Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 10:36 PM EDT

PDB ID	:	1XVD
Title	:	Soluble methane monooxygenase hydroxylase: 4-fluorophenol soaked structure
Authors	:	Sazinsky, M.H.; Lippard, S.J.
Deposited on	:	2004-10-27
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

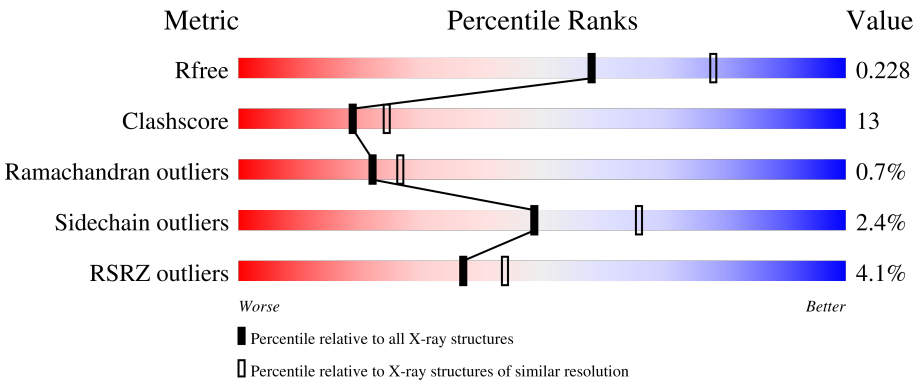
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	5% 70% 25% • •
1	B	527	4% 68% 27% • •
2	C	389	% 83% 16% •
2	D	389	6% 63% 36% •
3	E	170	% 86% 11% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	170	9% 58% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FPN	A	2666	-	X	-	-
5	FPN	B	2667	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18293 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
			Total	C	N	O	S			
1	A	510	4148	2655	713	762	18	0	0	0
1	B	510	4137	2646	711	762	18	0	0	0

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	388	3163	2036	545	574	8	0	0	0
2	D	388	3151	2028	543	572	8	0	0	0

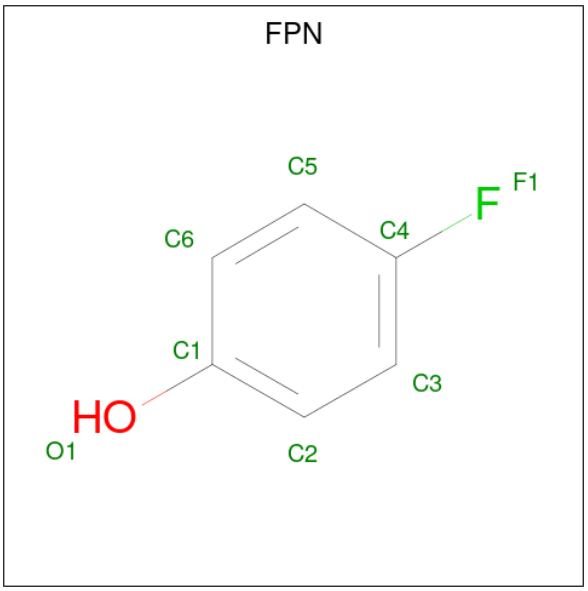
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	166	1364	864	245	250	5	0	0	0
3	F	166	1358	860	243	250	5	0	0	0

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

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

- Molecule 5 is 4-FLUOROPHENOL (three-letter code: FPN) (formula: C_6H_5FO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
5	A	1	8	6	1	1	0	0
			Total	C	F	O		
5	B	1	8	6	1	1	0	0

- Molecule 6 is water.

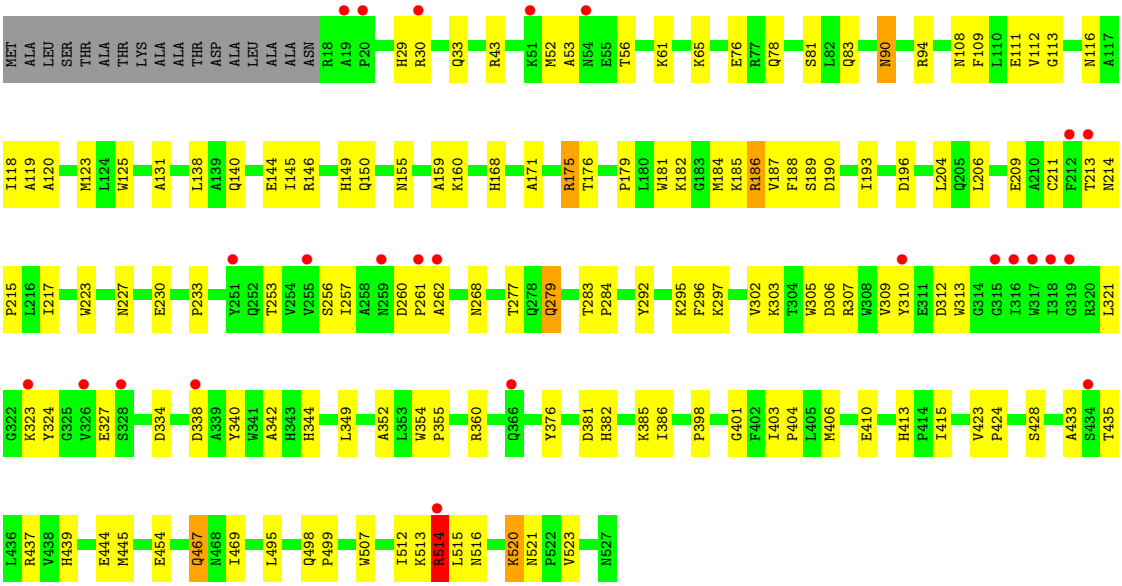
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	200	200	200	0	0
			Total	O		
6	B	198	198	198	0	0
			Total	O		
6	C	277	277	277	0	0
			Total	O		
6	D	105	105	105	0	0
			Total	O		
6	E	124	124	124	0	0
			Total	O		
6	F	48	48	48	0	0

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.

