



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:34 PM GMT

PDB ID : 1UM0
Title : Crystal structure of chorismate synthase complexed with FMN
Authors : Ahn, H.J.; Yoon, H.J.; Lee, B.; Suh, S.W.
Deposited on : 2003-09-18
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

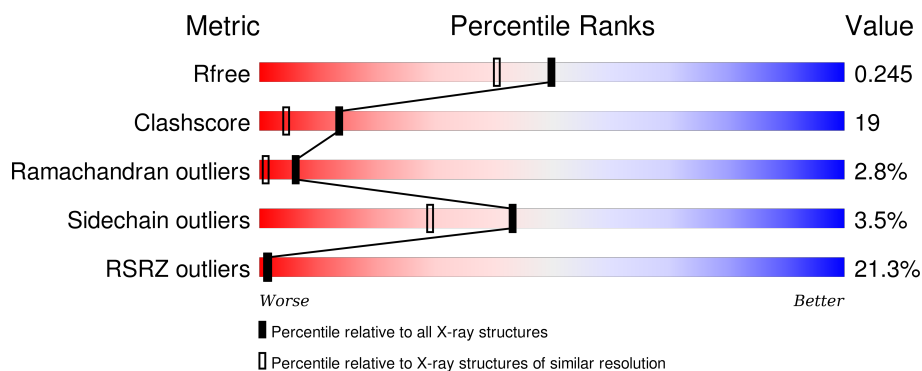
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	365	<div> <div>14%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	B	365	<div> <div>28%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	C	365	<div> <div>28%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	D	365	<div> <div>14%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	B	2400	-	-	-	X
2	FMN	C	3400	-	-	-	X

2 Entry composition [i](#)

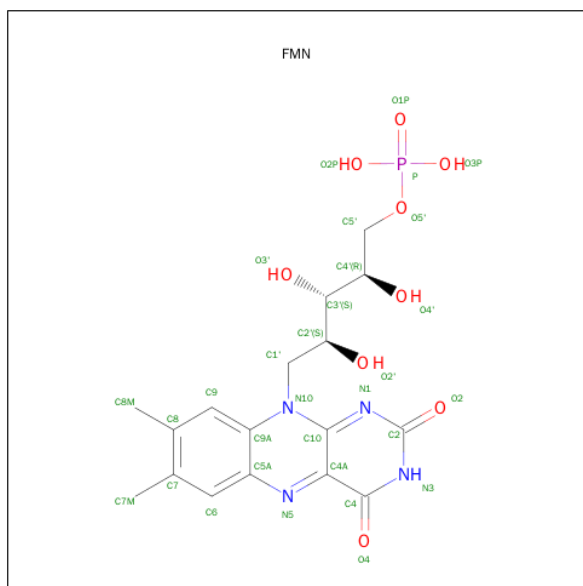
There are 3 unique types of molecules in this entry. The entry contains 11843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	B	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	C	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	D	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

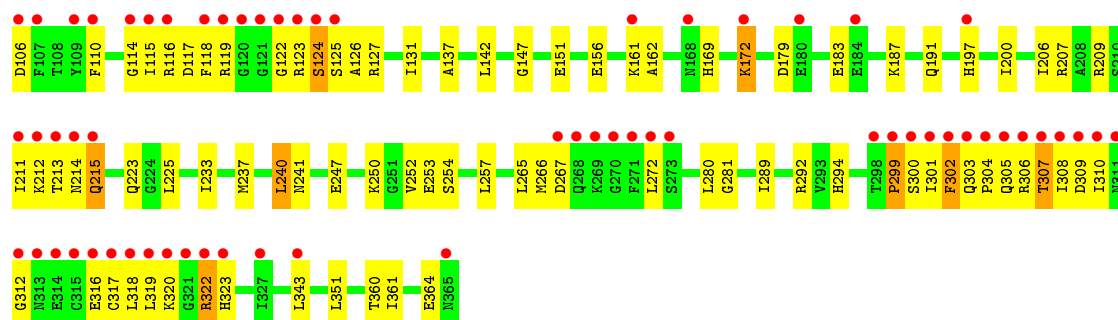
Continued on next page...

Continued from previous page...

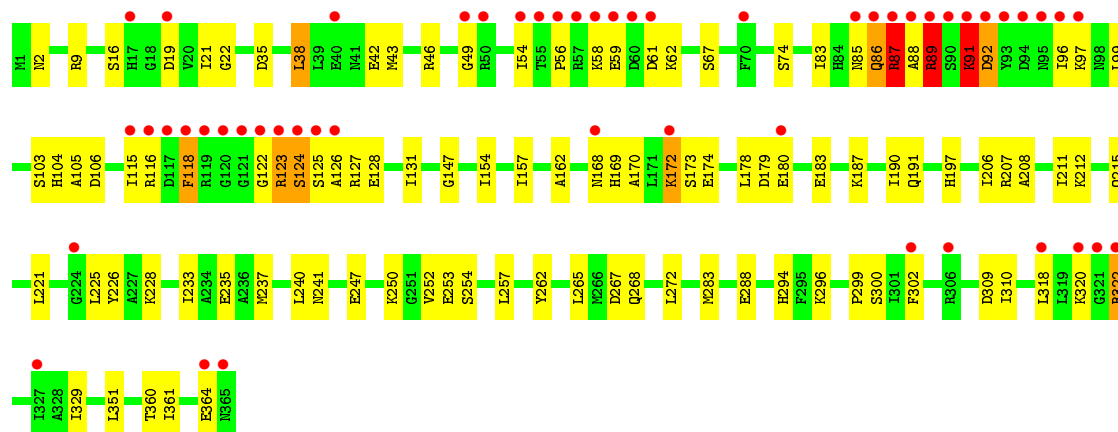
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	84	Total	O	0	0
			84	84		
3	C	76	Total	O	0	0
			76	76		
3	D	137	Total	O	0	0
			137	137		



• Molecule 1: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.69Å 146.69Å 132.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.95 29.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.90-1.95) 99.5 (29.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.243 0.216 , 0.245	Depositor DCC
R_{free} test set	10100 reflections (10.03%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.0	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 100703 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11843	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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	0.34	0/2857	0.63	2/3833 (0.1%)
1	B	0.31	0/2857	0.59	2/3833 (0.1%)
1	C	0.31	0/2857	0.58	2/3833 (0.1%)
1	D	0.33	0/2857	0.61	2/3833 (0.1%)
All	All	0.32	0/11428	0.60	8/15332 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	89	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	A	87	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	87	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	87	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	89	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	89	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	C	87	ARG	NE-CZ-NH2	7.23	123.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2816	0	2852	91	0
1	B	2816	0	2852	110	1
1	C	2816	0	2852	147	4
1	D	2816	0	2852	111	3
2	A	31	0	19	4	0
2	B	31	0	19	7	0
2	C	31	0	19	3	0
2	D	31	0	19	6	0
3	A	158	0	0	3	0
3	B	84	0	0	2	0
3	C	76	0	0	0	0
3	D	137	0	0	7	0
All	All	11843	0	11484	420	5

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 19.

