



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:26 pm BST

PDB ID : 1FZ3
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM III SOAK AT
PH 6.2 (0.1 M PIPES)
Authors : Whittington, D.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.03 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

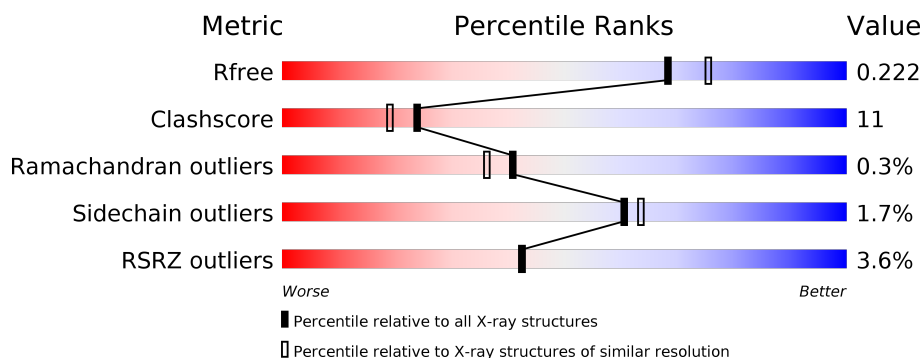
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>••</div> </div>
1	B	527	<div> <div>3%</div> <div>73%</div> <div>23%</div> <div>••</div> </div>
2	C	389	<div> <div>%</div> <div>80%</div> <div>19%</div> <div>•</div> </div>
2	D	389	<div> <div>7%</div> <div>71%</div> <div>28%</div> <div>•</div> </div>
3	E	170	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>••</div> </div>
3	F	170	<div> <div>11%</div> <div>70%</div> <div>27%</div> <div>••</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18782 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	388	Total	C	N	O	S	0	0	0
			3193	2054	551	580	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			

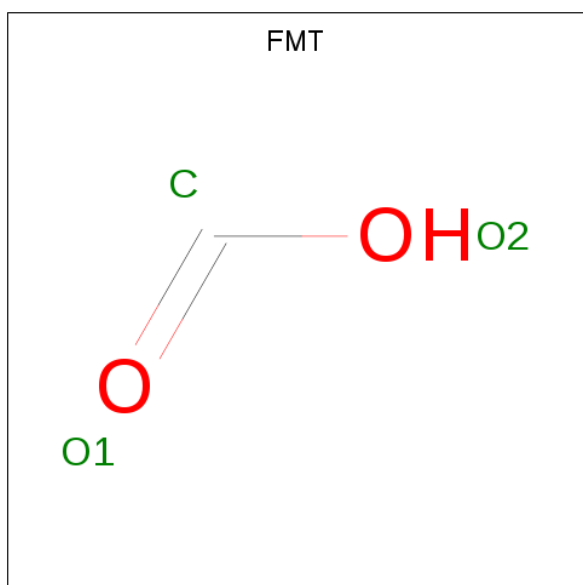
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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	2	Total Ca 2 2	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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	269	Total O 269 269	0	0
7	B	273	Total O 273 273	0	0

Continued on next page...

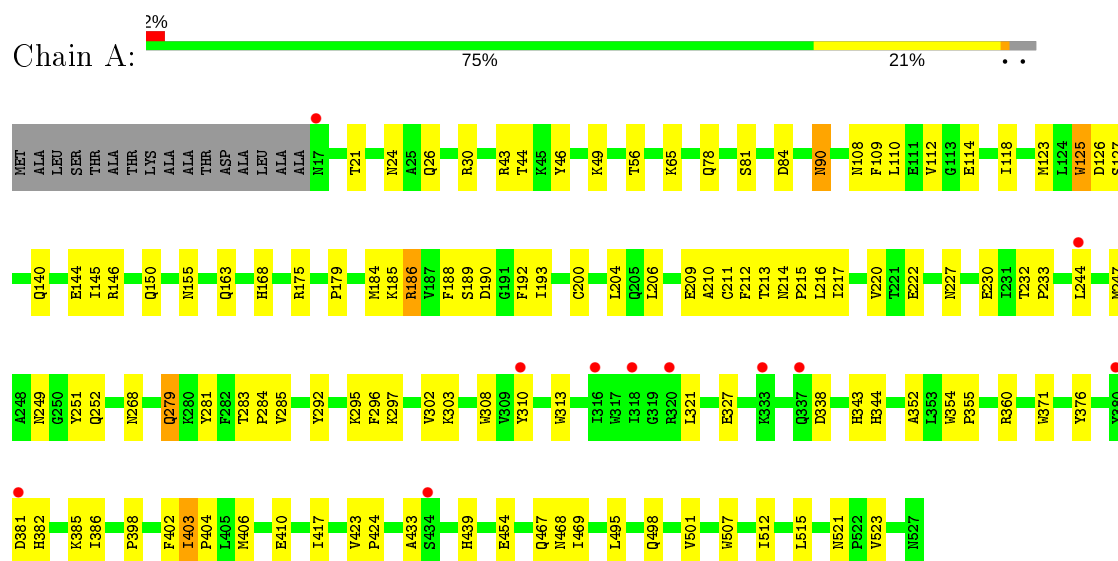
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	327	Total 327	O 327	0	0
7	D	165	Total 165	O 165	0	0
7	E	159	Total 159	O 159	0	0
7	F	69	Total 69	O 69	0	0

