



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1FZ2  
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II MIXED-  
VALENT GENERATED BY CRYSTAL 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

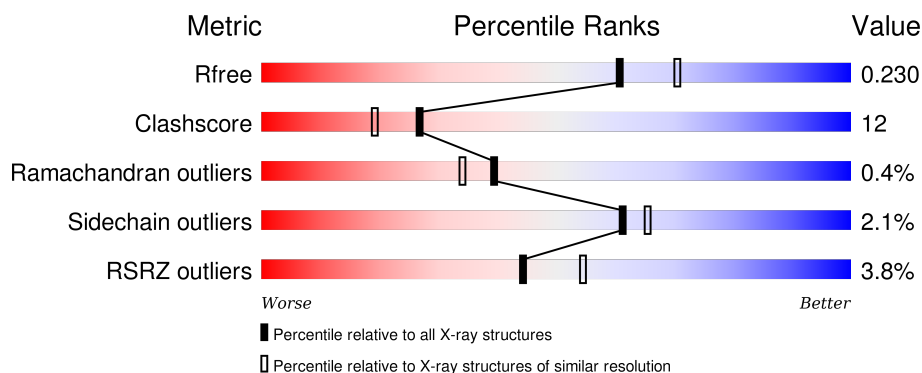
# 1 Overall quality at a glance

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> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	527	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
2	C	389	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>•</div> </div> </div>
2	D	389	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>31%</div> <div>• •</div> </div> </div>
3	E	170	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	170	<div><div></div><div>11%</div><div>71%</div><div>26%</div><div>..</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18664 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	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	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
			1382	875	249	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	3	Total 3	Ca 3	0	0

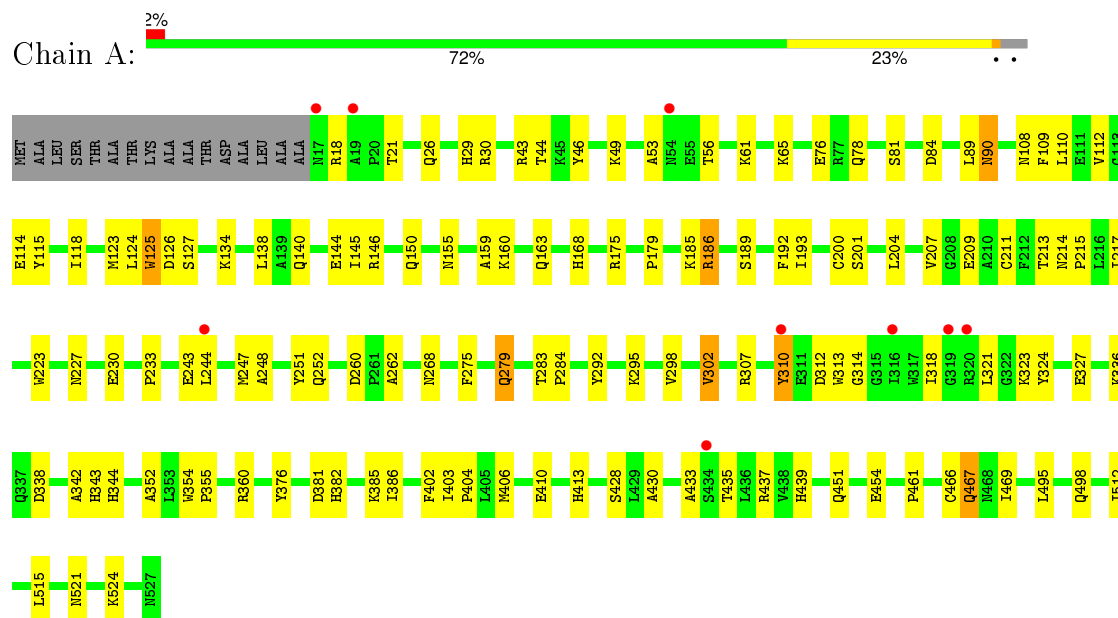
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	272	Total 272	O 272	0	0
6	B	251	Total 251	O 251	0	0
6	C	288	Total 288	O 288	0	0
6	D	133	Total 133	O 133	0	0
6	E	168	Total 168	O 168	0	0
6	F	49	Total 49	O 49	0	0

