Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:32 PM GMT

PDB ID	:	1FZ1
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM III OXIDIZED
Authors	:	Whittington, D.A.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	1.96 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

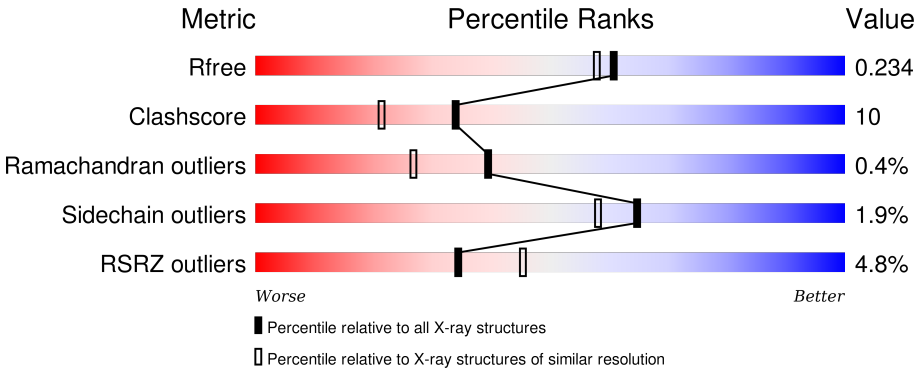
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.96 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 76% 20%
1	B	527	4% 74% 22%
2	C	389	2% 85% 14%
2	D	389	9% 74% 24%
3	E	170	2% 82% 14%

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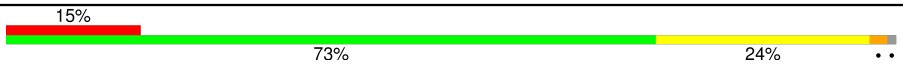
Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18852 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	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	F	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

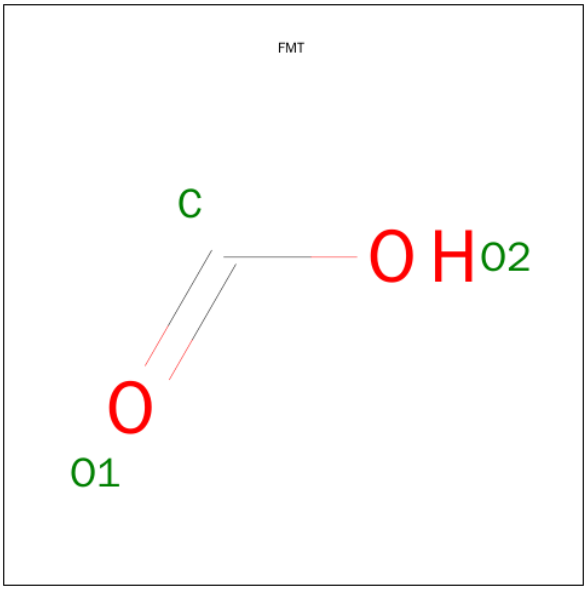
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Fe 2 2	0	0
4	A	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	3	Total Ca 3 3	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	300	Total O 300 300	0	0
7	B	290	Total O 290 290	0	0

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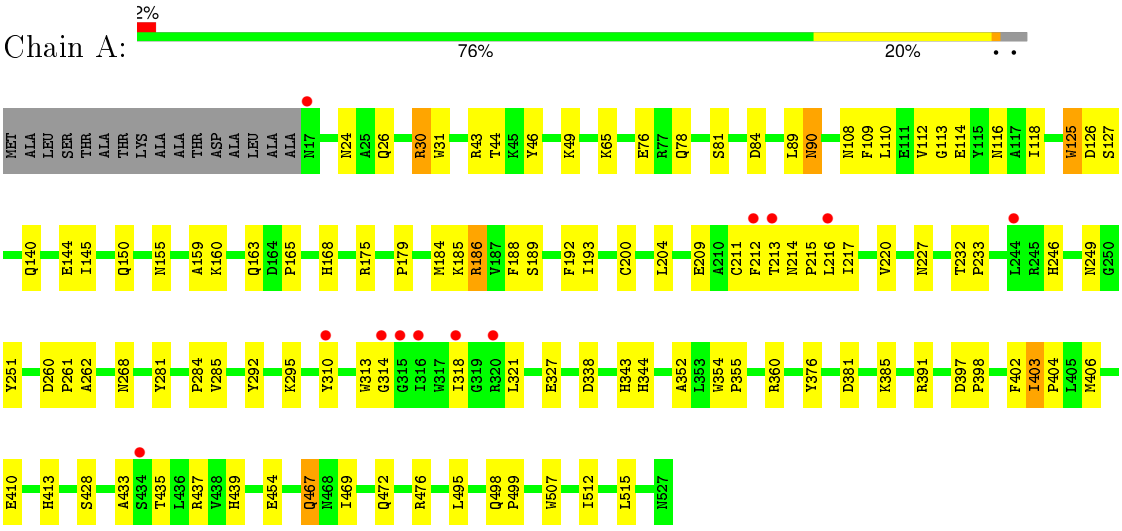
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	324	Total O 324 324	0	0
7	D	192	Total O 192 192	0	0
7	E	163	Total O 163 163	0	0
7	F	72	Total O 72 72	0	0

3 Residue-property plots (i)

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.