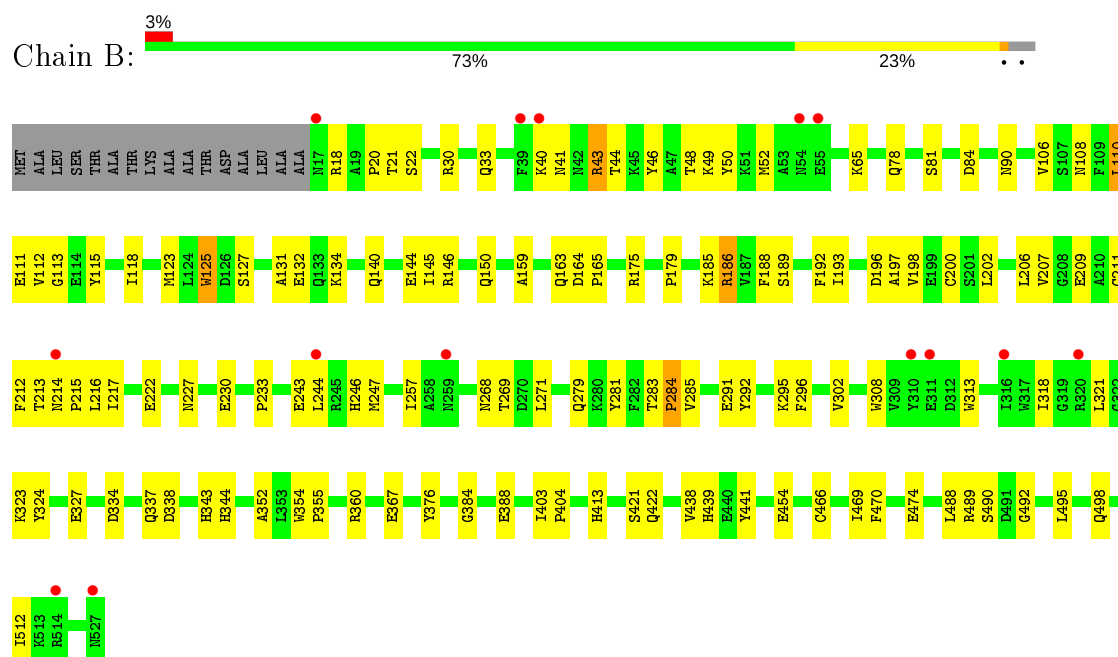
3 Residue-property plots

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

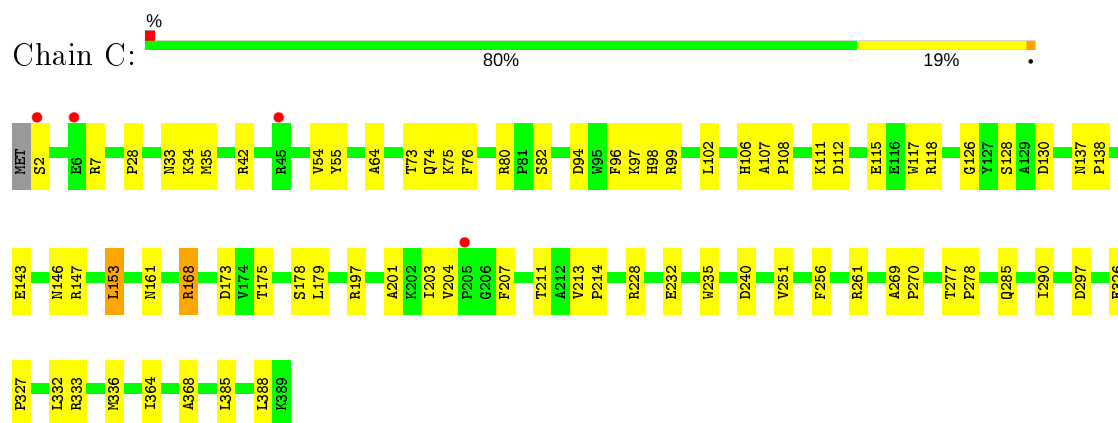
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



