



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2016 – 04:38 PM EDT

PDB ID : 1YCG
Title : X-ray Structures of Moorella thermoacetica FprA. Novel Diiron Site Structure and Mechanistic Insights into a Scavenging Nitric Oxide Reductase
Authors : Silaghi-Dumitrescu, R.; Kurtz, D.M.; Lanzilotta, W.N.
Deposited on : 2004-12-22
Resolution : 2.80 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-20027939
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-20027939

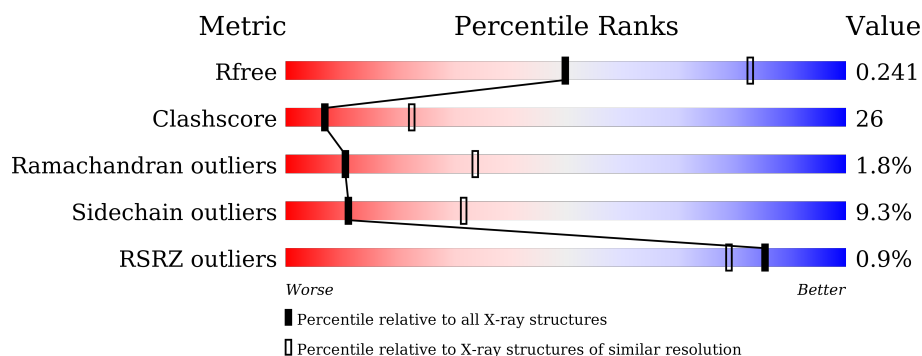
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	398	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>8%</div> </div> </div>
1	B	398	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>7%</div> </div> </div>
1	C	398	<div> <div></div> <div> <div>63%</div> <div>33%</div> </div> </div>
1	D	398	<div> <div></div> <div> <div>58%</div> <div>34%</div> <div>7%</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
3	FEO	A	501	-	-	X	-
3	FEO	B	511	-	-	X	-
3	FEO	D	531	-	-	X	-
4	EDO	A	602	-	-	X	X
4	EDO	B	612	-	-	X	X
4	EDO	C	622	-	-	X	X
4	EDO	D	632	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12758 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.

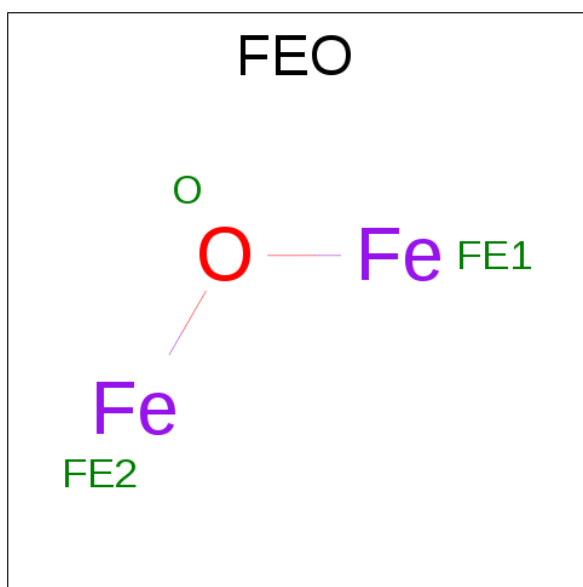
- Molecule 1 is a protein called Nitric oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	B	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	C	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			
1	D	398	Total	C	N	O	S	0	0	0
			3115	2006	525	572	12			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

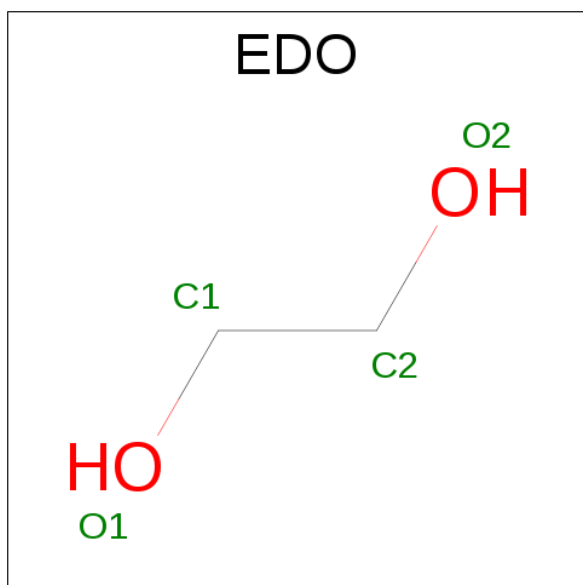
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Zn	0	0
			4	4		
2	A	4	Total	Zn	0	0
			4	4		
2	D	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



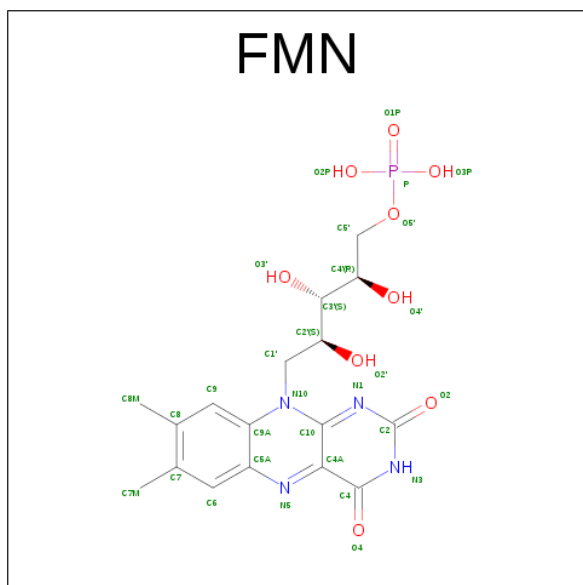
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	O	0	0
			3	2	1		
3	B	1	Total	Fe	O	0	0
			3	2	1		
3	C	1	Total	Fe	O	0	0
			3	2	1		
3	D	1	Total	Fe	O	0	0
			3	2	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



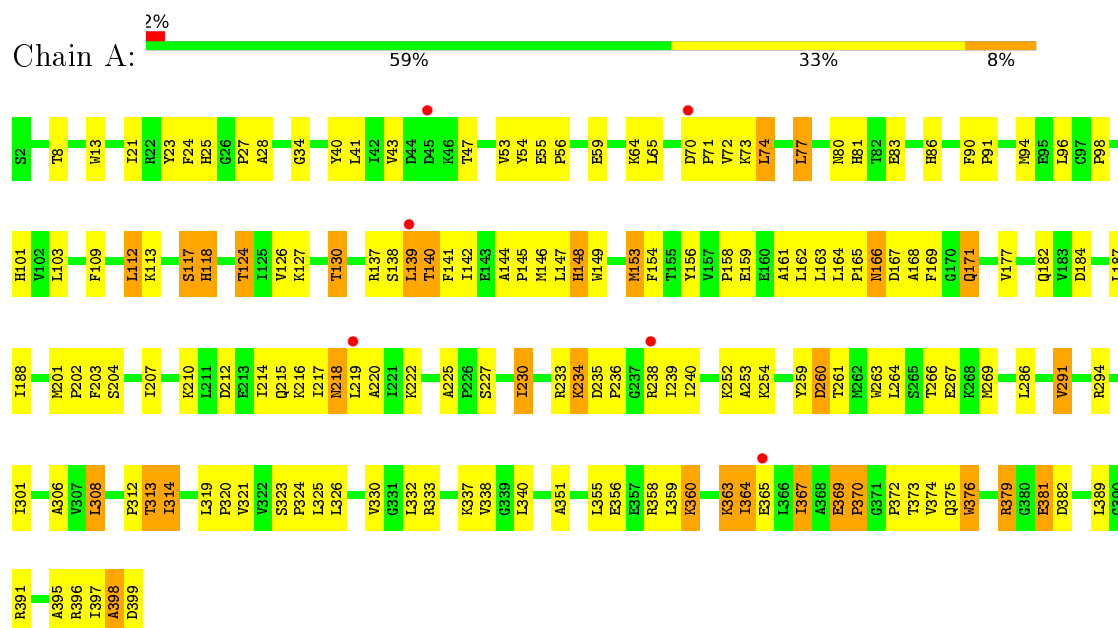
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	40	Total	O	0	0
			40	40		
6	D	35	Total	O	0	0
			35	35		

