Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 02:55 PM EST

PDB ID	:	1FZ4
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM III SOAKED AT PH 8.5 (0.1 M TRIS)
Authors	:	Whittington, D.A.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	2.38 Å(reported)

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

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

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

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

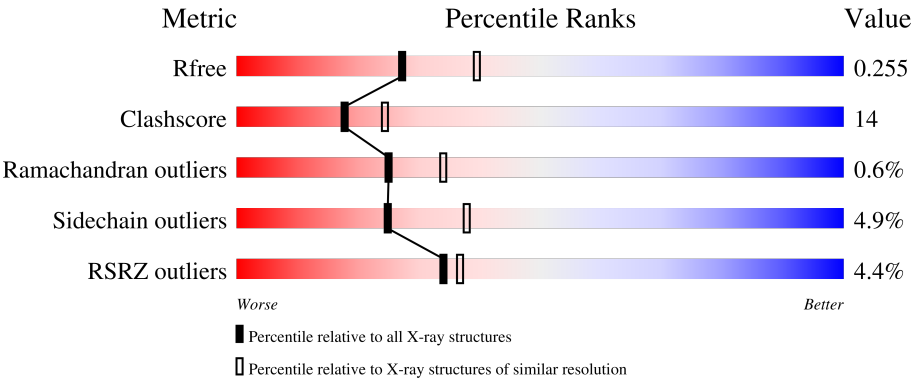
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	4% 69% 24%
1	B	527	3% 68% 26%
2	C	389	% 76% 22%
2	D	389	8% 74% 23%
3	E	170	% 66% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17975 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	18			
1	B	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	18			

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3193	2054	551	580	8			
2	D	387	Total	C	N	O	S	0	0	0
			3183	2048	549	578	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	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			

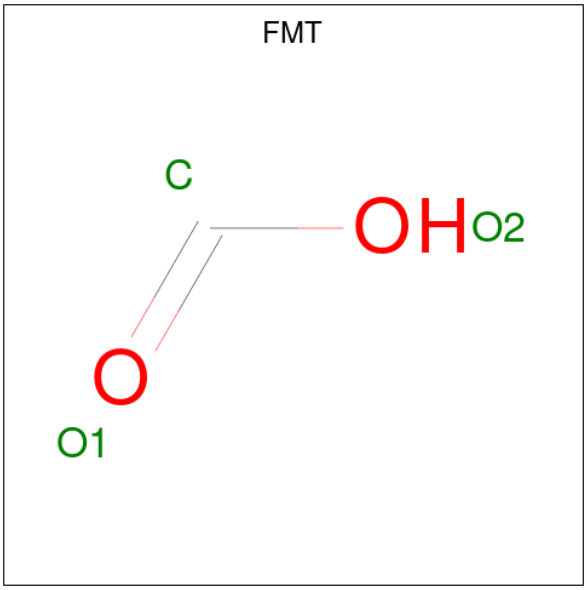
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

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

- Molecule 6 is 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	102	Total O 102 102	0	0
7	B	107	Total O 107 107	0	0

Continued on next page...

Continued from previous page...

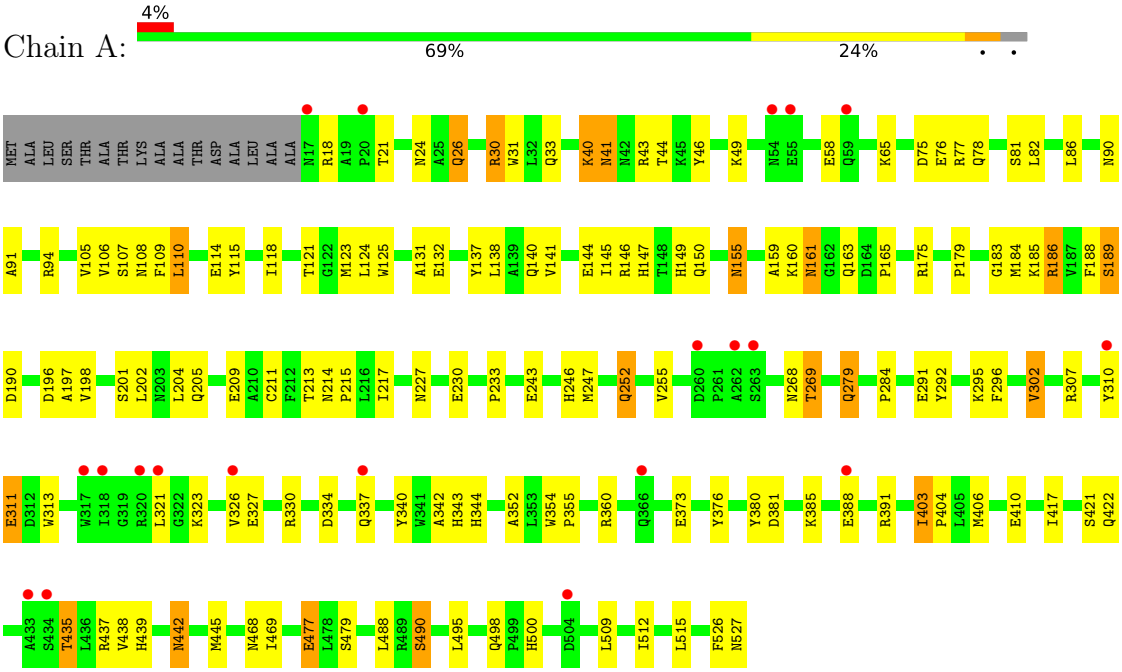
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	147	Total O 147 147	0	0
7	D	41	Total O 41 41	0	0
7	E	65	Total O 65 65	0	0
7	F	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

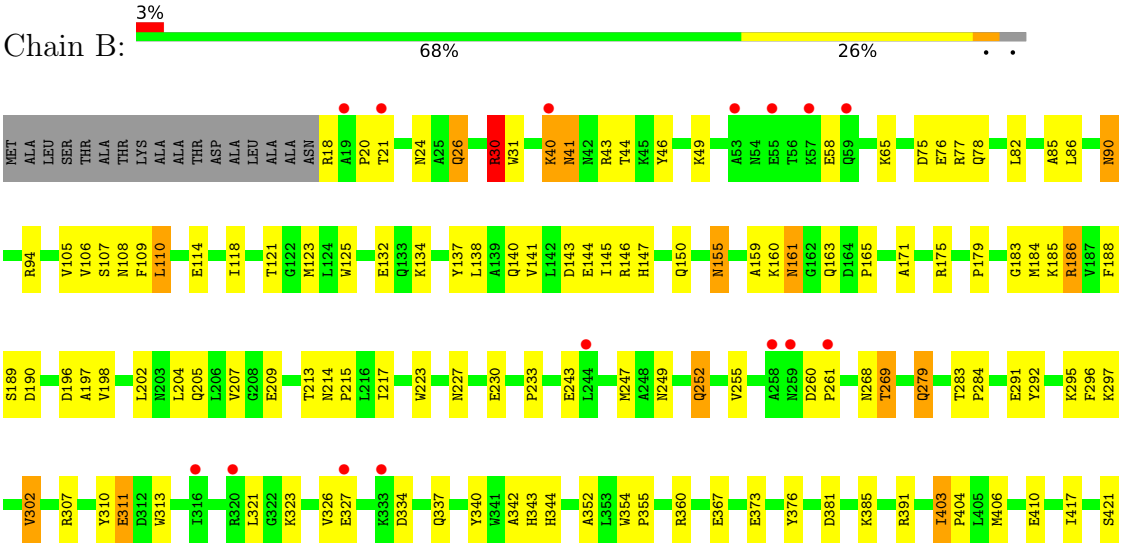
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