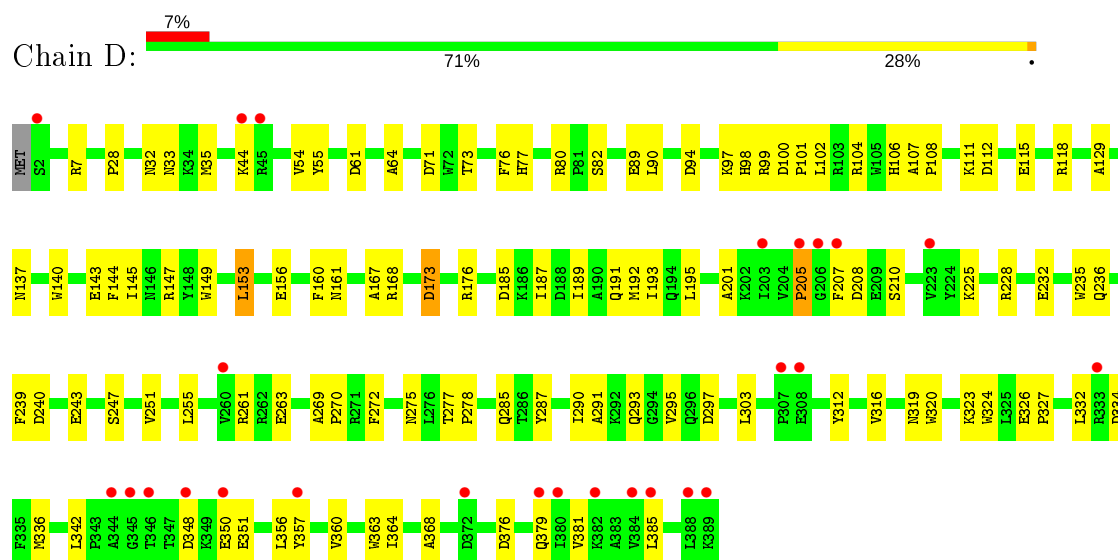
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



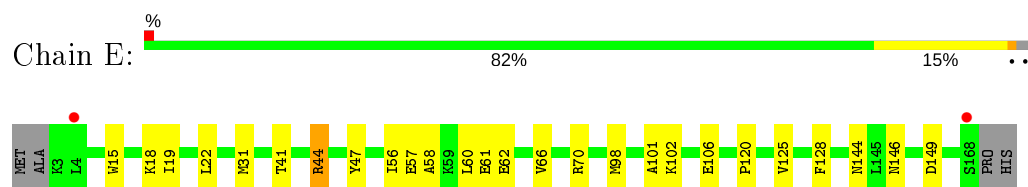
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



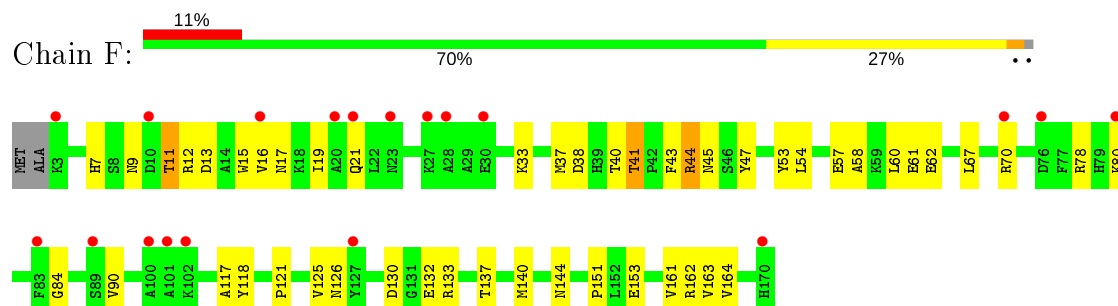
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• 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, α , β , γ	71.37Å 172.12Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.03 29.99 – 2.03	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.99-2.03) 92.9 (29.99-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.228 0.191 , 0.222	Depositor DCC
R_{free} test set	5809 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18782	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.57	0/4464
2	D	0.32	0/3289	0.53	0/4464
3	E	0.33	0/1396	0.59	0/1880
3	F	0.28	0/1416	0.50	0/1907
All	All	0.33	0/18010	0.55	0/24421

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	90	0
1	B	4185	0	3981	119	0
2	C	3193	0	3042	62	0
2	D	3193	0	3042	94	0
3	E	1368	0	1363	20	0
3	F	1386	0	1377	50	0
4	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

