.51	0.46
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.51	0.46
2:C:235:TRP:CD1	2:C:235:TRP:C	2.89	0.46
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.98	0.46
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.98	0.46
3:F:16:VAL:O	3:F:19:ILE:HG13	2.16	0.46
2:D:353:THR:O	2:D:357:TYR:HD1	1.99	0.46
1:B:196:ASP:HB2	3:F:140:MET:SD	2.56	0.46
3:E:4:LEU:CG	3:E:4:LEU:O	2.63	0.46
3:F:12:ARG:O	3:F:16:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.19	0.45
1:B:337:GLN:HG3	1:B:338:ASP:N	2.32	0.45
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.33	0.45
1:A:402:PHE:O	1:A:403:ILE:HD12	2.16	0.45
2:C:209:GLU:HG2	6:C:5044:HOH:O	2.15	0.45
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.70	0.45
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.52	0.45
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.97	0.45
2:D:77:HIS:CG	3:F:140:MET:HG2	2.52	0.45
2:C:153:LEU:HD12	2:C:153:LEU:C	2.37	0.45
1:B:43:ARG:HD2	1:B:43:ARG:C	2.37	0.45
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.99	0.45
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.99	0.44
1:B:320:ARG:CB	1:B:320:ARG:NH1	2.80	0.44
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.98	0.44
2:D:189:ILE:HD12	2:D:284:ALA:HB2	1.98	0.44
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.52	0.44
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.52	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.35	0.44
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.52	0.44
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.44
1:A:413:HIS:HD2	1:A:428:SER:OG	2.00	0.44
1:B:186:ARG:CZ	1:B:277:THR:HG23	2.48	0.44
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.15	0.44
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.52	0.44
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.99	0.44
2:C:4:LEU:HD23	6:D:454:HOH:O	2.17	0.44
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.18	0.44
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.18	0.44
3:F:46:SER:OG	3:F:48:GLU:HG2	2.18	0.44
1:B:155:ASN:OD1	1:B:168:HIS:HD2	2.01	0.44
1:A:466:CYS:HB2	2:C:73:THR:HA	1.98	0.44
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.53	0.44
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.52	0.44
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.18	0.43
1:B:140:GLN:O	1:B:144:GLU:HG2	2.18	0.43
1:B:184:MET:CE	1:B:188:PHE:HB2	2.47	0.43
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.43
3:F:61:GLU:O	3:F:121:PRO:HG2	2.17	0.43
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:GLU:HA	2:D:263:GLU:OE2	2.19	0.43
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.18	0.43
2:C:306:ASP:O	2:C:310:SER:HB2	2.17	0.43
1:B:184:MET:HE2	1:B:188:PHE:CG	2.54	0.43
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.00	0.43
1:A:146:ARG:HG2	1:A:150:GLN:OE1	2.19	0.43
1:B:33:GLN:NE2	1:B:33:GLN:HA	2.27	0.43
2:D:377:ARG:HH11	2:D:377:ARG:HG3	1.82	0.43
3:F:17:ASN:O	3:F:21:GLN:HG2	2.19	0.43
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.54	0.43
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.54	0.43
1:A:76:GLU:HG2	1:B:76:GLU:HG2	2.01	0.43
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	0.43
1:B:165:PRO:HG3	6:B:5118:HOH:O	2.19	0.43
2:D:227:ALA:O	2:D:231:VAL:HG23	2.18	0.43
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.01	0.43
1:B:288:MET:HE1	1:B:347:TYR:N	2.33	0.43
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.43
2:C:269:ALA:N	2:C:270:PRO:CD	2.82	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.60	0.42
1:B:320:ARG:HH11	1:B:320:ARG:CB	2.32	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.56	0.42
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.54	0.42
2:D:357:TYR:CZ	2:D:381:VAL:HG21	2.54	0.42