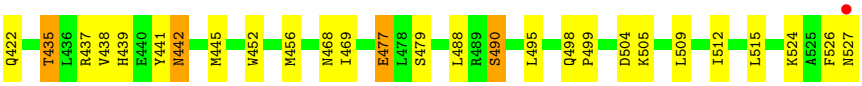
Chain A:



• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

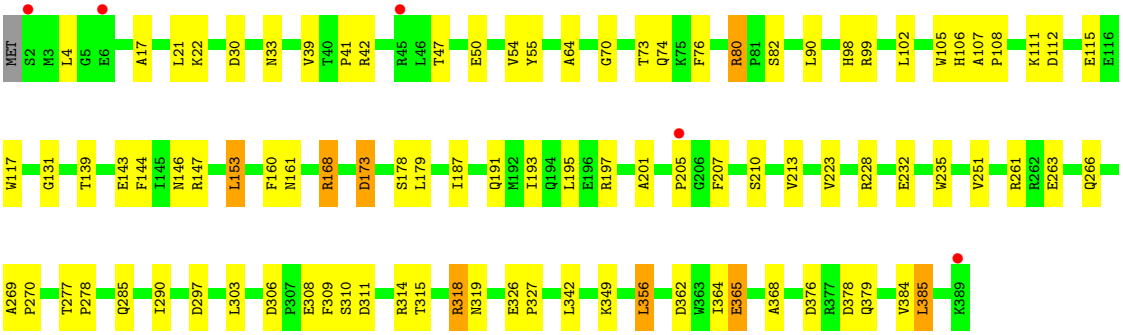
Chain B:





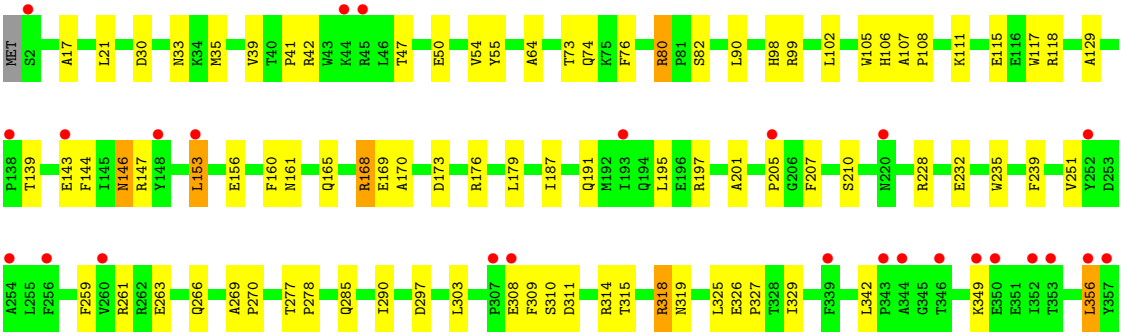
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:



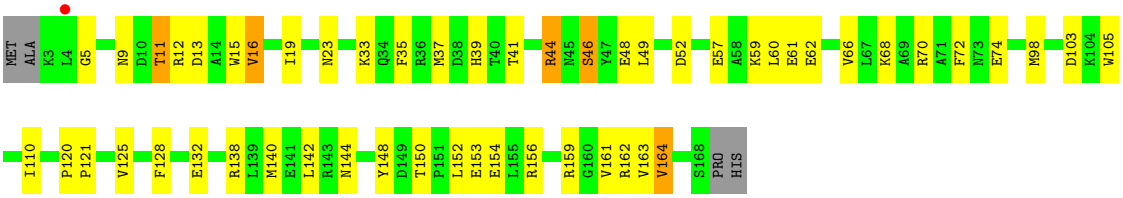
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



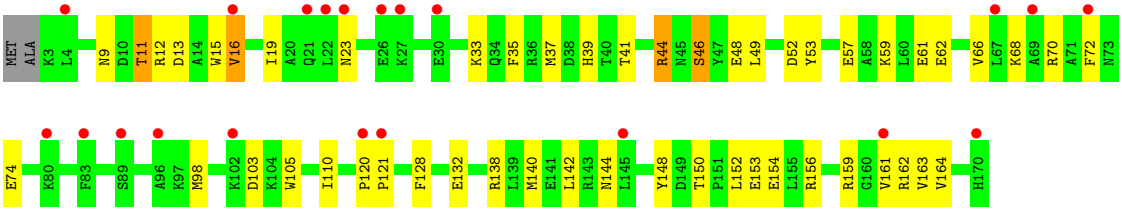
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:


MET ALA K3 L4 N9 D10 T11 R12 D13 A14 W15 V16 I19 A20 Q21 L22 N23 E26 K27 E30 K33 Q34 F35 R36 M37 D38 H39 T40 T41 R44 N45 S46 Y47 E48 L49 D52 Y53 E57 A58 K59 L60 E61 E62 V66 L67 K68 A69 R70 A71 F72 N73
E74 K80 F83 S89 A96 K97 M98 K102 D103 K104 W105 I110 P120 P121 F128 E132 R138 L139 M140 E141 L142 R143 N144 L145 Y148 D149 T150 P151 L152 E153 E154 L155 R156 R159 G160 V161 R162 V163 V164 H170

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.89Å 171.52Å 221.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.38 29.71 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.0 (29.70-2.38) 80.3 (29.71-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.256 0.220 , 0.255	Depositor DCC
R_{free} test set	3231 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17975	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: FE, CA, FMT

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	0.38	0/4310	0.72	10/5853 (0.2%)
1	B	0.38	0/4302	0.70	9/5842 (0.2%)
2	C	0.40	0/3289	0.58	0/4464
2	D	0.37	0/3279	0.57	0/4453
3	E	0.39	0/1396	0.60	0/1880
3	F	0.36	0/1416	0.58	0/1907
All	All	0.38	0/17992	0.65	19/24399 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	NE-CZ-NH1	-15.29	112.66	120.30
1	B	30	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	77	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	B	391	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	30	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	391	ARG	NE-CZ-NH1	-11.60	114.50	120.30
1	B	77	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	30	ARG	NE-CZ-NH2	10.96	125.78	120.30
1	B	391	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	B	30	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	391	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	B	77	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	30	ARG	CD-NE-CZ	6.64	132.89	123.60
1	B	30	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	279	GLN	CA-CB-CG	6.02	126.64	113.40
1	A	77	ARG	CD-NE-CZ	6.00	132.00	123.60
1	B	391	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	391	ARG	CD-NE-CZ	5.61	131.46	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	279	GLN	CA-CB-CG	5.17	124.78	113.40

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	125	0
1	B	4177	0	3975	133	0
2	C	3193	0	3042	87	0
2	D	3183	0	3029	87	0
3	E	1368	0	1363	49	0
3	F	1386	0	1377	48	0
4	A	2	0	0	0	0
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	102	0	0	4	0
7	B	107	0	0	4	0
7	C	147	0	0	4	0
7	D	41	0	0	1	0
7	E	65	0	0	0	0
7	F	11	0	0	1	0
All	All	17975	0	16768	466	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 14.