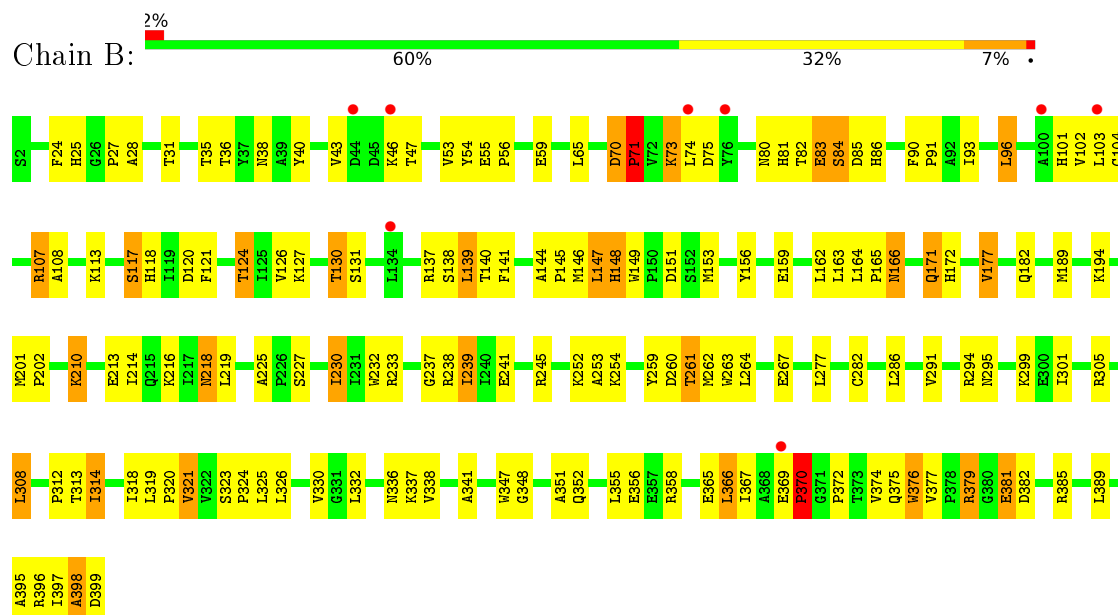
3 Residue-property plots

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

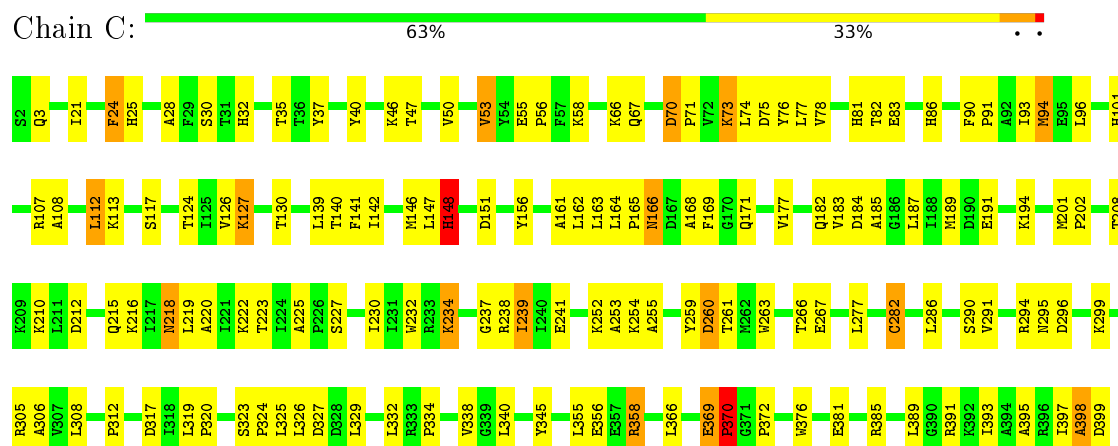
• Molecule 1: Nitric oxide reductase



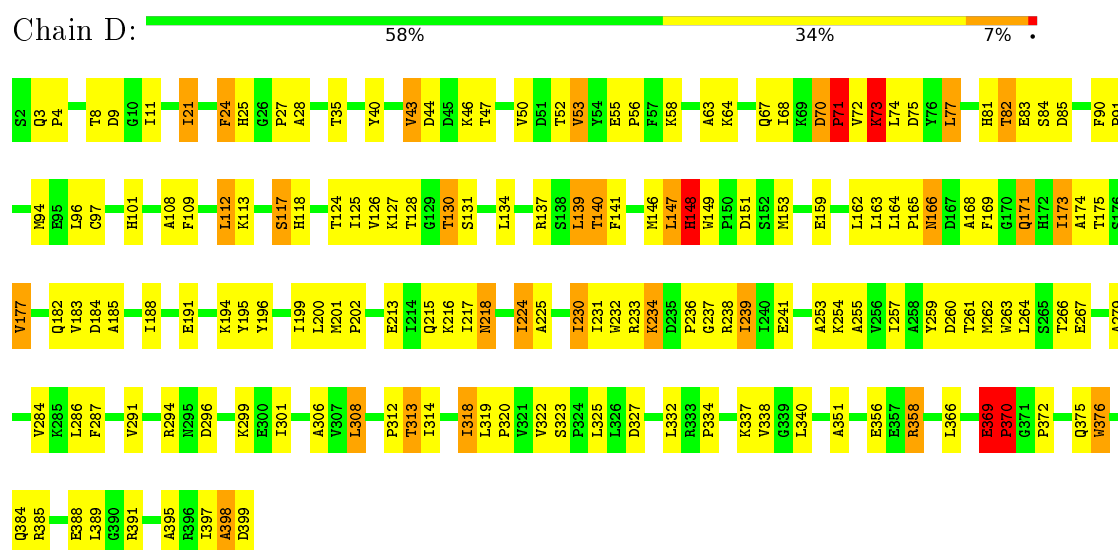
• Molecule 1: Nitric oxide reductase



- Molecule 1: Nitric oxide reductase



- Molecule 1: Nitric oxide reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.68Å 159.68Å 278.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.80 49.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.71-2.80) 99.9 (49.71-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.245 0.223 , 0.241	Depositor DCC
R_{free} test set	4459 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12758	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.55	2/3189 (0.1%)	0.82	7/4335 (0.2%)
1	B	0.50	0/3189	0.85	5/4335 (0.1%)
1	C	0.51	0/3189	0.90	7/4335 (0.2%)
1	D	0.54	1/3189 (0.0%)	0.88	7/4335 (0.2%)
All	All	0.53	3/12756 (0.0%)	0.86	26/17340 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SER	C-N	-8.93	1.13	1.34
1	D	73	LYS	C-O	-7.57	1.08	1.23
1	A	118	HIS	C-O	-7.39	1.09	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ASP	C-N-CD	-21.72	72.82	120.60
1	B	70	ASP	C-N-CD	-21.59	73.09	120.60
1	C	70	ASP	C-N-CD	-21.08	74.22	120.60
1	C	369	GLU	C-N-CD	-16.98	83.25	120.60
1	C	70	ASP	C-N-CA	13.71	179.60	122.00
1	A	70	ASP	C-N-CD	-12.88	92.27	120.60
1	B	70	ASP	C-N-CA	11.26	169.30	122.00
1	A	369	GLU	C-N-CD	-10.44	97.62	120.60
1	D	70	ASP	C-N-CA	9.90	163.58	122.00
1	D	369	GLU	C-N-CD	-9.58	99.52	120.60
1	B	71	PRO	CA-N-CD	-8.71	99.31	111.50
1	A	118	HIS	CA-C-N	-8.62	98.25	117.20
1	A	70	ASP	C-N-CA	8.51	157.76	122.00
1	A	118	HIS	CA-C-O	5.81	132.29	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	370	PRO	N-CA-C	-5.63	97.46	112.10
1	C	370	PRO	CA-N-CD	-5.54	103.74	111.50
1	D	71	PRO	CA-N-CD	-5.42	103.91	111.50
1	B	84	SER	N-CA-CB	-5.40	102.40	110.50
1	D	73	LYS	O-C-N	-5.32	114.18	122.70
1	B	117	SER	N-CA-C	5.30	125.31	111.00
1	D	369	GLU	N-CA-C	-5.30	96.69	111.00
1	A	369	GLU	N-CA-C	-5.26	96.80	111.00
1	A	117	SER	N-CA-C	5.25	125.18	111.00
1	D	370	PRO	CA-N-CD	-5.12	104.33	111.50
1	C	139	LEU	CA-CB-CG	5.09	127.01	115.30
1	C	369	GLU	CB-CA-C	5.08	120.56	110.40

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	3115	0	3130	187	0
1	B	3115	0	3131	170	0
1	C	3115	0	3131	144	0
1	D	3115	0	3131	184	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	3	0	0	4	0
3	B	3	0	0	5	0
3	C	3	0	0	1	0
3	D	3	0	0	2	0
4	A	4	0	6	8	0
4	B	4	0	6	12	0
4	C	4	0	6	9	0
4	D	4	0	6	12	0
5	A	31	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	19	2	0
5	C	31	0	19	2	0
5	D	31	0	19	0	0
6	A	31	0	0	3	0
6	B	26	0	0	6	0
6	C	40	0	0	6	3
6	D	35	0	0	5	1
All	All	12758	0	12623	664	3

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 26.