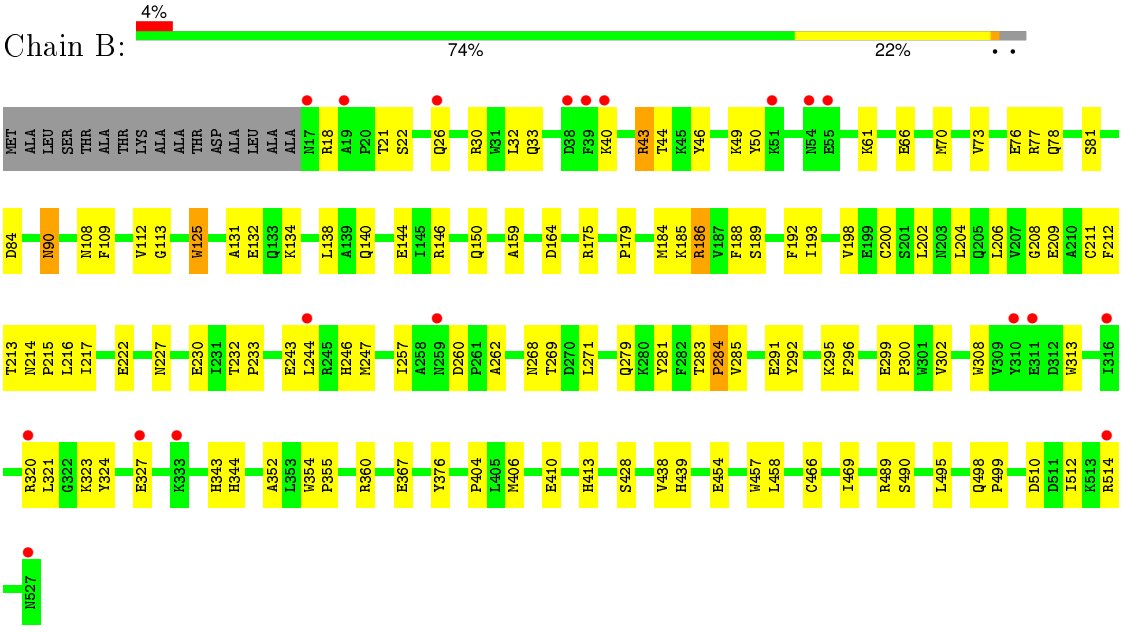
- Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain A:



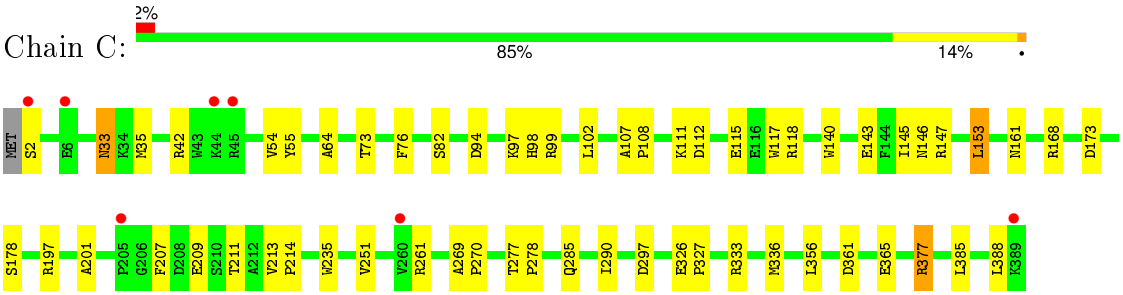
- Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:



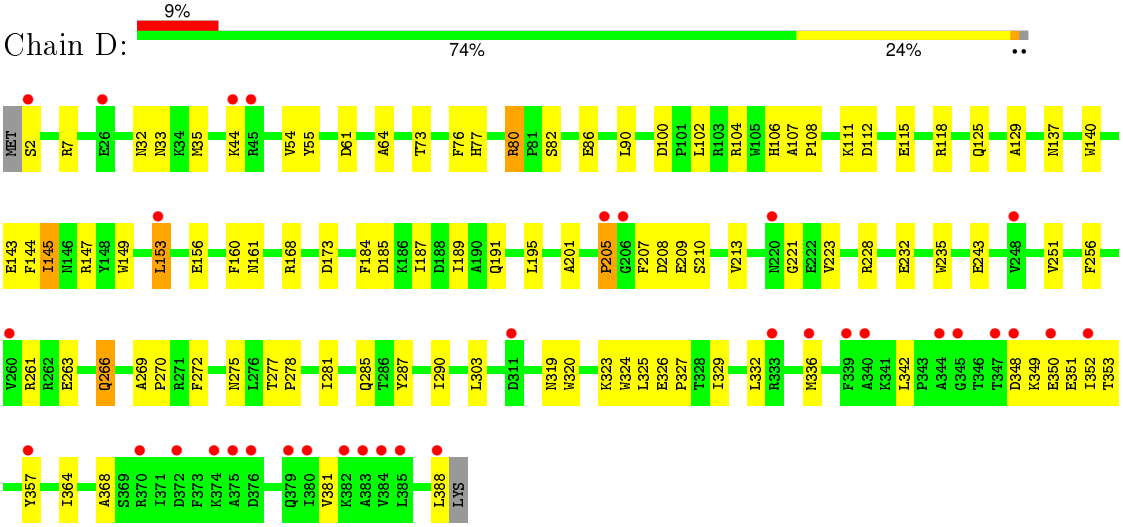
- Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:



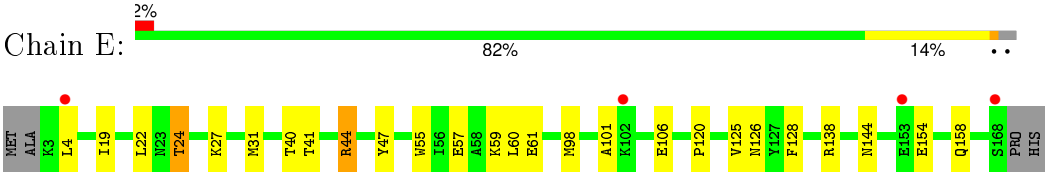
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



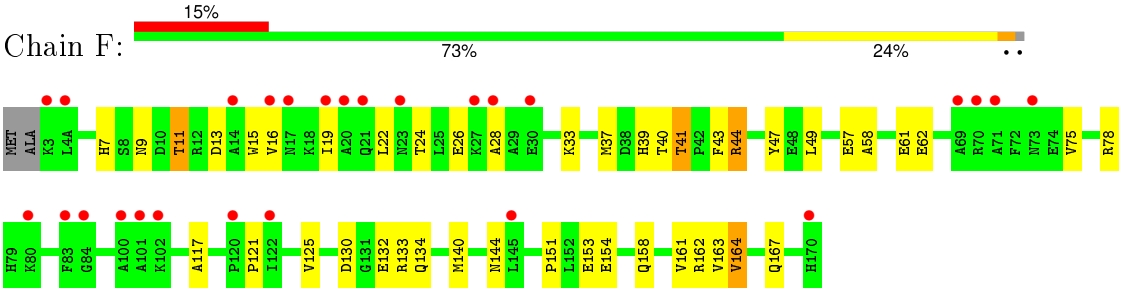
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.40Å 171.97Å 221.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.80 – 1.96 29.21 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.0 (22.80-1.96) 93.1 (29.21-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.18 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.234	Depositor DCC
R_{free} test set	6400 reflections (3.51%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 194705 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18852	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 2.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FMT, CA, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/4310	0.56	0/5853
1	B	0.32	0/4310	0.56	0/5853
2	C	0.37	0/3289	0.58	0/4464
2	D	0.32	0/3279	0.53	0/4453
3	E	0.33	0/1396	0.57	0/1880
3	F	0.28	0/1416	0.50	0/1907
All	All	0.33	0/18000	0.55	0/24410

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	84	0
1	B	4185	0	3981	110	0
2	C	3193	0	3042	46	0
2	D	3183	0	3029	82	0
3	E	1368	0	1363	20	0
3	F	1386	0	1377	40	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	3	0	1	0	0
7	A	300	0	0	6	0
7	B	290	0	0	6	0
7	C	324	0	0	6	0
7	D	192	0	0	6	0
7	E	163	0	0	1	0
7	F	72	0	0	7	0
All	All	18852	0	16774	346	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 10.