3:E:125:VAL:HG23	3:E:126:ASN:N	2.34	0.42
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.54	0.42
1:B:288:MET:HE3	1:B:346:LEU:HB3	2.00	0.42
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.42
2:C:102:LEU:HD13	2:C:290:ILE:HG23	2.02	0.42
1:B:288:MET:CE	1:B:347:TYR:N	2.82	0.42
3:F:125:VAL:HG22	6:F:1064:HOH:O	2.19	0.42
1:B:217:ILE:O	1:B:221:THR:HG23	2.19	0.42
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.49	0.42
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.35	0.42
1:A:159:ALA:O	2:C:33:ASN:HB2	2.19	0.42
2:C:33:ASN:HD22	2:C:33:ASN:N	2.16	0.42
1:B:190:ASP:HB3	2:D:74:GLN:O	2.20	0.42
1:A:214:ASN:ND2	1:A:247:MET:SD	2.93	0.42
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.01	0.42
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.42
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:ILE:HG22	3:F:60:LEU:HD13	2.02	0.41
1:A:382:HIS:CD2	1:A:431:LYS:HG3	2.55	0.41
1:B:208:GLY:C	1:B:213:THR:HG23	2.39	0.41
1:B:123:MET:CE	1:B:197:ALA:HA	2.50	0.41
2:D:235:TRP:CD1	2:D:235:TRP:C	2.93	0.41
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.03	0.41
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.55	0.41
1:B:288:MET:HE1	1:B:346:LEU:CB	2.51	0.41
1:A:192:PHE:O	1:A:200:CYS:HB3	2.20	0.41
2:D:291:ALA:O	2:D:295:VAL:HG23	2.21	0.41
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.03	0.41
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.85	0.41
2:C:184:PHE:O	2:C:187:ILE:HG22	2.21	0.41
2:D:176:ARG:HH11	2:D:176:ARG:HG3	1.86	0.41
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.55	0.41
2:D:336:MET:O	2:D:339:PHE:HD1	2.04	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.64	0.41
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.21	0.41
1:B:124:LEU:HD21	1:B:201:SER:HB2	2.03	0.41
1:A:365:ASP:OD2	1:A:365:ASP:C	2.59	0.41
1:A:109:PHE:CD2	1:A:184:MET:HE2	2.53	0.41
1:A:382:HIS:CB	1:A:431:LYS:HD2	2.51	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.60	0.41
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.56	0.41
2:D:185:ASP:O	2:D:189:ILE:HG12	2.21	0.40
3:F:102:LYS:HG2	3:F:106:GLU:OE1	2.20	0.40
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.35	0.40
1:A:44:THR:HG21	6:A:5166:HOH:O	2.21	0.40
1:A:167:GLY:O	1:A:171:ALA:HB2	2.21	0.40
2:D:262:ARG:O	2:D:266:GLN:HB3	2.21	0.40
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.56	0.40
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.21	0.40
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.56	0.40
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.56	0.40
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.03	0.40
2:D:153:LEU:HA	2:D:193:ILE:HD12	2.04	0.40
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.03	0.40
2:D:86:GLU:HG2	6:D:449:HOH:O	2.21	0.40
3:F:115:ARG:O	3:F:119:LYS:HB2	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	509/527 (97%)	487 (96%)	22 (4%)	0	100	100
1	B	509/527 (97%)	483 (95%)	24 (5%)	2 (0%)	39	34
2	C	386/389 (99%)	377 (98%)	8 (2%)	1 (0%)	46	42
2	D	385/389 (99%)	368 (96%)	14 (4%)	3 (1%)	24	15
3	E	165/170 (97%)	163 (99%)	2 (1%)	0	100	100
3	F	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
All	All	2120/2172 (98%)	2039 (96%)	75 (4%)	6 (0%)	46	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	D	251	VAL
1	B	284	PRO
2	C	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	433/442 (98%)	421 (97%)	12 (3%)	51	52
1	B	433/442 (98%)	426 (98%)	7 (2%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	322/323 (100%)	314 (98%)	8 (2%)	55	58
2	D	321/323 (99%)	314 (98%)	7 (2%)	60	63
3	E	145/147 (99%)	141 (97%)	4 (3%)	51	52
3	F	146/147 (99%)	142 (97%)	4 (3%)	52	53
All	All	1800/1824 (99%)	1758 (98%)	42 (2%)	58	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	90	ASN