All (664) 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:24:PHE:CE1	4:B:612:EDO:H11	1.50	1.44
1:A:24:PHE:CE1	4:A:602:EDO:H11	1.56	1.40
1:B:24:PHE:HE1	4:B:612:EDO:C1	1.53	1.21
1:A:261:THR:HG22	1:A:266:THR:HB	1.18	1.12
1:A:24:PHE:HE1	4:A:602:EDO:C1	1.65	1.09
1:A:369:GLU:HB3	1:A:370:PRO:HD2	1.28	1.08
1:B:381:GLU:CD	1:B:381:GLU:H	1.59	1.06
1:A:234:LYS:HE3	1:A:234:LYS:HA	1.38	1.06
1:A:314:ILE:HD11	1:A:319:LEU:HA	1.37	1.05
1:D:85:ASP:CG	4:D:632:EDO:H12	1.77	1.05
1:B:314:ILE:HD11	1:B:319:LEU:HA	1.41	1.01
1:A:381:GLU:CD	1:A:381:GLU:H	1.66	0.98
1:C:234:LYS:HE3	1:C:234:LYS:HA	1.44	0.97
1:B:171:GLN:HE22	1:B:230:ILE:H	0.98	0.96
1:A:379:ARG:HG3	1:A:381:GLU:OE2	1.67	0.95
1:B:369:GLU:HG3	1:B:370:PRO:HD2	1.49	0.95
1:C:56:PRO:HA	6:C:759:HOH:O	1.67	0.94
1:A:369:GLU:CB	1:A:370:PRO:HD2	1.96	0.94
1:D:101:HIS:HE1	1:D:124:THR:OG1	1.51	0.93
1:A:333:ARG:HH11	1:A:363:LYS:HZ3	0.97	0.93
1:A:171:GLN:HE22	1:A:230:ILE:H	1.14	0.93
1:D:261:THR:HG22	1:D:266:THR:HB	1.49	0.92
1:D:259:TYR:HE2	1:D:286:LEU:HD21	1.31	0.92
1:A:294:ARG:NH1	1:B:320:PRO:HB2	1.85	0.92
1:D:369:GLU:HB3	1:D:370:PRO:HD2	1.52	0.91
1:D:24:PHE:CE1	4:D:632:EDO:H11	2.05	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:HA	1:B:47:THR:HG22	1.51	0.91
1:A:127:LYS:O	1:A:130:THR:HG23	1.72	0.90
1:C:127:LYS:O	1:C:130:THR:HG22	1.72	0.90
1:A:320:PRO:HG2	1:B:294:ARG:HH12	1.36	0.89
1:D:171:GLN:HE22	1:D:230:ILE:H	0.94	0.88
1:D:171:GLN:HE22	1:D:230:ILE:N	1.72	0.87
1:B:202:PRO:HG3	1:B:332:LEU:HA	1.53	0.87
1:A:391:ARG:HH11	1:A:391:ARG:HG3	1.38	0.87
1:D:318:ILE:CD1	1:D:322:VAL:HB	2.05	0.87
1:A:320:PRO:HG2	1:B:294:ARG:NH1	1.90	0.86
1:D:85:ASP:OD1	4:D:632:EDO:H12	1.76	0.85
1:C:261:THR:CG2	1:C:266:THR:HB	2.07	0.84
1:B:305:ARG:HB3	1:B:397:ILE:HD12	1.59	0.84
1:C:320:PRO:HB2	1:D:294:ARG:NH1	1.92	0.84
1:D:109:PHE:CE2	1:D:113:LYS:HE2	2.11	0.84
1:D:369:GLU:CB	1:D:370:PRO:HD2	2.06	0.84
1:D:306:ALA:HB2	1:D:397:ILE:HD11	1.58	0.84
1:D:262:MET:HE3	1:D:314:ILE:HD12	1.57	0.83
1:D:127:LYS:O	1:D:130:THR:HG23	1.78	0.83
1:C:3:GLN:HE22	1:C:67:GLN:HE22	1.27	0.83
1:C:58:LYS:HE2	6:C:760:HOH:O	1.79	0.82
1:A:24:PHE:CE1	4:A:602:EDO:C1	2.51	0.82
1:A:261:THR:CG2	1:A:266:THR:HB	2.07	0.82
1:B:127:LYS:H	1:B:130:THR:CG2	1.93	0.82
1:B:314:ILE:HD11	1:B:319:LEU:CA	2.09	0.81
1:D:118:HIS:NE2	6:D:762:HOH:O	1.87	0.81
1:D:259:TYR:CE2	1:D:286:LEU:HD21	2.14	0.81
1:D:306:ALA:CB	1:D:397:ILE:HD11	2.11	0.80
1:C:3:GLN:NE2	1:C:67:GLN:HE22	1.80	0.80
3:A:501:FEO:O	4:A:602:EDO:H12	1.81	0.79
1:A:314:ILE:HD11	1:A:319:LEU:CA	2.12	0.79
1:D:171:GLN:NE2	1:D:230:ILE:H	1.77	0.79
1:A:333:ARG:HH11	1:A:363:LYS:NZ	1.80	0.79
1:B:313:THR:HG22	1:B:351:ALA:CB	2.13	0.78
1:A:259:TYR:HE2	1:A:286:LEU:HD21	1.48	0.78
1:A:202:PRO:HG3	1:A:332:LEU:HA	1.64	0.78
1:D:188:ILE:HD11	1:D:230:ILE:HB	1.66	0.78
1:C:259:TYR:HE2	1:C:286:LEU:HD21	1.47	0.77
1:A:308:LEU:HD13	1:A:340:LEU:HB3	1.64	0.77
1:B:381:GLU:N	1:B:381:GLU:CD	2.29	0.77
1:D:8:THR:HG23	1:D:11:ILE:HD13	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ILE:HD13	1:D:319:LEU:N	2.00	0.77
1:B:171:GLN:HE22	1:B:230:ILE:N	1.80	0.77
1:D:318:ILE:HD11	1:D:322:VAL:HB	1.66	0.76
1:C:294:ARG:NH1	1:D:320:PRO:HB2	2.01	0.76
3:C:521:FEO:O	4:C:622:EDO:H12	1.85	0.76
1:C:101:HIS:HE1	1:C:124:THR:OG1	1.68	0.75
1:C:202:PRO:HG3	1:C:332:LEU:HA	1.68	0.75
1:D:234:LYS:HA	1:D:234:LYS:HE3	1.67	0.75
1:A:90:PHE:HB3	1:A:91:PRO:HD3	1.68	0.74
1:D:261:THR:CG2	1:D:266:THR:HB	2.16	0.74
1:D:43:VAL:HA	1:D:47:THR:HG22	1.68	0.74
1:B:313:THR:HG22	1:B:351:ALA:HB3	1.68	0.74
1:C:126:VAL:HG13	1:C:130:THR:CG2	2.18	0.74
1:D:308:LEU:HD13	1:D:340:LEU:HB3	1.70	0.73
1:C:83:GLU:CD	4:C:622:EDO:O1	2.26	0.73
1:C:372:PRO:HG3	1:C:389:LEU:HD12	1.70	0.73
1:D:173:ILE:CD1	1:D:175:THR:HG23	2.19	0.73
1:A:381:GLU:N	1:A:381:GLU:CD	2.41	0.72
1:B:103:LEU:HD23	1:B:124:THR:HG23	1.71	0.72
1:B:83:GLU:OE1	4:B:612:EDO:O1	2.08	0.72
1:B:82:THR:O	1:B:83:GLU:O	2.06	0.72
1:A:127:LYS:H	1:A:130:THR:CG2	2.02	0.72
1:B:24:PHE:CE1	4:B:612:EDO:C1	2.43	0.72
1:A:98:PRO:HB2	1:D:279:ALA:O	1.89	0.72
1:B:372:PRO:HG3	1:B:389:LEU:CD1	2.20	0.72
1:C:320:PRO:CB	1:D:294:ARG:NH1	2.54	0.71
1:D:113:LYS:O	1:D:117:SER:HB3	1.91	0.71
1:D:25:HIS:HB2	1:D:28:ALA:HB3	1.72	0.71