All (466) 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:252:GLN:HA	1:B:252:GLN:HE21	1.12	1.08
1:A:252:GLN:HE21	1:A:252:GLN:HA	1.11	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:SER:HB3	1:B:155:ASN:HD21	1.16	1.06
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.39	1.04
1:A:107:SER:HB3	1:A:155:ASN:HD21	1.20	1.04
2:D:146:ASN:HD21	2:D:197:ARG:HH21	1.00	0.97
2:C:146:ASN:HD21	2:C:197:ARG:HH21	0.97	0.96
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.10	0.93
1:A:44:THR:HG22	1:A:46:TYR:H	1.32	0.93
2:C:319:ASN:HA	3:E:74:GLU:OE1	1.70	0.91
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.03	0.91
1:B:160:LYS:C	1:B:161:ASN:HD22	1.74	0.91
1:B:44:THR:HG22	1:B:46:TYR:H	1.32	0.90
1:A:209:GLU:HA	1:A:213:THR:HB	1.52	0.90
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.69	0.89
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.18	0.88
2:D:146:ASN:ND2	2:D:197:ARG:HH21	1.72	0.87
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.72	0.87
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.57	0.87
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.19	0.86
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.55	0.86
1:A:41:ASN:N	1:A:41:ASN:HD22	1.73	0.86
1:B:107:SER:CB	1:B:155:ASN:HD21	1.89	0.84
2:D:99:ARG:HH11	2:D:99:ARG:HG2	1.41	0.83
1:B:252:GLN:HA	1:B:252:GLN:NE2	1.92	0.83
1:A:252:GLN:HA	1:A:252:GLN:NE2	1.93	0.82
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.27	0.81
1:B:41:ASN:HD22	1:B:41:ASN:N	1.78	0.80
1:A:160:LYS:C	1:A:161:ASN:HD22	1.85	0.79
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.81	0.79
2:D:319:ASN:HA	3:F:74:GLU:OE1	1.84	0.78
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.15	0.77
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.32	0.77
2:C:146:ASN:HD21	2:C:197:ARG:NH2	1.81	0.77
1:B:107:SER:HB3	1:B:155:ASN:ND2	1.97	0.76
1:A:107:SER:CB	1:A:155:ASN:HD21	1.96	0.76
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.17	0.74
2:C:315:THR:HA	2:C:318:ARG:NH1	2.02	0.74
1:B:209:GLU:HA	1:B:213:THR:HB	1.68	0.74
2:C:315:THR:HA	2:C:318:ARG:HH12	1.53	0.74
1:A:355:PRO:HG2	1:A:403:ILE:HD11	1.70	0.73
3:F:98:MET:HE2	3:F:110:ILE:HB	1.70	0.73
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.84	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:98:MET:HE2	3:E:110:ILE:HB	1.70	0.73
2:D:377:ARG:HG2	7:D:422:HOH:O	1.88	0.73
2:D:315:THR:HA	2:D:318:ARG:NH1	2.03	0.72
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.69	0.72
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.88	0.72
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.88	0.71
1:A:155:ASN:N	1:A:155:ASN:HD22	1.87	0.71
2:D:315:THR:HA	2:D:318:ARG:HH12	1.55	0.70
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.25	0.69
1:B:161:ASN:HD22	1:B:161:ASN:N	1.86	0.69
2:C:99:ARG:HG2	2:C:99:ARG:HH11	1.58	0.69
3:F:41:THR:O	3:F:44:ARG:HD2	1.93	0.69
1:B:227:ASN:HD21	1:B:295:LYS:H	1.39	0.69
1:A:252:GLN:HE21	1:A:252:GLN:CA	1.98	0.69
3:F:57:GLU:O	3:F:61:GLU:HG3	1.93	0.68
1:A:40:LYS:HB3	1:A:41:ASN:HD22	1.59	0.67
2:C:146:ASN:HD22	2:C:197:ARG:HE	1.41	0.67
3:F:68:LYS:HG3	3:F:72:PHE:CD2	2.29	0.67
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.08	0.67
3:F:9:ASN:OD1	3:F:11:THR:HG22	1.95	0.67
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.75	0.66
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.61	0.66
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.41	0.66
2:C:376:ASP:HB3	2:C:379:GLN:HG3	1.78	0.66
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.76	0.66
2:D:376:ASP:HB3	2:D:379:GLN:HG3	1.78	0.65
3:E:57:GLU:O	3:E:61:GLU:HG3	1.97	0.65
1:A:107:SER:HB3	1:A:155:ASN:ND2	2.02	0.65
1:B:155:ASN:N	1:B:155:ASN:HD22	1.93	0.65
2:D:99:ARG:HG2	2:D:99:ARG:NH1	2.10	0.65
1:A:227:ASN:HD21	1:A:295:LYS:H	1.44	0.65
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.77	0.65
1:B:185:LYS:O	1:B:189:SER:HB2	1.97	0.64
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.78	0.64
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.32	0.64
1:B:269:THR:HG22	3:F:148:TYR:CE1	2.32	0.64
1:B:165:PRO:HG3	7:B:5010:HOH:O	1.96	0.64
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.81	0.63
1:B:268:ASN:HD21	1:B:327:GLU:H	1.46	0.63
3:E:138:ARG:HH21	3:E:142:LEU:HD21	1.62	0.63
1:B:31:TRP:CH2	2:D:210:SER:HA	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.80	0.63
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.79	0.63
2:C:47:THR:OG1	2:C:50:GLU:HG3	1.98	0.63
3:E:41:THR:O	3:E:44:ARG:HD2	1.97	0.63
3:E:68:LYS:HG3	3:E:72:PHE:CD2	2.33	0.63
2:D:47:THR:OG1	2:D:50:GLU:HG3	1.99	0.63
1:B:160:LYS:HG2	1:B:161:ASN:ND2	2.14	0.63
1:A:185:LYS:O	1:A:189:SER:HB2	1.99	0.62
1:A:108:ASN:ND2	1:A:175:ARG:HH11	1.98	0.62
1:A:268:ASN:HD21	1:A:327:GLU:H	1.47	0.62
2:D:111:LYS:O	2:D:115:GLU:HG3	1.98	0.62
2:D:146:ASN:HD22	2:D:197:ARG:HE	1.48	0.62
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.80	0.62
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.81	0.62
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.61
1:B:41:ASN:N	1:B:41:ASN:ND2	2.48	0.61