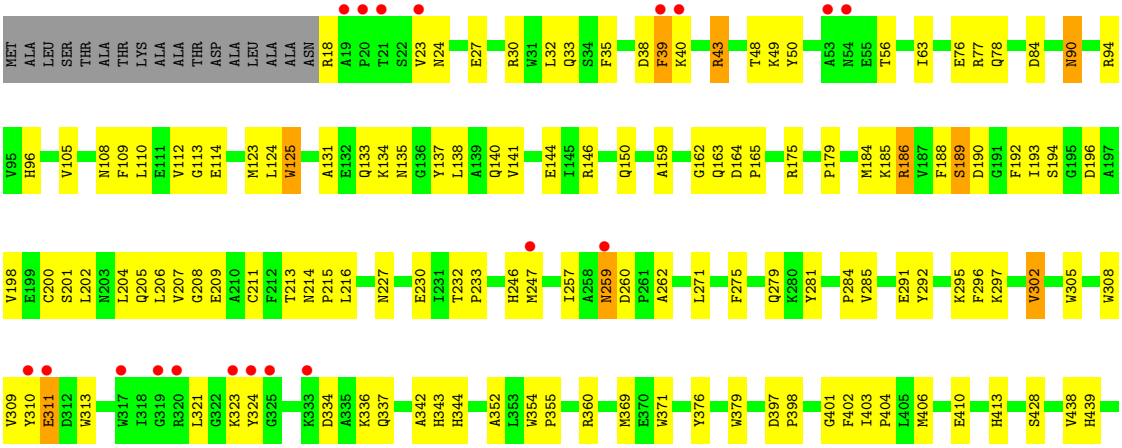
• Molecule 1: Methane monooxygenase component A alpha chain

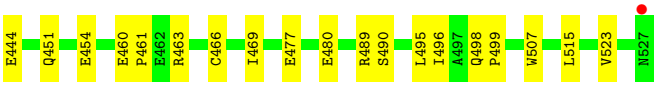
Chain A:



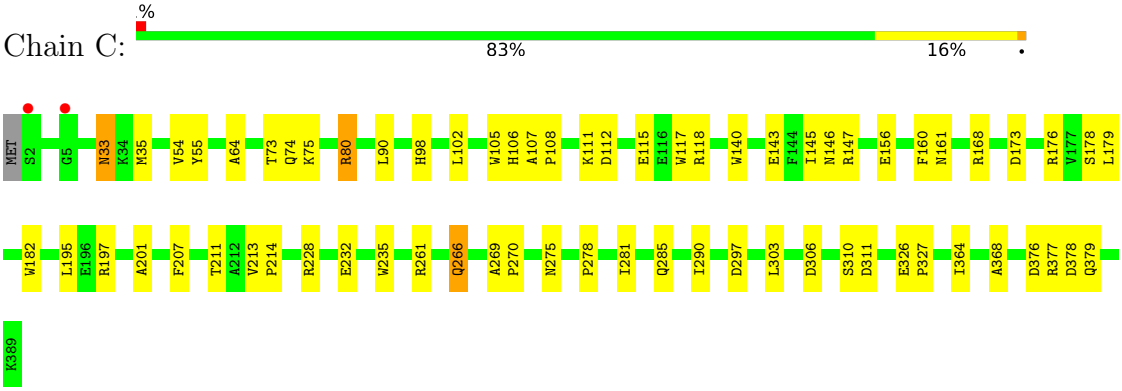
• Molecule 1: Methane monooxygenase component A alpha chain

Chain B:

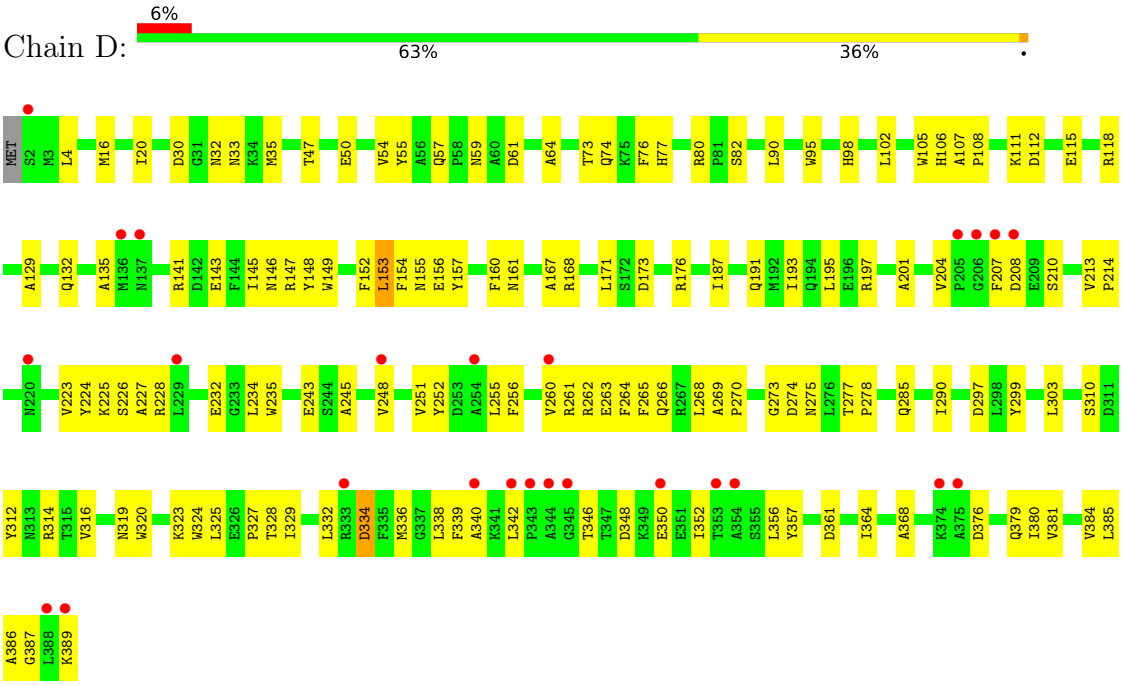




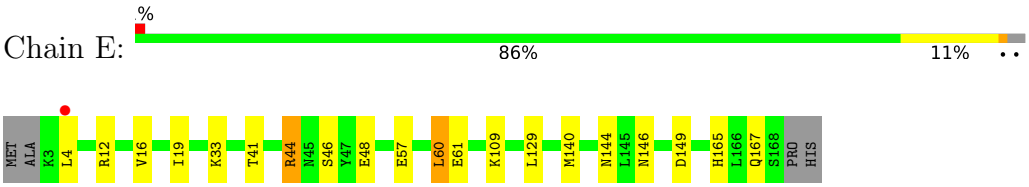
• Molecule 2: Methane monooxygenase component A beta chain



