Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 06:11 PM EST

PDB ID	:	1FZ0
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM II MIXED-VALENT GROWN ANAEROBICALLY
Authors	:	Whittington, D.A.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	2.07 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

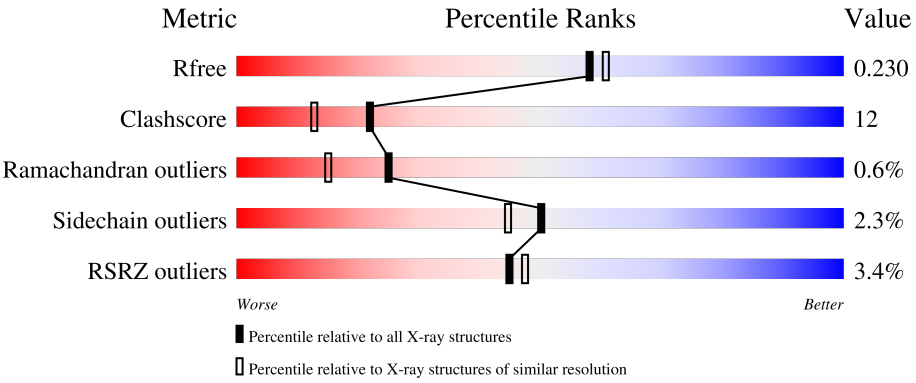
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	75% 20%
1	B	527	4% 71% 24%
2	C	389	80% 19%
2	D	389	6% 72% 26%
3	E	170	2% 79% 16%

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Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18857 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	A	2	Total Fe 2 2	0	0
4	B	2	Total Fe 2 2	0	0

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

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

- Molecule 6 is water.

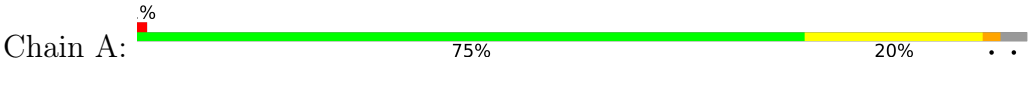
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	305	Total O 305 305	0	0
6	B	280	Total O 280 280	0	0
6	C	326	Total O 326 326	0	0
6	D	178	Total O 178 178	0	0
6	E	185	Total O 185 185	0	0
6	F	69	Total O 69 69	0	0

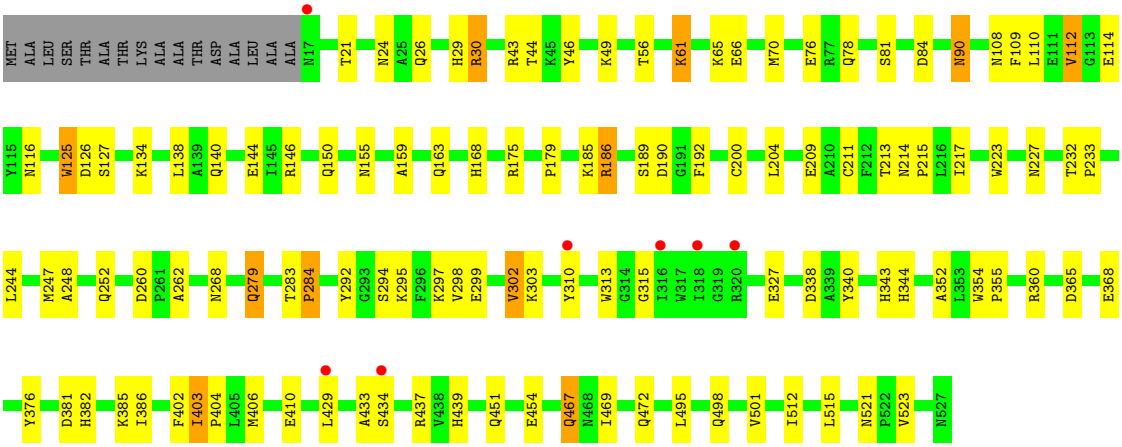
3 Residue-property plots (i)

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

• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

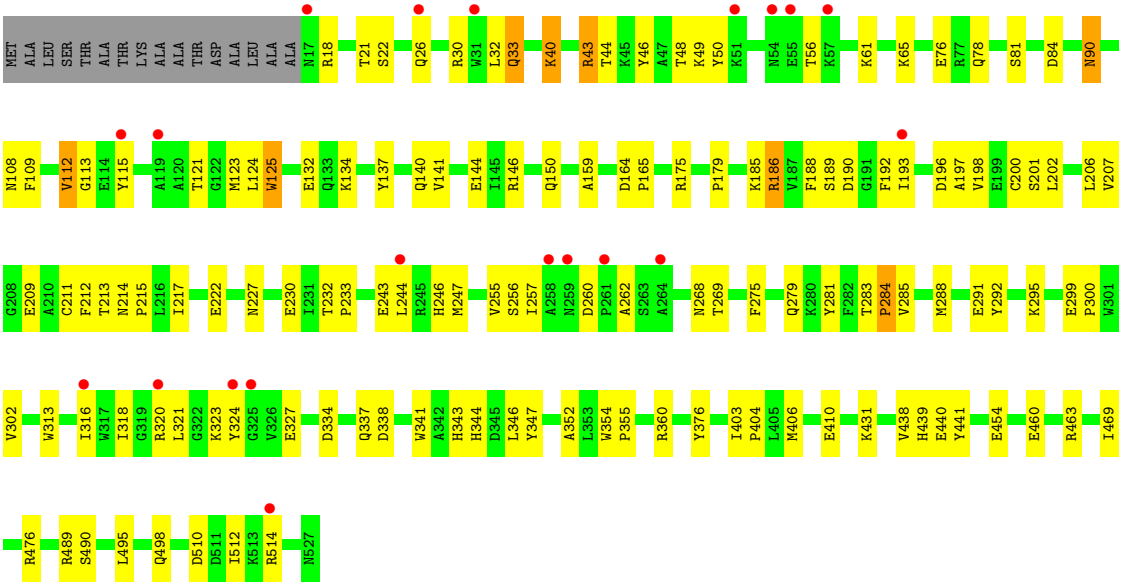
Chain A:





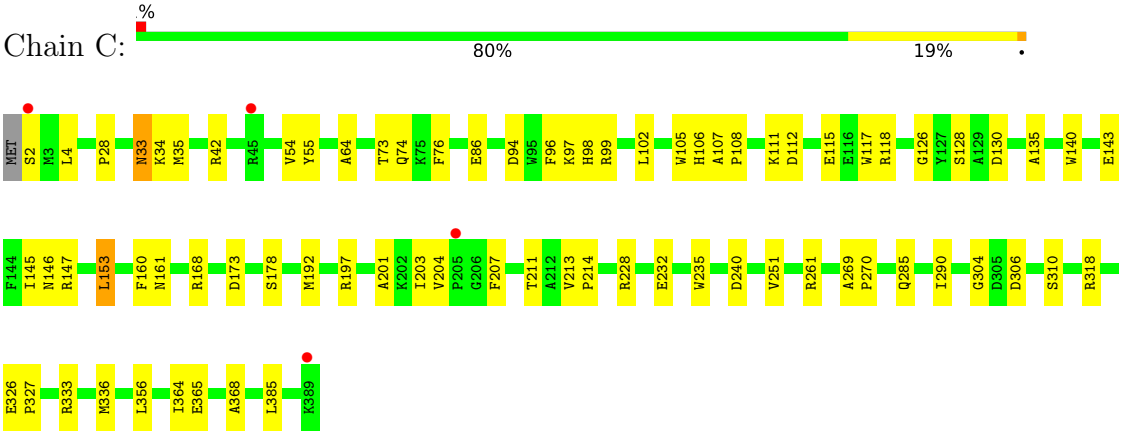
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:



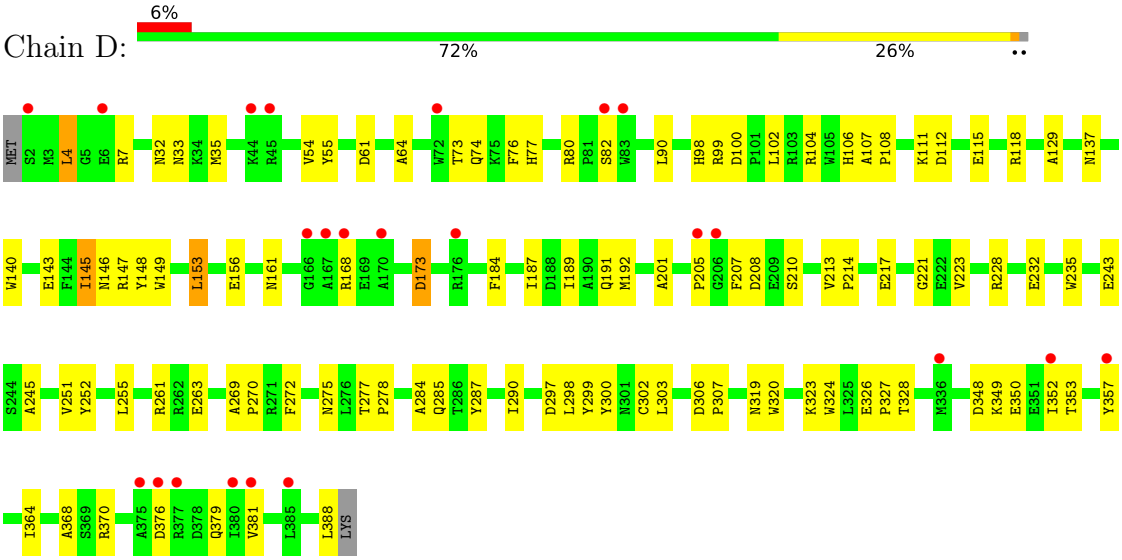
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:



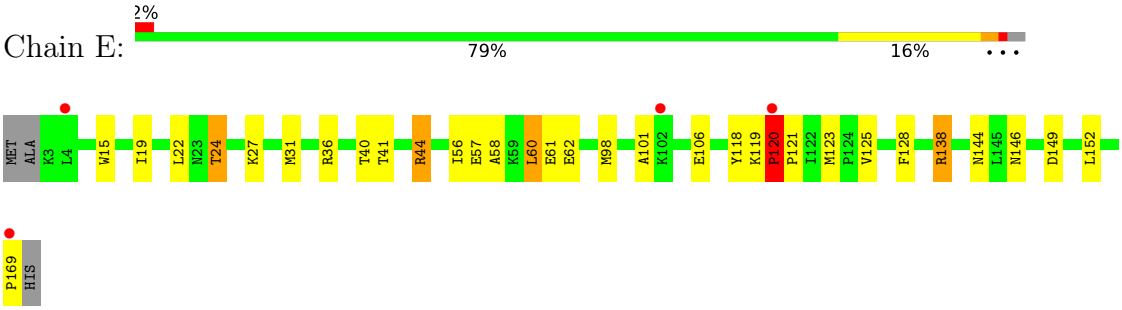
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



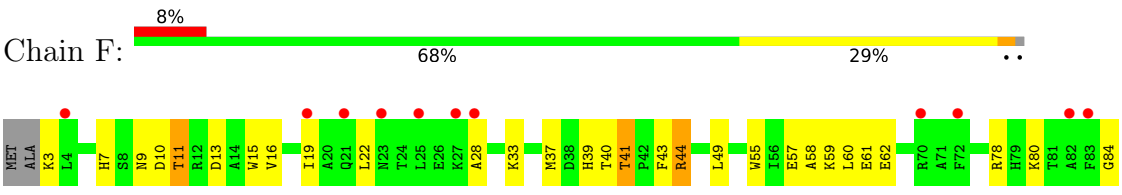
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

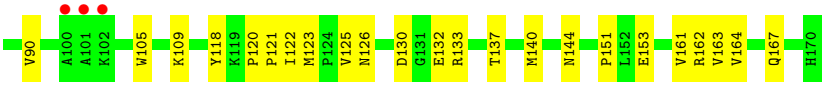
Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:




V90
A100
A101
K102
W105
K109
Y118
K119
P120
P121
I122
M123
P124
V125
N126
D130
G131
E132
R133
T137
M140
N144
P151
L152
E153
V161
R162
V163
V164
Q167
H170

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.42Å 171.71Å 221.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.07 49.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.07) 92.5 (49.19-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.230 0.194 , 0.230	Depositor DCC
R_{free} test set	5537 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18857	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.56	0/5853
1	B	0.33	0/4310	0.55	0/5853
2	C	0.37	0/3289	0.57	0/4464
2	D	0.32	0/3279	0.52	0/4453
3	E	0.34	0/1404	0.61	0/1892
3	F	0.28	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