1:B:127:LYS:O	1:B:130:THR:HG23	1.90	0.70
1:C:237:GLY:O	1:C:241:GLU:HG3	1.92	0.70
1:D:77:LEU:HD12	1:D:94:MET:HE3	1.72	0.70
1:A:113:LYS:O	1:A:117:SER:HB3	1.92	0.70
1:A:127:LYS:H	1:A:130:THR:HG21	1.57	0.70
1:D:128:THR:O	6:D:734:HOH:O	2.09	0.70
1:C:369:GLU:HB3	1:C:370:PRO:HD2	1.75	0.69
1:C:381:GLU:OE1	1:C:381:GLU:N	2.22	0.69
1:C:77:LEU:HD13	1:C:94:MET:HE1	1.75	0.69
1:D:82:THR:HG22	1:D:112:LEU:HD13	1.74	0.68
1:B:113:LYS:O	1:B:117:SER:HB3	1.93	0.68
1:C:90:PHE:HB3	1:C:91:PRO:HD3	1.76	0.68
1:A:379:ARG:CG	1:A:381:GLU:OE2	2.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:H	1:B:130:THR:HG21	1.56	0.68
1:C:177:VAL:HG22	1:C:182:GLN:OE1	1.94	0.68
1:B:107:ARG:NH1	1:B:107:ARG:HB3	2.09	0.68
1:B:80:ASN:HD22	1:B:153:MET:HG3	1.59	0.68
1:A:369:GLU:HB3	1:A:370:PRO:CD	2.16	0.67
1:D:73:LYS:O	1:D:73:LYS:CD	2.42	0.67
1:D:372:PRO:HG3	1:D:389:LEU:CD1	2.24	0.67
1:A:72:VAL:HB	1:A:96:LEU:HD11	1.77	0.67
1:B:117:SER:O	1:B:118:HIS:HD2	1.77	0.67
1:C:261:THR:HG23	1:C:266:THR:HB	1.76	0.67
1:A:379:ARG:HG2	1:A:382:ASP:OD2	1.94	0.66
1:D:127:LYS:H	1:D:130:THR:CG2	2.09	0.66
1:A:118:HIS:CE1	6:A:729:HOH:O	2.47	0.66
1:A:359:LEU:HD22	1:A:364:ILE:HG21	1.76	0.66
1:A:25:HIS:CD2	4:A:602:EDO:HO1	2.02	0.66
1:A:367:ILE:HD12	1:A:367:ILE:O	1.96	0.66
1:A:25:HIS:CD2	4:A:602:EDO:O1	2.46	0.65
1:D:82:THR:CG2	1:D:112:LEU:HD13	2.26	0.65
1:A:294:ARG:HH12	1:B:320:PRO:HB2	1.55	0.65
1:C:261:THR:HG22	1:C:266:THR:HB	1.76	0.65
3:D:531:FEO:O	4:D:632:EDO:C2	2.44	0.65
1:A:398:ALA:O	1:A:399:ASP:CB	2.43	0.65
1:C:185:ALA:HB1	1:C:238:ARG:NH1	2.12	0.65
1:D:259:TYR:HE2	1:D:286:LEU:CD2	2.06	0.65
1:C:372:PRO:HG3	1:C:389:LEU:CD1	2.27	0.65
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.61	0.65
1:B:372:PRO:HG3	1:B:389:LEU:HD13	1.78	0.65
3:B:511:FEO:O	4:B:612:EDO:H12	1.96	0.65
1:C:296:ASP:OD2	6:C:723:HOH:O	2.15	0.65
1:C:113:LYS:O	1:C:117:SER:HB3	1.96	0.64
1:C:47:THR:HG23	6:C:724:HOH:O	1.96	0.64
1:A:365:GLU:OE2	1:A:396:ARG:NH2	2.31	0.64
1:A:259:TYR:CE2	1:A:286:LEU:HD21	2.31	0.64
1:D:202:PRO:HG3	1:D:332:LEU:HA	1.79	0.64
3:D:531:FEO:O	4:D:632:EDO:H22	1.98	0.64
1:B:59:GLU:OE2	6:B:736:HOH:O	2.15	0.64
1:D:201:MET:HE3	1:D:334:PRO:HG3	1.79	0.64
1:D:164:LEU:HD23	1:D:225:ALA:HB3	1.80	0.64
1:B:366:LEU:N	1:B:366:LEU:HD23	2.12	0.63
3:B:511:FEO:O	4:B:612:EDO:C1	2.45	0.63
1:B:85:ASP:OD2	4:B:612:EDO:H12	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:THR:HG22	5:C:721:FMN:O1P	1.97	0.63
1:B:338:VAL:HG11	1:B:367:ILE:HD13	1.81	0.63
1:A:391:ARG:NH1	1:A:391:ARG:HG3	2.04	0.63
1:B:263:TRP:O	1:B:264:LEU:HB2	1.99	0.63
1:D:55:GLU:HB3	1:D:56:PRO:HD3	1.80	0.63
1:B:90:PHE:HB3	1:B:91:PRO:HD3	1.80	0.63
1:B:259:TYR:HE2	1:B:286:LEU:HD21	1.63	0.63
1:B:372:PRO:CG	1:B:389:LEU:HD13	2.29	0.63
1:B:313:THR:CG2	1:B:351:ALA:H	2.12	0.63
1:A:372:PRO:HG3	1:A:389:LEU:CD1	2.28	0.62
1:C:294:ARG:NH1	1:D:320:PRO:CB	2.62	0.62
1:D:24:PHE:CE1	4:D:632:EDO:C1	2.79	0.62
1:A:340:LEU:HD11	1:A:372:PRO:HD3	1.82	0.62
1:A:72:VAL:CG1	1:A:74:LEU:HD13	2.29	0.62
1:C:127:LYS:H	1:C:130:THR:CG2	2.12	0.62
1:B:381:GLU:HG2	1:B:385:ARG:HH21	1.65	0.62
1:C:185:ALA:HB1	1:C:238:ARG:HH12	1.64	0.62
1:B:171:GLN:NE2	1:B:230:ILE:H	1.83	0.62
1:C:320:PRO:HB2	1:D:294:ARG:HH12	1.65	0.62
3:A:501:FEO:O	4:A:602:EDO:C1	2.48	0.62
1:C:164:LEU:HD23	1:C:225:ALA:HB3	1.82	0.62
1:C:25:HIS:HB2	1:C:28:ALA:HB3	1.81	0.61
1:D:356:GLU:HG2	1:D:366:LEU:HD13	1.81	0.61
1:A:81:HIS:HE1	1:A:149:TRP:HB2	1.66	0.61
1:C:259:TYR:CE2	1:C:286:LEU:HD21	2.33	0.61
1:D:262:MET:CE	1:D:314:ILE:HD12	2.30	0.61
1:D:3:GLN:HE22	1:D:67:GLN:HE22	1.47	0.61
1:B:70:ASP:OD1	1:B:71:PRO:HD3	2.01	0.61
1:B:365:GLU:OE2	1:B:396:ARG:NH2	2.32	0.61
1:C:369:GLU:CB	1:C:370:PRO:HD2	2.27	0.60
1:D:3:GLN:NE2	1:D:67:GLN:HE22	1.98	0.60
1:B:126:VAL:HG11	1:B:141:PHE:CG	2.36	0.60
1:B:201:MET:HB3	1:B:202:PRO:HD3	1.83	0.60
1:C:127:LYS:H	1:C:130:THR:HG21	1.66	0.60
1:D:108:ALA:HB2	1:D:151:ASP:HB2	1.83	0.60
1:A:77:LEU:HD12	1:A:94:MET:CE	2.32	0.60
1:C:305:ARG:HB2	1:C:397:ILE:HG23	1.83	0.60
1:D:126:VAL:HG11	1:D:141:PHE:CG	2.37	0.60
1:A:372:PRO:HG3	1:A:389:LEU:HD13	1.83	0.60
1:D:96:LEU:HD13	1:D:96:LEU:O	2.01	0.60
1:B:141:PHE:HB3	1:B:153:MET:CE	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HG13	1:C:130:THR:HG23	1.83	0.60