All (346) 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	1.26	1.01
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.04	0.99
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.95	0.91
1:A:435:THR:HG21	1:A:437:ARG:HE	1.38	0.87
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.55	0.87
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.21	0.86
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.85
3:E:41:THR:O	3:E:44:ARG:HD2	1.76	0.85
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.22	0.83
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.82
1:B:268:ASN:HD21	1:B:327:GLU:H	1.24	0.82
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
3:F:40:THR:O	3:F:41:THR:HG22	1.83	0.79
1:A:435:THR:CG2	1:A:437:ARG:HE	1.95	0.79
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.82	0.79
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.65	0.79
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.64	0.79
1:B:209:GLU:HA	1:B:213:THR:OG1	1.83	0.79
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.79	0.77
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.78	0.77
3:F:41:THR:O	3:F:44:ARG:HD2	1.83	0.77
2:C:361:ASP:OD2	2:C:377:ARG:HD3	1.84	0.76
1:A:44:THR:HG22	1:A:46:TYR:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HG3	7:A:9288:HOH:O	1.84	0.76
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.16	0.75
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.36	0.74
1:B:406:MET:O	1:B:410:GLU:HG3	1.88	0.73
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.71	0.72
3:F:58:ALA:O	3:F:62:GLU:HG3	1.90	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.84	0.71
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.71	0.71
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.90	0.71
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.26	0.71
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.74	0.70
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.21	0.70
1:A:227:ASN:HD21	1:A:295:LYS:H	1.40	0.69
1:A:268:ASN:HD21	1:A:327:GLU:H	1.40	0.69
3:F:57:GLU:O	3:F:61:GLU:HG3	1.93	0.69
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.39	0.69
2:C:365:GLU:HG3	7:C:5249:HOH:O	1.93	0.69
1:B:244:LEU:HG	7:B:5024:HOH:O	1.92	0.69
1:B:33:GLN:NE2	1:B:132:GLU:H	1.91	0.68
1:B:367:GLU:HG3	7:B:5031:HOH:O	1.93	0.68
1:B:33:GLN:HE22	1:B:132:GLU:H	1.42	0.67
2:D:228:ARG:O	2:D:232:GLU:HG3	1.94	0.67
2:D:348:ASP:OD2	2:D:350:GLU:HB3	1.93	0.67
1:B:413:HIS:HD2	1:B:428:SER:OG	1.77	0.67
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.67
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.10	0.67
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.78	0.67
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.66
3:F:153:GLU:CD	3:F:153:GLU:H	1.99	0.66
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.78	0.65
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.95	0.65
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.77	0.65
1:A:109:PHE:HB3	1:A:184:MET:HE2	1.78	0.65
1:B:30:ARG:O	1:B:30:ARG:HD3	1.97	0.65
1:B:269:THR:HG23	7:B:5213:HOH:O	1.96	0.65
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.44	0.65
1:A:213:THR:O	1:A:217:ILE:HG12	1.98	0.64
3:F:13:ASP:O	3:F:16:VAL:HG22	1.97	0.64
3:E:98:MET:O	3:E:98:MET:HE2	1.97	0.63
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.63
1:A:140:GLN:O	1:A:144:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.47	0.63
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.82	0.62
1:B:227:ASN:HD21	1:B:295:LYS:H	1.46	0.62
3:E:22:LEU:HD11	3:E:31:MET:SD	2.39	0.62
1:B:489:ARG:HD2	1:B:495:LEU:O	1.99	0.62
1:B:269:THR:HG21	7:F:237:HOH:O	1.99	0.62
1:B:192:PHE:O	1:B:200:CYS:HB3	2.00	0.62
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.30	0.61
2:D:111:LYS:O	2:D:115:GLU:HG3	2.00	0.61
3:E:24:THR:HG22	3:E:27:LYS:H	1.65	0.61
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.82	0.61
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.01	0.61
1:B:213:THR:O	1:B:217:ILE:HG12	2.02	0.60
2:D:153:LEU:HD12	2:D:153:LEU:C	2.22	0.60
2:C:333:ARG:HD2	7:C:5327:HOH:O	2.01	0.60
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.83	0.60
3:F:24:THR:HG21	7:F:214:HOH:O	2.02	0.60
3:E:59:LYS:HE2	7:E:209:HOH:O	2.02	0.60
1:A:406:MET:O	1:A:410:GLU:HG3	2.02	0.59
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.02	0.59
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.84	0.59
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.84	0.59
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.82	0.59
1:B:268:ASN:ND2	1:B:327:GLU:H	1.95	0.59
2:D:44:LYS:HG3	7:D:499:HOH:O	2.01	0.59
1:B:26:GLN:HE21	1:B:61:LYS:HD2	1.66	0.59