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	97	0
1	B	4185	0	3981	138	0
2	C	3193	0	3042	66	0
2	D	3183	0	3029	85	0
3	E	1375	0	1370	30	0
3	F	1386	0	1377	44	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	305	0	0	6	0
6	B	280	0	0	7	0
6	C	326	0	0	10	0
6	D	178	0	0	1	0
6	E	185	0	0	0	0
6	F	69	0	0	3	0
All	All	18857	0	16780	403	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 (403) 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:78:GLN:HE22	1:A:150:GLN:HE21	1.06	0.99
3:F:41:THR:HG23	3:F:43:PHE:H	1.27	0.98
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.45	0.97
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.14	0.95
1:A:44:THR:HG22	1:A:46:TYR:H	1.37	0.88
1:B:44:THR:HG22	1:B:46:TYR:H	1.40	0.87
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.22	0.85
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.24	0.83
1:A:268:ASN:HD21	1:A:327:GLU:H	1.24	0.83
1:A:467:GLN:HG3	6:A:5266:HOH:O	1.78	0.82
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.59	0.81
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.63	0.80
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.30	0.79
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.63	0.78
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.33	0.77
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.82	0.77
1:A:30:ARG:O	1:A:30:ARG:HD3	1.86	0.76
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.87	0.75
1:A:209:GLU:HA	1:A:213:THR:HB	1.69	0.75
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.18	0.74
1:B:209:GLU:HA	1:B:213:THR:HB	1.68	0.73
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.69	0.73
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.71	0.73
3:F:40:THR:O	3:F:41:THR:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.71	0.72
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.72
3:E:41:THR:O	3:E:44:ARG:HD2	1.88	0.72
1:B:268:ASN:HD21	1:B:327:GLU:H	1.38	0.71
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.55	0.71
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.72	0.71
2:D:145:ILE:O	2:D:149:TRP:HB3	1.90	0.71
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.90	0.71
3:E:24:THR:HG22	3:E:27:LYS:H	1.54	0.71
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.21	0.70
1:B:227:ASN:HD21	1:B:295:LYS:H	1.39	0.69
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.74	0.69
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.74	0.69
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.56	0.68
1:A:29:HIS:ND1	1:A:61:LYS:HG3	2.08	0.68
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.39	0.68
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.24	0.68
1:B:26:GLN:HE21	1:B:61:LYS:HD2	1.58	0.68
3:E:98:MET:O	3:E:98:MET:HE2	1.93	0.68
1:B:489:ARG:HD2	1:B:495:LEU:O	1.95	0.67
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.77	0.67
1:A:76:GLU:HG3	1:B:76:GLU:HG2	1.76	0.67
1:A:406:MET:O	1:A:410:GLU:HG3	1.95	0.67
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.77	0.67
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.78	0.67
1:B:33:GLN:HE22	1:B:132:GLU:H	1.43	0.66
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.31	0.66
3:F:57:GLU:O	3:F:61:GLU:HG3	1.96	0.66
3:E:22:LEU:HD11	3:E:31:MET:SD	2.36	0.66
3:F:58:ALA:O	3:F:62:GLU:HG3	1.95	0.66
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.61	0.66
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.43	0.65
3:F:41:THR:O	3:F:44:ARG:HD2	1.97	0.65
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.32	0.65
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.89	0.64
2:C:318:ARG:HD2	6:C:5143:HOH:O	1.97	0.64
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.79	0.64
3:E:120:PRO:HA	3:E:123:MET:O	1.98	0.64
3:E:120:PRO:HD3	3:E:128:PHE:CD2	2.32	0.64
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.63	0.64
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.82	0.63
1:B:288:MET:HE1	1:B:346:LEU:HG	1.80	0.63
2:D:153:LEU:C	2:D:153:LEU:HD12	2.20	0.62
2:D:140:TRP:NE1	2:D:145:ILE:HD13	2.14	0.62
3:F:153:GLU:H	3:F:153:GLU:CD	2.03	0.62
2:C:336:MET:CE	2:C:385:LEU:HD23	2.29	0.62
2:D:228:ARG:O	2:D:232:GLU:HG3	2.00	0.62
1:A:30:ARG:HD3	1:A:30:ARG:C	2.20	0.61
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.65	0.61
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.01	0.61
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.00	0.61
1:B:18:ARG:O	2:D:129:ALA:HA	2.00	0.60
1:B:288:MET:CE	1:B:346:LEU:HB3	2.30	0.60
1:B:30:ARG:O	1:B:30:ARG:HD3	2.01	0.60
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.83	0.60
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.93	0.60
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.01	0.60
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.01	0.60
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.83	0.59
1:B:288:MET:HE1	1:B:346:LEU:CB	2.31	0.59
1:B:192:PHE:O	1:B:200:CYS:HB3	2.03	0.59
2:D:111:LYS:O	2:D:115:GLU:HG3	2.01	0.59
1:B:406:MET:O	1:B:410:GLU:HG3	2.02	0.59
1:B:123:MET:CE	1:B:197:ALA:HA	2.33	0.59
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.84	0.59
1:A:213:THR:O	1:A:217:ILE:HG12	2.02	0.58
1:A:268:ASN:ND2	1:A:327:GLU:H	1.99	0.58
1:A:140:GLN:O	1:A:144:GLU:HG2	2.04	0.58
2:D:187:ILE:O	2:D:191:GLN:HG3	2.03	0.58