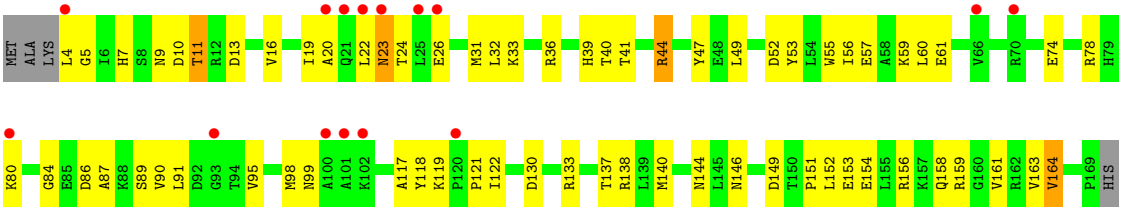
• Molecule 2: Methane monooxygenase component A beta chain



• Molecule 3: Methane monooxygenase component A gamma chain



• Molecule 3: Methane monooxygenase component A gamma chain


MET
ALA
LYS
L4
G5
I6
H7
S8
N9
D10
T11
R12
D13
V16
I19
A20
Q21
L22
N23
T24
L25
E26
M31
L32
K33
R36
H39
T40
T41
R44
Y47
E48
L49
D52
Y53
L54
W55
I56
E57
A58
K59
L60
E61
V66
R70
E74
R78
H79
K80
G84
E85
D86
A87
K88
S89
V90
L91
D92
G93
T94
V95
M98
N99
A100
A101
K102
A117
Y118
K119
P120
P121
I122
D130
R133
T137
R138
L139
M140
N144
L145
N146
D149
T150
P151
L152
E153
E154
L155
R156
K157
Q158
R159
G160
V161
R162
V163
V164
P169
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.18Å 171.50Å 221.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.30 29.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.94-2.30) 94.3 (29.94-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.229 0.193 , 0.228	Depositor DCC
R_{free} test set	4028 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18293	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FPN, 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	0.36	0/4273	0.58	1/5808 (0.0%)
1	B	0.35	0/4262	0.55	0/5796
2	C	0.39	0/3259	0.58	0/4430
2	D	0.34	0/3247	0.53	0/4417
3	E	0.37	0/1392	0.60	0/1876
3	F	0.30	0/1387	0.53	0/1873
All	All	0.36	0/17820	0.56	1/24200 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	514	ARG	NE-CZ-NH2	-5.33	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	514	ARG	Mainchain

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	4148	0	3919	114	0
1	B	4137	0	3888	140	0
2	C	3163	0	2986	60	0
2	D	3151	0	2960	114	0
3	E	1364	0	1352	17	0
3	F	1358	0	1335	57	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	5	0	0
5	B	8	0	5	0	0
6	A	200	0	0	4	0
6	B	198	0	0	5	0
6	C	277	0	0	1	0
6	D	105	0	0	0	0
6	E	124	0	0	2	0
6	F	48	0	0	0	0
All	All	18293	0	16450	441	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 13.