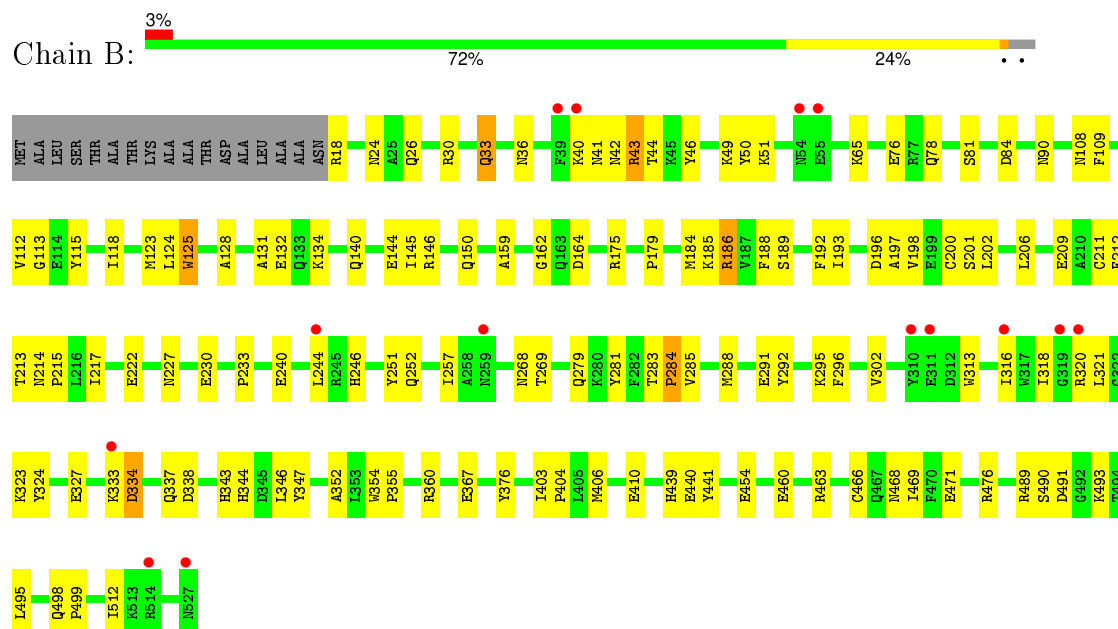
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

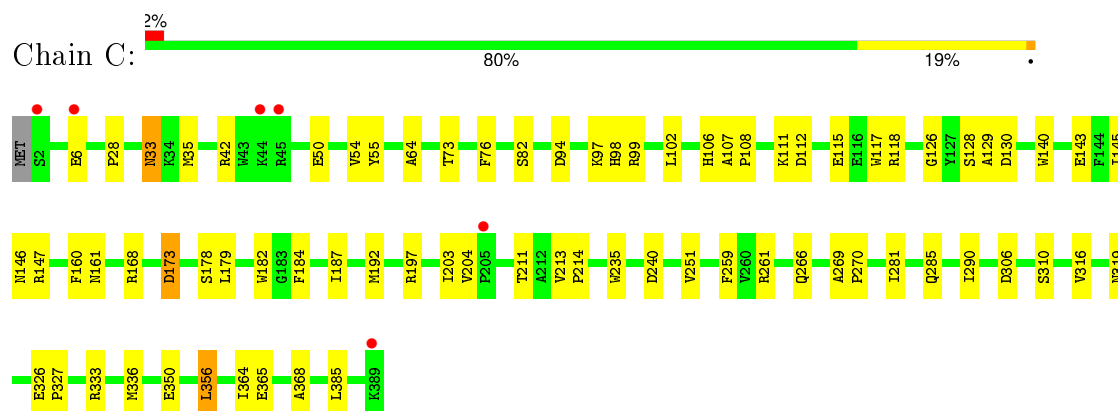
#### • Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



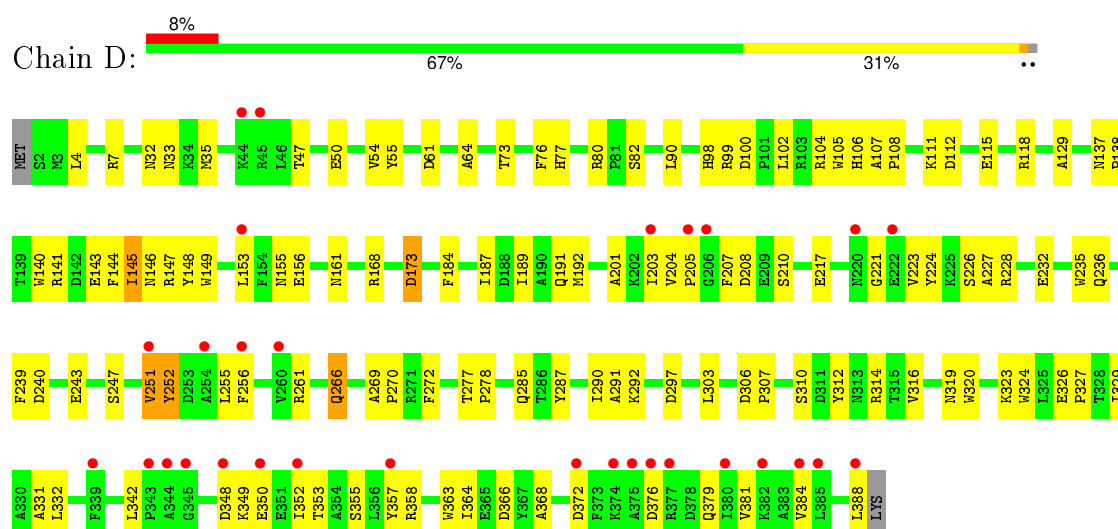
#### • Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