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.66	0.61
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.48	0.61
1:A:355:PRO:HG2	1:A:403:ILE:CD1	2.31	0.61
2:D:195:LEU:O	2:D:195:LEU:HD23	2.00	0.61
1:A:477:GLU:OE2	1:A:479:SER:N	2.34	0.60
2:D:146:ASN:HD21	2:D:197:ARG:NH2	1.85	0.60
2:C:111:LYS:O	2:C:115:GLU:HG3	2.00	0.60
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.84	0.60
1:B:161:ASN:N	1:B:161:ASN:ND2	2.49	0.60
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.84	0.60
3:E:39:HIS:CD2	3:E:49:LEU:HD12	2.36	0.60
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.84	0.59
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.37	0.59
1:B:252:GLN:HE21	1:B:252:GLN:CA	2.00	0.59
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.66	0.59
3:E:9:ASN:OD1	3:E:11:THR:HG22	2.03	0.59
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.85	0.59
1:A:438:VAL:HG12	3:E:164:VAL:CG2	2.32	0.59
2:C:223:VAL:HG23	7:C:5064:HOH:O	2.01	0.59
2:D:187:ILE:O	2:D:191:GLN:HG3	2.01	0.59
3:F:41:THR:HG22	7:F:176:HOH:O	2.03	0.59
1:A:40:LYS:HB3	1:A:41:ASN:ND2	2.18	0.59
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.85	0.59
1:B:477:GLU:OE2	1:B:479:SER:N	2.36	0.59
2:D:139:THR:O	2:D:143:GLU:HB3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:LEU:HD23	2:C:195:LEU:O	2.03	0.58
2:C:139:THR:O	2:C:143:GLU:HB3	2.03	0.58
1:B:227:ASN:HD21	1:B:296:PHE:H	1.51	0.58
2:C:376:ASP:CB	2:C:379:GLN:HG3	2.33	0.58
1:A:161:ASN:HD22	1:A:161:ASN:N	1.98	0.57
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.33	0.57
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.85	0.57
1:A:435:THR:CG2	1:A:437:ARG:HE	2.17	0.57
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.68	0.57
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.87	0.57
2:C:308:GLU:HG2	2:C:309:PHE:CE1	2.40	0.57
2:D:349:LYS:HE3	2:D:385:LEU:HD12	1.86	0.57
1:B:30:ARG:O	1:B:30:ARG:HD3	2.05	0.57
2:C:349:LYS:HE3	2:C:385:LEU:CD1	2.34	0.57
1:A:41:ASN:N	1:A:41:ASN:ND2	2.46	0.57
2:C:99:ARG:HG2	2:C:99:ARG:NH1	2.19	0.57
1:B:438:VAL:HG12	3:F:164:VAL:CG2	2.35	0.57
1:B:435:THR:CG2	1:B:437:ARG:HE	2.18	0.56
1:A:490:SER:OG	2:C:30:ASP:OD1	2.23	0.56
1:A:123:MET:CE	1:A:197:ALA:HA	2.35	0.56
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.91	0.56
1:B:526:PHE:O	1:B:527:ASN:ND2	2.36	0.56
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.85	0.56
2:C:105:TRP:O	2:C:108:PRO:HD2	2.06	0.56
2:D:376:ASP:CB	2:D:379:GLN:HG3	2.36	0.56
3:F:15:TRP:O	3:F:19:ILE:HG13	2.05	0.56
3:F:138:ARG:HH21	3:F:142:LEU:HD21	1.70	0.56
1:A:160:LYS:HG2	1:A:161:ASN:ND2	2.21	0.56
2:C:356:LEU:HD21	2:C:384:VAL:HG11	1.88	0.56
1:A:373:GLU:HA	1:A:373:GLU:OE1	2.05	0.56
3:F:13:ASP:HA	3:F:16:VAL:HG23	1.88	0.56
3:F:41:THR:O	3:F:44:ARG:CD	2.54	0.56
1:A:439:HIS:HD2	3:E:163:VAL:HA	1.70	0.56
1:A:58:GLU:HB3	1:A:132:GLU:O	2.05	0.56
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.89	0.56
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.02	0.55
1:A:49:LYS:CE	3:E:144:ASN:HD22	2.18	0.55
1:B:140:GLN:O	1:B:144:GLU:HG2	2.07	0.55
1:B:184:MET:HE1	1:B:188:PHE:CD2	2.41	0.55
1:B:373:GLU:OE1	1:B:373:GLU:HA	2.05	0.55
1:B:442:ASN:C	1:B:442:ASN:HD22	2.08	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LYS:HE3	2:D:385:LEU:CD1	2.36	0.55
3:E:35:PHE:CE1	3:E:39:HIS:HD2	2.24	0.55
3:E:41:THR:O	3:E:44:ARG:CD	2.55	0.55
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.40	0.55
1:B:227:ASN:ND2	1:B:295:LYS:H	2.04	0.54
3:F:46:SER:OG	3:F:48:GLU:HG2	2.08	0.54
1:A:91:ALA:HB1	7:A:6094:HOH:O	2.07	0.54
1:A:76:GLU:OE2	1:B:76:GLU:HG2	2.07	0.54
1:A:438:VAL:HG12	3:E:164:VAL:HG21	1.90	0.54
2:C:376:ASP:CG	2:C:379:GLN:HG3	2.27	0.54
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.43	0.54
3:E:161:VAL:HG23	3:E:162:ARG:N	2.23	0.54
3:F:33:LYS:O	3:F:37:MET:HG2	2.08	0.54
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.27	0.54
1:A:49:LYS:HE3	3:E:144:ASN:HD22	1.72	0.54
1:A:186:ARG:HA	2:C:73:THR:OG1	2.08	0.54
1:A:123:MET:HE1	1:A:197:ALA:HA	1.89	0.53
2:D:105:TRP:O	2:D:108:PRO:HD2	2.08	0.53
1:A:196:ASP:HB2	3:E:140:MET:SD	2.47	0.53
2:C:349:LYS:HE3	2:C:385:LEU:HD12	1.91	0.53
2:C:146:ASN:ND2	2:C:197:ARG:NH2	2.48	0.53
2:D:80:ARG:HB2	3:F:132:GLU:OE1	2.08	0.53
1:A:161:ASN:N	1:A:161:ASN:ND2	2.56	0.53
1:A:500:HIS:HB2	7:A:6060:HOH:O	2.09	0.53
2:D:153:LEU:C	2:D:153:LEU:HD12	2.29	0.53
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.91	0.53
1:B:160:LYS:HA	2:D:33:ASN:HB2	1.90	0.53
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.88	0.53
2:D:308:GLU:HG2	2:D:309:PHE:CE1	2.43	0.53
3:E:12:ARG:O	3:E:16:VAL:HG23	2.08	0.53
1:B:445:MET:HE1	1:B:526:PHE:O	2.09	0.52
2:C:187:ILE:O	2:C:191:GLN:HG3	2.09	0.52
3:F:159:ARG:HG3	3:F:161:VAL:HG12	1.91	0.52
3:E:15:TRP:O	3:E:19:ILE:HG13	2.08	0.52
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.92	0.52
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.91	0.52
1:A:442:ASN:HD22	1:A:442:ASN:C	2.11	0.52
1:B:490:SER:OG	2:D:30:ASP:OD1	2.27	0.52
7:B:5016:HOH:O	3:F:46:SER:HA	2.09	0.52
3:E:13:ASP:HA	3:E:16:VAL:HG23	1.92	0.52
1:A:209:GLU:HA	1:A:213:THR:CB	2.34	0.52