All (420) 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:C:307:THR:HG23	1:C:308:ILE:H	1.25	0.97
1:D:105:ALA:H	1:D:123:ARG:HH12	1.07	0.94
1:A:322:ARG:H	1:A:322:ARG:NH1	1.70	0.90
1:B:281:GLY:HA3	1:C:105:ALA:HB2	1.54	0.89
1:A:322:ARG:HH11	1:A:322:ARG:N	1.71	0.89
1:C:267:ASP:HB2	1:C:272:LEU:HD21	1.54	0.88
1:B:105:ALA:H	1:B:123:ARG:HH12	0.94	0.87
1:C:322:ARG:H	1:C:322:ARG:HH11	1.23	0.86
1:D:105:ALA:H	1:D:123:ARG:NH1	1.74	0.86
1:B:105:ALA:N	1:B:123:ARG:HH12	1.72	0.85
1:A:318:LEU:HD12	1:A:320:LYS:HE3	1.59	0.85
1:D:21:ILE:HG13	1:D:131:ILE:HD11	1.60	0.84
1:D:318:LEU:HD12	1:D:320:LYS:HE3	1.57	0.83
1:C:21:ILE:HG13	1:C:131:ILE:HD11	1.60	0.83
1:B:105:ALA:H	1:B:123:ARG:NH1	1.77	0.83
1:A:302:PHE:HE2	1:A:318:LEU:HD11	1.43	0.82
1:C:197:HIS:HB3	1:C:302:PHE:HB3	1.61	0.82
1:D:322:ARG:HH11	1:D:322:ARG:H	1.29	0.79
1:D:105:ALA:N	1:D:123:ARG:HH22	1.81	0.78
1:C:102:PRO:HG2	1:C:305:GLN:HB3	1.66	0.77
1:A:361:ILE:O	1:A:365:ASN:OXT	2.03	0.77
1:B:238:MET:HE3	1:B:243:VAL:O	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:O	1:A:172:LYS:HD3	1.86	0.76
1:C:122:GLY:O	1:C:123:ARG:HG2	1.85	0.76
1:A:123:ARG:HG3	1:A:124:SER:H	1.52	0.75
1:B:318:LEU:HD12	1:B:320:LYS:HE3	1.67	0.74
1:C:300:SER:HA	1:C:305:GLN:HE22	1.52	0.73
1:A:322:ARG:HH11	1:A:322:ARG:H	0.86	0.73
1:C:212:LYS:HD3	1:C:215:GLN:HG2	1.71	0.73
1:C:322:ARG:HH11	1:C:322:ARG:N	1.86	0.72
1:B:302:PHE:HE2	1:B:318:LEU:HD11	1.54	0.72
1:D:302:PHE:HE2	1:D:318:LEU:HD11	1.54	0.72
1:C:117:ASP:CG	1:C:118:PHE:H	1.93	0.72
1:B:169:HIS:HA	1:B:172:LYS:HE3	1.72	0.72
1:A:351:LEU:HD22	1:B:361:ILE:HD12	1.73	0.71
1:B:128:GLU:HG3	1:C:225:LEU:HD13	1.72	0.70
1:B:105:ALA:HB3	1:B:123:ARG:HH22	1.56	0.70
1:C:61:ASP:HA	1:C:84:HIS:O	1.91	0.70
1:A:75:THR:HA	1:C:115:ILE:HD12	1.74	0.70
1:A:45:ARG:HD2	3:A:1524:HOH:O	1.91	0.70
1:B:183:GLU:HG2	1:B:187:LYS:HE3	1.74	0.69
1:C:322:ARG:H	1:C:322:ARG:HD3	1.58	0.69
1:D:169:HIS:CD2	1:D:172:LYS:HE3	2.27	0.69
1:C:197:HIS:HB2	1:C:303:GLN:HG3	1.74	0.69
1:B:56:PRO:HA	1:B:59:GLU:HB2	1.74	0.69
1:C:307:THR:HG23	1:C:308:ILE:N	2.06	0.68
1:A:128:GLU:HG3	1:D:225:LEU:HD13	1.73	0.68
1:C:169:HIS:HA	1:C:172:LYS:NZ	2.09	0.68
1:B:104:HIS:HD2	1:B:123:ARG:HD2	1.59	0.68
1:A:302:PHE:CE2	1:A:318:LEU:HD11	2.26	0.67
1:A:169:HIS:CD2	1:A:172:LYS:HE3	2.29	0.67
1:D:253:GLU:O	1:D:257:LEU:HD13	1.94	0.67
1:C:102:PRO:HG2	1:C:305:GLN:CB	2.25	0.67
1:D:49:GLY:O	1:D:174:GLU:HA	1.95	0.67
1:D:322:ARG:NH1	1:D:322:ARG:HB2	2.10	0.67
1:A:300:SER:H	2:A:1400:FMN:HM82	1.59	0.67
1:D:105:ALA:N	1:D:123:ARG:HH12	1.87	0.66
1:A:225:LEU:HD13	1:D:128:GLU:HG3	1.77	0.66
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.61	0.65
1:C:322:ARG:HD3	1:C:322:ARG:N	2.11	0.65
1:D:85:ASN:ND2	1:D:86:GLN:HG3	2.11	0.65
2:B:2400:FMN:O3P	1:C:280:LEU:HD12	1.96	0.65
1:D:169:HIS:O	1:D:172:LYS:HD3	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:THR:H	1:C:56:PRO:CD	2.09	0.65
1:A:51:ASN:OD1	1:A:52:VAL:HG23	1.97	0.65
1:A:241:ASN:HB3	2:A:1400:FMN:H3'	1.79	0.65
1:B:100:PHE:HB2	1:C:266:MET:HE3	1.80	0.64
1:D:169:HIS:NE2	1:D:172:LYS:HE3	2.12	0.64
1:C:322:ARG:HB2	1:C:322:ARG:NH1	2.13	0.64
1:D:115:ILE:O	1:D:115:ILE:HD12	1.98	0.63
1:A:157:ILE:HD13	1:A:190:ILE:HD11	1.80	0.63
1:C:305:GLN:HB2	1:C:317:CYS:SG	2.39	0.63
1:B:247:GLU:OE1	1:B:294:HIS:HE1	1.82	0.63
1:C:97:LYS:HB2	1:C:97:LYS:NZ	2.14	0.62
1:A:241:ASN:ND2	1:D:228:LYS:NZ	2.47	0.62
1:C:247:GLU:OE2	1:C:252:VAL:HG22	1.99	0.62
1:C:52:VAL:HB	1:C:56:PRO:HB3	1.82	0.62
1:A:318:LEU:HD12	1:A:320:LYS:CE	2.29	0.62
1:B:320:LYS:H	1:B:320:LYS:HD2	1.63	0.62
1:C:301:ILE:H	1:C:305:GLN:NE2	1.98	0.61
1:C:247:GLU:HB2	1:C:292:ARG:HB2	1.82	0.61
1:D:128:GLU:HG2	3:D:4505:HOH:O	2.00	0.61
1:B:264:ASP:C	1:B:265:LEU:HD12	2.21	0.61
1:D:241:ASN:ND2	3:D:4433:HOH:O	2.34	0.60
1:C:318:LEU:HD12	1:C:320:LYS:HE3	1.81	0.60
1:B:253:GLU:O	1:B:257:LEU:HD13	2.01	0.60
1:D:322:ARG:HH11	1:D:322:ARG:N	1.99	0.60
1:A:330:ARG:HB3	1:A:330:ARG:HH21	1.65	0.60
1:A:54:ILE:HG22	1:A:55:THR:N	2.15	0.60
1:C:308:ILE:HG12	1:C:309:ASP:N	2.17	0.59
1:A:262:TYR:O	1:A:275:ARG:HD3	2.03	0.59
1:A:247:GLU:OE1	1:A:294:HIS:HE1	1.86	0.59
1:A:21:ILE:HG13	1:A:131:ILE:HD11	1.82	0.59
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.84	0.59
1:B:266:MET:H	1:C:307:THR:HA	1.68	0.58
1:A:161:LYS:HE2	3:A:1441:HOH:O	2.02	0.58
1:A:55:THR:O	1:A:59:GLU:HG2	2.02	0.58
1:B:116:ARG:HD3	1:B:310:ILE:HD13	1.86	0.58
1:D:21:ILE:HG23	1:D:83:ILE:HB	1.86	0.58
1:D:162:ALA:HB1	1:D:179:ASP:HB2	1.85	0.58
1:A:320:LYS:H	1:A:320:LYS:HD2	1.67	0.57
1:B:265:LEU:HG	1:C:306:ARG:O	2.04	0.57
1:A:361:ILE:HD12	1:B:351:LEU:HD22	1.87	0.57
1:A:300:SER:H	2:A:1400:FMN:C8M	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HB3	1:A:330:ARG:NH2	2.20	0.57
1:D:116:ARG:H	1:D:116:ARG:HD2	1.69	0.57
1:B:241:ASN:HD21	2:B:2400:FMN:H5'2	1.68	0.57
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.20	0.57
1:C:302:PHE:N	1:C:323:HIS:HD2	2.03	0.57
1:C:351:LEU:HD22	1:D:361:ILE:HD12	1.86	0.57
1:C:308:ILE:HD11	1:C:312:GLY:HA2	1.86	0.56
1:D:247:GLU:OE1	1:D:294:HIS:HE1	1.88	0.56
1:D:122:GLY:O	1:D:123:ARG:HG2	2.06	0.56
1:C:322:ARG:H	1:C:322:ARG:NH1	1.99	0.56
1:A:241:ASN:HD21	1:D:228:LYS:NZ	2.03	0.56
1:C:116:ARG:HD3	1:C:310:ILE:HG21	1.88	0.56
1:B:67:SER:HB3	1:D:16:SER:HB3	1.87	0.56
1:C:54:ILE:O	1:C:55:THR:HG23	2.06	0.56
1:A:296:LYS:HD2	1:D:262:TYR:CE1	2.41	0.56
1:C:316:GLU:HG2	1:C:318:LEU:H	1.71	0.56
1:C:253:GLU:O	1:C:257:LEU:HD13	2.04	0.56
1:B:271:PHE:H	1:B:271:PHE:HD1	1.54	0.56
1:C:106:ASP:HA	1:C:118:PHE:CZ	2.41	0.56
1:D:104:HIS:HB3	1:D:123:ARG:NH2	2.20	0.56
1:C:19:ASP:HA	1:C:86:GLN:OE1	2.06	0.56
1:C:124:SER:O	1:C:126:ALA:N	2.39	0.56
1:A:122:GLY:O	1:A:124:SER:N	2.39	0.56
1:C:55:THR:H	1:C:56:PRO:HD3	1.71	0.56
1:B:99:LEU:HA	1:B:309:ASP:HA	1.88	0.56
1:B:322:ARG:HD3	1:B:322:ARG:N	2.21	0.55
1:A:20:VAL:HG22	1:A:84:HIS:ND1	2.21	0.55
1:C:99:LEU:O	1:C:99:LEU:HD12	2.05	0.55
1:D:124:SER:HA	1:D:127:ARG:HD2	1.88	0.55
1:C:172:LYS:H	1:C:172:LYS:HD3	1.69	0.55
1:A:123:ARG:CG	1:A:124:SER:H	2.20	0.55
1:D:207:ARG:HG2	1:D:208:ALA:N	2.21	0.55
1:B:16:SER:HB3	1:D:67:SER:HB3	1.87	0.55
1:C:267:ASP:HB2	1:C:272:LEU:CD2	2.32	0.55
1:C:100:PHE:CE2	1:C:310:ILE:HA	2.42	0.55
1:D:21:ILE:HD12	1:D:22:GLY:H	1.71	0.54