1:C:3:GLN:HE22	1:C:67:GLN:NE2	1.97	0.60
1:D:90:PHE:HB3	1:D:91:PRO:HD3	1.84	0.60
1:B:117:SER:O	1:B:118:HIS:CD2	2.55	0.60
1:C:305:ARG:HB3	1:C:397:ILE:HD12	1.82	0.60
1:A:139:LEU:HD13	1:A:141:PHE:CZ	2.37	0.59
1:D:11:ILE:HD11	1:D:137:ARG:CZ	2.31	0.59
1:A:81:HIS:CE1	1:A:149:TRP:HB2	2.38	0.59
1:A:86:HIS:CE1	1:A:227:SER:HB2	2.37	0.59
1:D:318:ILE:HD11	1:D:322:VAL:CB	2.32	0.59
1:C:126:VAL:HG11	1:C:141:PHE:CG	2.38	0.59
1:B:369:GLU:CG	1:B:370:PRO:HD2	2.27	0.59
1:A:177:VAL:HG11	1:A:182:GLN:HB2	1.85	0.59
1:A:40:TYR:CZ	1:A:225:ALA:HB1	2.37	0.59
1:A:171:GLN:NE2	1:A:230:ILE:H	1.95	0.59
1:B:82:THR:C	1:B:83:GLU:O	2.40	0.59
1:D:312:PRO:HD2	1:D:319:LEU:HD22	1.84	0.59
1:A:72:VAL:CB	1:A:96:LEU:HD11	2.32	0.59
1:D:194:LYS:HB2	1:D:299:LYS:HD3	1.84	0.59
1:C:369:GLU:HG2	1:C:370:PRO:HD3	1.85	0.58
1:D:73:LYS:O	1:D:73:LYS:HD3	2.02	0.58
1:A:126:VAL:HG13	1:A:130:THR:OG1	2.03	0.58
1:D:72:VAL:HB	1:D:96:LEU:CD1	2.34	0.58
1:B:46:LYS:HA	1:B:75:ASP:OD2	2.02	0.58
1:A:294:ARG:NH1	1:B:320:PRO:CB	2.64	0.58
1:B:202:PRO:HG3	1:B:332:LEU:CA	2.31	0.58
1:D:56:PRO:HA	6:D:766:HOH:O	2.02	0.58
1:A:177:VAL:CG1	1:A:182:GLN:HB2	2.34	0.58
1:C:66:LYS:HE2	6:C:730:HOH:O	2.03	0.57
1:A:263:TRP:O	1:A:264:LEU:HB2	2.03	0.57
1:A:313:THR:HG22	1:A:351:ALA:HB3	1.87	0.57
1:A:77:LEU:HD12	1:A:94:MET:HE1	1.86	0.57
1:A:101:HIS:NE2	1:A:124:THR:HG22	2.19	0.57
1:A:103:LEU:HD23	1:A:124:THR:HG23	1.86	0.57
1:A:234:LYS:CE	1:A:234:LYS:HA	2.21	0.57
1:B:25:HIS:HB2	1:B:28:ALA:HB3	1.86	0.57
1:B:120:ASP:OD1	6:B:732:HOH:O	2.17	0.57
1:D:25:HIS:CB	1:D:28:ALA:HB3	2.34	0.57
1:D:232:TRP:CZ2	1:D:239:ILE:HG13	2.39	0.57
1:C:177:VAL:HG21	1:C:182:GLN:HB3	1.86	0.56
1:C:252:LYS:O	1:C:305:ARG:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD23	1:B:308:LEU:N	2.19	0.56
1:B:314:ILE:CD1	1:B:319:LEU:HA	2.27	0.56
1:A:109:PHE:O	1:A:113:LYS:HG2	2.05	0.56
1:B:28:ALA:O	1:B:294:ARG:NH2	2.38	0.56
1:A:333:ARG:NH1	1:A:363:LYS:HZ3	1.83	0.56
1:B:313:THR:HG22	1:B:351:ALA:H	1.69	0.56
1:A:261:THR:HG21	1:A:267:GLU:H	1.71	0.56
1:C:369:GLU:CB	1:C:370:PRO:CD	2.82	0.56
1:D:127:LYS:H	1:D:130:THR:HG21	1.70	0.56
1:A:149:TRP:CZ2	6:B:730:HOH:O	2.59	0.56
1:C:210:LYS:HE3	1:C:210:LYS:HA	1.87	0.56
1:C:55:GLU:HB3	1:C:56:PRO:HD3	1.86	0.56
1:A:21:ILE:HG23	1:A:34:GLY:HA2	1.86	0.56
1:D:213:GLU:HA	1:D:216:LYS:HE3	1.87	0.56
1:B:237:GLY:O	1:B:241:GLU:HG3	2.06	0.55
1:B:305:ARG:CB	1:B:397:ILE:HD12	2.32	0.55
1:C:381:GLU:HG2	1:C:385:ARG:NH2	2.22	0.55
1:B:101:HIS:NE2	1:B:124:THR:HG22	2.21	0.55
1:C:232:TRP:CZ2	1:C:239:ILE:HG13	2.42	0.55
1:C:189:MET:HE3	1:C:238:ARG:NE	2.20	0.55
1:C:323:SER:HB3	1:D:323:SER:HB3	1.87	0.55
1:B:305:ARG:HB2	1:B:397:ILE:HG23	1.87	0.55
1:D:188:ILE:HD11	1:D:230:ILE:CB	2.35	0.55
1:D:85:ASP:OD2	4:D:632:EDO:H12	2.06	0.55
1:D:191:GLU:HA	1:D:191:GLU:OE1	2.07	0.55
1:D:318:ILE:HD13	1:D:319:LEU:H	1.70	0.55
1:A:333:ARG:HD2	1:A:363:LYS:CE	2.36	0.55
1:D:101:HIS:CE1	1:D:124:THR:OG1	2.44	0.55
1:C:156:TYR:CE2	1:C:219:LEU:HD22	2.42	0.55
1:C:24:PHE:CE1	4:C:622:EDO:H11	2.41	0.55
1:A:314:ILE:HG12	1:A:319:LEU:CD1	2.37	0.55
1:A:306:ALA:HB2	1:A:397:ILE:HD11	1.89	0.55
1:A:55:GLU:HB3	1:A:56:PRO:HD3	1.89	0.55
1:C:163:LEU:HG	1:C:165:PRO:HG3	1.88	0.55
1:A:171:GLN:HE22	1:A:230:ILE:N	1.95	0.54
1:B:214:ILE:HG23	1:B:219:LEU:HD12	1.88	0.54
1:B:301:ILE:O	1:B:337:LYS:HE3	2.07	0.54
1:B:126:VAL:HG13	1:B:130:THR:HG23	1.90	0.54
1:D:398:ALA:O	1:D:399:ASP:CB	2.55	0.54
1:B:326:LEU:HD11	1:B:355:LEU:HD23	1.89	0.54
1:D:8:THR:CG2	1:D:11:ILE:HD13	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:O	1:D:67:GLN:HG3	2.08	0.54
1:B:338:VAL:CG1	1:B:367:ILE:HD13	2.37	0.54
1:D:72:VAL:HB	1:D:96:LEU:HD11	1.89	0.54
1:A:161:ALA:HB1	1:A:220:ALA:O	2.08	0.54
1:B:367:ILE:HD11	1:B:396:ARG:HD3	1.88	0.54
1:C:398:ALA:O	1:C:399:ASP:CB	2.56	0.54
1:D:173:ILE:HD13	1:D:174:ALA:N	2.23	0.54
1:A:146:MET:C	1:A:148:HIS:H	2.12	0.53
1:B:356:GLU:HG2	1:B:366:LEU:CD1	2.38	0.53
1:D:113:LYS:O	1:D:117:SER:CB	2.56	0.53
1:B:70:ASP:OD1	1:B:71:PRO:CD	2.57	0.53
1:C:81:HIS:CD2	1:C:166:ASN:HD21	2.25	0.53
1:A:25:HIS:HE2	4:A:602:EDO:C1	2.13	0.53
1:C:254:LYS:HG2	1:C:255:ALA:N	2.23	0.53
1:A:118:HIS:HD1	1:D:388:GLU:CD	2.11	0.53
1:A:165:PRO:O	1:A:166:ASN:HB3	2.08	0.53