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	2.10	0.52
2:C:54:VAL:O	2:C:55:TYR:HB2	2.09	0.52
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.94	0.51
2:C:310:SER:O	2:C:314:ARG:HG3	2.10	0.51
7:C:5017:HOH:O	3:E:125:VAL:HG22	2.10	0.51
3:E:159:ARG:HG3	3:E:161:VAL:HG12	1.91	0.51
1:A:184:MET:HE1	1:A:188:PHE:CD2	2.45	0.51
3:E:33:LYS:O	3:E:37:MET:HG2	2.10	0.51
1:A:190:ASP:HB3	2:C:74:GLN:O	2.10	0.51
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.91	0.51
2:C:309:PHE:CZ	3:E:62:GLU:HG2	2.45	0.51
1:A:155:ASN:N	1:A:155:ASN:ND2	2.57	0.51
1:A:435:THR:HG23	1:A:437:ARG:HE	1.74	0.51
2:D:82:SER:O	2:D:168:ARG:NH2	2.44	0.51
3:E:46:SER:OG	3:E:48:GLU:HG2	2.11	0.51
3:F:161:VAL:HG23	3:F:162:ARG:N	2.25	0.51
1:B:143:ASP:O	1:B:146:ARG:HB3	2.11	0.51
2:C:213:VAL:HG23	7:C:5068:HOH:O	2.11	0.50
1:B:252:GLN:HE22	1:B:255:VAL:HG21	1.75	0.50
2:C:365:GLU:HA	2:C:365:GLU:OE1	2.11	0.50
1:B:159:ALA:O	2:D:33:ASN:HB2	2.11	0.50
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.92	0.50
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.94	0.50
1:A:227:ASN:HD21	1:A:296:PHE:H	1.60	0.50
1:B:381:ASP:HA	1:B:385:LYS:HE2	1.93	0.50
1:A:140:GLN:O	1:A:144:GLU:HG2	2.12	0.50
1:B:107:SER:CB	1:B:155:ASN:ND2	2.68	0.50
1:B:160:LYS:HE3	1:B:161:ASN:HD21	1.77	0.50
2:C:365:GLU:OE1	2:C:365:GLU:CA	2.60	0.50
1:A:31:TRP:CH2	2:C:210:SER:HA	2.46	0.50
1:A:163:GLN:HG2	7:A:6095:HOH:O	2.12	0.50
1:A:439:HIS:CG	3:E:161:VAL:HG21	2.47	0.49
1:B:160:LYS:HG2	1:B:161:ASN:HD21	1.77	0.49
1:A:380:TYR:HE2	1:A:388:GLU:OE2	1.95	0.49
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.93	0.49
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.47	0.49
1:A:24:ASN:OD1	1:A:26:GLN:HG3	2.12	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
2:D:143:GLU:O	2:D:147:ARG:HB3	2.12	0.49
2:D:310:SER:O	2:D:314:ARG:HG3	2.12	0.49
1:B:24:ASN:OD1	1:B:26:GLN:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.48	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.49
2:D:228:ARG:O	2:D:232:GLU:HG3	2.12	0.49
3:F:152:LEU:O	3:F:156:ARG:HG3	2.12	0.49
1:A:227:ASN:ND2	1:A:295:LYS:H	2.11	0.49
1:B:307:ARG:HA	1:B:311:GLU:HG3	1.94	0.49
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.47	0.49
2:C:153:LEU:C	2:C:153:LEU:HD12	2.33	0.49
1:B:40:LYS:HB3	1:B:41:ASN:ND2	2.28	0.49
2:D:385:LEU:C	2:D:387:GLY:H	2.15	0.49
1:A:213:THR:O	1:A:217:ILE:HG12	2.13	0.49
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.13	0.49
2:C:143:GLU:O	2:C:147:ARG:HB3	2.12	0.49
1:A:137:TYR:O	1:A:141:VAL:HG23	2.13	0.49
1:A:230:GLU:C	1:A:233:PRO:HD2	2.34	0.49
1:A:417:ILE:HG13	1:A:468:ASN:HB2	1.95	0.49
1:A:488:LEU:HD21	1:A:509:LEU:HD13	1.95	0.49
1:B:284:PRO:HB3	1:B:342:ALA:HB1	1.94	0.49
1:B:367:GLU:HB2	7:B:5082:HOH:O	2.12	0.48
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.48	0.48
1:B:302:VAL:HG11	1:B:340:TYR:CE1	2.48	0.48
3:E:61:GLU:HB3	3:E:121:PRO:HD3	1.95	0.48
2:C:80:ARG:HB2	3:E:132:GLU:OE1	2.13	0.48
3:E:150:THR:HG23	3:E:154:GLU:HG2	1.94	0.48
1:A:252:GLN:HE22	1:A:255:VAL:HG21	1.78	0.48
1:A:269:THR:HG22	3:E:148:TYR:CE1	2.48	0.48
1:B:435:THR:HG23	1:B:437:ARG:HE	1.78	0.48
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.95	0.48
1:A:307:ARG:HA	1:A:311:GLU:HG3	1.94	0.48
1:B:30:ARG:HD3	1:B:30:ARG:C	2.33	0.48
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.96	0.48
1:B:118:ILE:HD13	1:B:145:ILE:HG12	1.96	0.48
1:B:141:VAL:O	1:B:145:ILE:HG13	2.14	0.48
1:B:196:ASP:HB2	3:F:140:MET:SD	2.54	0.48
2:D:146:ASN:ND2	2:D:197:ARG:NH2	2.52	0.48
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.79	0.48
1:B:198:VAL:O	1:B:202:LEU:HG	2.14	0.47
1:B:441:TYR:HE2	3:F:159:ARG:O	1.97	0.47
1:A:49:LYS:HD3	3:E:140:MET:HB3	1.96	0.47
1:B:165:PRO:HD2	2:D:30:ASP:HB3	1.96	0.47
3:F:98:MET:CE	3:F:110:ILE:HB	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ILE:HG13	1:B:468:ASN:HB2	1.96	0.47
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.95	0.47
3:E:103:ASP:OD1	3:E:105:TRP:HB2	2.14	0.47
1:A:110:LEU:O	1:A:114:GLU:HG2	2.14	0.47
2:C:82:SER:O	2:C:168:ARG:NH2	2.46	0.47
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.47
3:F:66:VAL:HG12	3:F:70:ARG:HH21	1.80	0.47
1:B:20:PRO:HG3	2:D:129:ALA:HB2	1.96	0.47
3:F:11:THR:CG2	3:F:12:ARG:N	2.78	0.47
2:C:277:THR:HB	2:C:278:PRO:HD3	1.96	0.47
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.14	0.47
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.97	0.47
1:B:524:LYS:O	1:B:527:ASN:HB2	2.14	0.47
3:F:35:PHE:CE1	3:F:39:HIS:HD2	2.33	0.47
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.50	0.47
1:A:165:PRO:HD2	2:C:30:ASP:HB3	1.96	0.47
1:A:243:GLU:O	1:A:247:MET:HG2	2.15	0.47
1:B:406:MET:O	1:B:410:GLU:HG3	2.15	0.47
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.48	0.47
2:D:39:VAL:O	2:D:41:PRO:HD3	2.15	0.47
2:D:235:TRP:CD1	2:D:235:TRP:C	2.88	0.47
3:F:153:GLU:H	3:F:153:GLU:CD	2.16	0.47
1:A:183:GLY:HA2	1:A:422:GLN:HB2	1.97	0.47
1:A:438:VAL:HB	3:E:164:VAL:HG23	1.96	0.47
1:B:230:GLU:C	1:B:233:PRO:HD2	2.35	0.47
3:E:152:LEU:O	3:E:156:ARG:HG3	2.15	0.47
1:B:137:TYR:O	1:B:141:VAL:HG23	2.15	0.46
3:F:13:ASP:HA	3:F:16:VAL:CG2	2.45	0.46
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.50	0.46
2:C:193:ILE:HA	7:C:5058:HOH:O	2.15	0.46
2:C:326:GLU:CB	2:C:327:PRO:HD3	2.46	0.46
7:A:6004:HOH:O	2:C:70:GLY:HA3	2.14	0.46
1:B:171:ALA:O	1:B:175:ARG:HD3	2.16	0.46
2:C:235:TRP:CD1	2:C:235:TRP:C	2.88	0.46
1:B:183:GLY:HA2	1:B:422:GLN:HB2	1.98	0.46
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.97	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
2:D:376:ASP:CG	2:D:379:GLN:HG3	2.36	0.46
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.46
1:B:488:LEU:HD21	1:B:509:LEU:HD13	1.98	0.46
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:120:PRO:HD3	3:F:128:PHE:CG	2.51	0.46
3:F:159:ARG:CG	3:F:161:VAL:HG12	2.46	0.46
3:F:103:ASP:OD1	3:F:105:TRP:HB2	2.16	0.46
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.99	0.45
1:A:321:LEU:O	1:A:326:VAL:HB	2.15	0.45
1:A:403:ILE:HD12	1:A:515:LEU:CD1	2.46	0.45
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.46	0.45
2:D:385:LEU:C	2:D:387:GLY:N	2.69	0.45
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.30	0.45
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.52	0.45
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.94	0.45
3:E:12:ARG:O	3:E:16:VAL:CG2	2.64	0.45
1:A:105:VAL:O	1:A:109:PHE:HB2	2.17	0.45
2:D:259:PHE:CE1	2:D:356:LEU:HD12	2.51	0.45