All (441) 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)
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.31	1.07
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.03	1.01
2:D:340:ALA:HA	2:D:389:LYS:HE2	1.47	0.96
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.70	0.91
3:F:41:THR:O	3:F:44:ARG:HD2	1.71	0.90
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.17	0.89
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.55	0.87
1:A:467:GLN:HG3	6:A:2865:HOH:O	1.76	0.85
1:A:209:GLU:HA	1:A:213:THR:HB	1.58	0.82
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.25	0.82
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.28	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.77	0.82
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.28	0.82
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.64	0.79
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.64	0.79
3:F:13:ASP:O	3:F:16:VAL:HG22	1.83	0.77
1:B:209:GLU:HA	1:B:213:THR:OG1	1.85	0.76
1:A:435:THR:CG2	1:A:437:ARG:HE	1.99	0.76
2:C:105:TRP:O	2:C:108:PRO:HD2	1.86	0.76
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.85	0.76
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.88	0.73
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.86	0.73
1:A:227:ASN:HD21	1:A:295:LYS:H	1.36	0.73
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.19	0.72
1:B:406:MET:O	1:B:410:GLU:HG3	1.88	0.72
1:A:435:THR:HG21	1:A:437:ARG:HE	1.55	0.72
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
1:B:477:GLU:OE2	1:B:480:GLU:HG2	1.91	0.70
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.22	0.70
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.74	0.70
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.90	0.70
3:F:91:LEU:O	3:F:95:VAL:HG23	1.92	0.68
1:A:204:LEU:O	1:A:209:GLU:HG3	1.93	0.68
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.76	0.68
1:A:513:LYS:O	1:A:514:ARG:C	2.33	0.67
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.43	0.67
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.76	0.67
1:B:196:ASP:HB2	3:F:140:MET:SD	2.35	0.67
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.77	0.67
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.26	0.66
3:F:52:ASP:O	3:F:56:ILE:HG12	1.96	0.66
1:A:401:GLY:HA2	1:A:515:LEU:HD21	1.78	0.66
2:D:325:LEU:O	2:D:329:ILE:HG12	1.95	0.66
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.11	0.66
3:E:57:GLU:O	3:E:61:GLU:HG3	1.96	0.66
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.78	0.65
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.79	0.65
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.79	0.65
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.60	0.65
1:A:349:LEU:HD22	1:A:415:ILE:HD12	1.78	0.65
3:F:153:GLU:H	3:F:153:GLU:CD	1.99	0.65
1:A:109:PHE:O	1:A:112:VAL:HG12	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HA	2:C:73:THR:OG1	1.97	0.65
1:A:213:THR:O	1:A:217:ILE:HG12	1.96	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.96	0.65
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.32	0.64
1:A:227:ASN:ND2	1:A:295:LYS:H	1.95	0.64
3:F:19:ILE:HD12	3:F:20:ALA:N	2.13	0.64
1:A:144:GLU:HA	1:A:144:GLU:OE2	1.98	0.64
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.11	0.64
2:D:153:LEU:C	2:D:153:LEU:HD12	2.18	0.64
1:B:38:ASP:O	1:B:39:PHE:HB3	1.97	0.64
2:D:153:LEU:HD12	2:D:154:PHE:N	2.12	0.64
1:B:23:VAL:HB	2:D:195:LEU:HD11	1.80	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.46	0.63
1:A:76:GLU:OE1	1:B:76:GLU:HG3	1.98	0.63
1:B:227:ASN:HD21	1:B:295:LYS:H	1.45	0.63
1:B:18:ARG:O	2:D:129:ALA:HA	1.98	0.63
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.62
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.80	0.62
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.62
1:B:489:ARG:HH11	1:B:496:ILE:HA	1.65	0.62
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.00	0.62
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.00	0.62
3:F:61:GLU:O	3:F:121:PRO:HG2	2.00	0.61
1:A:160:LYS:HE3	6:A:2857:HOH:O	2.01	0.61
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.96	0.61
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.82	0.61
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.48	0.61
2:D:255:LEU:HD12	2:D:328:THR:HG21	1.83	0.61
2:D:135:ALA:O	2:D:273:GLY:HA3	2.01	0.60
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.83	0.60
1:B:185:LYS:O	1:B:189:SER:HB2	2.02	0.60
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.83	0.60
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.00	0.60
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.37	0.60
1:A:401:GLY:HA2	1:A:515:LEU:CD2	2.32	0.59
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.03	0.59
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.59
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.49	0.59
3:F:57:GLU:O	3:F:61:GLU:HG3	2.02	0.59
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.83	0.59
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:ASN:C	2:D:278:PRO:HD2	2.21	0.59
1:B:402:PHE:C	1:B:403:ILE:HD12	2.23	0.59
3:E:41:THR:O	3:E:44:ARG:HD2	2.03	0.58
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.36	0.58
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.69	0.58
2:D:57:GLN:NE2	2:D:59:ASN:HD21	2.02	0.58
2:D:269:ALA:HB1	2:D:274:ASP:OD2	2.04	0.57
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.57
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.01	0.57
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.69	0.57
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.51	0.57
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.69	0.57
2:D:336:MET:CE	2:D:356:LEU:HD11	2.34	0.57
1:A:406:MET:O	1:A:410:GLU:HG3	2.05	0.57
1:A:185:LYS:O	1:A:189:SER:HB2	2.04	0.57
1:A:140:GLN:O	1:A:144:GLU:HG2	2.05	0.56
1:A:190:ASP:HB3	2:C:74:GLN:O	2.05	0.56
2:C:98:HIS:HE1	2:C:178:SER:OG	1.88	0.56
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.05	0.56
1:B:23:VAL:HB	2:D:195:LEU:CD1	2.35	0.56
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.40	0.56
1:A:413:HIS:HD2	1:A:428:SER:OG	1.88	0.56
2:D:105:TRP:O	2:D:108:PRO:HD2	2.04	0.56
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.39	0.56
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.88	0.56
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.06	0.56
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.87	0.56
1:A:184:MET:CE	1:A:188:PHE:HB2	2.35	0.56
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.88	0.56
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.40	0.56
1:B:43:ARG:HD2	1:B:43:ARG:C	2.26	0.55
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.06	0.55
1:A:171:ALA:O	1:A:175:ARG:HB3	2.06	0.55
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.88	0.55
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.87	0.55
1:B:109:PHE:O	1:B:112:VAL:HG12	2.07	0.55
1:A:116:ASN:CG	1:A:189:SER:HA	2.27	0.55
1:B:403:ILE:HD13	1:B:515:LEU:HD13	1.89	0.55
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.71	0.55
1:A:435:THR:HG22	1:A:437:ARG:HE	1.71	0.55
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.55
1:A:435:THR:HG21	1:A:437:ARG:HH21	1.73	0.54
1:B:137:TYR:O	1:B:141:VAL:HG23	2.08	0.54
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.90	0.54
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.88	0.54
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.72	0.54
1:B:403:ILE:HD11	1:B:507:TRP:CZ3	2.43	0.54
3:E:4:LEU:O	3:E:4:LEU:HG	2.07	0.54
2:D:157:TYR:O	2:D:160:PHE:HB3	2.07	0.54
1:B:227:ASN:ND2	1:B:295:LYS:H	2.05	0.54
2:D:336:MET:HE1	2:D:356:LEU:HD11	1.89	0.54
1:A:185:LYS:HA	1:A:189:SER:HB2	1.89	0.54