1:C:250:LYS:HE3	1:C:253:GLU:HB3	1.88	0.54
1:C:38:LEU:HD23	1:C:38:LEU:C	2.27	0.54
1:B:263:ASN:HD21	1:C:299:PRO:HA	1.72	0.54
1:C:197:HIS:O	1:C:303:GLN:HG3	2.08	0.54
1:B:197:HIS:HB3	1:B:302:PHE:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG22	1:A:55:THR:H	1.72	0.54
1:C:58:LYS:N	1:C:58:LYS:HD3	2.21	0.54
1:D:106:ASP:H	1:D:123:ARG:HH22	1.56	0.54
1:C:320:LYS:HD2	1:C:320:LYS:H	1.72	0.53
1:D:105:ALA:H	1:D:123:ARG:CZ	2.20	0.53
1:C:95:ASN:HB2	1:C:319:LEU:HD23	1.90	0.53
1:A:75:THR:HA	1:C:115:ILE:CD1	2.38	0.53
1:B:105:ALA:HB3	1:B:123:ARG:NH2	2.23	0.53
1:C:212:LYS:HD3	1:C:215:GLN:CG	2.36	0.53
1:B:54:ILE:HB	1:B:59:GLU:OE2	2.09	0.53
1:C:250:LYS:HB3	1:C:254:SER:OG	2.08	0.53
1:C:320:LYS:HD2	1:C:320:LYS:N	2.24	0.53
1:C:322:ARG:HB2	1:C:322:ARG:HH11	1.74	0.53
1:A:264:ASP:OD1	1:A:275:ARG:HD2	2.09	0.53
1:A:318:LEU:O	1:A:320:LYS:HD2	2.09	0.53
1:C:104:HIS:HB3	1:C:123:ARG:HH21	1.74	0.53
1:C:151:GLU:OE1	1:C:209:ARG:NH1	2.42	0.53
1:C:307:THR:CG2	1:C:308:ILE:H	2.08	0.53
1:D:105:ALA:N	1:D:123:ARG:NH2	2.55	0.53
1:D:300:SER:H	2:D:4400:FMN:HM82	1.74	0.52
1:B:206:ILE:N	1:B:206:ILE:HD12	2.25	0.52
1:D:97:LYS:NZ	1:D:97:LYS:HB2	2.24	0.52
1:D:106:ASP:N	1:D:123:ARG:HH22	2.08	0.52
1:D:169:HIS:NE2	1:D:180:GLU:HB3	2.24	0.52
1:A:330:ARG:CB	1:A:330:ARG:HH21	2.22	0.52
1:C:101:ARG:HD2	1:C:319:LEU:HD11	1.90	0.52
1:D:206:ILE:HD12	1:D:206:ILE:N	2.24	0.52
1:D:54:ILE:HG22	1:D:58:LYS:HD2	1.92	0.52
1:D:302:PHE:CE2	1:D:318:LEU:HD11	2.41	0.52
1:B:169:HIS:HE1	1:B:183:GLU:OE2	1.92	0.52
1:C:187:LYS:O	1:C:191:GLN:HG3	2.09	0.52
1:D:58:LYS:HG3	1:D:59:GLU:HG2	1.91	0.52
1:C:265:LEU:N	1:C:265:LEU:HD22	2.25	0.52
1:B:151:GLU:OE1	1:B:209:ARG:NH1	2.41	0.52
1:D:174:GLU:H	1:D:174:GLU:CD	2.14	0.52
1:B:123:ARG:HE	1:B:124:SER:H	1.58	0.51
1:D:250:LYS:HB3	1:D:254:SER:OG	2.10	0.51
1:D:169:HIS:HE1	1:D:183:GLU:OE2	1.93	0.51
1:C:48:GLY:HA2	1:C:52:VAL:HG21	1.93	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.43	0.51
1:B:20:VAL:HG22	1:B:84:HIS:ND1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:O	1:C:237:MET:HG2	2.10	0.51
1:A:48:GLY:O	1:A:49:GLY:C	2.48	0.51
1:D:322:ARG:N	1:D:322:ARG:HD3	2.26	0.51
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.26	0.51
1:A:169:HIS:HE1	1:A:183:GLU:OE2	1.94	0.51
1:C:50:ARG:NH2	1:C:323:HIS:HA	2.26	0.50
1:C:183:GLU:HG2	1:C:187:LYS:HE3	1.92	0.50
1:C:147:GLY:HA2	1:C:211:ILE:HD12	1.92	0.50
1:B:183:GLU:CG	1:B:187:LYS:HE3	2.40	0.50
1:C:169:HIS:HA	1:C:172:LYS:HZ2	1.76	0.50
1:A:241:ASN:ND2	1:D:228:LYS:HZ3	2.08	0.50
1:B:98:ASN:O	1:B:310:ILE:HG13	2.10	0.50
1:A:162:ALA:HB1	1:A:179:ASP:HB2	1.93	0.50
1:C:162:ALA:HB1	1:C:179:ASP:HB2	1.92	0.50
1:B:267:ASP:OD2	1:B:268:GLN:HG3	2.11	0.50
1:B:250:LYS:HE2	1:B:257:LEU:HD21	1.94	0.50
1:B:162:ALA:HB1	1:B:179:ASP:HB2	1.94	0.50
1:D:105:ALA:H	1:D:123:ARG:NH2	2.10	0.50
1:A:128:GLU:HG3	1:D:225:LEU:CD1	2.40	0.50
1:B:9:ARG:HD2	3:B:2423:HOH:O	2.11	0.50
3:B:2470:HOH:O	1:D:115:ILE:HD11	2.12	0.50
1:A:304:PRO:HB3	1:A:316:GLU:OE1	2.11	0.50
1:B:258:LYS:HG2	1:C:200:ILE:HG22	1.93	0.50
1:C:52:VAL:HB	1:C:56:PRO:CB	2.42	0.49
1:D:211:ILE:O	1:D:211:ILE:HG22	2.12	0.49
1:A:320:LYS:HD2	1:A:320:LYS:N	2.28	0.49
1:C:156:GLU:OE1	1:C:161:LYS:HG2	2.12	0.49
1:A:67:SER:HB3	1:C:16:SER:HB3	1.94	0.49
1:A:9:ARG:HD2	3:A:1447:HOH:O	2.12	0.49
1:D:123:ARG:NH2	3:D:4478:HOH:O	2.45	0.49
1:C:100:PHE:CD1	1:C:106:ASP:HB3	2.47	0.49
1:D:169:HIS:CE1	1:D:172:LYS:HE3	2.48	0.49
1:D:116:ARG:N	1:D:116:ARG:HD2	2.27	0.49
1:B:54:ILE:HG22	1:B:55:THR:N	2.27	0.49
1:D:104:HIS:CE1	1:D:299:PRO:HB2	2.47	0.49
1:B:47:GLN:HE22	1:B:60:ASP:HB2	1.78	0.49
1:D:296:LYS:HE3	1:D:299:PRO:HG3	1.95	0.49
1:C:100:PHE:HB3	1:C:106:ASP:HB2	1.95	0.49
1:B:172:LYS:H	1:B:172:LYS:HD3	1.77	0.49
1:C:54:ILE:O	1:C:55:THR:OG1	2.27	0.49
1:B:262:TYR:HD1	1:B:263:ASN:N	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:SER:HB3	1:C:67:SER:HB3	1.95	0.48
1:B:115:ILE:HD12	1:D:74:SER:O	2.12	0.48
1:B:241:ASN:CG	2:B:2400:FMN:H3'	2.34	0.48
1:B:101:ARG:HD2	1:B:319:LEU:HD21	1.94	0.48
1:D:187:LYS:O	1:D:191:GLN:HG3	2.13	0.48
1:A:262:TYR:CE1	1:D:296:LYS:HD2	2.48	0.48
1:C:104:HIS:HD2	1:C:123:ARG:HE	1.61	0.48
1:C:117:ASP:CG	1:C:118:PHE:N	2.64	0.48
1:B:169:HIS:O	1:B:172:LYS:HD3	2.13	0.48
1:D:9:ARG:HD2	3:D:4468:HOH:O	2.12	0.48
1:C:247:GLU:OE1	1:C:294:HIS:HE1	1.96	0.48
1:C:100:PHE:CE1	1:C:310:ILE:HG12	2.48	0.48
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.48
1:C:142:LEU:C	1:C:142:LEU:HD23	2.34	0.48
1:A:314:GLU:HG3	1:D:268:GLN:HG3	1.95	0.48
1:A:169:HIS:NE2	1:A:172:LYS:HE3	2.29	0.48
1:D:87:ARG:HB2	1:D:88:ALA:H	1.47	0.48
1:A:21:ILE:HG23	1:A:83:ILE:HB	1.96	0.48
1:D:320:LYS:H	1:D:320:LYS:HD2	1.79	0.47
1:A:46:ARG:NH1	1:A:330:ARG:HH12	2.11	0.47
1:D:124:SER:O	1:D:126:ALA:N	2.46	0.47
1:D:322:ARG:HD3	1:D:322:ARG:H	1.78	0.47
1:A:241:ASN:HD21	1:D:228:LYS:HZ1	1.61	0.47
1:C:48:GLY:HA2	1:C:52:VAL:CG2	2.44	0.47
1:C:200:ILE:HD12	1:C:200:ILE:O	2.14	0.47
1:D:360:THR:HG23	1:D:364:GLU:OE1	2.14	0.47
1:C:322:ARG:CB	1:C:322:ARG:HH11	2.28	0.47
1:C:213:THR:O	1:C:214:ASN:HB2	2.14	0.47
1:C:304:PRO:HG3	1:C:318:LEU:CD2	2.45	0.47
1:C:302:PHE:CE2	1:C:320:LYS:HA	2.49	0.47
1:B:299:PRO:HD2	2:B:2400:FMN:H9	1.96	0.47
1:C:305:GLN:O	1:C:317:CYS:HB3	2.15	0.47
1:C:100:PHE:HD1	1:C:106:ASP:HB3	1.79	0.47
1:D:97:LYS:HA	3:D:4500:HOH:O	2.13	0.47
1:C:123:ARG:O	1:C:124:SER:HB2	2.15	0.47
1:D:154:ILE:HG21	1:D:157:ILE:HD11	1.97	0.47
1:C:104:HIS:CD2	1:C:123:ARG:HE	2.33	0.47
1:B:157:ILE:HD12	1:B:175:ILE:HD12	1.96	0.47
1:D:170:ALA:HB2	1:D:178:LEU:HD23	1.97	0.47
1:B:207:ARG:HA	1:B:289:ILE:O	2.15	0.46
1:A:322:ARG:N	1:A:322:ARG:HD3	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LYS:N	1:C:58:LYS:CD	2.79	0.46
1:C:38:LEU:HD22	1:C:137:ALA:HB1	1.96	0.46
1:D:241:ASN:HB3	2:D:4400:FMN:H3'	1.98	0.46
1:B:104:HIS:CD2	1:B:123:ARG:HD2	2.46	0.46
1:B:241:ASN:ND2	2:B:2400:FMN:H3'	2.30	0.46
1:B:110:PHE:O	1:B:114:GLY:HA2	2.15	0.46
1:B:247:GLU:OE1	1:B:294:HIS:CE1	2.66	0.46
1:B:265:LEU:HD23	1:C:306:ARG:HB2	1.97	0.46
1:B:258:LYS:NZ	1:B:261:GLU:OE1	2.48	0.46
1:B:330:ARG:NH2	1:B:330:ARG:HB3	2.31	0.46
1:D:91:LYS:HB2	1:D:92:ASP:H	1.57	0.46
1:D:123:ARG:NH1	2:D:4400:FMN:O4'	2.50	0.45
1:B:101:ARG:NH1	1:B:101:ARG:HG3	2.29	0.45
1:C:206:ILE:N	1:C:206:ILE:HD12	2.30	0.45