1	A	125	TRP
1	A	186	ARG
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	391	ARG
1	A	403	ILE
1	A	467	GLN
1	A	520	LYS
1	B	33	GLN
1	B	43	ARG
1	B	90	ASN
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	310	TYR
2	C	33	ASN
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	378	ASP
2	C	382	LYS
2	D	4	LEU
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP

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Mol	Chain	Res	Type
2	D	205	PRO
2	D	301	ASN
3	E	24	THR
3	E	44	ARG
3	E	60	LEU
3	E	138	ARG
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) 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	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	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	17	ASN
1	B	33	GLN
1	B	36	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	155	ASN
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	214	ASN
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	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
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	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	F	7	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN

### 5.3.3 RNA ⓘ

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 7 ligands modelled in this entry, 7 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, 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	511/527 (96%)	-0.12	10 (1%) 68 75	18, 28, 49, 67	0
1	B	511/527 (96%)	-0.19	16 (3%) 52 62	19, 29, 50, 70	0
2	C	388/389 (99%)	-0.40	6 (1%) 76 82	15, 22, 39, 57	0
2	D	387/389 (99%)	0.33	33 (8%) 13 19	21, 38, 61, 70	0
3	E	167/170 (98%)	-0.33	2 (1%) 81 85	17, 25, 40, 68	0
3	F	168/170 (98%)	0.72	20 (11%) 6 10	31, 48, 66, 74	0
All	All	2132/2172 (98%)	-0.06	87 (4%) 41 51	15, 30, 56, 74	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	ASN	5.5
3	E	4	LEU	4.8
2	D	44	LYS	4.0
3	F	23	ASN	4.0
2	D	385	LEU	3.9
2	D	380	ILE	3.9
2	D	205	PRO	3.8
3	F	83	PHE	3.7
3	F	100	ALA	3.5
3	E	169	PRO	3.4
2	D	45	ARG	3.4
2	D	382	LYS	3.4
3	F	19	ILE	3.4
2	C	2	SER	3.3
1	B	316	ILE	3.3
3	F	72	PHE	3.2
2	D	206	GLY	3.2
1	B	54	ASN	3.1
1	A	316	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	45	ARG	3.1
2	D	375	ALA	3.1
2	D	348	ASP	3.0
3	F	170	HIS	3.0
1	B	320	ARG	2.9
1	A	17	ASN	2.8
1	B	244	LEU	2.8
1	A	310	TYR	2.7
2	C	6	GLU	2.7
1	B	311	GLU	2.7
2	D	344	ALA	2.7
3	F	120	PRO	2.7
2	D	338	LEU	2.7
2	D	374	LYS	2.7
1	B	514	ARG	2.7
1	A	244	LEU	2.6
1	B	40	LYS	2.6
2	C	389	LYS	2.6
2	D	345	GLY	2.6
1	B	39	PHE	2.6
2	D	339	PHE	2.6
3	F	4	LEU	2.6
3	F	101	ALA	2.6
2	C	205	PRO	2.5
3	F	21	GLN	2.5
3	F	73	ASN	2.5
1	B	527	ASN	2.5
3	F	27	LYS	2.5
1	A	251	TYR	2.4
2	D	343	PRO	2.4
3	F	17	ASN	2.4
2	D	357	TYR	2.4
3	F	80	LYS	2.4
2	D	254	ALA	2.4
2	D	347	THR	2.3
1	B	310	TYR	2.3
2	D	388	LEU	2.3
1	B	19	ALA	2.3
1	B	251	TYR	2.3
1	B	55	GLU	2.3
2	D	384	VAL	2.3
3	F	16	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	320	ARG	2.3
1	B	443	GLY	2.2
3	F	122	ILE	2.2
3	F	20	ALA	2.2
2	D	365	GLU	2.2
2	C	44	LYS	2.2
2	D	352	ILE	2.2
3	F	26	GLU	2.2
1	A	318	ILE	2.2
1	A	366	GLN	2.1
2	D	2	SER	2.1
2	D	350	GLU	2.1
2	D	370	ARG	2.1
1	B	51	LYS	2.1
1	A	377	PRO	2.1
2	D	340	ALA	2.1
2	D	377	ARG	2.1
2	D	137	ASN	2.1
3	F	25	LEU	2.1
2	D	270	PRO	2.1
2	D	379	GLN	2.1
1	A	319	GLY	2.0
3	F	30	GLU	2.0
2	D	369	SER	2.0
2	D	203	ILE	2.0
2	D	372	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FE2	A	5001	1/1	0.99	0.05	-2.07	30,30,30,30	0
4	FE2	B	5004	1/1	0.98	0.05	-2.77	43,43,43,43	0
4	FE2	B	5003	1/1	0.99	0.05	-2.90	29,29,29,29	0
5	CA	A	5005	1/1	0.99	0.03	-3.28	34,34,34,34	0
4	FE2	A	5002	1/1	0.98	0.03	-3.50	39,39,39,39	0
5	CA	C	5007	1/1	0.98	0.07	-	38,38,38,38	0
5	CA	C	5006	1/1	0.89	0.05	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.