1:A:338:ASP:OD1	1:A:433:ALA:HB2	2.03	0.58
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.86	0.58
3:F:13:ASP:O	3:F:16:VAL:HG22	2.03	0.58
1:B:288:MET:HE1	1:B:346:LEU:CG	2.33	0.58
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.01	0.58
3:E:120:PRO:O	3:E:121:PRO:C	2.40	0.57
2:C:333:ARG:HD2	6:C:5283:HOH:O	2.04	0.57
2:C:365:GLU:HG2	6:C:5224:HOH:O	2.02	0.57
1:B:213:THR:O	1:B:217:ILE:HG12	2.04	0.57
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.34	0.57
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.85	0.57
2:D:145:ILE:HG22	2:D:146:ASN:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.39	0.57
1:A:227:ASN:HD21	1:A:295:LYS:H	1.51	0.57
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.68	0.57
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.87	0.57
1:B:227:ASN:ND2	1:B:295:LYS:H	2.02	0.57
3:F:3:LYS:HG3	3:F:10:ASP:OD2	2.05	0.57
2:C:118:ARG:NH2	2:D:111:LYS:HD3	2.20	0.57
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.05	0.57
1:A:76:GLU:CG	1:B:76:GLU:HG2	2.35	0.56
2:C:111:LYS:O	2:C:115:GLU:HG3	2.05	0.56
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.87	0.56
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.87	0.56
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.41	0.56
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.05	0.56
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.40	0.56
2:C:211:THR:O	2:C:214:PRO:HD2	2.06	0.56
1:B:244:LEU:HB2	6:B:5188:HOH:O	2.06	0.56
1:A:244:LEU:HB2	6:A:5302:HOH:O	2.06	0.56
3:F:61:GLU:O	3:F:121:PRO:HG2	2.07	0.55
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.90	0.55
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.88	0.55
2:C:97:LYS:HD2	6:C:5117:HOH:O	2.06	0.55
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.06	0.55
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.04	0.55
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.07	0.54
1:B:33:GLN:NE2	1:B:132:GLU:H	2.04	0.54
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.39	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	2.01	0.54
1:A:44:THR:OG1	1:A:127:SER:HA	2.08	0.54
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.90	0.54
1:A:252:GLN:HB3	6:A:5171:HOH:O	2.06	0.54
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.23	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.54
3:E:58:ALA:O	3:E:62:GLU:HG3	2.08	0.54
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.08	0.54
3:E:41:THR:O	3:E:44:ARG:CD	2.54	0.54
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.53
1:B:214:ASN:OD1	1:B:243:GLU:HG3	2.08	0.53
3:F:15:TRP:O	3:F:19:ILE:HG23	2.08	0.53
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.42	0.53
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.91	0.53
3:E:36:ARG:CZ	3:E:119:LYS:HB3	2.39	0.53
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.90	0.53
2:C:86:GLU:HB2	3:E:120:PRO:HG2	1.91	0.52
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.37	0.52
1:B:206:LEU:HB2	6:B:5202:HOH:O	2.09	0.52
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.90	0.52
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.56	0.52
6:D:452:HOH:O	3:F:125:VAL:HG22	2.09	0.52
1:B:288:MET:HE1	1:B:346:LEU:C	2.29	0.52
2:D:54:VAL:O	2:D:55:TYR:HB2	2.09	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.91	0.52
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.28	0.52
1:B:212:PHE:O	1:B:215:PRO:HD2	2.10	0.52
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.92	0.52
3:E:57:GLU:O	3:E:61:GLU:HG3	2.08	0.52
1:A:186:ARG:HA	2:C:73:THR:OG1	2.10	0.52
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.91	0.52
3:F:33:LYS:O	3:F:37:MET:HG2	2.09	0.52
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.13	0.51
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.75	0.51
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.44	0.51
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.41	0.51
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.11	0.51
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.45	0.51
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.93	0.51
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.46	0.51
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.26	0.51
1:A:163:GLN:O	2:C:28:PRO:HA	2.10	0.51
1:B:269:THR:HG21	6:F:185:HOH:O	2.11	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.11	0.51
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.58	0.51
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.46	0.51
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.11	0.51
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.10	0.50
2:D:82:SER:O	2:D:168:ARG:NH2	2.44	0.50
3:F:105:TRP:O	3:F:109:LYS:HG3	2.12	0.50
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.93	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.77	0.50
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.94	0.50
2:C:96:PHE:O	2:C:99:ARG:NH2	2.44	0.50
1:A:472:GLN:NE2	6:A:5266:HOH:O	2.45	0.50
1:B:198:VAL:O	1:B:202:LEU:HG	2.12	0.50
2:C:34:LYS:HD3	6:C:5264:HOH:O	2.12	0.50
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.93	0.50
1:B:123:MET:HE3	1:B:197:ALA:HA	1.94	0.50
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.92	0.50
1:B:185:LYS:O	1:B:189:SER:HB2	2.11	0.49