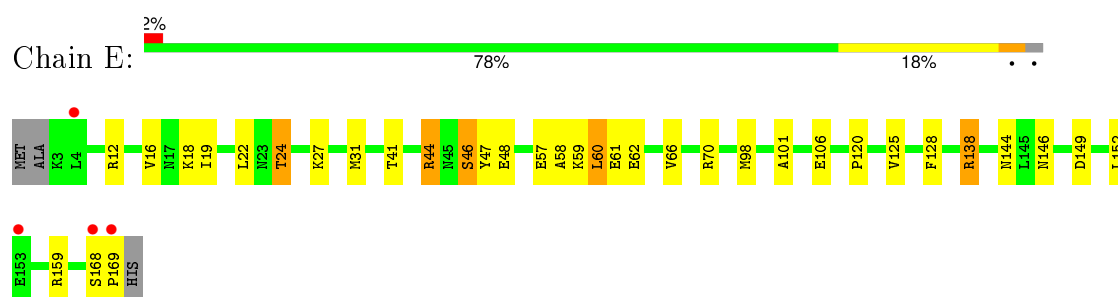
- Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



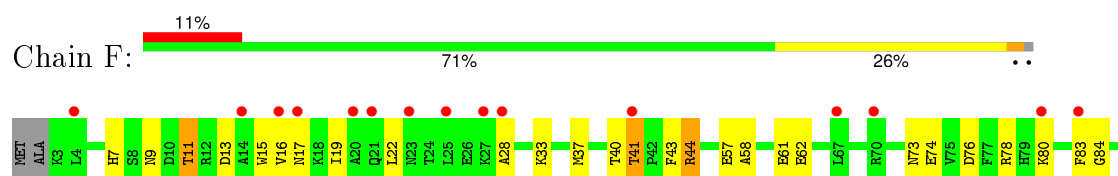
- Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

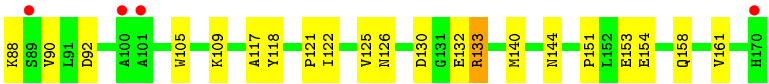


- Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



- 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, $\alpha$ , $\beta$ , $\gamma$	71.37Å 171.89Å 221.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.15 29.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.83-2.15) 94.9 (29.83-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.50 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.191 , 0.229 0.193 , 0.230	Depositor DCC
$R_{free}$ test set	5021 reflections (3.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.4	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 148377 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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	0/4302	0.55	0/5842
2	C	0.36	0/3289	0.57	0/4464
2	D	0.32	0/3279	0.52	0/4453
3	E	0.34	0/1404	0.59	0/1892
3	F	0.28	0/1412	0.49	0/1903
All	All	0.33	0/17996	0.55	0/24407