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	3	0	1	0	0
7	A	269	0	0	3	0
7	B	273	0	0	8	0
7	C	327	0	0	5	0
7	D	165	0	0	4	0
7	E	159	0	0	0	0
7	F	69	0	0	2	0
All	All	18782	0	16787	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (381) 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	1.11	0.94
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.51	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.09	0.89
1:B:209:GLU:HA	1:B:213:THR:HB	1.53	0.88
1:A:44:THR:HG22	1:A:46:TYR:H	1.39	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.86
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.21	0.85
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.56	0.85
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.62	0.82
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.27	0.80
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.64	0.79
3:E:41:THR:O	3:E:44:ARG:HD2	1.83	0.78
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.66	0.78
1:A:209:GLU:HA	1:A:213:THR:OG1	1.84	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.77
1:B:44:THR:HG22	1:B:46:TYR:H	1.50	0.77
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.00	0.77
3:F:41:THR:O	3:F:44:ARG:HD2	1.84	0.76
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.69	0.75
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.30	0.75
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.69	0.75
1:A:268:ASN:HD21	1:A:327:GLU:H	1.34	0.75
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.17	0.74
3:F:41:THR:CG2	3:F:43:PHE:H	2.00	0.73
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.38	0.71
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.72	0.71
3:F:58:ALA:O	3:F:62:GLU:HG3	1.90	0.71
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.37	0.71
1:B:367:GLU:HG3	7:B:5010:HOH:O	1.91	0.70
1:B:244:LEU:HG	7:B:5100:HOH:O	1.92	0.70
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.72	0.70
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.74	0.69
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.90	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.21	0.69
3:F:13:ASP:O	3:F:16:VAL:HG22	1.93	0.69
3:F:41:THR:HG22	3:F:43:PHE:H	1.56	0.68
3:F:57:GLU:O	3:F:61:GLU:HG3	1.92	0.68
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.42	0.67
1:B:227:ASN:HD21	1:B:295:LYS:H	1.42	0.67
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.66
1:A:244:LEU:HG	7:A:9115:HOH:O	1.95	0.66
2:C:333:ARG:HD2	7:C:5162:HOH:O	1.95	0.66
3:F:15:TRP:O	3:F:19:ILE:HG23	1.95	0.66
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.88	0.65
3:E:98:MET:O	3:E:98:MET:HE2	1.97	0.65
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.79	0.65
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.61	0.65
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.32	0.65
1:A:140:GLN:O	1:A:144:GLU:HG2	1.97	0.64
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.64
2:D:228:ARG:O	2:D:232:GLU:HG3	1.97	0.64
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.63	0.64
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.81	0.63
1:B:30:ARG:O	1:B:30:ARG:HD3	1.98	0.63
1:B:243:GLU:O	1:B:247:MET:HG2	1.99	0.63
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.63
1:A:406:MET:O	1:A:410:GLU:HG3	1.98	0.63
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.00	0.62
1:A:338:ASP:OD1	1:A:433:ALA:HB2	1.99	0.62
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.82	0.62
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.83	0.62
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:O	1:B:217:ILE:HG12	2.00	0.61
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.82	0.61
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.82	0.61
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.82	0.61
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.31	0.61
1:B:192:PHE:O	1:B:200:CYS:HB3	2.02	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.84	0.60
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.82	0.60
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.99	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.48	0.60
1:B:33:GLN:HE22	1:B:132:GLU:H	1.48	0.60
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.83	0.59
1:B:244:LEU:HB2	7:B:5172:HOH:O	2.02	0.59
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.85	0.59
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.91	0.59
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.83	0.59
2:D:153:LEU:HD12	2:D:153:LEU:C	2.23	0.59
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.03	0.59
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.02	0.59
2:D:44:LYS:HG3	7:D:491:HOH:O	2.02	0.59
1:A:227:ASN:ND2	1:A:295:LYS:H	2.00	0.59
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.84	0.58
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.68	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.03	0.58
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.86	0.58
1:B:227:ASN:HD21	1:B:296:PHE:H	1.52	0.57