2:C:2:SER:HB2	6:C:5259:HOH:O	2.12	0.49
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.93	0.49
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.76	0.49
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.46	0.49
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.29	0.49
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.93	0.49
1:A:84:ASP:HB3	1:B:81:SER:OG	2.13	0.49
1:B:140:GLN:O	1:B:144:GLU:HG2	2.12	0.49
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.45	0.49
1:A:185:LYS:O	1:A:189:SER:HB2	2.13	0.49
1:A:434:SER:OG	3:E:169:PRO:HG3	2.12	0.49
2:C:143:GLU:O	2:C:147:ARG:HB3	2.13	0.49
3:E:120:PRO:O	3:E:123:MET:O	2.30	0.49
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.95	0.49
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.49
3:F:162:ARG:NH1	3:F:164:VAL:HG12	2.28	0.49
1:B:337:GLN:HG3	1:B:338:ASP:N	2.29	0.48
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.48
3:F:132:GLU:HG3	6:F:226:HOH:O	2.12	0.48
1:A:21:THR:HG22	2:C:128:SER:CB	2.43	0.48
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.48
2:D:298:LEU:O	2:D:302:CYS:HB2	2.14	0.48
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.95	0.47
2:C:153:LEU:C	2:C:153:LEU:HD12	2.34	0.47
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.95	0.47
1:A:61:LYS:HD3	1:A:61:LYS:N	2.29	0.47
1:B:334:ASP:HA	1:B:337:GLN:HG2	1.96	0.47
2:D:189:ILE:HD12	2:D:284:ALA:HB2	1.95	0.47
1:B:214:ASN:HD21	1:B:247:MET:CE	2.27	0.47
1:B:269:THR:HG23	6:B:5182:HOH:O	2.13	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HE2	2:C:192:MET:HE2	1.96	0.47
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.50	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.47
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.96	0.47
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.79	0.47
2:C:54:VAL:O	2:C:55:TYR:HB2	2.15	0.47
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.47
2:D:353:THR:O	2:D:357:TYR:HD1	1.97	0.47
1:B:123:MET:HE2	1:B:197:ALA:HA	1.96	0.47
1:B:196:ASP:HB2	3:F:140:MET:SD	2.55	0.47
2:D:98:HIS:CD2	2:D:99:ARG:N	2.82	0.47
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.15	0.47
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.68	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.50	0.47
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.15	0.47
6:C:5137:HOH:O	3:E:125:VAL:HG22	2.15	0.47
2:D:277:THR:HB	2:D:278:PRO:HD3	1.97	0.47
1:A:192:PHE:O	1:A:200:CYS:HB3	2.15	0.46
1:A:204:LEU:O	1:A:209:GLU:HG3	2.14	0.46
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.80	0.46
1:B:115:TYR:OH	2:D:173:ASP:HA	2.15	0.46
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.80	0.46
1:B:43:ARG:HD2	1:B:43:ARG:C	2.36	0.46
2:D:352:ILE:HG13	2:D:353:THR:N	2.30	0.46
1:A:66:GLU:O	1:A:70:MET:HG2	2.15	0.46
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.51	0.46
1:B:109:PHE:O	1:B:112:VAL:HG12	2.16	0.46
2:D:217:GLU:O	2:D:221:GLY:HA3	2.16	0.46
2:D:235:TRP:CD1	2:D:235:TRP:C	2.89	0.46
3:E:40:THR:C	3:E:41:THR:HG23	2.35	0.46
2:C:105:TRP:O	2:C:108:PRO:HD2	2.15	0.46
2:D:300:TYR:CE1	2:D:370:ARG:HG3	2.50	0.46
2:D:184:PHE:O	2:D:187:ILE:HG22	2.16	0.46
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.80	0.45
2:C:228:ARG:O	2:C:232:GLU:HG3	2.17	0.45
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.46	0.45
3:E:119:LYS:CG	3:E:120:PRO:HD2	2.46	0.45
3:F:39:HIS:HD2	6:F:231:HOH:O	1.99	0.45
2:C:306:ASP:O	2:C:310:SER:HB2	2.15	0.45
2:C:318:ARG:HG2	6:C:5277:HOH:O	2.17	0.45
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.80	0.45
2:D:269:ALA:N	2:D:270:PRO:CD	2.80	0.45
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.12	0.45
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.51	0.45
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.47	0.45
3:E:118:TYR:O	3:E:119:LYS:C	2.55	0.45
1:A:227:ASN:ND2	1:A:295:LYS:H	2.13	0.45
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.45
2:C:146:ASN:O	2:C:214:PRO:HG3	2.17	0.45
2:D:324:TRP:O	2:D:327:PRO:HD2	2.17	0.45
1:B:190:ASP:HB3	2:D:74:GLN:O	2.17	0.45
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.52	0.45
6:B:5026:HOH:O	2:C:365:GLU:HG3	2.17	0.45
1:B:283:THR:HB	1:B:284:PRO:HD3	1.98	0.44
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.44
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.32	0.44
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.52	0.44
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.52	0.44
1:A:214:ASN:ND2	1:A:247:MET:CE	2.80	0.44
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.99	0.44
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.98	0.44
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.02	0.44
3:F:19:ILE:HG21	3:F:60:LEU:HD12	2.00	0.44
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.31	0.44
1:B:232:THR:HB	1:B:233:PRO:HD3	1.99	0.44
1:A:44:THR:HG21	6:A:5173:HOH:O	2.18	0.44
1:B:44:THR:HG21	6:B:5171:HOH:O	2.17	0.44
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.51	0.44
1:B:209:GLU:HA	1:B:213:THR:CB	2.42	0.44
1:B:510:ASP:O	1:B:514:ARG:HG3	2.18	0.44
3:E:36:ARG:HH22	3:E:121:PRO:HD2	1.83	0.44
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.44
2:D:143:GLU:O	2:D:147:ARG:HB3	2.18	0.44
1:A:360:ARG:NH2	1:A:501:VAL:O	2.50	0.44
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.99	0.44