1:B:101:ARG:HD2	1:B:319:LEU:HD11	1.98	0.45
1:C:54:ILE:O	1:C:54:ILE:HG22	2.15	0.45
1:D:116:ARG:HG2	1:D:310:ILE:HD13	1.97	0.45
1:B:112:LYS:HZ3	1:C:223:GLN:NE2	2.15	0.45
1:D:265:LEU:HB2	1:D:272:LEU:HD12	1.97	0.45
1:D:99:LEU:HA	1:D:309:ASP:HA	1.97	0.45
1:B:320:LYS:HD2	1:B:320:LYS:N	2.30	0.45
1:B:104:HIS:CE1	1:B:300:SER:HG	2.35	0.45
1:B:85:ASN:O	1:B:86:GLN:HB2	2.17	0.45
1:B:233:ILE:O	1:B:237:MET:HG2	2.17	0.45
1:C:318:LEU:HD12	1:C:320:LYS:CE	2.47	0.45
1:D:318:LEU:O	1:D:320:LYS:HD2	2.16	0.45
1:D:267:ASP:HA	3:D:4515:HOH:O	2.15	0.45
1:C:102:PRO:HG3	1:C:307:THR:HG22	1.98	0.45
1:B:9:ARG:NH1	1:D:2:ASN:OD1	2.49	0.45
1:A:318:LEU:HD13	1:A:318:LEU:C	2.37	0.45
1:A:9:ARG:NH1	1:C:2:ASN:OD1	2.49	0.45
1:B:101:ARG:O	1:B:104:HIS:HB2	2.17	0.44
1:C:102:PRO:N	1:C:307:THR:HG21	2.32	0.44
1:C:93:TYR:HA	1:C:320:LYS:O	2.17	0.44
1:B:212:LYS:HB2	1:B:215:GLN:CB	2.47	0.44
1:B:215:GLN:OE1	1:B:216:LYS:N	2.50	0.44
1:B:170:ALA:HB2	1:B:178:LEU:HD23	1.99	0.44
1:A:99:LEU:HA	1:A:309:ASP:HA	1.99	0.44
1:D:147:GLY:HA3	1:D:212:LYS:HD3	1.98	0.44
1:B:105:ALA:HB2	1:C:281:GLY:HA3	1.99	0.44
1:D:247:GLU:OE2	1:D:252:VAL:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:OE2	1:A:207:ARG:NH1	2.39	0.44
1:D:61:ASP:O	1:D:62:LYS:HB2	2.18	0.44
1:C:127:ARG:HG2	1:C:127:ARG:NH1	2.32	0.44
1:D:38:LEU:HD22	1:D:42:GLU:HG2	1.99	0.44
1:A:101:ARG:NH1	1:A:106:ASP:OD2	2.50	0.44
1:B:47:GLN:HE22	1:B:60:ASP:CB	2.30	0.44
1:B:101:ARG:NH1	1:B:118:PHE:CZ	2.85	0.44
1:C:117:ASP:O	1:C:118:PHE:HB2	2.17	0.44
1:B:112:LYS:NZ	1:C:223:GLN:NE2	2.66	0.44
1:A:296:LYS:HE3	1:A:299:PRO:HG3	1.99	0.44
1:D:123:ARG:CG	1:D:124:SER:N	2.81	0.43
2:D:4400:FMN:H2'	2:D:4400:FMN:H9	2.00	0.43
1:C:169:HIS:HA	1:C:172:LYS:CE	2.47	0.43
1:B:262:TYR:CD1	1:B:263:ASN:N	2.86	0.43
1:B:263:ASN:ND2	1:C:299:PRO:HA	2.33	0.43
1:D:54:ILE:CG2	1:D:58:LYS:HD2	2.48	0.43
1:C:207:ARG:HA	1:C:289:ILE:O	2.18	0.43
1:C:102:PRO:HA	1:C:307:THR:HB	2.00	0.43
1:B:330:ARG:CB	1:B:330:ARG:HH21	2.32	0.43
1:A:125:SER:O	1:A:126:ALA:C	2.57	0.43
1:A:123:ARG:HG3	1:A:124:SER:N	2.27	0.43
1:B:272:LEU:HD23	1:B:272:LEU:N	2.33	0.43
1:C:77:THR:HB	1:C:78:PRO:CD	2.49	0.43
1:D:172:LYS:NZ	1:D:173:SER:HA	2.34	0.43
1:B:169:HIS:CD2	1:B:180:GLU:HB3	2.53	0.43
1:A:59:GLU:OE1	1:A:59:GLU:HA	2.18	0.43
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.84	0.43
1:C:308:ILE:HG12	1:C:309:ASP:H	1.84	0.43
1:D:106:ASP:H	1:D:123:ARG:NH2	2.17	0.43
1:D:300:SER:H	2:D:4400:FMN:C8M	2.30	0.43
2:B:2400:FMN:P	1:C:281:GLY:H	2.41	0.43
1:D:318:LEU:HD12	1:D:320:LYS:CE	2.38	0.43
1:C:265:LEU:HD22	1:C:265:LEU:H	1.84	0.43
1:B:261:GLU:O	1:B:275:ARG:NH1	2.52	0.43
1:A:235:GLU:HB2	1:D:235:GLU:HB2	2.00	0.43
1:D:221:LEU:O	1:D:283:MET:HA	2.18	0.43
1:C:47:GLN:HE22	1:C:60:ASP:CB	2.31	0.43
1:B:129:SER:O	1:B:133:VAL:HG23	2.19	0.43
1:B:262:TYR:O	1:B:263:ASN:O	2.37	0.42
1:A:45:ARG:HH22	1:A:336:GLU:CD	2.22	0.42
1:C:172:LYS:H	1:C:172:LYS:CD	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD22	2:A:1400:FMN:O2	2.18	0.42
1:B:117:ASP:OD1	1:B:118:PHE:N	2.52	0.42
1:D:21:ILE:CG2	1:D:83:ILE:HB	2.47	0.42
1:A:124:SER:O	1:A:126:ALA:N	2.53	0.42
1:A:142:LEU:C	1:A:142:LEU:HD23	2.39	0.42
1:D:299:PRO:HG2	2:D:4400:FMN:H4'	2.02	0.42
1:C:110:PHE:O	1:C:114:GLY:N	2.52	0.42
1:C:21:ILE:HG23	1:C:83:ILE:HB	2.02	0.42
1:D:233:ILE:O	1:D:237:MET:HG2	2.20	0.42
1:C:320:LYS:CD	1:C:320:LYS:H	2.32	0.42
1:D:106:ASP:OD1	1:D:123:ARG:NH2	2.50	0.42
1:B:300:SER:H	2:B:2400:FMN:C8M	2.32	0.42
1:C:169:HIS:HE1	1:C:183:GLU:OE2	2.02	0.42
1:D:35:ASP:CG	1:D:38:LEU:HB2	2.40	0.42
1:B:117:ASP:O	1:B:118:PHE:O	2.38	0.42
1:B:123:ARG:HG3	1:B:124:SER:N	2.34	0.42
1:D:322:ARG:CZ	1:D:322:ARG:HB2	2.49	0.42
1:D:19:ASP:HB2	1:D:85:ASN:O	2.20	0.42
1:C:47:GLN:HE22	1:C:60:ASP:CG	2.23	0.42
1:A:4:LEU:HB2	1:D:226:TYR:CD1	2.54	0.42
1:C:59:GLU:O	1:C:59:GLU:HG2	2.20	0.42
1:D:190:ILE:HD11	1:D:329:ILE:HD11	2.02	0.42
1:B:125:SER:O	1:B:126:ALA:HB3	2.19	0.42
1:C:317:CYS:O	1:C:317:CYS:SG	2.77	0.42
1:A:47:GLN:HE22	1:A:60:ASP:CB	2.32	0.42
1:A:170:ALA:O	1:A:176:PHE:HA	2.20	0.42
1:A:101:ARG:NH2	1:A:123:ARG:HE	2.18	0.42
1:B:265:LEU:N	1:B:265:LEU:HD12	2.35	0.42
1:D:106:ASP:N	1:D:123:ARG:NH2	2.68	0.41
1:B:250:LYS:HE3	1:B:253:GLU:HB3	2.02	0.41
1:A:96:ILE:O	1:A:99:LEU:HG	2.19	0.41
1:D:43:MET:O	1:D:46:ARG:HG2	2.19	0.41
1:C:240:LEU:HD22	2:C:3400:FMN:O2	2.19	0.41
1:D:197:HIS:HB3	1:D:302:PHE:HB3	2.03	0.41
1:A:225:LEU:HD13	1:D:128:GLU:CG	2.48	0.41
1:A:21:ILE:CG2	1:A:83:ILE:HB	2.50	0.41
1:C:99:LEU:HA	1:C:309:ASP:HA	2.01	0.41
1:A:169:HIS:CE1	1:A:172:LYS:HE3	2.56	0.41
1:C:20:VAL:HG22	1:C:84:HIS:ND1	2.35	0.41
1:B:39:LEU:O	1:B:43:MET:HG2	2.20	0.41
1:C:361:ILE:HD12	1:D:351:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:CG	1:A:172:LYS:HE3	2.56	0.41
1:C:54:ILE:O	1:C:55:THR:CB	2.67	0.41
1:C:53:PHE:O	1:C:54:ILE:C	2.58	0.41
1:A:54:ILE:CG2	1:A:55:THR:N	2.82	0.41
1:B:104:HIS:HB3	1:B:123:ARG:NH1	2.34	0.41
1:B:322:ARG:N	1:B:322:ARG:CD	2.84	0.41
1:B:208:ALA:HB3	1:B:289:ILE:HB	2.02	0.41
1:B:169:HIS:NE2	1:B:180:GLU:HB3	2.36	0.41
1:C:300:SER:HB3	2:C:3400:FMN:C8M	2.51	0.41
1:B:123:ARG:CG	1:B:124:SER:N	2.84	0.41
1:C:97:LYS:HB2	1:C:97:LYS:HZ2	1.85	0.41
1:B:250:LYS:HE3	1:B:253:GLU:CB	2.51	0.41
1:A:247:GLU:OE1	1:A:294:HIS:CE1	2.71	0.41
1:C:57:ARG:HG3	1:C:57:ARG:HH11	1.86	0.41
1:A:233:ILE:O	1:A:237:MET:HG2	2.20	0.41
1:C:50:ARG:HH12	2:C:3400:FMN:HM72	1.86	0.40
1:D:288:GLU:HG3	3:D:4520:HOH:O	2.20	0.40
1:A:175:ILE:HG21	1:A:190:ILE:HD12	2.04	0.40
1:C:360:THR:HG23	1:C:364:GLU:OE1	2.21	0.40
1:A:65:ILE:HD13	1:A:65:ILE:HG21	1.88	0.40
1:B:77:THR:HB	1:B:78:PRO:CD	2.52	0.40
1:A:362:TYR:CE2	1:B:347:VAL:HG13	2.56	0.40
1:C:38:LEU:HD23	1:C:38:LEU:O	2.20	0.40
1:B:330:ARG:HH21	1:B:330:ARG:HB3	1.86	0.40
1:C:60:ASP:O	1:C:62:LYS:HD2	2.22	0.40
1:C:318:LEU:O	1:C:320:LYS:HD2	2.21	0.40
1:C:53:PHE:N	1:C:53:PHE:CD1	2.89	0.40
1:B:247:GLU:HB2	1:B:292:ARG:HB2	2.04	0.40
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.85	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:OE1	1:D:89:ARG:NE[6_555]	1.85	0.35
1:B:272:LEU:CD2	1:B:272:LEU:CD2[2_655]	1.87	0.33
1:C:71:GLU:CB	1:D:89:ARG:NH2[6_555]	1.91	0.29
1:C:316:GLU:OE1	1:C:316:GLU:OE1[2_655]	1.98	0.22
1:C:71:GLU:OE1	1:D:89:ARG:CZ[6_555]	2.09	0.11