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.21	0.54
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.16	0.54
2:D:143:GLU:O	2:D:147:ARG:HB3	2.08	0.54
2:D:262:ARG:O	2:D:266:GLN:HB3	2.08	0.54
1:B:402:PHE:O	1:B:403:ILE:HD12	2.08	0.53
2:D:224:TYR:O	2:D:227:ALA:N	2.42	0.53
1:B:110:LEU:O	1:B:114:GLU:HG2	2.09	0.53
2:C:146:ASN:O	2:C:214:PRO:HG3	2.09	0.53
3:E:46:SER:OG	3:E:48:GLU:HG2	2.09	0.53
1:A:382:HIS:O	1:A:386:ILE:HG12	2.08	0.53
1:B:208:GLY:O	1:B:213:THR:HG23	2.08	0.53
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.90	0.53
1:B:205:GLN:HA	1:B:209:GLU:HB2	1.91	0.53
2:D:54:VAL:O	2:D:55:TYR:HB2	2.09	0.53
2:D:141:ARG:HD2	2:D:204:VAL:HG21	1.91	0.53
1:B:403:ILE:HD13	1:B:515:LEU:CD1	2.39	0.53
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.01	0.53
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.90	0.53
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.25	0.52
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.91	0.52
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.91	0.52
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.75	0.52
1:B:310:TYR:CZ	1:B:336:LYS:HD2	2.45	0.52
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.91	0.52
3:E:109:LYS:HE2	6:E:274:HOH:O	2.09	0.52
1:B:48:THR:O	3:F:137:THR:HG23	2.10	0.52
1:B:96:HIS:HB2	2:D:20:ILE:CD1	2.39	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.52
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.92	0.51
6:A:2832:HOH:O	3:E:144:ASN:HB3	2.10	0.51
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.09	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.10	0.51
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.45	0.51
2:C:228:ARG:O	2:C:232:GLU:HG3	2.10	0.51
2:C:306:ASP:O	2:C:310:SER:HB2	2.10	0.51
2:C:377:ARG:HG2	6:C:593:HOH:O	2.09	0.51
3:F:130:ASP:O	3:F:133:ARG:HG2	2.10	0.51
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.08	0.51
1:A:355:PRO:HG2	1:A:403:ILE:HD13	1.91	0.51
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.46	0.51
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.40	0.51
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.46	0.51
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.93	0.51
1:B:230:GLU:C	1:B:233:PRO:HD2	2.32	0.51
2:D:324:TRP:C	2:D:327:PRO:HD2	2.30	0.51
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.47	0.50
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.09	0.50
1:B:403:ILE:HD11	1:B:507:TRP:HZ3	1.76	0.50
2:D:77:HIS:CG	3:F:140:MET:HG2	2.46	0.50
2:D:167:ALA:O	2:D:176:ARG:NH1	2.44	0.50
3:F:19:ILE:HD12	3:F:19:ILE:C	2.32	0.50
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.76	0.50
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.46	0.50
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.91	0.50
1:B:192:PHE:O	1:B:200:CYS:HB3	2.12	0.50
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.93	0.50
1:B:198:VAL:O	1:B:202:LEU:HG	2.11	0.50
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.41	0.50
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.45	0.50
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.94	0.50
1:B:202:LEU:HD22	1:B:206:LEU:HD22	1.94	0.50
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.91	0.50
1:A:182:LYS:O	2:C:73:THR:HG21	2.12	0.50
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.50
2:D:145:ILE:O	2:D:149:TRP:HB3	2.12	0.50
2:D:260:VAL:O	2:D:265:PHE:HD1	1.94	0.50
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.25	0.50
2:D:152:PHE:O	2:D:155:ASN:HB3	2.12	0.50
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HA	2:D:73:THR:OG1	2.12	0.49
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.92	0.49
2:D:329:ILE:CD1	2:D:380:ILE:HG23	2.43	0.49
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.47	0.49
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.30	0.49
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.94	0.49
1:A:53:ALA:HB3	1:A:56:THR:OG1	2.13	0.49
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.13	0.49
3:F:22:LEU:HD11	3:F:31:MET:SD	2.52	0.49
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.94	0.49
2:D:339:PHE:CE2	2:D:352:ILE:HD12	2.48	0.49
2:D:340:ALA:HB2	2:D:389:LYS:HG2	1.94	0.49
2:D:277:THR:HB	2:D:278:PRO:HD3	1.95	0.49
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.48	0.48
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.94	0.48
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.48
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.48	0.48
1:B:401:GLY:HA2	1:B:515:LEU:HD21	1.95	0.48
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.78	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.13	0.48
3:F:24:THR:HG22	3:F:26:GLU:HB3	1.95	0.48
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.48
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.95	0.48
3:E:12:ARG:O	3:E:16:VAL:HG23	2.14	0.48
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.29	0.48
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.49	0.48
2:C:111:LYS:O	2:C:115:GLU:HG3	2.13	0.48
2:C:266:GLN:NE2	2:D:132:GLN:OE1	2.47	0.48
1:B:162:GLY:HA3	6:B:2789:HOH:O	2.14	0.47
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.49	0.47
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.44	0.47
2:C:211:THR:C	2:C:214:PRO:HD2	2.34	0.47
2:D:376:ASP:OD1	2:D:379:GLN:HB2	2.14	0.47
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.44	0.47
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.49	0.47
1:B:515:LEU:HD21	6:B:2831:HOH:O	2.14	0.47
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.47
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.80	0.47
1:B:413:HIS:HD2	1:B:428:SER:OG	1.97	0.47
1:A:120:ALA:HA	1:A:193:ILE:HG22	1.95	0.47
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:O	2:C:33:ASN:HB2	2.14	0.47
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.29	0.47
2:D:208:ASP:OD1	2:D:210:SER:HB3	2.14	0.47
3:F:32:LEU:HD13	3:F:60:LEU:HB3	1.96	0.47
1:A:206:LEU:HB2	6:A:2863:HOH:O	2.15	0.47
2:D:357:TYR:CD2	2:D:381:VAL:HG21	2.49	0.47
1:A:230:GLU:C	1:A:233:PRO:HD2	2.35	0.47
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.15	0.47
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.50	0.47
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.97	0.47
1:A:196:ASP:HB2	3:E:140:MET:SD	2.55	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46
1:B:24:ASN:OD1	1:B:27:GLU:HG3	2.14	0.46
1:B:310:TYR:CE1	1:B:336:LYS:HD2	2.50	0.46
1:B:466:CYS:HB2	2:D:73:THR:HA	1.96	0.46
2:C:75:LYS:HB3	2:C:80:ARG:O	2.14	0.46
1:A:435:THR:HG23	3:E:167:GLN:O	2.15	0.46
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.80	0.46
1:B:190:ASP:HB3	2:D:74:GLN:O	2.16	0.46
1:B:227:ASN:HD21	1:B:296:PHE:H	1.63	0.46
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.98	0.46
2:D:310:SER:O	2:D:314:ARG:HG3	2.15	0.46
1:A:185:LYS:CA	1:A:189:SER:HB2	2.45	0.46
1:B:43:ARG:HD2	1:B:43:ARG:O	2.16	0.46
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.50	0.46
2:C:98:HIS:CD2	2:C:297:ASP:OD1	2.68	0.46
2:D:385:LEU:C	2:D:387:GLY:H	2.19	0.46
1:A:306:ASP:O	1:A:310:TYR:HB2	2.16	0.46
1:B:56:THR:HG21	1:B:133:GLN:OE1	2.16	0.46
1:B:146:ARG:HG2	1:B:150:GLN:OE1	2.14	0.46
2:C:235:TRP:CD1	2:C:235:TRP:C	2.89	0.46
1:A:175:ARG:HG2	1:A:176:THR:N	2.28	0.46
2:D:16:MET:O	2:D:20:ILE:HG12	2.15	0.46
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.98	0.46
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.51	0.46
2:D:324:TRP:O	2:D:327:PRO:HD2	2.15	0.46
1:A:513:LYS:O	1:A:515:LEU:N	2.49	0.45
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.51	0.45
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.15	0.45
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.51	0.45