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	108	0
1	B	4177	0	3975	133	0
2	C	3193	0	3042	61	0
2	D	3183	0	3029	94	0
3	E	1375	0	1370	26	0
3	F	1382	0	1366	48	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	3	0	0	0	0
6	A	272	0	0	8	0
6	B	251	0	0	9	0
6	C	288	0	0	6	0
6	D	133	0	0	1	0
6	E	168	0	0	0	0
6	F	49	0	0	2	0
All	All	18664	0	16763	412	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 (412) 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:B:78:GLN:HE22	1:B:150:GLN:HE21	1.03	1.01
3:F:41:THR:HG23	3:F:43:PHE:H	1.27	1.00
1:B:268:ASN:HD21	1:B:327:GLU:H	1.09	0.98
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.13	0.89
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.21	0.88
1:A:44:THR:HG22	1:A:46:TYR:H	1.37	0.88
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.54	0.87
3:F:40:THR:O	3:F:41:THR:HG22	1.75	0.87
1:B:209:GLU:HA	1:B:213:THR:HB	1.56	0.85
1:A:467:GLN:HG3	6:A:5243:HOH:O	1.79	0.82
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.26	0.82
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.63	0.80
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.61	0.80
1:B:44:THR:HG22	1:B:46:TYR:H	1.47	0.80
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.64	0.79
1:A:209:GLU:HA	1:A:213:THR:HB	1.63	0.79
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.79
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.63	0.79
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.64	0.79
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.65	0.79
3:E:41:THR:O	3:E:44:ARG:HD2	1.85	0.76
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.86	0.76
1:A:268:ASN:HD21	1:A:327:GLU:H	1.30	0.76
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:MET:O	1:B:410:GLU:HG3	1.85	0.76
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.51	0.75
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.70	0.73
1:A:406:MET:O	1:A:410:GLU:HG3	1.89	0.73
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.82	0.73
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.36	0.73
3:F:133:ARG:HH11	3:F:133:ARG:HB3	1.55	0.72
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.73	0.71
3:E:24:THR:HG22	3:E:27:LYS:H	1.56	0.71
1:A:227:ASN:HD21	1:A:295:LYS:H	1.39	0.71
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.70
1:B:244:LEU:HG	6:B:5195:HOH:O	1.92	0.69
2:C:6:GLU:HG3	6:C:5263:HOH:O	1.91	0.69
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.22	0.69
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.93	0.69
1:B:24:ASN:OD1	1:B:26:GLN:HG2	1.94	0.68
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.58	0.68
1:B:227:ASN:HD21	1:B:295:LYS:H	1.40	0.68
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.40	0.67
1:B:288:MET:HE1	1:B:346:LEU:CB	2.24	0.67
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.75	0.67
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.67
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.43	0.66
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.93	0.66
2:D:111:LYS:O	2:D:115:GLU:HG3	1.95	0.66
3:F:41:THR:O	3:F:44:ARG:HD2	1.96	0.66
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.66
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.95	0.65
1:B:268:ASN:ND2	1:B:327:GLU:H	1.91	0.65
1:B:288:MET:CE	1:B:346:LEU:HB3	2.26	0.65
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.79	0.65
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.27	0.64
3:F:58:ALA:O	3:F:62:GLU:HG3	1.97	0.64
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.64
3:E:98:MET:O	3:E:98:MET:HE2	1.97	0.64
3:F:153:GLU:CD	3:F:153:GLU:H	2.02	0.63
1:B:288:MET:HE1	1:B:346:LEU:CG	2.29	0.63
2:D:145:ILE:O	2:D:149:TRP:HB3	1.98	0.63
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.98	0.63
2:D:217:GLU:O	2:D:221:GLY:HA3	1.99	0.63
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.99	0.63
1:A:244:LEU:HG	6:A:5166:HOH:O	1.98	0.63
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.80	0.62
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.00	0.62
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.63	0.62
1:A:140:GLN:O	1:A:144:GLU:HG2	2.00	0.62
1:A:268:ASN:ND2	1:A:327:GLU:H	1.98	0.62
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.64	0.62
1:B:288:MET:HE1	1:B:346:LEU:HG	1.81	0.62
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.30	0.61
1:B:240:GLU:HG2	6:B:5194:HOH:O	1.99	0.61
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.61
3:E:57:GLU:O	3:E:61:GLU:HG3	1.98	0.61
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.82	0.61
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.82	0.61
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.61
3:F:15:TRP:O	3:F:19:ILE:HG23	2.01	0.60
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.34	0.60
2:C:111:LYS:O	2:C:115:GLU:HG3	2.01	0.60
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.35	0.60
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.83	0.59
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.65	0.59
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.02	0.59
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.83	0.59
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.02	0.59
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.03	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.02	0.59
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.03	0.59
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.94	0.59
1:B:212:PHE:O	1:B:215:PRO:HD2	2.03	0.58
1:B:333:LYS:HG3	6:B:5108:HOH:O	2.02	0.58