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	363/365 (100%)	327 (90%)	25 (7%)	11 (3%)	5	1
1	B	363/365 (100%)	323 (89%)	29 (8%)	11 (3%)	5	1
1	C	363/365 (100%)	321 (88%)	32 (9%)	10 (3%)	6	1
1	D	363/365 (100%)	336 (93%)	18 (5%)	9 (2%)	7	1
All	All	1452/1460 (100%)	1307 (90%)	104 (7%)	41 (3%)	6	1

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	95	ASN
1	A	116	ARG
1	A	123	ARG
1	A	125	SER
1	B	61	ASP
1	B	95	ASN
1	B	118	PHE
1	B	125	SER
1	B	262	TYR
1	B	263	ASN
1	B	271	PHE
1	C	54	ILE
1	C	55	THR
1	C	124	SER
1	C	125	SER
1	C	307	THR
1	D	124	SER
1	A	49	GLY
1	A	52	VAL
1	B	124	SER
1	C	61	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	56	PRO
1	D	92	ASP
1	D	118	PHE
1	D	125	SER
1	B	88	ALA
1	A	87	ARG
1	A	89	ARG
1	A	97	LYS
1	A	117	ASP
1	C	119	ARG
1	D	86	GLN
1	D	89	ARG
1	B	86	GLN
1	B	267	ASP
1	D	91	LYS
1	C	299	PRO
1	C	48	GLY
1	C	52	VAL
1	D	96	ILE