1:B:210:LYS:HE2	1:B:213:GLU:OE2	2.09	0.53
1:C:40:TYR:CZ	1:C:225:ALA:HB1	2.44	0.53
1:C:312:PRO:HD2	1:C:319:LEU:HD22	1.89	0.53
1:D:44:ASP:H	1:D:47:THR:HG22	1.73	0.53
1:B:127:LYS:O	1:B:130:THR:CG2	2.55	0.53
1:D:73:LYS:NZ	1:D:73:LYS:HB2	2.24	0.53
1:C:28:ALA:O	1:C:294:ARG:NH2	2.42	0.53
1:C:25:HIS:NE2	4:C:622:EDO:O2	2.41	0.52
1:D:177:VAL:HG21	1:D:182:GLN:HB3	1.91	0.52
1:D:286:LEU:HD23	1:D:287:PHE:N	2.24	0.52
1:B:286:LEU:C	1:B:286:LEU:HD23	2.30	0.52
1:D:257:ILE:HD13	1:D:284:VAL:HG13	1.91	0.52
1:A:375:GLN:O	1:A:376:TRP:HB2	2.10	0.52
1:D:372:PRO:HG3	1:D:389:LEU:HD12	1.89	0.52
1:A:210:LYS:HA	1:A:210:LYS:HE3	1.92	0.52
1:C:329:LEU:HD22	1:C:334:PRO:HG2	1.92	0.52
1:D:24:PHE:CE1	4:D:632:EDO:H21	2.45	0.52
1:B:259:TYR:CE2	1:B:286:LEU:HD21	2.43	0.52
1:A:320:PRO:CG	1:B:294:ARG:NH1	2.67	0.52
1:A:398:ALA:O	1:A:399:ASP:HB2	2.07	0.52
1:B:146:MET:C	1:B:148:HIS:H	2.13	0.52
1:C:21:ILE:HG21	1:C:35:THR:HG22	1.92	0.52
1:D:146:MET:C	1:D:148:HIS:H	2.13	0.52
1:D:71:PRO:HD2	1:D:71:PRO:O	2.08	0.52
1:D:85:ASP:OD2	4:D:632:EDO:H22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:HE2	1:A:286:LEU:CD2	2.20	0.52
1:A:321:VAL:HG21	1:B:27:PRO:CB	2.38	0.52
1:C:340:LEU:HD11	1:C:372:PRO:HD3	1.92	0.52
1:D:173:ILE:HD11	1:D:175:THR:HG23	1.91	0.52
1:D:318:ILE:HD12	1:D:322:VAL:HB	1.88	0.52
1:A:323:SER:HB3	1:B:323:SER:HB3	1.91	0.52
1:B:102:VAL:HG12	1:B:104:CYS:SG	2.49	0.52
1:C:146:MET:C	1:C:148:HIS:H	2.12	0.52
1:C:308:LEU:HD22	1:C:340:LEU:HB3	1.92	0.52
1:D:215:GLN:HA	1:D:215:GLN:OE1	2.10	0.52
1:B:81:HIS:CE1	1:B:149:TRP:HB2	2.45	0.52
1:A:164:LEU:HD23	1:A:225:ALA:HB3	1.91	0.51
1:A:214:ILE:HG23	1:A:219:LEU:HD12	1.92	0.51
1:D:296:ASP:OD2	6:D:741:HOH:O	2.18	0.51
1:A:326:LEU:HD11	1:A:355:LEU:HD23	1.92	0.51
1:C:398:ALA:O	1:C:399:ASP:HB3	2.10	0.51
1:C:46:LYS:HA	1:C:75:ASP:OD2	2.10	0.51
1:D:391:ARG:HH11	1:D:391:ARG:HG3	1.76	0.51
1:B:379:ARG:HG3	1:B:382:ASP:OD2	2.11	0.51
1:B:156:TYR:CZ	1:B:219:LEU:HD22	2.44	0.51
1:C:194:LYS:HB2	1:C:299:LYS:HD3	1.91	0.51
1:D:21:ILE:HG21	1:D:35:THR:HG22	1.91	0.51
1:D:185:ALA:HB1	1:D:238:ARG:NH1	2.25	0.51
1:D:257:ILE:CD1	1:D:284:VAL:HG13	2.41	0.51
1:D:3:GLN:CD	1:D:67:GLN:HE22	2.14	0.51
1:B:261:THR:HG21	1:B:267:GLU:HB2	1.92	0.51
1:D:40:TYR:CZ	1:D:225:ALA:HB1	2.46	0.51
1:C:3:GLN:OE1	1:C:67:GLN:NE2	2.43	0.51
1:C:77:LEU:HD13	1:C:94:MET:CE	2.39	0.51
1:D:259:TYR:CD1	1:D:260:ASP:N	2.78	0.51
1:B:194:LYS:HB2	1:B:299:LYS:HD3	1.92	0.51
1:B:395:ALA:O	1:B:398:ALA:HB2	2.10	0.51
1:B:262:MET:CE	5:B:711:FMN:HM83	2.41	0.51
1:A:137:ARG:HA	1:A:159:GLU:HG2	1.93	0.51
1:B:189:MET:HE3	1:B:238:ARG:HD3	1.92	0.51
1:B:277:LEU:O	1:B:282:CYS:HB3	2.10	0.51
1:C:25:HIS:NE2	4:C:622:EDO:O1	2.41	0.51
1:A:72:VAL:HB	1:A:96:LEU:CD1	2.41	0.50
1:A:118:HIS:ND1	1:D:388:GLU:OE1	2.42	0.50
1:A:306:ALA:CB	1:A:397:ILE:HD11	2.40	0.50
1:C:358:ARG:NH2	1:D:327:ASP:OD2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:ND2	1:A:167:ASP:H	2.08	0.50
1:D:384:GLN:O	1:D:388:GLU:HG3	2.12	0.50
1:C:77:LEU:CD1	1:C:94:MET:HE1	2.42	0.50
1:D:127:LYS:H	1:D:130:THR:HG23	1.75	0.50
1:D:257:ILE:HD13	1:D:284:VAL:CG1	2.42	0.50
1:D:73:LYS:CG	1:D:73:LYS:O	2.59	0.50
1:D:46:LYS:HA	1:D:75:ASP:OD2	2.12	0.50
1:B:381:GLU:HG2	1:B:385:ARG:NH2	2.27	0.50
1:C:305:ARG:CB	1:C:397:ILE:HD12	2.41	0.50
1:D:177:VAL:HG22	1:D:182:GLN:CD	2.32	0.50
1:B:137:ARG:HA	1:B:159:GLU:CD	2.32	0.50
1:D:131:SER:OG	1:D:140:THR:HB	2.12	0.50
1:A:203:PHE:O	1:A:207:ILE:HG12	2.11	0.50
3:B:511:FEO:O	4:B:612:EDO:C2	2.60	0.50
1:D:398:ALA:O	1:D:399:ASP:HB3	2.12	0.50
1:A:291:VAL:CG1	1:A:291:VAL:O	2.60	0.50
1:C:73:LYS:HE2	1:C:73:LYS:HA	1.94	0.50
1:A:379:ARG:HH11	1:A:382:ASP:CG	2.15	0.49
1:D:11:ILE:HD12	1:D:11:ILE:N	2.27	0.49
1:D:306:ALA:HB3	1:D:397:ILE:HD11	1.92	0.49
1:D:224:ILE:HG13	1:D:236:PRO:HB3	1.94	0.49
1:D:24:PHE:CZ	4:D:632:EDO:H11	2.47	0.49
1:D:366:LEU:HD12	1:D:369:GLU:OE1	2.12	0.49
1:D:24:PHE:HE1	4:D:632:EDO:H21	1.77	0.49
1:B:81:HIS:HE1	1:B:149:TRP:HB2	1.78	0.49
1:D:173:ILE:C	1:D:173:ILE:HD13	2.33	0.49
1:D:356:GLU:HG2	1:D:366:LEU:CD1	2.43	0.49
1:A:330:VAL:O	1:A:333:ARG:NE	2.46	0.49
1:B:164:LEU:HD23	1:B:225:ALA:HB3	1.93	0.49
1:D:301:ILE:O	1:D:337:LYS:HE3	2.13	0.49
1:B:126:VAL:HG13	1:B:130:THR:CG2	2.43	0.49
1:D:3:GLN:OE1	1:D:67:GLN:NE2	2.46	0.49