2:C:97:LYS:HD2	6:C:5135:HOH:O	2.03	0.58
1:B:269:THR:HG23	6:B:5224:HOH:O	2.02	0.58
3:F:13:ASP:O	3:F:16:VAL:HG22	2.03	0.58
1:B:227:ASN:ND2	1:B:295:LYS:H	2.01	0.58
1:A:109:PHE:O	1:A:112:VAL:HG12	2.04	0.58
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.38	0.58
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.13	0.57
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.86	0.57
2:D:228:ARG:O	2:D:232:GLU:HG3	2.04	0.57
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.85	0.57
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.50	0.57
1:B:192:PHE:O	1:B:200:CYS:HB3	2.05	0.57
1:B:18:ARG:O	2:D:129:ALA:HA	2.04	0.57
1:B:51:LYS:HG3	6:B:5199:HOH:O	2.04	0.57
1:A:313:TRP:CZ3	1:A:318:ILE:HD11	2.40	0.56
1:B:33:GLN:HE22	1:B:132:GLU:H	1.50	0.56
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.88	0.56
1:B:123:MET:CE	1:B:197:ALA:HA	2.34	0.56
2:D:153:LEU:HD12	2:D:153:LEU:C	2.26	0.56
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.88	0.56
2:C:179:LEU:HD12	2:C:182:TRP:CE3	2.41	0.56
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.71	0.56
3:F:41:THR:HG23	3:F:43:PHE:N	2.10	0.56
3:E:58:ALA:O	3:E:62:GLU:HG3	2.06	0.56
1:A:227:ASN:ND2	1:A:295:LYS:H	2.04	0.55
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.41	0.55
1:B:268:ASN:HD21	1:B:327:GLU:N	1.92	0.55
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.40	0.55
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.87	0.55
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.07	0.55
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.89	0.55
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.37	0.55
1:A:213:THR:O	1:A:217:ILE:HG12	2.06	0.55
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.89	0.54
1:B:337:GLN:HG3	1:B:338:ASP:N	2.23	0.54
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.07	0.54
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.72	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.36	0.54
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.54
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.42	0.54
1:B:33:GLN:NE2	1:B:132:GLU:H	2.05	0.54
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.90	0.54
1:A:314:GLY:HA2	1:A:318:ILE:HD12	1.89	0.54
6:C:5103:HOH:O	3:E:125:VAL:HG22	2.07	0.54
3:E:18:LYS:HB2	3:E:18:LYS:NZ	2.23	0.54
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.23	0.53
2:C:350:GLU:HB3	6:C:5197:HOH:O	2.08	0.53
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.08	0.53
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:HD21	1:A:327:GLU:N	2.05	0.53
3:F:61:GLU:O	3:F:121:PRO:HG2	2.08	0.53
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.43	0.53
1:B:115:TYR:OH	2:D:173:ASP:HA	2.08	0.53
1:B:198:VAL:O	1:B:202:LEU:HG	2.08	0.53
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.09	0.53
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.90	0.53
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.91	0.53
2:D:143:GLU:O	2:D:147:ARG:HB3	2.09	0.53
1:B:244:LEU:HB2	6:B:5234:HOH:O	2.09	0.53
1:B:123:MET:HE3	1:B:197:ALA:HA	1.90	0.53
1:A:53:ALA:HB1	6:A:5184:HOH:O	2.09	0.52
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.09	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.92	0.52
2:C:333:ARG:HD2	6:C:5230:HOH:O	2.08	0.52
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.10	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.05	0.52
1:A:313:TRP:CH2	1:A:318:ILE:HD11	2.44	0.52
1:A:110:LEU:O	1:A:114:GLU:HG2	2.09	0.52
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.52
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.91	0.52
1:B:269:THR:HG21	6:F:369:HOH:O	2.08	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.91	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.44	0.52
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.44	0.52
2:D:187:ILE:O	2:D:191:GLN:HG3	2.10	0.52
1:B:30:ARG:HH11	1:B:30:ARG:HG2	1.75	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.92	0.51
3:F:125:VAL:HG23	3:F:126:ASN:N	2.25	0.51
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.93	0.51
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.88	0.51
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.28	0.51
2:D:240:ASP:HB2	3:F:125:VAL:HG21	1.92	0.51
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.92	0.51
3:F:57:GLU:O	3:F:61:GLU:HG3	2.11	0.51
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.76	0.51
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.93	0.51
3:E:41:THR:O	3:E:44:ARG:CD	2.56	0.51
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.25	0.51
1:B:288:MET:HE1	1:B:346:LEU:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:365:GLU:HG3	6:C:5210:HOH:O	2.09	0.51
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.93	0.51
1:A:204:LEU:O	1:A:209:GLU:HG3	2.10	0.50
1:B:490:SER:OG	2:D:32:ASN:HB2	2.10	0.50
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.11	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.10	0.50
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.47	0.50
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.45	0.50
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.47	0.50
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.26	0.50
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.09	0.50
1:A:252:GLN:HB3	6:A:5045:HOH:O	2.11	0.50
1:A:160:LYS:HE3	6:A:5061:HOH:O	2.10	0.50
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.12	0.50
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.46	0.50