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	300/300 (100%)	290 (97%)	10 (3%)	45	32
1	B	300/300 (100%)	290 (97%)	10 (3%)	45	32
1	C	300/300 (100%)	290 (97%)	10 (3%)	45	32
1	D	300/300 (100%)	288 (96%)	12 (4%)	38	23
All	All	1200/1200 (100%)	1158 (96%)	42 (4%)	43	29

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	61	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89	ARG
1	A	93	TYR
1	A	103	SER
1	A	168	ASN
1	A	172	LYS
1	A	214	ASN
1	A	240	LEU
1	A	322	ARG
1	B	87	ARG
1	B	89	ARG
1	B	119	ARG
1	B	172	LYS
1	B	215	GLN
1	B	240	LEU
1	B	241	ASN
1	B	302	PHE
1	B	322	ARG
1	B	343	LEU
1	C	58	LYS
1	C	87	ARG
1	C	89	ARG
1	C	172	LYS
1	C	215	GLN
1	C	240	LEU
1	C	241	ASN
1	C	302	PHE
1	C	322	ARG
1	C	343	LEU
1	D	38	LEU
1	D	87	ARG
1	D	89	ARG
1	D	91	LYS
1	D	103	SER
1	D	118	PHE
1	D	123	ARG
1	D	168	ASN
1	D	172	LYS
1	D	215	GLN
1	D	240	LEU
1	D	322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	85	ASN
1	A	104	HIS
1	A	111	HIS
1	A	168	ASN
1	A	169	HIS
1	A	186	GLN
1	A	191	GLN
1	A	214	ASN
1	A	215	GLN
1	A	223	GLN
1	A	241	ASN
1	A	294	HIS
1	A	313	ASN
1	B	47	GLN
1	B	51	ASN
1	B	111	HIS
1	B	168	ASN
1	B	186	GLN
1	B	191	GLN
1	B	196	ASN
1	B	214	ASN
1	B	223	GLN
1	B	241	ASN
1	B	263	ASN
1	B	294	HIS
1	B	313	ASN
1	C	47	GLN
1	C	51	ASN
1	C	168	ASN
1	C	169	HIS
1	C	186	GLN
1	C	191	GLN
1	C	192	ASN
1	C	214	ASN
1	C	223	GLN
1	C	241	ASN
1	C	294	HIS
1	C	303	GLN
1	C	305	GLN
1	C	313	ASN
1	C	323	HIS
1	D	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	104	HIS
1	D	111	HIS
1	D	168	ASN
1	D	186	GLN
1	D	191	GLN
1	D	215	GLN
1	D	223	GLN
1	D	241	ASN
1	D	294	HIS

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](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	FMN	A	1400	-	32,33,33	2.13	11 (34%)	34,50,50	3.25	13 (38%)
2	FMN	B	2400	-	32,33,33	2.16	9 (28%)	34,50,50	3.25	14 (41%)
2	FMN	C	3400	-	32,33,33	2.12	11 (34%)	34,50,50	3.23	11 (32%)
2	FMN	D	4400	-	32,33,33	2.13	11 (34%)	34,50,50	3.23	13 (38%)