1:A:365:GLU:CD	1:A:396:ARG:HH22	2.17	0.49
1:B:25:HIS:CB	1:B:28:ALA:HB3	2.43	0.49
1:C:108:ALA:HB2	1:C:151:ASP:HB2	1.93	0.49
1:A:142:ILE:HD11	1:A:219:LEU:HD11	1.95	0.49
1:D:183:VAL:HG12	1:D:184:ASP:N	2.28	0.49
1:D:261:THR:HG21	1:D:267:GLU:H	1.78	0.49
1:A:80:ASN:HD22	1:A:153:MET:CG	2.25	0.48
1:C:294:ARG:HH11	1:D:320:PRO:CB	2.24	0.48
1:A:146:MET:C	1:A:148:HIS:N	2.66	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ALA:HB3	1:B:352:GLN:NE2	2.28	0.48
1:C:86:HIS:CE1	1:C:227:SER:HB2	2.49	0.48
1:A:139:LEU:HD13	1:A:141:PHE:HZ	1.79	0.48
1:A:83:GLU:OE2	3:A:501:FEO:O	2.30	0.48
1:B:163:LEU:HG	1:B:165:PRO:HG3	1.96	0.48
1:A:72:VAL:CG2	1:A:96:LEU:HD11	2.43	0.48
1:A:25:HIS:HB2	1:A:28:ALA:HB3	1.94	0.48
1:A:261:THR:HG21	1:A:267:GLU:N	2.28	0.48
1:A:372:PRO:CG	1:A:389:LEU:HD13	2.41	0.48
1:D:58:LYS:HE2	6:D:763:HOH:O	2.14	0.48
1:A:140:THR:HG23	1:A:156:TYR:HB3	1.96	0.48
1:A:163:LEU:O	1:A:165:PRO:HD3	2.13	0.48
1:A:333:ARG:HD2	1:A:363:LYS:HG3	1.95	0.48
1:B:101:HIS:CD2	1:B:124:THR:HG22	2.48	0.48
1:C:306:ALA:HA	1:C:338:VAL:O	2.14	0.48
1:B:305:ARG:HD2	1:B:397:ILE:HG23	1.96	0.48
1:D:188:ILE:HD13	1:D:230:ILE:HG21	1.96	0.48
1:C:25:HIS:CE1	4:C:622:EDO:O2	2.67	0.48
1:A:301:ILE:O	1:A:337:LYS:HE3	2.14	0.48
1:C:261:THR:HG21	1:C:267:GLU:H	1.79	0.48
1:B:398:ALA:O	1:B:399:ASP:CB	2.61	0.47
1:B:144:ALA:N	1:B:145:PRO:HD3	2.29	0.47
1:B:263:TRP:O	1:B:264:LEU:CB	2.62	0.47
1:D:82:THR:C	1:D:83:GLU:O	2.52	0.47
1:B:146:MET:C	1:B:148:HIS:N	2.67	0.47
1:C:259:TYR:HE2	1:C:286:LEU:CD2	2.22	0.47
1:D:237:GLY:O	1:D:241:GLU:HG3	2.15	0.47
1:C:294:ARG:HH12	1:D:320:PRO:HB2	1.78	0.47
1:D:385:ARG:HD2	1:D:385:ARG:HA	1.81	0.47
1:B:294:ARG:HH21	1:B:295:ASN:HD21	1.62	0.47
1:D:81:HIS:CE1	1:D:149:TRP:HB2	2.49	0.47
1:B:141:PHE:CD2	1:B:153:MET:CE	2.97	0.47
1:C:146:MET:C	1:C:148:HIS:N	2.67	0.47
1:C:216:LYS:C	1:C:218:ASN:N	2.67	0.47
1:D:163:LEU:HG	1:D:165:PRO:HG3	1.96	0.47
1:B:291:VAL:CG1	1:B:291:VAL:O	2.63	0.47
1:B:326:LEU:O	1:B:330:VAL:HG23	2.14	0.47
1:A:263:TRP:O	1:A:264:LEU:CB	2.63	0.47
1:B:31:THR:HG22	1:B:172:HIS:HB3	1.97	0.47
1:A:216:LYS:C	1:A:218:ASN:N	2.69	0.47
1:B:85:ASP:CG	4:B:612:EDO:H12	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:TRP:CZ2	1:B:239:ILE:HG12	2.50	0.47
1:D:147:LEU:HD12	1:D:147:LEU:HA	1.44	0.47
1:C:393:ILE:O	1:C:397:ILE:HG12	2.15	0.46
1:A:291:VAL:O	1:A:291:VAL:HG13	2.15	0.46
1:B:323:SER:HB2	1:B:324:PRO:HD3	1.98	0.46
1:A:314:ILE:CD1	1:A:319:LEU:HA	2.28	0.46
1:B:141:PHE:HB3	1:B:153:MET:HE2	1.96	0.46
1:C:82:THR:HG22	1:C:112:LEU:HD13	1.98	0.46
1:A:321:VAL:HG21	1:B:27:PRO:HB2	1.98	0.46
1:A:391:ARG:NH1	1:A:391:ARG:CG	2.76	0.46
1:A:72:VAL:HG21	1:A:96:LEU:HD11	1.97	0.46
1:B:55:GLU:HB3	1:B:56:PRO:HD3	1.97	0.46
1:C:70:ASP:OD2	1:C:70:ASP:C	2.54	0.46
1:B:102:VAL:HG21	1:B:121:PHE:CD2	2.51	0.46
1:B:314:ILE:CD1	1:B:318:ILE:O	2.64	0.46
1:C:212:ASP:O	1:C:215:GLN:HB3	2.15	0.46
1:B:139:LEU:HD13	1:B:141:PHE:CZ	2.50	0.46
1:B:253:ALA:HB2	1:B:399:ASP:HB2	1.98	0.46
1:B:252:LYS:O	1:B:254:LYS:N	2.47	0.46
1:C:25:HIS:CB	1:C:28:ALA:HB3	2.46	0.46
1:A:163:LEU:HG	1:A:165:PRO:HG3	1.98	0.46
1:D:196:TYR:HA	1:D:200:LEU:HD12	1.98	0.46
1:A:103:LEU:CD2	1:A:124:THR:HG23	2.47	0.45
1:B:120:ASP:CG	6:B:732:HOH:O	2.54	0.45
1:B:141:PHE:HD2	1:B:153:MET:HE2	1.81	0.45
1:B:24:PHE:HE1	4:B:612:EDO:H11	0.58	0.45
1:B:375:GLN:O	1:B:376:TRP:HB2	2.16	0.45
1:C:253:ALA:HB2	1:C:399:ASP:HB2	1.98	0.45
1:C:25:HIS:HE2	4:C:622:EDO:C1	2.29	0.45
1:C:30:SER:H	1:C:295:ASN:ND2	2.13	0.45
1:D:146:MET:C	1:D:148:HIS:N	2.68	0.45
1:D:254:LYS:HG2	1:D:255:ALA:N	2.31	0.45
1:B:96:LEU:HD13	1:B:96:LEU:O	2.16	0.45
1:C:76:TYR:CD1	1:C:101:HIS:HB3	2.51	0.45
1:B:138:SER:N	1:B:159:GLU:OE1	2.40	0.45
1:B:35:THR:OG1	1:B:36:THR:N	2.49	0.45
1:B:141:PHE:CD2	1:B:153:MET:HE1	2.51	0.45
1:B:216:LYS:C	1:B:218:ASN:N	2.68	0.45
1:C:82:THR:CG2	1:C:112:LEU:HD13	2.46	0.45
1:C:323:SER:HB2	1:C:324:PRO:HD3	1.99	0.45
1:C:90:PHE:CE1	1:C:94:MET:HE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:GLN:HE22	1:D:67:GLN:NE2	2.15	0.45
1:A:113:LYS:NZ	6:A:705:HOH:O	2.50	0.45
1:B:40:TYR:CZ	1:B:225:ALA:HB1	2.51	0.45
1:D:188:ILE:CD1	1:D:230:ILE:HG21	2.46	0.45
1:D:372:PRO:CG	1:D:389:LEU:CD1	2.95	0.45
1:A:27:PRO:HG2	1:B:321:VAL:HG21	1.99	0.45