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.83	0.59
2:D:352:ILE:HG13	2:D:353:THR:N	2.18	0.59
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.36	0.59
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.85	0.58
1:A:209:GLU:HA	1:A:213:THR:HB	1.85	0.58
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.83	0.58
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.38	0.58
2:C:361:ASP:OD2	2:C:377:ARG:CD	2.50	0.58
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.68	0.58
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.03	0.58
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.84	0.58
3:F:15:TRP:O	3:F:19:ILE:HG23	2.04	0.58
1:B:18:ARG:O	2:D:129:ALA:HA	2.04	0.58
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.85	0.57
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.37	0.57
3:F:41:THR:HG23	3:F:43:PHE:N	2.09	0.57
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.85	0.57
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.39	0.57
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.50	0.57
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.12	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.87	0.57
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.86	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.05	0.56
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.87	0.56
1:A:338:ASP:OD1	1:A:433:ALA:HB2	2.06	0.56
3:F:132:GLU:HG3	7:F:185:HOH:O	2.05	0.56
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.88	0.56
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.06	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.56
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.56
1:B:44:THR:HG21	7:B:5140:HOH:O	2.05	0.55
2:C:211:THR:O	2:C:214:PRO:HD2	2.06	0.55
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.87	0.55
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.55
1:A:227:ASN:ND2	1:A:295:LYS:H	2.04	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.54
1:B:244:LEU:HB2	7:B:5176:HOH:O	2.06	0.54
1:A:185:LYS:O	1:A:189:SER:HB2	2.07	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.89	0.54
1:A:268:ASN:ND2	1:A:327:GLU:H	2.06	0.53
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.53
1:B:212:PHE:O	1:B:215:PRO:HD2	2.09	0.53
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.41	0.53
2:D:324:TRP:C	2:D:327:PRO:HD2	2.28	0.53
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.12	0.53
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.73	0.53
1:A:163:GLN:HG2	7:A:9078:HOH:O	2.09	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.90	0.52
1:B:206:LEU:HB2	7:B:5218:HOH:O	2.09	0.52
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.45	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.08	0.52
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.44	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.04	0.52
3:F:61:GLU:O	3:F:121:PRO:HG2	2.08	0.52
2:D:324:TRP:O	2:D:327:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.43	0.52
1:B:43:ARG:HD2	1:B:43:ARG:O	2.10	0.52
2:D:187:ILE:O	2:D:191:GLN:HG3	2.10	0.52
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.40	0.51
1:B:198:VAL:O	1:B:202:LEU:HG	2.09	0.51
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.92	0.51
1:B:109:PHE:O	1:B:112:VAL:HG12	2.10	0.51
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.40	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.92	0.51
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.51
1:B:227:ASN:ND2	1:B:295:LYS:H	2.07	0.51
2:C:2:SER:HB2	7:C:5189:HOH:O	2.09	0.51
2:D:184:PHE:O	2:D:187:ILE:HG22	2.11	0.51
1:A:160:LYS:HE3	7:A:9243:HOH:O	2.11	0.51
3:E:4:LEU:HG	3:E:4:LEU:O	2.11	0.50
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.09	0.50
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.93	0.50
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.12	0.50
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.47	0.50
7:D:518:HOH:O	3:F:125:VAL:HG22	2.11	0.49
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.94	0.49
2:D:213:VAL:HG23	7:D:569:HOH:O	2.12	0.49
3:E:57:GLU:O	3:E:61:GLU:HG3	2.12	0.49
2:D:348:ASP:OD1	2:D:351:GLU:HG3	2.12	0.49
7:C:5020:HOH:O	3:E:125:VAL:HG22	2.12	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.43	0.49
2:C:97:LYS:HD2	7:C:5246:HOH:O	2.12	0.49
2:D:145:ILE:O	2:D:149:TRP:HB3	2.13	0.49
1:A:84:ASP:HB3	1:B:81:SER:OG	2.13	0.49
1:B:43:ARG:HD2	1:B:43:ARG:C	2.33	0.48
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.95	0.48
3:F:33:LYS:O	3:F:37:MET:HG2	2.12	0.48
1:A:212:PHE:O	1:A:215:PRO:HD2	2.13	0.48