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
2	FMN	A	1400	-	-	0/18/18/18	0/3/3/3
2	FMN	B	2400	-	-	0/18/18/18	0/3/3/3
2	FMN	C	3400	-	-	0/18/18/18	0/3/3/3
2	FMN	D	4400	-	-	0/18/18/18	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3400	FMN	C9A-N10	-3.79	1.33	1.38
2	B	2400	FMN	C9A-N10	-3.27	1.34	1.38
2	D	4400	FMN	C9A-N10	-3.07	1.34	1.38
2	A	1400	FMN	C9A-N10	-3.05	1.34	1.38
2	A	1400	FMN	C2-N3	2.00	1.42	1.38
2	C	3400	FMN	C6-C7	2.05	1.43	1.37
2	C	3400	FMN	C2-N3	2.12	1.42	1.38
2	D	4400	FMN	C9A-C5A	2.12	1.47	1.42
2	D	4400	FMN	C2'-C3'	2.14	1.57	1.53
2	B	2400	FMN	P-O3P	2.14	1.62	1.54
2	D	4400	FMN	C2-N3	2.14	1.42	1.38
2	D	4400	FMN	P-O3P	2.15	1.62	1.54
2	A	1400	FMN	P-O3P	2.16	1.62	1.54
2	A	1400	FMN	C9A-C5A	2.20	1.47	1.42
2	A	1400	FMN	C4A-N5	2.26	1.36	1.33
2	C	3400	FMN	C5'-C4'	2.30	1.55	1.51
2	D	4400	FMN	C4A-N5	2.32	1.36	1.33
2	C	3400	FMN	C8-C7	2.39	1.47	1.41
2	D	4400	FMN	C8-C7	2.41	1.47	1.41
2	C	3400	FMN	P-O3P	2.41	1.63	1.54
2	B	2400	FMN	C8-C7	2.43	1.47	1.41
2	A	1400	FMN	C4-C4A	2.44	1.46	1.41
2	A	1400	FMN	C8-C7	2.47	1.47	1.41
2	A	1400	FMN	C5'-C4'	2.51	1.55	1.51
2	B	2400	FMN	C4-C4A	2.53	1.46	1.41
2	D	4400	FMN	C4-C4A	2.53	1.46	1.41
2	C	3400	FMN	C4-C4A	2.66	1.46	1.41
2	B	2400	FMN	C4A-N5	2.67	1.37	1.33
2	C	3400	FMN	C4A-N5	2.71	1.37	1.33
2	C	3400	FMN	C1'-N10	3.00	1.51	1.48
2	B	2400	FMN	C5'-C4'	3.20	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3400	FMN	C4A-C10	4.15	1.48	1.40
2	B	2400	FMN	C4A-C10	4.17	1.48	1.40
2	D	4400	FMN	C4A-C10	4.18	1.48	1.40
2	B	2400	FMN	C1'-N10	4.20	1.52	1.48
2	A	1400	FMN	C4A-C10	4.26	1.48	1.40
2	A	1400	FMN	C1'-N10	4.73	1.53	1.48
2	D	4400	FMN	C1'-N10	4.76	1.53	1.48
2	D	4400	FMN	C4-N3	6.00	1.43	1.33
2	B	2400	FMN	C4-N3	6.01	1.43	1.33
2	A	1400	FMN	C4-N3	6.03	1.43	1.33
2	C	3400	FMN	C4-N3	6.16	1.44	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3400	FMN	C4A-C4-N3	-6.59	114.90	123.52
2	A	1400	FMN	C4A-C4-N3	-6.52	115.00	123.52
2	D	4400	FMN	C4A-C4-N3	-6.51	115.01	123.52
2	B	2400	FMN	C4A-C4-N3	-6.43	115.12	123.52
2	C	3400	FMN	C4A-C10-N10	-6.24	115.98	120.52
2	B	2400	FMN	C4A-C10-N10	-5.60	116.45	120.52
2	D	4400	FMN	C4A-C10-N10	-5.36	116.62	120.52
2	A	1400	FMN	C4A-C10-N10	-5.28	116.69	120.52
2	B	2400	FMN	N3-C2-N1	-4.81	119.59	127.69
2	C	3400	FMN	N3-C2-N1	-4.80	119.60	127.69
2	A	1400	FMN	N3-C2-N1	-4.77	119.66	127.69
2	D	4400	FMN	N3-C2-N1	-4.77	119.66	127.69
2	C	3400	FMN	C9A-C5A-N5	-3.44	116.57	122.18
2	B	2400	FMN	C9A-C5A-N5	-3.31	116.80	122.18
2	A	1400	FMN	C9A-C5A-N5	-3.26	116.86	122.18
2	D	4400	FMN	C9A-C5A-N5	-3.25	116.89	122.18
2	B	2400	FMN	C4-C4A-C10	-2.48	118.35	119.94
2	A	1400	FMN	C4-C4A-C10	-2.41	118.40	119.94
2	C	3400	FMN	C4-C4A-C10	-2.39	118.41	119.94
2	D	4400	FMN	C9-C9A-C5A	-2.26	115.59	119.65
2	D	4400	FMN	C4-C4A-C10	-2.19	118.54	119.94
2	A	1400	FMN	C9-C9A-C5A	-2.18	115.73	119.65
2	B	2400	FMN	C9-C9A-C5A	-2.11	115.86	119.65
2	B	2400	FMN	C8M-C8-C9	-2.06	114.51	120.33
2	A	1400	FMN	C8M-C8-C9	-2.03	114.58	120.33
2	B	2400	FMN	O2P-P-O1P	2.11	117.51	110.63
2	D	4400	FMN	O2P-P-O1P	2.12	117.54	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2400	FMN	O4'-C4'-C3'	2.35	115.01	108.96
2	A	1400	FMN	O4'-C4'-C3'	2.52	115.44	108.96
2	C	3400	FMN	O4'-C4'-C3'	2.54	115.49	108.96
2	D	4400	FMN	O4'-C4'-C3'	2.63	115.73	108.96
2	C	3400	FMN	C4A-N5-C5A	3.05	120.32	116.72
2	A	1400	FMN	C4A-N5-C5A	3.16	120.45	116.72
2	B	2400	FMN	C4A-N5-C5A	3.26	120.56	116.72
2	C	3400	FMN	C1'-N10-C9A	3.27	122.62	118.83
2	D	4400	FMN	C4A-N5-C5A	3.40	120.73	116.72
2	B	2400	FMN	C1'-N10-C9A	3.80	123.23	118.83
2	C	3400	FMN	C6-C5A-C9A	4.00	123.53	119.11
2	B	2400	FMN	C6-C5A-C9A	4.09	123.62	119.11
2	D	4400	FMN	C6-C5A-C9A	4.28	123.83	119.11
2	D	4400	FMN	C1'-N10-C9A	4.31	123.83	118.83
2	A	1400	FMN	C6-C5A-C9A	4.36	123.91	119.11
2	A	1400	FMN	C1'-N10-C9A	4.44	123.98	118.83
2	C	3400	FMN	C5A-C9A-N10	6.36	122.35	117.58
2	D	4400	FMN	C5A-C9A-N10	6.63	122.55	117.58
2	A	1400	FMN	C5A-C9A-N10	6.77	122.65	117.58
2	B	2400	FMN	C5A-C9A-N10	6.92	122.76	117.58
2	D	4400	FMN	C4-N3-C2	10.84	124.20	115.16
2	A	1400	FMN	C4-N3-C2	10.88	124.24	115.16
2	B	2400	FMN	C4-N3-C2	10.94	124.29	115.16
2	C	3400	FMN	C4-N3-C2	11.09	124.41	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1400	FMN	4	0
2	B	2400	FMN	7	0
2	C	3400	FMN	3	0
2	D	4400	FMN	6	0

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, 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	365/365 (100%)	1.32	52 (14%) 4 6	16, 26, 116, 158	9 (2%)
1	B	365/365 (100%)	2.17	104 (28%) 1 0	20, 36, 129, 154	9 (2%)
1	C	365/365 (100%)	2.79	103 (28%) 1 0	19, 34, 147, 162	9 (2%)
1	D	365/365 (100%)	1.07	52 (14%) 4 6	17, 28, 100, 134	9 (2%)
All	All	1460/1460 (100%)	1.84	311 (21%) 1 1	16, 30, 130, 162	36 (2%)