1:A:435:THR:HG22	3:E:168:SER:HA	1.93	0.50
1:A:413:HIS:HD2	1:A:428:SER:OG	1.95	0.50
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.76	0.50
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.04	0.50
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.12	0.50
3:F:33:LYS:O	3:F:37:MET:HG2	2.11	0.50
1:A:186:ARG:HA	2:C:73:THR:OG1	2.12	0.50
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.94	0.50
2:D:54:VAL:O	2:D:55:TYR:HB2	2.11	0.50
2:C:54:VAL:O	2:C:55:TYR:HB2	2.12	0.50
1:A:338:ASP:OD1	1:A:433:ALA:HB2	2.11	0.49
2:D:82:SER:O	2:D:168:ARG:NH2	2.45	0.49
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.30	0.49
2:C:98:HIS:HE1	2:C:178:SER:OG	1.94	0.49
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.47	0.49
1:A:26:GLN:HG2	6:A:5178:HOH:O	2.10	0.49
1:B:367:GLU:HG3	6:B:5018:HOH:O	2.12	0.49
3:F:19:ILE:C	3:F:19:ILE:HD12	2.33	0.49
2:D:324:TRP:C	2:D:327:PRO:HD2	2.33	0.49
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.49
1:A:243:GLU:O	1:A:247:MET:HG2	2.13	0.49
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.49
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.27	0.48
2:C:211:THR:C	2:C:214:PRO:HD2	2.34	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.13	0.48
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.96	0.48
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.44	0.48
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.95	0.48
3:E:22:LEU:HD11	3:E:31:MET:SD	2.53	0.48
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.44	0.48
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.78	0.48
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.49	0.48
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.77	0.48
3:E:46:SER:OG	3:E:48:GLU:HG2	2.14	0.48
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.77	0.48
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.48	0.48
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.49	0.48
1:A:402:PHE:O	1:A:403:ILE:HD12	2.14	0.48
1:B:186:ARG:HD3	1:B:186:ARG:C	2.34	0.48
1:A:192:PHE:O	1:A:200:CYS:HB3	2.14	0.48
1:A:159:ALA:O	2:C:33:ASN:HB2	2.14	0.47
1:A:466:CYS:HB2	2:C:73:THR:HA	1.95	0.47
1:A:451:GLN:HB2	3:E:152:LEU:HD11	1.95	0.47
1:B:196:ASP:HB2	3:F:140:MET:SD	2.55	0.47
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.47
1:B:128:ALA:O	1:B:134:LYS:HE2	2.14	0.47
2:D:184:PHE:O	2:D:187:ILE:HG22	2.15	0.47
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.47
1:B:251:TYR:HE2	1:B:320:ARG:HH12	1.62	0.47
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.50	0.47
2:C:118:ARG:NH2	2:D:111:LYS:HD3	2.29	0.47
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.49	0.47
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.97	0.47
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.50	0.47
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.50	0.46
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.50	0.46
3:F:105:TRP:O	3:F:109:LYS:HG3	2.15	0.46
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.97	0.46
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.97	0.46
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.97	0.46
1:B:213:THR:O	1:B:217:ILE:HG12	2.14	0.46
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.50	0.46
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.46
1:A:81:SER:OG	1:B:84:ASP:HB3	2.15	0.46
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:THR:HB	2:D:278:PRO:HD3	1.98	0.46
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.51	0.46
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.69	0.46
1:A:248:ALA:O	1:A:252:GLN:HB2	2.16	0.46
1:B:49:LYS:CD	3:F:144:ASN:HD22	2.29	0.45
1:B:334:ASP:HA	1:B:337:GLN:HG2	1.99	0.45
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.46	0.45
1:A:163:GLN:O	2:C:28:PRO:HA	2.16	0.45
1:A:163:GLN:HG2	6:A:5119:HOH:O	2.15	0.45
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.45
1:B:41:ASN:O	2:D:236:GLN:HB3	2.17	0.45
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.98	0.45
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.50	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.32	0.45
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:A:343:HIS:H	1:A:343:HIS:CD2	2.35	0.45
3:F:132:GLU:HG3	6:F:352:HOH:O	2.16	0.45
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.52	0.44
2:D:98:HIS:CD2	2:D:99:ARG:N	2.84	0.44
1:A:115:TYR:OH	2:C:173:ASP:HA	2.17	0.44
2:D:329:ILE:HG23	2:D:384:VAL:HG22	1.98	0.44
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.52	0.44
1:B:230:GLU:C	1:B:233:PRO:HD2	2.37	0.44
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.29	0.44
1:A:435:THR:HG22	3:E:169:PRO:HD3	2.00	0.44
1:B:403:ILE:HG22	1:B:406:MET:SD	2.58	0.44
2:D:105:TRP:O	2:D:108:PRO:HD2	2.16	0.44
1:B:30:ARG:NH1	1:B:30:ARG:HG2	2.32	0.44
1:B:125:TRP:C	1:B:125:TRP:CD1	2.90	0.44
2:D:292:LYS:HE3	2:D:366:ASP:OD2	2.18	0.44
1:A:521:ASN:HB3	1:A:524:LYS:HG2	2.00	0.44
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.44
1:B:252:GLN:HG3	6:B:5206:HOH:O	2.18	0.44
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.52	0.44
2:D:324:TRP:O	2:D:327:PRO:HD2	2.18	0.44
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.47	0.44
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.44
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.53	0.44
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.43
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:74:GLU:O	3:F:78:ARG:HG3	2.17	0.43
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.33	0.43