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:ARG:HA	3:F:40:THR:HG23	1.98	0.45
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.51	0.45
1:B:165:PRO:HD2	2:D:30:ASP:HB3	1.99	0.45
2:C:266:GLN:HB2	2:C:281:ILE:HG21	1.98	0.45
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.31	0.45
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.50	0.45
1:B:216:LEU:HA	1:B:308:TRP:HH2	1.81	0.45
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.98	0.45
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.98	0.45
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.99	0.45
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.16	0.45
1:A:186:ARG:HD3	1:A:186:ARG:C	2.37	0.45
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.60	0.45
2:D:339:PHE:O	2:D:342:LEU:HB2	2.16	0.45
2:D:381:VAL:O	2:D:385:LEU:HB2	2.17	0.45
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.98	0.45
1:A:268:ASN:HD21	1:A:327:GLU:H	1.65	0.45
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.99	0.44
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.44
1:A:227:ASN:HD21	1:A:296:PHE:H	1.64	0.44
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.20	0.44
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.51	0.44
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.52	0.44
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.51	0.44
2:D:153:LEU:HB3	2:D:193:ILE:HG21	1.99	0.44
3:F:86:ASP:O	3:F:89:SER:HB2	2.17	0.44
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.98	0.44
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.44
2:D:312:TYR:O	2:D:316:VAL:HG23	2.18	0.44
1:A:113:GLY:HA2	1:A:188:PHE:O	2.18	0.44
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.85	0.44
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.52	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:B:369:MET:HE2	1:B:379:TRP:HH2	1.83	0.44
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.48	0.44
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.48	0.44
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.82	0.44
2:D:111:LYS:O	2:D:115:GLU:HG3	2.17	0.44
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.18	0.43
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.45	0.43
1:B:50:TYR:CD1	1:B:50:TYR:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.43
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.70	0.43
2:C:90:LEU:HD13	2:C:303:LEU:HD13	2.00	0.43
1:B:460:GLU:N	1:B:461:PRO:HD3	2.34	0.43
2:D:197:ARG:HB3	2:D:197:ARG:NH1	2.34	0.43
1:B:184:MET:HE1	1:B:188:PHE:CD2	2.54	0.43
2:C:54:VAL:O	2:C:55:TYR:HB2	2.18	0.43
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.54	0.43
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.53	0.43
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.43
1:B:209:GLU:HB3	1:B:247:MET:HE3	2.00	0.43
3:F:23:ASN:H	3:F:23:ASN:ND2	2.17	0.43
2:D:226:SER:HB2	2:D:334:ASP:CG	2.40	0.42
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.48	0.42
1:B:124:LEU:HD21	1:B:201:SER:HB2	2.00	0.42
1:B:185:LYS:HA	1:B:189:SER:HB2	2.01	0.42
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.53	0.42
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.48	0.42
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.55	0.42
2:D:357:TYR:O	2:D:361:ASP:HB2	2.19	0.42
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.54	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.00	0.42
1:B:165:PRO:HG3	6:B:2823:HOH:O	2.19	0.42
1:B:207:VAL:HG11	1:B:275:PHE:HA	2.02	0.42
2:C:115:GLU:HB3	2:D:115:GLU:HB3	2.01	0.42
2:D:340:ALA:CA	2:D:389:LYS:HE2	2.33	0.42
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.56	0.42
1:A:175:ARG:HG3	1:A:181:TRP:CG	2.54	0.42
1:B:49:LYS:HD3	3:F:140:MET:CB	2.47	0.42
2:D:223:VAL:HA	2:D:334:ASP:O	2.20	0.42
1:A:187:VAL:HG12	1:A:277:THR:HG22	2.01	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.83	0.42
2:D:235:TRP:CD1	2:D:235:TRP:C	2.90	0.42
3:E:33:LYS:NZ	6:E:229:HOH:O	2.48	0.42
1:A:302:VAL:HG23	1:A:303:LYS:H	1.85	0.42
1:A:323:LYS:HE2	1:A:324:TYR:CZ	2.54	0.42
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.20	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.16	0.42
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.42
1:A:279:GLN:HE21	1:A:279:GLN:HB3	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.54	0.42
1:B:451:GLN:HG2	6:B:2845:HOH:O	2.18	0.42
2:C:176:ARG:HB2	2:C:176:ARG:NH1	2.35	0.41
2:D:336:MET:HE2	2:D:356:LEU:HD11	2.01	0.41
2:D:342:LEU:HD13	2:D:346:THR:HG21	2.02	0.41
1:B:63:ILE:HA	2:D:191:GLN:HE22	1.85	0.41
3:F:23:ASN:C	3:F:23:ASN:HD22	2.24	0.41
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.41
1:A:260:ASP:HA	1:A:261:PRO:HD3	1.95	0.41
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.14	0.41
2:D:153:LEU:C	2:D:153:LEU:CD1	2.89	0.41
3:F:23:ASN:H	3:F:23:ASN:HD22	1.69	0.41
1:B:259:ASN:HD22	1:B:259:ASN:HA	1.70	0.41
2:D:95:TRP:CE2	2:D:171:LEU:HD12	2.56	0.41
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.51	0.41
1:A:118:ILE:HG21	2:C:176:ARG:HD3	2.02	0.41
1:B:163:GLN:HG2	6:B:2675:HOH:O	2.21	0.41
2:D:146:ASN:HB2	2:D:207:PHE:CZ	2.56	0.41
3:F:154:GLU:HG3	3:F:158:GLN:NE2	2.35	0.41
1:A:119:ALA:HB1	2:C:168:ARG:HD2	2.02	0.41
1:A:253:THR:O	1:A:257:ILE:HG12	2.20	0.41
1:A:520:LYS:HB3	1:A:520:LYS:NZ	2.36	0.41
1:B:334:ASP:O	1:B:337:GLN:HB3	2.20	0.41
1:B:444:GLU:HA	1:B:444:GLU:OE2	2.21	0.41
3:F:23:ASN:ND2	3:F:23:ASN:N	2.69	0.41
1:A:52:MET:HA	1:A:256:SER:O	2.21	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.02	0.41
1:B:413:HIS:CD2	1:B:428:SER:OG	2.74	0.41
2:D:224:TYR:O	2:D:225:LYS:C	2.59	0.41
3:E:129:LEU:HD23	3:E:129:LEU:HA	1.90	0.41
1:A:108:ASN:ND2	1:A:175:ARG:HE	2.18	0.41
1:A:109:PHE:HB3	1:A:184:MET:SD	2.61	0.41
1:A:283:THR:HB	1:A:284:PRO:CD	2.50	0.41
1:A:435:THR:HG21	1:A:437:ARG:NE	2.28	0.41
1:A:444:GLU:HG3	1:A:445:MET:N	2.35	0.41
1:B:32:LEU:HD12	1:B:35:PHE:CD2	2.56	0.41
1:B:194:SER:HA	2:D:76:PHE:CE1	2.56	0.41
1:B:202:LEU:CD2	1:B:206:LEU:HD22	2.51	0.41
1:B:232:THR:N	1:B:233:PRO:CD	2.83	0.41
3:F:152:LEU:O	3:F:156:ARG:HG3	2.20	0.41
2:C:275:ASN:C	2:C:278:PRO:HD2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:ASP:HB3	2:C:379:GLN:HB2	2.02	0.41
2:D:228:ARG:O	2:D:232:GLU:HG3	2.21	0.41
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.30	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.40
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.40
1:B:284:PRO:HB3	1:B:342:ALA:HB1	2.04	0.40
2:D:385:LEU:HD12	2:D:385:LEU:HA	1.95	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.91	0.40
1:B:30:ARG:HG2	1:B:30:ARG:NH1	2.36	0.40
1:B:305:TRP:CE2	1:B:309:VAL:HG21	2.56	0.40
2:C:146:ASN:ND2	2:C:197:ARG:NH2	2.62	0.40
2:D:187:ILE:O	2:D:191:GLN:HG3	2.21	0.40
3:F:80:LYS:HE3	3:F:84:GLY:HA2	2.01	0.40
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.56	0.40
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.56	0.40
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.20	0.40
2:D:213:VAL:N	2:D:214:PRO:HD2	2.37	0.40
2:D:234:LEU:HD13	2:D:248:VAL:HG22	2.04	0.40
2:D:264:PHE:O	2:D:268:LEU:HG	2.22	0.40
2:D:336:MET:C	2:D:338:LEU:H	2.24	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	508/527 (96%)	482 (95%)	24 (5%)	2 (0%)	34	42
1	B	508/527 (96%)	479 (94%)	25 (5%)	4 (1%)	19	23
2	C	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	41	50
2	D	386/389 (99%)	354 (92%)	29 (8%)	3 (1%)	19	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	164/170 (96%)	151 (92%)	9 (6%)	4 (2%)	6	4
All	All	2116/2172 (97%)	2000 (94%)	102 (5%)	14 (1%)	22	26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	B	311	GLU
2	D	251	VAL
1	B	39	PHE
2	D	64	ALA
2	C	64	ALA
3	F	74	GLU
3	F	87	ALA
1	A	94	ARG
1	A	340	TYR
1	B	94	ARG
3	F	122	ILE
2	D	386	ALA
3	F	5	GLY