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.38	0.57
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.34	0.57
2:D:111:LYS:O	2:D:115:GLU:HG3	2.03	0.57
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.50	0.57
3:F:61:GLU:O	3:F:121:PRO:HG2	2.05	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.04	0.57
1:B:227:ASN:ND2	1:B:295:LYS:H	2.02	0.57
1:B:268:ASN:CG	1:B:327:GLU:HG2	2.25	0.57
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.87	0.57
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.86	0.57
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.39	0.56
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.05	0.56
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.71	0.56
1:B:269:THR:HG21	7:F:940:HOH:O	2.06	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:LYS:O	3:F:37:MET:HG2	2.05	0.56
1:B:33:GLN:NE2	1:B:132:GLU:H	2.03	0.56
1:B:18:ARG:O	2:D:129:ALA:HA	2.05	0.56
1:B:44:THR:HG21	7:B:5112:HOH:O	2.06	0.56
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.41	0.55
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.88	0.55
1:B:159:ALA:O	2:D:33:ASN:HB2	2.07	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.98	0.55
1:A:268:ASN:HD21	1:A:327:GLU:N	2.03	0.55
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.42	0.55
2:C:175:THR:O	2:C:179:LEU:HD13	2.07	0.55
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.89	0.55
2:D:225:LYS:HE2	2:D:334:ASP:OD2	2.07	0.54
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.89	0.54
2:C:228:ARG:O	2:C:232:GLU:HG3	2.08	0.54
2:C:336:MET:CE	2:C:388:LEU:HG	2.38	0.54
2:C:34:LYS:HD3	7:C:5283:HOH:O	2.07	0.54
1:A:186:ARG:HA	2:C:73:THR:OG1	2.07	0.54
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.07	0.54
2:D:140:TRP:O	2:D:145:ILE:HD13	2.08	0.54
1:A:44:THR:OG1	1:A:127:SER:HA	2.07	0.54
1:B:20:PRO:HG2	7:B:5143:HOH:O	2.08	0.54
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.54
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.56	0.54
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.42	0.54
2:D:145:ILE:O	2:D:149:TRP:HB3	2.08	0.54
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.91	0.53
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.90	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.42	0.53
1:B:212:PHE:O	1:B:215:PRO:HD2	2.08	0.53
3:F:162:ARG:NH1	3:F:164:VAL:HG12	2.24	0.53
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.91	0.53
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.07	0.53
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.09	0.53
1:A:213:THR:O	1:A:217:ILE:HG12	2.10	0.52
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.38	0.52
3:E:58:ALA:O	3:E:62:GLU:HG3	2.10	0.52
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.42	0.52
3:F:41:THR:HG23	3:F:43:PHE:H	1.73	0.52
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:GLU:O	3:E:61:GLU:HG3	2.08	0.52
1:A:268:ASN:ND2	1:A:327:GLU:H	2.04	0.52
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.92	0.52
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.93	0.52
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.91	0.52
1:B:268:ASN:HD21	1:B:327:GLU:H	1.56	0.52
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.52
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.43	0.51
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.44	0.51
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.45	0.51
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.38	0.51
1:B:52:MET:HE3	1:B:127:SER:HB3	1.92	0.51
2:C:211:THR:O	2:C:214:PRO:HD2	2.10	0.51
2:D:71:ASP:HB2	3:F:54:LEU:HD11	1.93	0.51
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.11	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
1:B:185:LYS:O	1:B:189:SER:HB2	2.11	0.51
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.44	0.51
1:A:297:LYS:HG2	1:A:371:TRP:CE2	2.46	0.50
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.45	0.50
2:C:97:LYS:HD2	7:C:5103:HOH:O	2.10	0.50
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.92	0.50
1:A:109:PHE:O	1:A:112:VAL:HG12	2.10	0.50
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.50
1:B:48:THR:O	3:F:137:THR:HG23	2.12	0.50
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.92	0.50
1:B:43:ARG:HD2	1:B:43:ARG:O	2.12	0.50
2:C:96:PHE:O	2:C:99:ARG:NH2	2.44	0.50
2:D:82:SER:O	2:D:168:ARG:NH2	2.44	0.50
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.93	0.50
3:F:153:GLU:CD	3:F:153:GLU:H	2.15	0.50
2:C:336:MET:HE3	2:C:388:LEU:HG	1.92	0.50
3:F:40:THR:O	3:F:41:THR:HB	2.11	0.50
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.12	0.49
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.75	0.49
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.95	0.49
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.76	0.49
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.15	0.49
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.13	0.49
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.49