1:B:490:SER:OG	2:D:32:ASN:HB2	2.13	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.13	0.48
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.48
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.31	0.48
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.09	0.48
2:D:223:VAL:HG23	7:D:577:HOH:O	2.14	0.48
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:MET:HE1	2:C:356:LEU:HD11	1.95	0.48
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.94	0.48
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.44	0.47
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.97	0.47
1:B:227:ASN:HD21	1:B:296:PHE:H	1.62	0.47
2:C:211:THR:C	2:C:214:PRO:HD2	2.35	0.47
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.49	0.47
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.79	0.47
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.50	0.47
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.80	0.47
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.14	0.47
3:F:33:LYS:HE3	3:F:117:ALA:HA	1.95	0.47
2:C:111:LYS:O	2:C:115:GLU:HG3	2.14	0.47
1:A:314:GLY:O	1:A:318:ILE:HD11	2.15	0.47
2:C:98:HIS:HE1	2:C:178:SER:OG	1.97	0.47
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.50	0.47
1:B:32:LEU:C	1:B:32:LEU:HD23	2.34	0.47
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.47
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.80	0.46
1:B:232:THR:HB	1:B:233:PRO:HD3	1.97	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.15	0.46
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.14	0.46
2:D:143:GLU:O	2:D:147:ARG:HB3	2.16	0.46
3:F:162:ARG:NH1	3:F:164:VAL:HG12	2.31	0.46
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.51	0.46
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.10	0.46
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.46	0.46
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.46
1:A:343:HIS:H	1:A:343:HIS:CD2	2.31	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
2:D:54:VAL:O	2:D:55:TYR:HB2	2.15	0.46
1:A:109:PHE:O	1:A:112:VAL:HG12	2.16	0.46
1:A:268:ASN:HD21	1:A:327:GLU:N	2.11	0.46
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.16	0.45
1:B:510:ASP:O	1:B:514:ARG:HG3	2.15	0.45
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.52	0.45
1:A:472:GLN:NE2	7:A:9288:HOH:O	2.49	0.45
1:B:159:ALA:O	2:D:33:ASN:HB2	2.16	0.45
1:A:44:THR:HG21	7:A:9010:HOH:O	2.16	0.45
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:LEU:HD12	2:C:153:LEU:C	2.37	0.45
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.98	0.45
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.99	0.45
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.51	0.45
1:A:81:SER:OG	1:B:84:ASP:HB3	2.16	0.45
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.98	0.45
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.32	0.45
2:C:143:GLU:O	2:C:147:ARG:HB3	2.17	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.45
1:A:232:THR:HB	1:A:233:PRO:HD3	1.97	0.44
1:A:159:ALA:O	2:C:33:ASN:HB2	2.18	0.44
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.32	0.44
1:B:30:ARG:HD3	1:B:30:ARG:C	2.37	0.44
2:D:275:ASN:C	2:D:278:PRO:HD2	2.38	0.44
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.18	0.44
1:B:208:GLY:O	1:B:213:THR:HG23	2.17	0.44
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.98	0.44
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.53	0.44
2:C:54:VAL:O	2:C:55:TYR:HB2	2.17	0.44
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.52	0.44
2:D:140:TRP:CE2	2:D:145:ILE:HD11	2.53	0.44
2:C:146:ASN:O	2:C:214:PRO:HG3	2.18	0.44
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.53	0.44
2:D:324:TRP:HA	2:D:327:PRO:HD2	2.00	0.43
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.82	0.43
1:B:184:MET:HE1	1:B:188:PHE:CG	2.53	0.43
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.99	0.43
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.43
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.51	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.43
2:C:209:GLU:HG2	7:C:5188:HOH:O	2.18	0.43
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.16	0.43
1:A:44:THR:OG1	1:A:127:SER:HA	2.18	0.43
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.47	0.43
1:B:66:GLU:O	1:B:70:MET:HG2	2.18	0.43
1:A:249:ASN:HD22	1:A:249:ASN:HA	1.64	0.43
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.32	0.43
3:E:4:LEU:CG	3:E:4:LEU:O	2.66	0.43
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.18	0.43
3:E:154:GLU:O	3:E:158:GLN:HG3	2.18	0.43
2:D:209:GLU:HG2	7:D:461:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ALA:N	2:D:270:PRO:CD	2.82	0.43