2:D:239:PHE:HB2	3:F:126:ASN:HA	2.00	0.43
1:B:288:MET:CE	1:B:347:TYR:N	2.82	0.43
1:A:323:LYS:HE2	1:A:324:TYR:CZ	2.53	0.43
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.19	0.43
1:B:468:ASN:OD1	1:B:471:GLU:HG3	2.18	0.43
2:D:352:ILE:HD11	2:D:388:LEU:HD11	2.01	0.43
2:D:138:PRO:HA	2:D:141:ARG:HH12	1.82	0.43
1:A:56:THR:CG2	1:A:252:GLN:HE21	2.32	0.43
1:A:89:LEU:HD21	1:B:230:GLU:HG3	2.00	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.65	0.43
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.43
1:B:476:ARG:HH11	1:B:476:ARG:HG3	1.83	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.52	0.42
1:A:44:THR:OG1	1:A:127:SER:HA	2.19	0.42
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.83	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.19	0.42
1:B:227:ASN:HD21	1:B:296:PHE:H	1.67	0.42
2:C:33:ASN:HD22	2:C:33:ASN:N	2.16	0.42
1:B:468:ASN:CG	1:B:471:GLU:HG3	2.40	0.42
1:B:36:ASN:HD21	1:B:42:ASN:HD21	1.66	0.42
2:D:226:SER:HB2	2:D:331:ALA:HA	2.01	0.42
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.54	0.42
1:B:140:GLN:O	1:B:144:GLU:HG2	2.19	0.42
3:E:66:VAL:CG1	3:E:70:ARG:HH21	2.31	0.42
3:F:33:LYS:HE3	3:F:117:ALA:HB2	2.02	0.42
2:D:312:TYR:O	2:D:316:VAL:HG23	2.20	0.42
3:E:12:ARG:O	3:E:16:VAL:HG23	2.19	0.42
3:F:40:THR:O	3:F:41:THR:CG2	2.58	0.42
3:E:98:MET:HE2	3:E:138:ARG:HG2	2.00	0.42
1:B:123:MET:HE2	1:B:197:ALA:HA	2.00	0.42
2:D:352:ILE:HG13	2:D:353:THR:N	2.34	0.42
1:A:84:ASP:HB3	1:B:81:SER:OG	2.20	0.42
2:D:357:TYR:CE1	2:D:381:VAL:HG21	2.55	0.42
2:D:266:GLN:HA	2:D:266:GLN:HE21	1.84	0.42
1:B:316:ILE:O	1:B:320:ARG:HG3	2.20	0.42
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.54	0.42
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.42
2:D:291:ALA:HB2	6:D:431:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.37	0.42
1:B:209:GLU:HA	1:B:213:THR:CB	2.40	0.42
1:B:460:GLU:HB3	1:B:463:ARG:HG3	2.02	0.42
1:A:21:THR:HG22	2:C:128:SER:CB	2.50	0.42
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.55	0.42
2:D:98:HIS:CD2	2:D:99:ARG:H	2.38	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.02	0.42
1:A:430:ALA:HA	6:A:5265:HOH:O	2.19	0.42
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.17	0.41
1:B:491:ASP:O	1:B:493:LYS:HG3	2.20	0.41
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.01	0.41
1:B:162:GLY:HA3	6:B:5040:HOH:O	2.19	0.41
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.56	0.41
1:A:18:ARG:O	2:C:129:ALA:HA	2.20	0.41
1:A:284:PRO:HB3	1:A:342:ALA:HB1	2.02	0.41
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.50	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
1:A:207:VAL:HG11	1:A:275:PHE:HA	2.02	0.41
2:D:310:SER:O	2:D:314:ARG:HG3	2.21	0.41
1:B:403:ILE:HG23	1:B:406:MET:HG3	2.02	0.41
1:A:283:THR:HB	1:A:284:PRO:HD3	2.03	0.41
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.86	0.41
1:A:193:ILE:HD11	2:C:82:SER:HB3	2.02	0.41
2:C:184:PHE:O	2:C:187:ILE:HG22	2.20	0.41
1:A:90:ASN:HA	1:A:90:ASN:HD22	1.61	0.41
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.01	0.41
3:F:88:LYS:O	3:F:92:ASP:OD1	2.38	0.41
2:C:306:ASP:O	2:C:310:SER:HB2	2.19	0.41
2:D:256:PHE:HA	2:D:332:LEU:HD21	2.03	0.41
1:A:124:LEU:HD21	1:A:201:SER:HB2	2.02	0.41
1:B:288:MET:HE1	1:B:347:TYR:N	2.36	0.41
1:B:246:HIS:N	1:B:246:HIS:CD2	2.88	0.41
1:A:65:LYS:HE2	2:C:192:MET:HE2	2.02	0.41
1:A:123:MET:SD	2:C:168:ARG:NH1	2.94	0.41
2:D:226:SER:CB	2:D:331:ALA:HA	2.50	0.41
1:A:354:TRP:N	1:A:355:PRO:CD	2.84	0.41
2:C:316:VAL:O	2:C:319:ASN:HB3	2.21	0.41
3:F:73:ASN:ND2	3:F:76:ASP:OD2	2.54	0.41
2:D:355:SER:O	2:D:358:ARG:HB2	2.21	0.41
2:D:102:LEU:HB2	2:D:104:ARG:HD2	2.04	0.41
3:F:16:VAL:HG23	3:F:17:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.56	0.41
3:E:59:LYS:HA	3:E:59:LYS:HD3	1.93	0.41
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.02	0.41
2:D:145:ILE:HG22	2:D:146:ASN:N	2.36	0.40
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.03	0.40
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.49	0.40
3:F:33:LYS:HB2	3:F:83:PHE:HZ	1.86	0.40
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.56	0.40
1:B:320:ARG:HB3	1:B:320:ARG:NH1	2.35	0.40
2:C:266:GLN:HB2	2:C:281:ILE:HG21	2.04	0.40
2:D:306:ASP:HA	2:D:307:PRO:HD3	1.90	0.40
1:B:403:ILE:CG2	1:B:406:MET:HG3	2.52	0.40
2:D:224:TYR:O	2:D:227:ALA:HB3	2.21	0.40
1:A:230:GLU:C	1:A:233:PRO:HD2	2.42	0.40
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.70	0.40
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.56	0.40
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.56	0.40
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.51	0.40
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.54	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	509/527 (97%)	486 (96%)	23 (4%)	0	100	100
1	B	508/527 (96%)	480 (94%)	26 (5%)	2 (0%)	39	34
2	C	386/389 (99%)	376 (97%)	8 (2%)	2 (0%)	34	26
2	D	385/389 (99%)	362 (94%)	19 (5%)	4 (1%)	19	11
3	E	165/170 (97%)	162 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	166/170 (98%)	160 (96%)	5 (3%)	1 (1%)	30	21
All	All	2119/2172 (98%)	2026 (96%)	84 (4%)	9 (0%)	39	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	64	ALA
3	F	122	ILE
1	B	40	LYS
2	D	252	TYR
2	C	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%)	424 (98%)	9 (2%)	61	65
1	B	432/442 (98%)	424 (98%)	8 (2%)	65	69
2	C	322/323 (100%)	318 (99%)	4 (1%)	78	83
2	D	321/323 (99%)	314 (98%)	7 (2%)	60	63
3	E	145/147 (99%)	140 (97%)	5 (3%)	44	42
3	F	145/147 (99%)	141 (97%)	4 (3%)	51	52
All	All	1798/1824 (99%)	1761 (98%)	37 (2%)	61	65