1:A:185:LYS:O	1:A:189:SER:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:OD1	1:B:327:GLU:HG2	2.13	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.13	0.49
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.94	0.49
1:B:52:MET:CE	1:B:127:SER:HB3	2.43	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
2:C:277:THR:HB	2:C:278:PRO:HD3	1.94	0.49
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.48	0.48
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.48
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.95	0.48
1:B:123:MET:CE	1:B:197:ALA:HA	2.43	0.48
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.95	0.48
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.95	0.48
3:E:18:LYS:HB2	3:E:18:LYS:NZ	2.28	0.48
1:B:106:VAL:O	1:B:110:LEU:HB2	2.13	0.48
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.48
3:F:19:ILE:C	3:F:19:ILE:HD12	2.33	0.48
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.42	0.48
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.48	0.48
1:A:163:GLN:HG2	7:A:9175:HOH:O	2.14	0.48
2:D:381:VAL:O	2:D:385:LEU:HB2	2.14	0.48
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.48
2:D:332:LEU:O	2:D:336:MET:HG2	2.14	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.47
3:E:102:LYS:HG2	3:E:106:GLU:OE1	2.13	0.47
7:C:5122:HOH:O	3:E:125:VAL:HG22	2.14	0.47
2:D:89:GLU:OE2	3:F:125:VAL:HG13	2.13	0.47
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.49	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
2:D:195:LEU:O	2:D:195:LEU:HD23	2.14	0.47
2:D:235:TRP:CD1	2:D:235:TRP:C	2.88	0.47
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.96	0.47
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.50	0.47
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.32	0.47
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.47
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.47
1:A:227:ASN:HD21	1:A:296:PHE:H	1.60	0.47
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.48	0.47
2:D:101:PRO:HG2	2:D:293:GLN:HB3	1.95	0.47
7:D:497:HOH:O	3:F:125:VAL:HG22	2.14	0.47
2:C:126:GLY:O	2:C:130:ASP:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:HIS:HE1	2:C:178:SER:OG	1.97	0.46
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.51	0.46
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.46
1:B:209:GLU:HA	1:B:213:THR:CB	2.35	0.46
2:C:7:ARG:HH11	2:C:7:ARG:HG3	1.81	0.46
1:B:206:LEU:HB2	7:B:5239:HOH:O	2.16	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.46
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.80	0.46
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.97	0.46
2:C:75:LYS:HB3	2:C:80:ARG:O	2.15	0.46
3:F:17:ASN:O	3:F:21:GLN:HG2	2.15	0.46
2:C:111:LYS:O	2:C:115:GLU:HG3	2.15	0.46
1:B:41:ASN:O	2:D:236:GLN:HB3	2.16	0.46
2:C:153:LEU:HD12	2:C:153:LEU:C	2.37	0.46
2:C:2:SER:HB2	7:C:5256:HOH:O	2.15	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.16	0.46
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.98	0.45
1:A:184:MET:HE1	1:A:188:PHE:CG	2.51	0.45
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.45
2:D:187:ILE:O	2:D:191:GLN:HG3	2.16	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
1:A:21:THR:HG22	2:C:128:SER:CB	2.46	0.45
1:B:337:GLN:HG3	1:B:338:ASP:N	2.32	0.45
1:A:186:ARG:HD3	1:A:186:ARG:O	2.17	0.45
1:B:230:GLU:C	1:B:233:PRO:HD2	2.36	0.45
1:B:123:MET:SD	2:D:168:ARG:NH1	2.89	0.45
1:B:186:ARG:HD3	1:B:186:ARG:C	2.37	0.45
1:B:198:VAL:O	1:B:202:LEU:HG	2.16	0.45
1:B:413:HIS:HE1	7:B:5261:HOH:O	1.99	0.45
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.98	0.45
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:B:123:MET:HE2	1:B:197:ALA:HA	1.99	0.45
1:B:21:THR:HG22	1:B:22:SER:N	2.32	0.45
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.51	0.45
1:B:334:ASP:HA	1:B:337:GLN:HG2	1.99	0.45
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.52	0.45
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.99	0.45
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.52	0.44
1:B:186:ARG:HA	2:D:73:THR:OG1	2.16	0.44
1:A:216:LEU:O	1:A:220:VAL:HG23	2.16	0.44
1:A:81:SER:OG	1:B:84:ASP:HB3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.53	0.44
2:D:143:GLU:O	2:D:147:ARG:HB3	2.17	0.44
2:D:277:THR:HB	2:D:278:PRO:HD3	1.98	0.44
1:B:196:ASP:HB2	3:F:140:MET:SD	2.58	0.44
3:F:41:THR:HG22	3:F:43:PHE:N	2.30	0.44
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.00	0.44
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.48	0.44
2:D:324:TRP:C	2:D:327:PRO:HD2	2.37	0.44
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.52	0.44
3:F:12:ARG:O	3:F:16:VAL:HG13	2.17	0.44
1:A:163:GLN:O	2:C:28:PRO:HA	2.18	0.44
1:A:206:LEU:HB2	7:A:9036:HOH:O	2.18	0.44
1:B:384:GLY:O	1:B:388:GLU:HG3	2.18	0.44
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.99	0.44
2:C:235:TRP:CD1	2:C:235:TRP:C	2.91	0.44
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.53	0.44
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.52	0.44