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.99	0.43
2:D:332:LEU:O	2:D:336:MET:HG2	2.19	0.43
1:B:186:ARG:HA	2:D:73:THR:OG1	2.18	0.43
1:A:30:ARG:HD3	1:A:31:TRP:CD1	2.54	0.43
1:B:73:VAL:HG12	1:B:77:ARG:HH22	1.83	0.43
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.53	0.43
1:A:402:PHE:O	1:A:403:ILE:HD12	2.18	0.43
1:A:193:ILE:HD11	2:C:82:SER:HB3	2.01	0.43
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.47	0.43
1:A:186:ARG:HD3	1:A:186:ARG:C	2.39	0.43
1:B:186:ARG:HD3	1:B:186:ARG:C	2.39	0.43
1:A:413:HIS:HD2	1:A:428:SER:OG	2.01	0.43
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.54	0.43
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.42
2:D:325:LEU:O	2:D:329:ILE:HG13	2.20	0.42
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.35	0.42
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.54	0.42
3:F:49:LEU:HA	7:F:178:HOH:O	2.18	0.42
2:D:77:HIS:CG	3:F:140:MET:HG2	2.54	0.42
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.54	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.42
3:F:26:GLU:HB2	7:F:213:HOH:O	2.19	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.00	0.42
1:A:192:PHE:O	1:A:200:CYS:HB3	2.19	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.38	0.42
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.37	0.42
2:D:80:ARG:HG2	2:D:86:GLU:OE1	2.18	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.02	0.42
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.99	0.42
1:A:360:ARG:HG2	1:A:498:GLN:HB2	2.01	0.42
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.55	0.42
1:A:165:PRO:HG3	7:A:9076:HOH:O	2.20	0.42
2:C:235:TRP:CD1	2:C:235:TRP:C	2.93	0.42
2:C:336:MET:HE3	2:C:388:LEU:HG	2.02	0.42
3:F:39:HIS:HD2	7:F:225:HOH:O	2.02	0.42
1:A:110:LEU:O	1:A:114:GLU:HG2	2.19	0.42
1:B:125:TRP:C	1:B:125:TRP:CD1	2.93	0.42
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.19	0.41
2:C:277:THR:HB	2:C:278:PRO:HD3	2.01	0.41
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:GLN:HE21	2:D:125:GLN:HB3	1.74	0.41
1:A:116:ASN:CG	1:A:189:SER:HA	2.41	0.41
3:E:55:TRP:CZ2	3:E:59:LYS:HE3	2.54	0.41
1:B:457:TRP:CZ3	1:B:458:LEU:HD23	2.55	0.41
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.56	0.41
2:D:349:LYS:HA	2:D:352:ILE:HG12	2.02	0.41
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.81	0.41
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.56	0.41
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.20	0.41
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.55	0.41
2:D:266:GLN:HA	2:D:266:GLN:HE21	1.84	0.41
2:D:349:LYS:HG3	2:D:352:ILE:HD11	2.03	0.41
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.21	0.41
3:E:40:THR:C	3:E:41:THR:HG23	2.40	0.41
1:B:202:LEU:HD22	1:B:206:LEU:HD23	2.03	0.41
2:C:269:ALA:N	2:C:270:PRO:CD	2.84	0.41
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.56	0.41
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.86	0.41
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.03	0.41
2:D:2:SER:HB2	7:D:466:HOH:O	2.21	0.41
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.55	0.41
3:F:75:VAL:HG23	7:F:217:HOH:O	2.20	0.41
1:A:216:LEU:O	1:A:220:VAL:HG23	2.20	0.41
1:B:184:MET:HE2	1:B:188:PHE:HB2	2.03	0.41
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.56	0.41
2:D:195:LEU:O	2:D:195:LEU:HD23	2.21	0.41
2:C:201:ALA:HA	2:C:207:PHE:HB3	2.01	0.41
3:E:125:VAL:HG23	3:E:126:ASN:N	2.36	0.40
1:A:354:TRP:N	1:A:355:PRO:CD	2.85	0.40
1:B:21:THR:HG22	1:B:22:SER:N	2.37	0.40
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.40
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.60	0.40
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.64	0.40
2:D:352:ILE:CG1	2:D:353:THR:N	2.84	0.40
2:D:266:GLN:HB2	2:D:281:ILE:HG21	2.03	0.40
1:B:299:GLU:HA	1:B:300:PRO:HD3	1.98	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%)	490 (96%)	18 (4%)	1 (0%)	52 43
1	B	509/527 (97%)	489 (96%)	18 (4%)	2 (0%)	39 27
2	C	386/389 (99%)	378 (98%)	6 (2%)	2 (0%)	34 21
2	D	385/389 (99%)	365 (95%)	16 (4%)	4 (1%)	19 8
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100 100
3	F	166/170 (98%)	162 (98%)	4 (2%)	0	100 100
All	All	2119/2172 (98%)	2046 (97%)	64 (3%)	9 (0%)	39 27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	D	221	GLY
1	A	284	PRO
2	C	64	ALA
1	B	284	PRO
2	C	251	VAL
2	D	251	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	433/442 (98%)	424 (98%)	9 (2%)	61 53
1	B	433/442 (98%)	428 (99%)	5 (1%)	78 75
2	C	322/323 (100%)	317 (98%)	5 (2%)	70 66
2	D	321/323 (99%)	314 (98%)	7 (2%)	60 51
3	E	144/147 (98%)	141 (98%)	3 (2%)	61 53
3	F	146/147 (99%)	141 (97%)	5 (3%)	44 30
All	All	1799/1824 (99%)	1765 (98%)	34 (2%)	65 58