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.53	0.43
1:A:299:GLU:HG3	1:A:303:LYS:HD3	1.99	0.43
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.43
1:A:352:ALA:HA	1:A:404:PRO:CB	2.32	0.43
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.47	0.43
2:D:349:LYS:HA	2:D:352:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:CE1	1:A:61:LYS:HG3	2.52	0.43
1:B:316:ILE:O	1:B:320:ARG:HG3	2.19	0.43
2:C:135:ALA:HB3	6:C:5319:HOH:O	2.18	0.43
2:D:98:HIS:CD2	2:D:99:ARG:H	2.36	0.43
1:A:429:LEU:HG	1:A:429:LEU:O	2.19	0.43
1:B:165:PRO:HG3	6:B:5134:HOH:O	2.18	0.43
1:B:202:LEU:HD22	1:B:206:LEU:HD23	2.00	0.43
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.19	0.43
1:A:159:ALA:O	2:C:33:ASN:HB2	2.18	0.43
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.83	0.43
1:B:288:MET:CE	1:B:347:TYR:N	2.82	0.43
3:E:119:LYS:HG2	3:E:120:PRO:HD2	2.01	0.43
1:B:65:LYS:CE	2:D:192:MET:HE2	2.47	0.43
1:B:146:ARG:HB2	2:D:106:HIS:CD2	2.54	0.43
2:C:86:GLU:O	3:E:120:PRO:HG2	2.19	0.43
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.54	0.43
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.19	0.43
2:C:304:GLY:HA3	6:C:5113:HOH:O	2.19	0.43
2:D:255:LEU:HB2	2:D:328:THR:HG21	2.01	0.43
1:A:402:PHE:O	1:A:403:ILE:HD12	2.18	0.42
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.16	0.42
1:B:48:THR:O	3:F:137:THR:HG23	2.18	0.42
3:F:41:THR:O	3:F:44:ARG:CD	2.66	0.42
1:B:186:ARG:HD3	1:B:186:ARG:C	2.39	0.42
1:B:207:VAL:HG11	1:B:275:PHE:HA	2.01	0.42
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.98	0.42
2:C:270:PRO:HB3	2:D:270:PRO:HB3	2.01	0.42
2:D:306:ASP:HA	2:D:307:PRO:HD3	1.89	0.42
1:A:232:THR:HB	1:A:233:PRO:HD3	2.00	0.42
1:B:255:VAL:HG22	1:B:324:TYR:CZ	2.54	0.42
1:A:109:PHE:O	1:A:112:VAL:HG12	2.20	0.42
1:A:343:HIS:CD2	1:A:343:HIS:H	2.37	0.42
2:C:235:TRP:CD1	2:C:235:TRP:C	2.93	0.42
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.55	0.42
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.54	0.42
1:A:163:GLN:HG2	6:A:5220:HOH:O	2.19	0.42
1:A:248:ALA:O	1:A:252:GLN:HB2	2.20	0.42
1:A:294:SER:O	1:A:297:LYS:NZ	2.53	0.42
1:B:121:THR:HG21	1:B:140:GLN:HB3	2.01	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.15	0.42
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:C	1:B:32:LEU:HD23	2.40	0.42
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.19	0.42
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.50	0.42
1:B:30:ARG:HD3	1:B:30:ARG:C	2.41	0.42
1:B:49:LYS:HD3	3:F:140:MET:HB3	2.02	0.42
1:B:230:GLU:C	1:B:233:PRO:HD2	2.40	0.42
2:D:324:TRP:C	2:D:327:PRO:HD2	2.40	0.42
1:A:76:GLU:HG3	1:B:76:GLU:OE2	2.20	0.41
1:B:21:THR:HG22	1:B:22:SER:N	2.35	0.41
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.55	0.41
1:A:110:LEU:O	1:A:114:GLU:HG2	2.19	0.41
1:B:268:ASN:ND2	1:B:327:GLU:H	2.11	0.41
1:B:137:TYR:O	1:B:141:VAL:HG23	2.20	0.41
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.56	0.41
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.21	0.41
1:B:33:GLN:HA	1:B:33:GLN:NE2	2.34	0.41
2:C:269:ALA:N	2:C:270:PRO:CD	2.83	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.62	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.65	0.41
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.21	0.41
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.56	0.41
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.55	0.41
2:D:213:VAL:N	2:D:214:PRO:HD2	2.36	0.41
1:A:451:GLN:HB2	3:E:152:LEU:HD11	2.01	0.41
1:B:441:TYR:HB2	3:F:161:VAL:HG23	2.01	0.41
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.02	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.55	0.41
3:F:120:PRO:HG3	3:F:123:MET:O	2.21	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.56	0.41
1:A:190:ASP:HB3	2:C:74:GLN:O	2.20	0.41
1:B:246:HIS:CD2	1:B:246:HIS:N	2.89	0.41
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.03	0.41
2:D:326:GLU:HB2	2:D:327:PRO:HD3	2.02	0.41
1:A:186:ARG:C	1:A:186:ARG:HD3	2.41	0.40
1:B:56:THR:HG21	1:B:256:SER:OG	2.21	0.40
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.40
1:B:299:GLU:HA	1:B:300:PRO:HD3	1.98	0.40
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.02	0.40
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.56	0.40
1:A:116:ASN:CG	1:A:189:SER:HA	2.42	0.40
1:A:283:THR:HB	1:A:284:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:HIS:H	1:B:343:HIS:CD2	2.40	0.40
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.39	0.40
2:C:126:GLY:O	2:C:130:ASP:HB2	2.21	0.40
2:D:4:LEU:HD12	2:D:4:LEU:HA	1.93	0.40
1:B:40:LYS:HG3	6:B:5166:HOH:O	2.21	0.40
3:E:98:MET:HE2	3:E:138:ARG:HG2	2.02	0.40
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.20	0.40
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.22	0.40
2:C:336:MET:HE2	2:C:385:LEU:HD23	2.02	0.40
3:F:125:VAL:HG23	3:F:126:ASN:N	2.36	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%)	485 (95%)	22 (4%)	2 (0%)	34	25
1	B	509/527 (97%)	484 (95%)	23 (4%)	2 (0%)	34	25
2	C	386/389 (99%)	375 (97%)	9 (2%)	2 (0%)	29	19
2	D	385/389 (99%)	363 (94%)	18 (5%)	4 (1%)	15	6
3	E	165/170 (97%)	160 (97%)	4 (2%)	1 (1%)	25	15
3	F	166/170 (98%)	161 (97%)	4 (2%)	1 (1%)	25	15
All	All	2120/2172 (98%)	2028 (96%)	80 (4%)	12 (1%)	25	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	120	PRO
1	A	315	GLY