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.02	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
1:A:193:ILE:HD11	2:C:82:SER:HB3	1.99	0.43
2:D:360:VAL:O	2:D:364:ILE:HG13	2.17	0.43
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.43
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.18	0.43
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.00	0.43
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.53	0.43
2:D:348:ASP:OD1	2:D:351:GLU:HG3	2.18	0.43
3:F:132:GLU:HG3	7:F:1113:HOH:O	2.18	0.43
1:A:216:LEU:HA	1:A:308:TRP:CH2	2.53	0.43
1:A:65:LYS:HD2	2:C:117:TRP:HB2	2.00	0.43
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.47	0.43
1:A:212:PHE:O	1:A:215:PRO:HD2	2.18	0.43
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.53	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.82	0.43
3:E:22:LEU:HD21	3:E:31:MET:SD	2.58	0.43
2:D:326:GLU:HG3	7:D:441:HOH:O	2.18	0.43
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:190:ASP:HB3	2:C:74:GLN:O	2.18	0.43
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.83	0.43
2:D:193:ILE:HA	7:D:553:HOH:O	2.19	0.43
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.53	0.43
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:HB3	1:B:81:SER:OG	2.18	0.42
2:C:240:ASP:OD1	3:E:125:VAL:HG21	2.19	0.42
3:F:40:THR:HG22	3:F:53:TYR:CD1	2.54	0.42
1:A:402:PHE:O	1:A:403:ILE:HD12	2.19	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.82	0.42
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.49	0.42
1:B:488:LEU:HD13	1:B:492:GLY:O	2.19	0.42
1:B:490:SER:OG	2:D:32:ASN:HB2	2.19	0.42
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.69	0.42
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.30	0.42
2:D:324:TRP:O	2:D:327:PRO:HD2	2.19	0.42
1:A:184:MET:HE1	1:A:188:PHE:CD2	2.55	0.42
1:A:343:HIS:H	1:A:343:HIS:CD2	2.37	0.42
1:B:140:GLN:O	1:B:144:GLU:HG2	2.20	0.42
2:D:167:ALA:O	2:D:176:ARG:NH1	2.51	0.42
1:A:210:ALA:HA	1:A:247:MET:CE	2.49	0.42
1:A:417:ILE:HG13	1:A:468:ASN:HB2	2.02	0.42
1:B:207:VAL:O	1:B:211:CYS:HB3	2.20	0.42
1:A:222:GLU:OE1	2:C:7:ARG:NH1	2.52	0.42
2:D:140:TRP:CE2	2:D:145:ILE:HD11	2.54	0.42
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.55	0.42
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.20	0.42
1:B:421:SER:O	1:B:422:GLN:HB2	2.20	0.42
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.06	0.42
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.20	0.42
2:D:275:ASN:C	2:D:278:PRO:HD2	2.40	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.01	0.41
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.02	0.41
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.55	0.41
1:B:438:VAL:HB	3:F:164:VAL:CG2	2.50	0.41
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.55	0.41
3:F:19:ILE:HG21	3:F:60:LEU:CD1	2.50	0.41
2:C:146:ASN:O	2:C:214:PRO:HG3	2.20	0.41
1:A:232:THR:HB	1:A:233:PRO:HD3	2.01	0.41
1:B:113:GLY:HA2	1:B:188:PHE:HB3	2.01	0.41
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.41
3:F:38:ASP:HA	3:F:45:ASN:HB2	2.02	0.41
1:B:65:LYS:CE	2:D:192:MET:HE2	2.48	0.41
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.55	0.41
1:B:163:GLN:O	2:D:28:PRO:HA	2.20	0.41
3:E:66:VAL:CG1	3:E:70:ARG:HH21	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:HD22	1:A:249:ASN:HA	1.68	0.41
1:B:355:PRO:HG2	1:B:403:ILE:HD12	2.01	0.41
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.85	0.41
1:A:90:ASN:HA	1:A:90:ASN:HD22	1.61	0.41
1:B:470:PHE:O	1:B:474:GLU:HB2	2.20	0.41
2:D:94:ASP:HB3	2:D:97:LYS:HG3	2.02	0.41
2:D:98:HIS:CD2	2:D:99:ARG:N	2.89	0.41
1:A:192:PHE:O	1:A:200:CYS:HB3	2.20	0.41
1:A:230:GLU:C	1:A:233:PRO:HD2	2.42	0.41
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.20	0.41
2:D:240:ASP:HB2	3:F:125:VAL:HG21	2.02	0.41
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.56	0.41
2:D:291:ALA:O	2:D:295:VAL:HG23	2.21	0.41
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.86	0.41
1:B:108:ASN:O	1:B:111:GLU:HB3	2.21	0.41
2:D:312:TYR:O	2:D:316:VAL:HG23	2.21	0.41
3:E:15:TRP:O	3:E:19:ILE:HG13	2.21	0.41
1:B:125:TRP:C	1:B:125:TRP:CD1	2.94	0.40
1:A:110:LEU:O	1:A:114:GLU:HG2	2.20	0.40
1:B:246:HIS:CD2	1:B:246:HIS:N	2.88	0.40
2:C:256:PHE:HA	2:C:332:LEU:HD21	2.03	0.40
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.92	0.40
1:A:360:ARG:NH2	1:A:501:VAL:O	2.54	0.40
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.48	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.94	0.40
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.35	0.40
2:D:140:TRP:NE1	2:D:145:ILE:CD1	2.81	0.40
1:B:165:PRO:HG3	7:B:5025:HOH:O	2.22	0.40
1:B:227:ASN:ND2	1:B:296:PHE:H	2.17	0.40
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	487 (96%)	21 (4%)	1 (0%)	47	43
1	B	509/527 (97%)	484 (95%)	23 (4%)	2 (0%)	34	28
2	C	386/389 (99%)	374 (97%)	10 (3%)	2 (0%)	29	22
2	D	386/389 (99%)	367 (95%)	17 (4%)	2 (0%)	29	22
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
All	All	2120/2172 (98%)	2033 (96%)	80 (4%)	7 (0%)	41	36