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	425/442 (96%)	413 (97%)	12 (3%)	43	60
1	B	422/442 (96%)	412 (98%)	10 (2%)	49	66
2	C	315/323 (98%)	307 (98%)	8 (2%)	47	65
2	D	312/323 (97%)	306 (98%)	6 (2%)	57	73
3	E	143/147 (97%)	141 (99%)	2 (1%)	67	81
3	F	142/147 (97%)	137 (96%)	5 (4%)	36	50
All	All	1759/1824 (96%)	1716 (98%)	43 (2%)	49	66

All (43) 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	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	334	ASP
1	A	467	GLN
1	A	514	ARG
1	A	516	ASN
1	A	520	LYS
1	B	43	ARG
1	B	90	ASN
1	B	125	TRP
1	B	186	ARG
1	B	189	SER
1	B	259	ASN
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	523	VAL
2	C	33	ASN
2	C	35	MET
2	C	80	ARG
2	C	173	ASP
2	C	195	LEU
2	C	266	GLN
2	C	311	ASP
2	C	378	ASP
2	D	4	LEU
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	334	ASP
3	E	44	ARG
3	E	60	LEU
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	53	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	164	VAL

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	54	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	168	HIS
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	259	ASN
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	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	516	ASN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	337	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	301	ASN
2	D	57	GLN
2	D	98	HIS
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	F	7	HIS
3	F	23	ASN
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	FPN	B	2667	-	8,8,8	2.35	5 (62%)	10,10,10	2.04	3 (30%)
5	FPN	A	2666	-	8,8,8	2.49	5 (62%)	10,10,10	2.09	3 (30%)