2:C:146:ASN:ND2	2:C:197:ARG:HE	2.13	0.45
2:D:356:LEU:HD21	2:D:384:VAL:HG11	1.99	0.45
1:A:186:ARG:HD3	1:A:186:ARG:C	2.36	0.45
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.00	0.45
1:B:155:ASN:ND2	1:B:155:ASN:N	2.61	0.45
1:A:198:VAL:O	1:A:202:LEU:HG	2.17	0.45
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.52	0.45
2:C:39:VAL:O	2:C:41:PRO:HD3	2.16	0.45
2:C:362:ASP:O	2:C:365:GLU:HB2	2.17	0.44
3:E:153:GLU:CD	3:E:153:GLU:H	2.20	0.44
3:F:11:THR:HG21	3:F:52:ASP:OD2	2.18	0.44
3:F:12:ARG:O	3:F:16:VAL:HG23	2.16	0.44
1:A:160:LYS:HE3	1:A:161:ASN:HD21	1.80	0.44
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.47	0.44
1:A:445:MET:HE1	1:A:526:PHE:O	2.17	0.44
1:B:123:MET:CE	1:B:197:ALA:HA	2.47	0.44
1:B:213:THR:O	1:B:217:ILE:HG12	2.18	0.44
1:B:321:LEU:O	1:B:326:VAL:HB	2.17	0.44
3:F:98:MET:HG3	3:F:138:ARG:HG2	2.00	0.44
3:E:98:MET:HG3	3:E:138:ARG:HG2	2.00	0.44
1:A:18:ARG:HD2	2:C:131:GLY:HA3	1.99	0.44
1:A:477:GLU:OE2	1:A:477:GLU:C	2.56	0.44
1:A:81:SER:HB3	1:B:85:ALA:HB2	2.00	0.44
1:A:106:VAL:O	1:A:110:LEU:HB2	2.18	0.44
1:A:115:TYR:OH	2:C:173:ASP:HA	2.17	0.44
3:E:159:ARG:CG	3:E:161:VAL:HG12	2.48	0.44
3:F:150:THR:HG23	3:F:154:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:O	1:A:144:GLU:HB3	2.18	0.44
2:D:98:HIS:CD2	2:D:297:ASP:OD1	2.70	0.44
1:B:186:ARG:HD3	1:B:186:ARG:C	2.38	0.43
3:E:11:THR:CG2	3:E:12:ARG:N	2.81	0.43
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.18	0.43
1:B:106:VAL:O	1:B:110:LEU:HB2	2.18	0.43
1:A:406:MET:O	1:A:410:GLU:HG3	2.18	0.43
1:B:243:GLU:O	1:B:247:MET:HG2	2.18	0.43
3:F:12:ARG:O	3:F:16:VAL:CG2	2.66	0.43
1:A:108:ASN:HD21	1:A:175:ARG:CD	2.32	0.43
1:B:438:VAL:HG12	3:F:164:VAL:HG21	2.00	0.43
1:B:190:ASP:HB3	2:D:74:GLN:O	2.18	0.43
2:C:144:PHE:CZ	2:C:342:LEU:HD23	2.53	0.43
2:D:195:LEU:HD23	2:D:195:LEU:C	2.38	0.43
2:D:269:ALA:HB3	2:D:270:PRO:HD3	2.00	0.43
2:D:365:GLU:OE1	2:D:365:GLU:HA	2.18	0.43
3:E:19:ILE:HG12	3:E:60:LEU:HD13	2.01	0.43
3:F:13:ASP:CA	3:F:16:VAL:HG23	2.48	0.43
1:A:204:LEU:HG	1:A:205:GLN:HG3	2.01	0.43
1:B:40:LYS:HB3	1:B:41:ASN:HD22	1.81	0.43
2:D:146:ASN:ND2	2:D:197:ARG:HE	2.16	0.43
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.54	0.43
2:C:270:PRO:CB	2:D:270:PRO:HB3	2.28	0.43
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.49	0.42
1:B:186:ARG:HA	2:D:73:THR:OG1	2.19	0.42
1:B:421:SER:O	1:B:422:GLN:HB2	2.19	0.42
2:C:98:HIS:CD2	2:C:297:ASP:OD1	2.72	0.42
2:C:228:ARG:O	2:C:232:GLU:HG3	2.19	0.42
2:D:309:PHE:CZ	3:F:62:GLU:HG2	2.54	0.42
2:D:325:LEU:O	2:D:329:ILE:HG13	2.19	0.42
3:E:59:LYS:HA	3:E:59:LYS:HD3	1.86	0.42
1:A:146:ARG:HB2	2:C:106:HIS:NE2	2.33	0.42
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.71	0.42
1:A:421:SER:O	1:A:422:GLN:HB2	2.20	0.42
1:B:82:LEU:HD23	1:B:86:LEU:HD12	2.01	0.42
2:D:17:ALA:O	2:D:21:LEU:HG	2.19	0.42
2:D:176:ARG:NH1	2:D:176:ARG:HB2	2.35	0.42
3:E:11:THR:HG21	3:E:52:ASP:OD2	2.19	0.42
2:C:195:LEU:HD23	2:C:195:LEU:C	2.39	0.42
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.99	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:59:LYS:HD3	3:F:59:LYS:HA	1.87	0.42
1:A:124:LEU:HB3	1:A:137:TYR:CE1	2.55	0.42
1:A:527:ASN:O	3:E:162:ARG:NH2	2.53	0.42
1:B:58:GLU:HB3	1:B:132:GLU:O	2.19	0.42
1:B:269:THR:HG22	3:F:148:TYR:HE1	1.84	0.42
1:B:442:ASN:C	1:B:442:ASN:ND2	2.73	0.42
1:B:403:ILE:HD12	1:B:515:LEU:CD1	2.50	0.42
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.01	0.42
2:D:365:GLU:OE1	2:D:365:GLU:CA	2.68	0.42
1:B:260:ASP:HA	1:B:261:PRO:HD3	1.94	0.42
2:C:17:ALA:O	2:C:21:LEU:HG	2.20	0.42
1:B:163:GLN:HG2	7:B:5009:HOH:O	2.19	0.42
1:B:268:ASN:HD22	1:B:268:ASN:HA	1.65	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.56	0.42
2:D:385:LEU:O	2:D:387:GLY:N	2.53	0.42
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.54	0.42
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.66	0.41
1:A:159:ALA:O	2:C:33:ASN:HB2	2.20	0.41
1:B:121:THR:HG21	1:B:140:GLN:CD	2.41	0.41
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.55	0.41
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.20	0.41
1:A:121:THR:HG21	1:A:140:GLN:CD	2.40	0.41
1:A:82:LEU:HD23	1:A:86:LEU:HD12	2.02	0.41
1:A:204:LEU:O	1:A:209:GLU:HG3	2.19	0.41
1:A:330:ARG:NH1	3:E:148:TYR:HB2	2.35	0.41
2:C:263:GLU:HA	2:C:263:GLU:OE2	2.20	0.41
3:E:11:THR:HG22	3:E:12:ARG:N	2.36	0.41
1:B:204:LEU:HG	1:B:205:GLN:HG3	2.02	0.41
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.86	0.41
1:B:477:GLU:OE2	1:B:477:GLU:C	2.59	0.41
1:B:18:ARG:O	2:D:129:ALA:HA	2.21	0.41
1:B:26:GLN:HE21	1:B:26:GLN:HB2	1.70	0.41
1:B:123:MET:HB2	2:D:168:ARG:HD3	2.03	0.41
1:B:249:ASN:HD22	1:B:249:ASN:HA	1.63	0.41
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.28	0.41
2:D:269:ALA:N	2:D:270:PRO:CD	2.84	0.41
1:A:442:ASN:C	1:A:442:ASN:ND2	2.74	0.41
1:A:246:HIS:CD2	1:A:246:HIS:N	2.89	0.40
2:C:4:LEU:HD12	2:C:4:LEU:HA	1.79	0.40
2:C:22:LYS:O	2:C:22:LYS:HG3	2.21	0.40
3:E:13:ASP:HA	3:E:16:VAL:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:THR:HG22	3:F:12:ARG:N	2.37	0.40
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.56	0.40
1:B:452:TRP:O	1:B:456:MET:HG3	2.21	0.40
2:C:306:ASP:O	2:C:310:SER:HB2	2.21	0.40
2:C:364:ILE:HA	2:C:368:ALA:HB3	2.03	0.40
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.40
1:B:114:GLU:OE1	1:B:147:HIS:CB	2.69	0.40
1:B:283:THR:HB	1:B:284:PRO:HD3	2.03	0.40
2:C:261:ARG:NE	2:C:285:GLN:NE2	2.63	0.40
3:E:120:PRO:HG2	3:E:125:VAL:HG12	2.04	0.40
1:B:504:ASP:O	1:B:505:LYS:HB2	2.22	0.40
2:C:98:HIS:HE1	2:C:178:SER:OG	2.04	0.40
2:C:356:LEU:HD21	2:C:384:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	477 (94%)	30 (6%)	2 (0%)	34	46
1	B	508/527 (96%)	479 (94%)	27 (5%)	2 (0%)	34	46
2	C	386/389 (99%)	365 (95%)	18 (5%)	3 (1%)	19	27
2	D	385/389 (99%)	360 (94%)	21 (6%)	4 (1%)	15	21
3	E	164/170 (96%)	158 (96%)	5 (3%)	1 (1%)	25	34
3	F	166/170 (98%)	158 (95%)	8 (5%)	0	100	100
All	All	2118/2172 (98%)	1997 (94%)	109 (5%)	12 (1%)	25	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	B	40	LYS
2	C	205	PRO
2	D	205	PRO
1	A	94	ARG
1	B	94	ARG
2	C	64	ALA
2	D	64	ALA
3	E	5	GLY
2	D	251	VAL
2	D	386	ALA
2	C	251	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/442 (98%)	407 (94%)	26 (6%)	19	28
1	B	432/442 (98%)	407 (94%)	25 (6%)	20	30
2	C	322/323 (100%)	310 (96%)	12 (4%)	34	50
2	D	321/323 (99%)	307 (96%)	14 (4%)	28	42
3	E	144/147 (98%)	138 (96%)	6 (4%)	30	44
3	F	146/147 (99%)	140 (96%)	6 (4%)	30	45
All	All	1798/1824 (99%)	1709 (95%)	89 (5%)	25	38