All (7) Ramachandran outliers are listed below:

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

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%)	53	55
1	B	433/442 (98%)	426 (98%)	7 (2%)	62	66
2	C	322/323 (100%)	317 (98%)	5 (2%)	62	66
2	D	322/323 (100%)	316 (98%)	6 (2%)	57	59
3	E	144/147 (98%)	143 (99%)	1 (1%)	84	87
3	F	146/147 (99%)	143 (98%)	3 (2%)	53	55
All	All	1800/1824 (99%)	1769 (98%)	31 (2%)	60	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	90	ASN
1	A	125	TRP
1	A	186	ARG
1	A	279	GLN
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
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	168	ARG
2	C	173	ASP
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	160	PHE
2	D	173	ASP
2	D	205	PRO
3	E	44	ARG
3	F	11	THR
3	F	41	THR
3	F	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
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	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
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	293	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	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	F	7	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN

5.3.3 RNA [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 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	-

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, 95th 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%)	-0.04	11 (2%) 62 61	17, 28, 49, 65	0
1	B	511/527 (96%)	-0.09	14 (2%) 54 54	19, 30, 50, 66	0
2	C	388/389 (99%)	-0.38	4 (1%) 82 82	14, 21, 36, 55	0
2	D	388/389 (99%)	0.33	26 (6%) 17 17	21, 36, 55, 71	0
3	E	166/170 (97%)	-0.23	2 (1%) 79 78	17, 25, 40, 61	0
3	F	168/170 (98%)	0.80	19 (11%) 5 4	30, 45, 62, 69	0
All	All	2132/2172 (98%)	0.00	76 (3%) 42 42	14, 30, 52, 71	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	4.4
1	A	310	TYR	4.4
3	F	100	ALA	4.3
3	E	4	LEU	4.2
1	B	17	ASN	4.0
1	A	316	ILE	3.9
2	D	380	ILE	3.9
3	E	168	SER	3.7
2	D	205	PRO	3.6
2	D	45	ARG	3.5
2	D	388	LEU	3.5
3	F	101	ALA	3.5
2	D	44	LYS	3.5
1	B	40	LYS	3.4
3	F	170	HIS	3.3
2	D	260	VAL	3.3
2	D	348	ASP	3.2
2	D	385	LEU	3.1
1	A	17	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	2	SER	3.1
1	B	54	ASN	3.1
1	B	310	TYR	3.1
1	B	214	ASN	3.0
2	D	389	LYS	3.0
1	B	39	PHE	3.0
3	F	23	ASN	3.0
1	A	381	ASP	3.0
2	D	333	ARG	2.9
3	F	21	GLN	2.9
3	F	102	LYS	2.8
1	A	380	TYR	2.8
1	B	311	GLU	2.8
1	A	318	ILE	2.7
2	D	357	TYR	2.7
3	F	20	ALA	2.7
1	B	259	ASN	2.7
1	B	527	ASN	2.7
3	F	27	LYS	2.7
1	B	316	ILE	2.7
2	C	6	GLU	2.7
2	D	345	GLY	2.7
1	B	244	LEU	2.7
3	F	3	LYS	2.6
3	F	10	ASP	2.6
2	D	350	GLU	2.6
2	D	379	GLN	2.6
1	B	320	ARG	2.5
3	F	16	VAL	2.5
2	D	206	GLY	2.5
3	F	80	LYS	2.5
2	D	207	PHE	2.5
3	F	83	PHE	2.5
2	D	344	ALA	2.5
2	D	307	PRO	2.4
1	A	333	LYS	2.4
2	D	382	LYS	2.4
1	A	337	GLN	2.3
2	C	45	ARG	2.3
1	B	55	GLU	2.3
1	A	320	ARG	2.3
3	F	70	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	372	ASP	2.3
1	B	514	ARG	2.2
3	F	28	ALA	2.2
2	C	205	PRO	2.2
2	D	223	VAL	2.2
1	A	434	SER	2.2
3	F	127	TYR	2.2
2	D	384	VAL	2.2
2	D	308	GLU	2.2
2	D	346	THR	2.2
3	F	89	SER	2.1
2	D	2	SER	2.1
3	F	30	GLU	2.0
2	D	203	ILE	2.0
3	F	76	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
6	FMT	A	9001	3/3	0.92	0.15	41,41,48,53	0
5	CA	C	5006	1/1	0.96	0.09	51,51,51,51	0
5	CA	A	5005	1/1	0.98	0.08	46,46,46,46	0
5	CA	C	5007	1/1	0.98	0.08	35,35,35,35	0
4	FE	B	5004	1/1	0.98	0.03	39,39,39,39	0
4	FE	A	5002	1/1	0.99	0.03	36,36,36,36	0
4	FE	A	5001	1/1	1.00	0.03	28,28,28,28	0
4	FE	B	5003	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.