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
5	FPN	B	2667	-	-	-	0/1/1/1
5	FPN	A	2666	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2666	FPN	C6-C5	3.71	1.45	1.38
5	B	2667	FPN	C6-C5	3.62	1.45	1.38
5	A	2666	FPN	C3-C2	3.28	1.44	1.38
5	B	2667	FPN	C3-C2	2.82	1.43	1.38
5	A	2666	FPN	C3-C4	2.70	1.42	1.37
5	B	2667	FPN	C3-C4	2.68	1.42	1.37
5	A	2666	FPN	C2-C1	2.59	1.43	1.38
5	B	2667	FPN	C5-C4	2.56	1.42	1.37
5	A	2666	FPN	C5-C4	2.50	1.42	1.37
5	B	2667	FPN	C2-C1	2.44	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2666	FPN	C3-C2-C1	-3.50	116.03	119.88
5	B	2667	FPN	C3-C2-C1	-3.43	116.12	119.88
5	B	2667	FPN	C6-C1-C2	3.39	125.48	119.77
5	A	2666	FPN	C6-C1-C2	3.35	125.41	119.77
5	A	2666	FPN	C5-C6-C1	-3.09	116.48	119.88
5	B	2667	FPN	C5-C6-C1	-2.99	116.59	119.88

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	510/527 (96%)	0.05	25 (4%)	29	36	21, 39, 68, 80	0
1	B	510/527 (96%)	-0.09	20 (3%)	39	46	23, 37, 68, 79	0
2	C	388/389 (99%)	-0.52	2 (0%)	91	94	17, 26, 41, 61	0
2	D	388/389 (99%)	0.28	25 (6%)	19	25	26, 48, 73, 93	0
3	E	166/170 (97%)	-0.44	1 (0%)	89	92	20, 30, 48, 68	0
3	F	166/170 (97%)	0.67	15 (9%)	9	12	37, 57, 77, 83	0
All	All	2128/2172 (97%)	-0.03	88 (4%)	37	44	17, 37, 70, 93	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	5.8
2	D	205	PRO	5.7
2	C	2	SER	4.3
2	D	375	ALA	4.0
1	B	39	PHE	4.0
1	A	328	SER	4.0
1	A	316	ILE	3.9
2	D	344	ALA	3.8
1	B	53	ALA	3.8
2	D	350	GLU	3.7
1	A	19	ALA	3.7
1	B	310	TYR	3.5
1	A	310	TYR	3.4
1	A	318	ILE	3.4
1	A	319	GLY	3.4
3	F	80	LYS	3.3
1	A	54	ASN	3.2
1	A	326	VAL	3.1
1	A	213	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	434	SER	3.1
1	B	527	ASN	3.0
3	F	101	ALA	2.9
2	D	136	MET	2.9
1	A	251	TYR	2.9
1	A	20	PRO	2.9
3	F	120	PRO	2.9
2	D	388	LEU	2.8
1	B	320	ARG	2.7
1	B	311	GLU	2.7
1	B	20	PRO	2.7
3	F	21	GLN	2.7
1	B	323	LYS	2.7
2	D	220	ASN	2.7
2	D	342	LEU	2.7
3	F	70	ARG	2.7
3	F	22	LEU	2.7
1	A	262	ALA	2.7
1	B	54	ASN	2.7
2	D	206	GLY	2.7
3	F	26	GLU	2.6
1	B	19	ALA	2.6
1	A	212	PHE	2.6
3	F	100	ALA	2.6
3	F	23	ASN	2.6
2	D	354	ALA	2.6
2	C	5	GLY	2.6
2	D	254	ALA	2.6
2	D	2	SER	2.6
1	A	255	VAL	2.5
3	F	102	LYS	2.5
1	B	40	LYS	2.5
2	D	260	VAL	2.5
1	B	259	ASN	2.5
2	D	374	LYS	2.4
1	A	315	GLY	2.4
1	A	259	ASN	2.4
1	A	338	ASP	2.4
2	D	343	PRO	2.4
2	D	208	ASP	2.3
1	A	317	TRP	2.3
1	B	21	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	514	ARG	2.3
2	D	353	THR	2.3
1	A	30	ARG	2.3
2	D	137	ASN	2.3
1	B	324	TYR	2.3
1	A	366	GLN	2.2
3	F	25	LEU	2.2
2	D	333	ARG	2.2
1	A	323	LYS	2.2
1	B	317	TRP	2.2
2	D	340	ALA	2.2
1	B	333	LYS	2.2
3	E	4	LEU	2.2
3	F	4	LEU	2.2
1	B	247	MET	2.2
2	D	345	GLY	2.2
3	F	93	GLY	2.2
2	D	229	LEU	2.1
1	B	325	GLY	2.1
1	B	319	GLY	2.1
1	A	261	PRO	2.1
2	D	248	VAL	2.1
2	D	207	PHE	2.1
3	F	66	VAL	2.0
1	A	51	LYS	2.0
1	B	23	VAL	2.0
3	F	20	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 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, 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(Å^2)	Q<0.9
4	FE	B	529	1/1	0.94	0.03	72,72,72,72	0
5	FPN	B	2667	8/8	0.94	0.18	34,35,37,41	0
4	FE	A	529	1/1	0.96	0.03	78,78,78,78	0
4	FE	B	528	1/1	0.96	0.06	63,63,63,63	0
5	FPN	A	2666	8/8	0.97	0.15	30,33,36,39	0
4	FE	A	528	1/1	0.98	0.05	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.