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	26	GLN
1	A	30	ARG
1	A	41	ASN
1	A	43	ARG
1	A	90	ASN
1	A	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	TRP
1	A	155	ASN
1	A	161	ASN
1	A	186	ARG
1	A	189	SER
1	A	252	GLN
1	A	269	THR
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	311	GLU
1	A	323	LYS
1	A	334	ASP
1	A	337	GLN
1	A	403	ILE
1	A	435	THR
1	A	442	ASN
1	A	477	GLU
1	A	490	SER
1	B	21	THR
1	B	26	GLN
1	B	30	ARG
1	B	41	ASN
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	125	TRP
1	B	155	ASN
1	B	161	ASN
1	B	186	ARG
1	B	252	GLN
1	B	269	THR
1	B	279	GLN
1	B	302	VAL
1	B	310	TYR
1	B	311	GLU
1	B	323	LYS
1	B	334	ASP
1	B	337	GLN
1	B	403	ILE
1	B	435	THR
1	B	442	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	477	GLU
1	B	490	SER
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	179	LEU
2	C	266	GLN
2	C	311	ASP
2	C	318	ARG
2	C	356	LEU
2	C	365	GLU
2	C	378	ASP
2	C	385	LEU
2	D	35	MET
2	D	80	ARG
2	D	146	ASN
2	D	153	LEU
2	D	168	ARG
2	D	173	ASP
2	D	179	LEU
2	D	266	GLN
2	D	311	ASP
2	D	318	ARG
2	D	356	LEU
2	D	365	GLU
2	D	378	ASP
2	D	385	LEU
3	E	11	THR
3	E	16	VAL
3	E	23	ASN
3	E	44	ARG
3	E	46	SER
3	E	164	VAL
3	F	11	THR
3	F	16	VAL
3	F	23	ASN
3	F	44	ARG
3	F	46	SER
3	F	53	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	108	ASN
1	A	155	ASN
1	A	161	ASN
1	A	168	HIS
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	451	GLN
1	B	26	GLN
1	B	41	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	155	ASN
1	B	161	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	252	GLN
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	382	HIS
1	B	413	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	439	HIS
1	B	442	ASN
1	B	451	GLN
1	B	527	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	D	98	HIS
2	D	146	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
3	E	39	HIS
3	E	45	ASN
3	E	144	ASN
3	E	167	GLN
3	F	39	HIS
3	F	45	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	6001	-	2,2,2	0.64	0	1,1,1	0.61	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