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	CYS	29.1
1	C	307	THR	29.0
1	C	301	ILE	26.5
1	C	302	PHE	24.9
1	B	121	GLY	22.9
1	C	88	ALA	22.3
1	C	305	GLN	22.1
1	B	53	PHE	21.9
1	B	270	GLY	21.7
1	B	271	PHE	21.7
1	A	53	PHE	20.9
1	B	272	LEU	20.5
1	C	121	GLY	20.1
1	A	88	ALA	18.6
1	B	265	LEU	18.5
1	B	118	PHE	17.7
1	C	99	LEU	17.4
1	C	317	CYS	17.2
1	D	121	GLY	17.0
1	C	118	PHE	16.7
1	A	55	THR	16.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	16.5
1	B	88	ALA	16.4
1	A	93	TYR	16.1
1	C	303	GLN	16.0
1	A	52	VAL	15.6
1	B	52	VAL	15.3
1	D	89	ARG	15.3
1	B	56	PRO	15.2
1	C	52	VAL	15.0
1	C	314	GLU	14.5
1	B	51	ASN	14.5
1	A	120	GLY	14.5
1	C	120	GLY	13.9
1	B	54	ILE	13.1
1	C	54	ILE	13.1
1	A	56	PRO	13.0
1	D	87	ARG	13.0
1	C	90	SER	13.0
1	C	304	PRO	12.9
1	A	50	ARG	12.9
1	A	119	ARG	12.8
1	C	89	ARG	12.8
1	C	101	ARG	12.8
1	C	102	PRO	12.7
1	C	56	PRO	12.6
1	B	266	MET	12.5
1	C	93	TYR	12.4
1	D	90	SER	12.3
1	C	96	ILE	12.2
1	C	103	SER	12.1
1	C	98	ASN	12.0
1	C	119	ARG	12.0
1	B	90	SER	11.9
1	B	93	TYR	11.9
1	C	86	GLN	11.5
1	C	58	LYS	11.5
1	A	51	ASN	11.4
1	A	58	LYS	11.4
1	C	318	LEU	11.2
1	A	49	GLY	11.2
1	A	89	ARG	11.1
1	D	88	ALA	11.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	55	THR	10.9
1	A	91	LYS	10.8
1	C	95	ASN	10.7
1	C	87	ARG	10.6
1	A	92	ASP	10.5
1	B	57	ARG	10.5
1	C	309	ASP	10.5
1	B	263	ASN	10.4
1	C	320	LYS	10.3
1	C	49	GLY	10.3
1	B	120	GLY	10.3
1	C	321	GLY	10.3
1	B	87	ARG	10.1
1	A	95	ASN	10.1
1	D	119	ARG	10.0
1	C	92	ASP	10.0
1	D	91	LYS	9.9
1	C	300	SER	9.8
1	B	264	ASP	9.8
1	C	97	LYS	9.7
1	A	57	ARG	9.7
1	D	123	ARG	9.7
1	C	308	ILE	9.5
1	A	60	ASP	9.4
1	B	49	GLY	9.4
1	C	213	THR	9.4
1	C	310	ILE	9.2
1	A	365	ASN	9.1
1	D	56	PRO	9.1
1	D	93	TYR	9.1
1	D	59	GLU	9.0
1	C	59	GLU	8.9
1	D	57	ARG	8.8
1	C	311	ASN	8.8
1	C	57	ARG	8.8
1	A	118	PHE	8.7
1	C	91	LYS	8.7
1	C	124	SER	8.7
1	C	313	ASN	8.7
1	D	58	LYS	8.7
1	B	268	GLN	8.7
1	B	119	ARG	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	92	ASP	8.6
1	D	122	GLY	8.6
1	B	273	SER	8.5
1	C	319	LEU	8.4
1	C	322	ARG	8.4
1	B	214	ASN	8.4
1	D	365	ASN	8.4
1	C	122	GLY	8.3
1	B	60	ASP	8.2
1	C	214	ASN	8.2
1	C	104	HIS	8.2
1	C	55	THR	8.2
1	C	100	PHE	8.2
1	D	120	GLY	8.1
1	B	50	ARG	8.0
1	C	123	ARG	7.9
1	B	58	LYS	7.9
1	A	121	GLY	7.9
1	A	123	ARG	7.9
1	B	89	ARG	7.7
1	D	60	ASP	7.5
1	C	105	ALA	7.4
1	C	306	ARG	7.4
1	B	123	ARG	7.2
1	A	86	GLN	7.2
1	C	269	LYS	7.1
1	C	53	PHE	7.1
1	C	94	ASP	7.0
1	B	116	ARG	6.8
1	D	92	ASP	6.8
1	B	267	ASP	6.8
1	B	86	GLN	6.7
1	B	302	PHE	6.7
1	C	272	LEU	6.7
1	B	61	ASP	6.5
1	C	312	GLY	6.5
1	D	96	ILE	6.5
1	C	365	ASN	6.4
1	A	87	ARG	6.3
1	C	51	ASN	6.3
1	A	94	ASP	6.3
1	B	315	CYS	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	59	GLU	6.3
1	B	313	ASN	6.2
1	B	365	ASN	6.2
1	B	269	LYS	6.1
1	A	96	ILE	6.1
1	D	118	PHE	6.1
1	A	124	SER	6.0
1	B	213	THR	6.0
1	D	115	ILE	6.0
1	A	90	SER	6.0
1	D	94	ASP	6.0
1	D	124	SER	5.9
1	D	95	ASN	5.9
1	C	50	ARG	5.8
1	A	17	HIS	5.8
1	C	17	HIS	5.8
1	B	322	ARG	5.8
1	A	117	ASP	5.8
1	C	267	ASP	5.8
1	D	49	GLY	5.7
1	B	94	ASP	5.7
1	D	97	LYS	5.6
1	B	91	LYS	5.5
1	B	97	LYS	5.4
1	B	17	HIS	5.4
1	B	122	GLY	5.4
1	B	321	GLY	5.4
1	A	122	GLY	5.3
1	B	85	ASN	5.3
1	C	316	GLU	5.2
1	D	321	GLY	5.1
1	C	323	HIS	5.0
1	A	85	ASN	4.9
1	C	48	GLY	4.8
1	B	309	ASP	4.8
1	B	59	GLU	4.8
1	A	115	ILE	4.7
1	D	364	GLU	4.7
1	B	96	ILE	4.7
1	C	85	ASN	4.7
1	C	268	GLN	4.7
1	D	116	ARG	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	125	SER	4.6
1	B	319	LEU	4.6
1	C	270	GLY	4.5
1	B	95	ASN	4.5
1	C	60	ASP	4.5
1	B	312	GLY	4.5
1	C	211	ILE	4.4
1	D	322	ARG	4.4
1	D	55	THR	4.4
1	B	172	LYS	4.3
1	B	320	LYS	4.3
1	A	19	ASP	4.3
1	D	86	GLN	4.2
1	B	318	LEU	4.2
1	D	19	ASP	4.1
1	D	125	SER	4.1
1	C	19	ASP	4.0
1	C	20	VAL	4.0
1	B	98	ASN	3.9
1	C	61	ASP	3.9
1	C	116	ARG	3.8
1	A	214	ASN	3.7
1	A	322	ARG	3.7
1	B	306	ARG	3.7
1	D	17	HIS	3.7
1	C	172	LYS	3.7
1	D	320	LYS	3.6
1	D	302	PHE	3.6
1	B	62	LYS	3.6
1	B	300	SER	3.6
1	D	85	ASN	3.5
1	D	117	ASP	3.5
1	A	116	ARG	3.5
1	B	212	LYS	3.5
1	C	106	ASP	3.5
1	A	364	GLU	3.5
1	B	307	THR	3.5
1	B	308	ILE	3.4
1	D	318	LEU	3.4
1	B	341	LEU	3.4
1	B	168	ASN	3.3
1	A	241	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	125	SER	3.3
1	A	125	SER	3.2
1	A	126	ALA	3.2
1	A	320	LYS	3.2
1	A	224	GLY	3.2
1	B	126	ALA	3.2
1	D	172	LYS	3.2
1	B	19	ASP	3.1
1	C	109	TYR	3.1
1	B	48	GLY	3.1
1	C	299	PRO	3.1
1	C	215	GLN	3.1
1	B	124	SER	3.1
1	B	21	ILE	3.1
1	B	301	ILE	3.0
1	C	62	LYS	3.0
1	C	115	ILE	3.0
1	B	99	LEU	3.0
1	B	115	ILE	3.0
1	B	311	ASN	2.9
1	C	212	LYS	2.9
1	B	174	GLU	2.8
1	A	47	GLN	2.8
1	B	164	ASN	2.8
1	C	110	PHE	2.7
1	D	61	ASP	2.7
1	B	310	ILE	2.7
1	C	197	HIS	2.7
1	C	271	PHE	2.7
1	C	15	GLU	2.7
1	B	317	CYS	2.6
1	B	197	HIS	2.6
1	B	334	VAL	2.6
1	B	240	LEU	2.6
1	A	61	ASP	2.6
1	D	126	ALA	2.6
1	D	180	GLU	2.6
1	D	168	ASN	2.6
1	D	70	PHE	2.5
1	D	224	GLY	2.5
1	A	97	LYS	2.5
1	D	40	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	110	PHE	2.5
1	C	180	GLU	2.5
1	B	338	LEU	2.5
1	A	62	LYS	2.5
1	B	262	TYR	2.4
1	D	50	ARG	2.4
1	B	100	PHE	2.4
1	C	107	PHE	2.4
1	B	44	LYS	2.4
1	B	314	GLU	2.4
1	B	47	GLN	2.4
1	B	206	ILE	2.4
1	B	180	GLU	2.3
1	B	323	HIS	2.3
1	A	321	GLY	2.3
1	A	334	VAL	2.3
1	B	15	GLU	2.3
1	C	273	SER	2.3
1	B	364	GLU	2.2
1	D	54	ILE	2.2
1	D	327	ILE	2.2
1	C	298	THR	2.2
1	C	114	GLY	2.2
1	B	327	ILE	2.2
1	B	316	GLU	2.2
1	B	163	LYS	2.1
1	C	161	LYS	2.1
1	A	318	LEU	2.1
1	B	102	PRO	2.1
1	C	47	GLN	2.1
1	C	184	GLU	2.1
1	C	327	ILE	2.1
1	B	304	PRO	2.1
1	B	72	ASP	2.1
1	B	117	ASP	2.1
1	C	168	ASN	2.1
1	D	306	ARG	2.0
1	C	343	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FMN	B	2400	31/31	0.45	0.40	1.94	62,69,82,82	0
2	FMN	C	3400	31/31	0.36	0.58	1.43	71,73,87,87	0
2	FMN	D	4400	31/31	0.61	0.29	0.96	45,61,70,71	0
2	FMN	A	1400	31/31	0.66	0.30	0.67	30,57,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.