All (34) 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	310	TYR
1	A	391	ARG
1	A	403	ILE
1	A	467	GLN
1	B	43	ARG
1	B	90	ASN
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
2	C	33	ASN
2	C	35	MET
2	C	153	LEU
2	C	173	ASP
2	C	377	ARG
2	D	35	MET
2	D	80	ARG
2	D	145	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	266	GLN
3	E	24	THR
3	E	44	ARG
3	E	138	ARG
3	F	11	THR

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Mol	Chain	Res	Type
3	F	41	THR
3	F	44	ARG
3	F	164	VAL
3	F	167	GLN

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	116	ASN
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	343	HIS
1	A	344	HIS
1	A	411	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	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN
1	B	133	GLN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	268	ASN
1	B	273	ASN

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Mol	Chain	Res	Type
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	155	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	293	GLN
2	D	296	GLN
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	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FMT	A	9001	4	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FMT	A	9001	4	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.17	12 (2%) 64 73	16, 27, 45, 63	0
1	B	511/527 (96%)	0.12	19 (3%) 45 56	16, 27, 45, 62	0
2	C	388/389 (99%)	-0.16	7 (1%) 71 80	13, 21, 35, 52	0
2	D	387/389 (99%)	0.53	34 (8%) 12 20	18, 33, 51, 58	0
3	E	166/170 (97%)	-0.08	4 (2%) 62 72	17, 24, 38, 56	0
3	F	168/170 (98%)	1.03	26 (15%) 3 4	30, 42, 57, 64	0
All	All	2131/2172 (98%)	0.21	102 (4%) 34 45	13, 28, 48, 64	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	100	ALA	5.1
1	B	17	ASN	5.0
3	E	4	LEU	4.7
2	D	205	PRO	4.4
1	A	310	TYR	4.2
3	F	20	ALA	4.2
2	D	388	LEU	4.1
2	D	44	LYS	4.0
1	A	244	LEU	4.0
1	B	40	LYS	3.9
3	F	170	HIS	3.9
1	A	316	ILE	3.8
1	B	527	ASN	3.8
3	F	80	LYS	3.8
2	D	352	ILE	3.8
1	B	39	PHE	3.7
2	D	45	ARG	3.7
2	D	385	LEU	3.6
1	A	17	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	21	GLN	3.6
2	D	380	ILE	3.5
1	B	311	GLU	3.5
3	F	23	ASN	3.5
1	B	244	LEU	3.4
2	C	2	SER	3.4
2	D	348	ASP	3.4
2	D	26	GLU	3.3
2	C	6	GLU	3.2
3	F	102	LYS	3.2
2	C	205	PRO	3.2
3	F	27	LYS	3.1
2	C	389	LYS	3.1
3	F	70	ARG	3.1
2	D	376	ASP	3.1
2	D	374	LYS	3.1
1	A	318	ILE	3.0
2	D	345	GLY	3.0
2	C	45	ARG	3.0
2	D	372	ASP	3.0
2	D	344	ALA	2.9
1	B	316	ILE	2.9
3	F	69	ALA	2.9
1	B	38	ASP	2.9
3	F	19	ILE	2.8
3	F	16	VAL	2.8
1	B	333	LYS	2.8
3	F	84	GLY	2.8
1	B	54	ASN	2.7
1	B	26	GLN	2.7
1	B	55	GLU	2.6
3	F	17	ASN	2.6
2	D	375	ALA	2.6
1	A	315	GLY	2.6
2	D	339	PHE	2.6
2	D	2	SER	2.6
3	F	28	ALA	2.6
1	B	51	LYS	2.5
1	A	434	SER	2.5
1	B	19	ALA	2.5
3	F	101	ALA	2.5
3	F	83	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	73	ASN	2.4
2	D	357	TYR	2.4
1	A	320	ARG	2.4
1	A	213	THR	2.4
2	C	44	LYS	2.4
2	D	333	ARG	2.3
3	F	71	ALA	2.3
2	D	347	THR	2.3
3	E	102	LYS	2.3
3	E	168	SER	2.3
3	F	3	LYS	2.3
1	A	212	PHE	2.3
1	A	314	GLY	2.3
2	D	206	GLY	2.3
1	A	216	LEU	2.2
2	D	311	ASP	2.2
1	B	259	ASN	2.2
2	D	260	VAL	2.2
2	D	153	LEU	2.2
3	F	145	LEU	2.2
3	E	153	GLU	2.2
1	B	310	TYR	2.2
2	D	350	GLU	2.1
3	F	4(A)	LEU	2.1
3	F	30	GLU	2.1
2	D	384	VAL	2.1
1	B	327	GLU	2.1
1	B	320	ARG	2.1
2	D	382	LYS	2.1
3	F	122	ILE	2.1
2	D	340	ALA	2.1
2	D	370	ARG	2.1
1	B	514	ARG	2.1
2	C	260	VAL	2.1
2	D	336	MET	2.1
3	F	120	PRO	2.1
2	D	220	ASN	2.0
2	D	248	VAL	2.0
3	F	14	ALA	2.0
2	D	379	GLN	2.0
2	D	383	ALA	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^{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	LLDF	B-factors(Å^2)	Q<0.9
6	FMT	A	9001	3/3	0.87	0.10	-0.18	40,40,45,49	0
4	FE	A	5001	1/1	1.00	0.02	-1.77	25,25,25,25	0
4	FE	A	5002	1/1	0.99	0.02	-1.79	36,36,36,36	0
4	FE	B	5003	1/1	0.99	0.04	-3.05	26,26,26,26	0
4	FE	B	5004	1/1	0.98	0.04	-3.13	36,36,36,36	0
5	CA	A	5005	1/1	0.99	0.04	-3.57	37,37,37,37	0
5	CA	C	5008	1/1	0.96	0.13	-	44,44,44,44	0
5	CA	C	5007	1/1	0.99	0.10	-	36,36,36,36	0
5	CA	C	5006	1/1	0.97	0.09	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.