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%)	0.10	20 (3%) 39 42	22, 43, 70, 86	0
1	B	510/527 (96%)	0.00	16 (3%) 49 51	23, 40, 71, 84	0
2	C	388/389 (99%)	-0.39	5 (1%) 77 78	18, 29, 47, 70	0
2	D	387/389 (99%)	0.45	31 (8%) 12 13	26, 51, 78, 86	0
3	E	166/170 (97%)	-0.22	1 (0%) 89 89	21, 34, 53, 66	0
3	F	168/170 (98%)	0.91	21 (12%) 3 4	40, 61, 82, 90	0
All	All	2130/2172 (98%)	0.09	94 (4%) 34 37	18, 41, 74, 90	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	205	PRO	5.5
2	D	2	SER	5.5
2	C	2	SER	4.9
2	D	353	THR	4.8
1	A	434	SER	4.4
2	D	344	ALA	4.2
2	D	375	ALA	4.2
3	F	72	PHE	4.1
2	C	205	PRO	3.9
1	A	262	ALA	3.8
1	B	40	LYS	3.7
1	B	244	LEU	3.7
1	A	55	GLU	3.7
1	A	326	VAL	3.6
2	D	343	PRO	3.6
2	C	6	GLU	3.5
3	F	27	LYS	3.4
1	A	54	ASN	3.4
1	B	55	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	349	LYS	3.3
1	B	261	PRO	3.3
1	A	310	TYR	3.3
1	B	333	LYS	3.3
1	B	527	ASN	3.3
3	F	89	SER	3.2
1	A	260	ASP	3.2
1	A	17	ASN	3.2
2	D	352	ILE	3.1
3	F	170	HIS	3.1
2	D	254	ALA	3.1
3	F	80	LYS	3.0
3	F	26	GLU	3.0
1	B	21	THR	3.0
1	B	259	ASN	3.0
1	B	258	ALA	2.9
3	F	102	LYS	2.9
2	D	339	PHE	2.8
1	B	316	ILE	2.8
2	D	379	GLN	2.7
2	D	260	VAL	2.7
1	B	59	GLN	2.7
3	E	4	LEU	2.6
2	D	256	PHE	2.6
2	D	307	PRO	2.6
1	B	19	ALA	2.5
2	D	388	LEU	2.5
3	F	67	LEU	2.5
2	D	44	LYS	2.5
2	D	45	ARG	2.4
3	F	96	ALA	2.4
2	D	138	PRO	2.4
2	C	389	LYS	2.4
3	F	83	PHE	2.4
2	D	153	LEU	2.4
2	D	357	TYR	2.4
3	F	21	GLN	2.4
3	F	23	ASN	2.3
1	A	320	ARG	2.3
1	A	20	PRO	2.3
2	D	252	TYR	2.3
2	D	193	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	2.3
2	D	356	LEU	2.3
1	B	57	LYS	2.2
2	D	374	LYS	2.2
3	F	145	LEU	2.2
2	D	143	GLU	2.2
1	B	53	ALA	2.2
1	B	320	ARG	2.2
2	D	220	ASN	2.2
1	A	366	GLN	2.2
3	F	22	LEU	2.2
1	A	388	GLU	2.2
3	F	30	GLU	2.2
1	A	59	GLN	2.1
1	A	263	SER	2.1
2	D	148	TYR	2.1
3	F	16	VAL	2.1
3	F	4	LEU	2.1
1	B	327	GLU	2.1
1	A	433	ALA	2.1
2	D	383	ALA	2.1
1	A	317	TRP	2.1
2	C	45	ARG	2.0
3	F	121	PRO	2.0
1	A	504	ASP	2.0
3	F	161	VAL	2.0
1	A	318	ILE	2.0
2	D	308	GLU	2.0
1	A	337	GLN	2.0
3	F	69	ALA	2.0
3	F	120	PRO	2.0
2	D	350	GLU	2.0
2	D	346	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	5007	1/1	0.84	0.07	72,72,72,72	0
6	FMT	A	6001	3/3	0.90	0.17	60,60,61,63	0
5	CA	A	5005	1/1	0.93	0.05	57,57,57,57	0
5	CA	C	5006	1/1	0.94	0.08	62,62,62,62	0
4	FE	B	5004	1/1	0.96	0.04	59,59,59,59	0
4	FE	A	5002	1/1	0.97	0.04	67,67,67,67	0
4	FE	B	5003	1/1	0.98	0.05	48,48,48,48	0
4	FE	A	5001	1/1	0.99	0.02	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.