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Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	C	64	ALA
2	D	251	VAL
2	D	252	TYR
3	F	122	ILE
1	B	284	PRO
2	D	205	PRO
1	A	284	PRO
2	C	251	VAL

5.3.2 Protein sidechains (i)

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%)	43	37
1	B	433/442 (98%)	425 (98%)	8 (2%)	59	55
2	C	322/323 (100%)	316 (98%)	6 (2%)	57	53
2	D	321/323 (99%)	315 (98%)	6 (2%)	57	53
3	E	145/147 (99%)	140 (97%)	5 (3%)	37	30
3	F	146/147 (99%)	142 (97%)	4 (3%)	44	39
All	All	1800/1824 (99%)	1759 (98%)	41 (2%)	50	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	61	LYS
1	A	90	ASN
1	A	112	VAL
1	A	125	TRP
1	A	186	ARG
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	B	33	GLN
1	B	43	ARG
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	440	GLU
2	C	4	LEU
2	C	33	ASN
2	C	35	MET
2	C	153	LEU
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	153	LEU
2	D	173	ASP
3	E	24	THR
3	E	44	ARG
3	E	60	LEU
3	E	120	PRO
3	E	138	ARG
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) 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

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	168	HIS
1	A	214	ASN
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	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	133	GLN
1	B	155	ASN
1	B	168	HIS
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	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN

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Mol	Chain	Res	Type
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	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	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	511/527 (96%)	-0.08	7 (1%)	75	76	15, 26, 45, 63	0
1	B	511/527 (96%)	-0.02	20 (3%)	39	41	16, 28, 47, 62	0
2	C	388/389 (99%)	-0.35	4 (1%)	82	83	11, 19, 34, 54	0
2	D	387/389 (99%)	0.35	23 (5%)	22	23	18, 35, 54, 64	0
3	E	167/170 (98%)	-0.41	4 (2%)	59	61	15, 22, 36, 71	0
3	F	168/170 (98%)	0.65	14 (8%)	11	11	28, 44, 59, 66	0
All	All	2132/2172 (98%)	-0.01	72 (3%)	45	47	11, 27, 51, 71	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	120	PRO	4.5
2	D	380	ILE	4.2
3	F	100	ALA	4.0
3	F	82	ALA	4.0
1	A	310	TYR	3.8
2	D	83	TRP	3.6
1	B	54	ASN	3.4
3	F	23	ASN	3.4
3	F	102	LYS	3.3
2	D	44	LYS	3.3
1	B	17	ASN	3.3
2	D	82	SER	3.1
3	E	169	PRO	3.1
1	B	193	ILE	2.9
2	C	45	ARG	2.9
1	B	325	GLY	2.8
1	B	55	GLU	2.8
1	A	318	ILE	2.7
2	D	205	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	83	PHE	2.7
2	D	385	LEU	2.7
2	D	168	ARG	2.7
3	F	4	LEU	2.6
1	A	429	LEU	2.6
2	D	352	ILE	2.6
1	B	261	PRO	2.6
2	D	176	ARG	2.5
1	B	57	LYS	2.5
3	F	21	GLN	2.5
2	D	375	ALA	2.5
1	B	259	ASN	2.5
2	D	357	TYR	2.5
3	E	102	LYS	2.5
2	D	72	TRP	2.5
3	F	70	ARG	2.5
3	F	25	LEU	2.5
2	D	376	ASP	2.5
1	A	17	ASN	2.4
3	F	27	LYS	2.4
3	F	28	ALA	2.4
2	C	389	LYS	2.4
1	B	258	ALA	2.4
2	D	45	ARG	2.3
2	D	2	SER	2.3
3	F	101	ALA	2.3
2	D	166	GLY	2.3
1	B	316	ILE	2.3
1	A	316	ILE	2.3
2	C	205	PRO	2.3
2	D	206	GLY	2.3
2	D	377	ARG	2.3
1	B	51	LYS	2.3
3	F	72	PHE	2.2
1	B	264	ALA	2.2
3	F	19	ILE	2.2
2	D	170	ALA	2.2
1	B	320	ARG	2.2
1	B	31	TRP	2.1
1	A	320	ARG	2.1
1	B	119	ALA	2.1
2	C	2	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	167	ALA	2.1
1	A	434	SER	2.1
1	B	514	ARG	2.1
3	E	4	LEU	2.1
1	B	26	GLN	2.1
1	B	115	TYR	2.1
1	B	324	TYR	2.1
2	D	336	MET	2.1
1	B	244	LEU	2.1
2	D	6	GLU	2.0
2	D	381	VAL	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 monosaccharides 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^{th} 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(Å^2)	Q<0.9
5	CA	C	5006	1/1	0.93	0.07	46,46,46,46	0
5	CA	C	5007	1/1	0.94	0.07	51,51,51,51	0
4	FE2	A	5002	1/1	0.95	0.06	49,49,49,49	0
4	FE2	B	5004	1/1	0.97	0.05	53,53,53,53	0
5	CA	A	5005	1/1	0.99	0.03	35,35,35,35	0
4	FE2	A	5001	1/1	1.00	0.06	30,30,30,30	0
4	FE2	B	5003	1/1	1.00	0.04	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.