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG

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Mol	Chain	Res	Type
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	467	GLN
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	334	ASP
1	B	440	GLU
2	C	33	ASN
2	C	35	MET
2	C	173	ASP
2	C	356	LEU
2	D	4	LEU
2	D	35	MET
2	D	80	ARG
2	D	145	ILE
2	D	173	ASP
2	D	266	GLN
2	D	372	ASP
3	E	24	THR
3	E	44	ARG
3	E	46	SER
3	E	60	LEU
3	E	138	ARG
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	83	GLN

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Mol	Chain	Res	Type
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	411	ASN
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	26	GLN
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
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

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Mol	Chain	Res	Type
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	125	GLN
2	D	155	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
2	D	379	GLN
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	99	ASN
3	F	144	ASN
3	F	158	GLN
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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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	511/527 (96%)	-0.14	9 (1%) 71 79	18, 30, 51, 74	0
1	B	510/527 (96%)	-0.19	14 (2%) 58 67	19, 32, 52, 66	0
2	C	388/389 (99%)	-0.41	6 (1%) 76 82	15, 23, 39, 58	0
2	D	387/389 (99%)	0.34	30 (7%) 16 22	20, 40, 64, 73	0
3	E	167/170 (98%)	-0.41	4 (2%) 62 71	17, 26, 41, 74	0
3	F	168/170 (98%)	0.69	19 (11%) 7 11	32, 50, 68, 76	0
All	All	2131/2172 (98%)	-0.07	82 (3%) 44 54	15, 32, 58, 76	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	380	ILE	5.2
1	B	316	ILE	4.4
3	E	169	PRO	4.1
1	A	244	LEU	4.1
2	D	205	PRO	4.0
2	D	44	LYS	3.7
3	F	67	LEU	3.7
3	F	83	PHE	3.6
1	A	17	ASN	3.6
3	F	23	ASN	3.3
2	D	352	ILE	3.3
2	D	388	LEU	3.3
1	B	244	LEU	3.2
2	C	389	LYS	3.2
2	D	348	ASP	3.1
2	D	385	LEU	3.1
2	C	2	SER	3.1
2	D	375	ALA	3.0
3	F	28	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	100	ALA	3.0
1	A	316	ILE	3.0
3	F	25	LEU	3.0
3	F	70	ARG	3.0
3	F	20	ALA	2.9
1	A	310	TYR	2.9
2	D	45	ARG	2.8
1	B	40	LYS	2.8
1	B	54	ASN	2.8
2	C	6	GLU	2.7
3	F	80	LYS	2.7
3	E	4	LEU	2.7
1	A	19	ALA	2.7
2	C	45	ARG	2.7
1	B	311	GLU	2.7
2	D	345	GLY	2.6
3	F	101	ALA	2.6
1	B	39	PHE	2.6
1	B	55	GLU	2.6
1	B	527	ASN	2.5
2	D	339	PHE	2.5
3	F	4	LEU	2.5
2	D	374	LYS	2.5
2	D	203	ILE	2.5
3	F	17	ASN	2.4
1	A	319	GLY	2.4
1	B	333	LYS	2.4
3	F	27	LYS	2.4
3	F	170	HIS	2.4
3	F	14	ALA	2.3
2	D	254	ALA	2.3
3	E	168	SER	2.3
2	D	153	LEU	2.3
1	B	320	ARG	2.3
2	D	343	PRO	2.2
3	F	16	VAL	2.2
1	B	259	ASN	2.2
1	A	320	ARG	2.2
2	C	205	PRO	2.2
2	D	350	GLU	2.2
2	D	256	PHE	2.2
2	D	382	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	21	GLN	2.2
1	B	514	ARG	2.2
2	D	357	TYR	2.2
2	C	44	LYS	2.2
1	A	54	ASN	2.1
2	D	260	VAL	2.1
2	D	376	ASP	2.1
3	F	41	THR	2.1
2	D	377	ARG	2.1
3	E	153	GLU	2.1
1	A	434	SER	2.1
2	D	206	GLY	2.1
2	D	344	ALA	2.1
2	D	251	VAL	2.1
3	F	89	SER	2.1
2	D	220	ASN	2.1
2	D	222	GLU	2.0
2	D	384	VAL	2.0
1	B	319	GLY	2.0
2	D	372	ASP	2.0
1	B	310	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
4	FE2	A	5002	1/1	0.58	0.08	-1.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	A	5005	1/1	0.98	0.07	-1.35	37,37,37,37	0
4	FE2	A	5001	1/1	0.95	0.04	-2.05	37,37,37,37	0
4	FE2	B	5004	1/1	0.94	0.06	-3.45	66,66,66,66	0
4	FE2	B	5003	1/1	0.98	0.03	-6.74	34,34,34,34	0
5	CA	C	5006	1/1	0.92	0.07	-	53,53,53,53	0
5	CA	C	5008	1/1	0.91	0.08	-	55,55,55,55	0
5	CA	C	5007	1/1	0.98	0.05	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.