1:D:294:ARG:HE	1:D:294:ARG:HB3	1.46	0.45
1:A:59:GLU:H	1:A:59:GLU:CD	2.20	0.45
1:D:81:HIS:HE1	1:D:149:TRP:HB2	1.82	0.45
1:A:269:MET:CE	1:A:374:VAL:HB	2.47	0.45
1:B:107:ARG:HA	1:B:107:ARG:HH11	1.81	0.45
1:B:314:ILE:HD11	1:B:319:LEU:N	2.31	0.45
1:A:188:ILE:HA	1:A:188:ILE:HD12	1.87	0.44
1:A:259:TYR:CD1	1:A:260:ASP:N	2.85	0.44
1:A:306:ALA:HA	1:A:338:VAL:O	2.17	0.44
1:A:13:TRP:CZ3	1:A:64:LYS:HE2	2.52	0.44
1:B:38:ASN:HB2	1:B:227:SER:HA	1.99	0.44
1:B:85:ASP:OD1	3:B:511:FEO:O	2.36	0.44
1:D:201:MET:N	1:D:202:PRO:CD	2.80	0.44
1:A:127:LYS:H	1:A:130:THR:HG23	1.79	0.44
1:A:159:GLU:H	1:A:159:GLU:CD	2.21	0.44
1:B:107:ARG:HB3	1:B:107:ARG:HH11	1.82	0.44
1:B:54:TYR:CD2	1:B:56:PRO:HD2	2.53	0.44
1:C:326:LEU:HD11	1:C:355:LEU:HD23	2.00	0.44
1:D:159:GLU:H	1:D:159:GLU:CD	2.20	0.44
1:D:261:THR:HG22	1:D:266:THR:CB	2.33	0.44
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.49	0.44
1:A:216:LYS:C	1:A:218:ASN:H	2.20	0.44
1:B:53:VAL:CG1	1:B:54:TYR:N	2.80	0.44
1:A:333:ARG:HD3	1:A:333:ARG:HA	1.75	0.44
1:A:308:LEU:CD1	1:A:340:LEU:HB3	2.40	0.44
1:B:367:ILE:CD1	1:B:396:ARG:HH11	2.30	0.44
1:B:73:LYS:HE2	1:B:73:LYS:HA	1.99	0.44
1:D:168:ALA:O	1:D:169:PHE:HB2	2.17	0.44
1:D:397:ILE:O	1:D:397:ILE:HG22	2.15	0.44
1:A:333:ARG:HD2	1:A:363:LYS:HE2	1.99	0.44
1:A:53:VAL:CG1	1:A:54:TYR:N	2.81	0.44
1:A:72:VAL:HG12	1:A:74:LEU:HD13	1.99	0.44
1:B:177:VAL:HG22	1:B:182:GLN:CD	2.38	0.44
1:C:184:ASP:OD2	1:C:187:LEU:HD13	2.18	0.44
1:A:149:TRP:CH2	6:B:730:HOH:O	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HG22	1:A:158:PRO:HD3	1.99	0.44
1:A:379:ARG:NH1	1:A:382:ASP:OD1	2.51	0.44
1:B:165:PRO:O	1:B:166:ASN:HB3	2.17	0.44
1:B:379:ARG:HB2	1:B:381:GLU:OE2	2.17	0.44
1:B:83:GLU:HG2	1:B:84:SER:H	1.83	0.44
1:A:156:TYR:CE2	1:A:219:LEU:HD22	2.53	0.44
1:A:395:ALA:O	1:A:398:ALA:HB2	2.18	0.44
1:B:347:TRP:CD1	1:B:348:GLY:N	2.86	0.44
1:C:77:LEU:HD11	1:C:93:ILE:HG21	1.99	0.44
1:A:184:ASP:CG	1:A:187:LEU:HD13	2.38	0.44
1:A:83:GLU:CD	3:A:501:FEO:O	2.56	0.44
1:B:291:VAL:O	1:B:291:VAL:HG13	2.17	0.44
1:C:177:VAL:HG21	1:C:182:GLN:CB	2.47	0.44
1:C:32:HIS:NE2	6:C:723:HOH:O	2.36	0.44
1:D:232:TRP:CZ2	1:D:239:ILE:CG1	3.01	0.44
1:D:395:ALA:O	1:D:398:ALA:HB2	2.17	0.44
1:C:320:PRO:CB	1:D:294:ARG:HH12	2.24	0.43
1:D:217:ILE:O	1:D:217:ILE:HG22	2.18	0.43
1:A:234:LYS:HE3	1:A:234:LYS:CA	2.28	0.43
1:A:252:LYS:O	1:A:254:LYS:N	2.49	0.43
1:C:261:THR:HG22	1:C:266:THR:CB	2.44	0.43
1:D:306:ALA:HA	1:D:338:VAL:O	2.18	0.43
1:D:73:LYS:HE3	1:D:73:LYS:O	2.18	0.43
1:A:101:HIS:CD2	1:A:124:THR:HG22	2.53	0.43
1:A:81:HIS:HE1	1:A:149:TRP:CG	2.36	0.43
1:C:3:GLN:CD	1:C:67:GLN:HE22	2.22	0.43
1:D:183:VAL:CG1	1:D:184:ASP:N	2.81	0.43
1:D:24:PHE:CE1	4:D:632:EDO:C2	3.01	0.43
1:C:201:MET:N	1:C:202:PRO:CD	2.81	0.43
1:D:134:LEU:HD11	1:D:139:LEU:HD21	2.00	0.43
1:D:216:LYS:C	1:D:218:ASN:N	2.71	0.43
1:B:241:GLU:O	1:B:245:ARG:HG3	2.18	0.43
1:B:312:PRO:HD2	1:B:319:LEU:HD22	1.99	0.43
1:C:183:VAL:HG12	1:C:184:ASP:N	2.34	0.43
1:C:216:LYS:C	1:C:218:ASN:H	2.21	0.43
1:C:277:LEU:O	1:C:282:CYS:HB2	2.19	0.43
1:D:165:PRO:O	1:D:166:ASN:HB3	2.18	0.43
1:D:52:THR:OG1	1:D:53:VAL:N	2.52	0.43
1:A:126:VAL:HG12	1:A:127:LYS:N	2.33	0.43
1:A:77:LEU:HD12	1:A:94:MET:HE3	2.00	0.43
1:B:216:LYS:C	1:B:218:ASN:H	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:H	1:C:130:THR:HG22	1.84	0.43
1:C:24:PHE:HE1	4:C:622:EDO:H11	1.83	0.43
1:D:308:LEU:CD1	1:D:340:LEU:HB3	2.44	0.43
1:D:77:LEU:HD12	1:D:94:MET:CE	2.44	0.43
1:A:391:ARG:NH1	6:A:720:HOH:O	2.50	0.43
1:A:41:LEU:HD13	1:A:65:LEU:CD2	2.49	0.43
1:B:365:GLU:CD	1:B:396:ARG:HH22	2.21	0.43
1:C:77:LEU:CD1	1:C:93:ILE:HG21	2.49	0.43
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.28	0.43
1:C:222:LYS:O	1:C:223:THR:HG22	2.19	0.43
1:C:263:TRP:CE3	1:D:84:SER:OG	2.72	0.43
1:C:327:ASP:OD2	1:D:358:ARG:NH2	2.52	0.43
1:D:4:PRO:HG3	1:D:64:LYS:HB3	2.00	0.43
1:A:43:VAL:HG13	1:A:47:THR:HG22	2.01	0.43
1:A:25:HIS:HB3	1:B:262:MET:HE2	2.01	0.42
1:B:43:VAL:CA	1:B:47:THR:HG22	2.36	0.42
1:D:70:ASP:OD1	1:D:70:ASP:C	2.57	0.42
1:B:260:ASP:HB3	1:B:319:LEU:HD23	2.01	0.42
1:D:313:THR:HG22	1:D:351:ALA:HB3	2.01	0.42
1:A:236:PRO:O	1:A:240:ILE:HG13	2.19	0.42
1:B:141:PHE:HD2	1:B:153:MET:CE	2.32	0.42
1:B:262:MET:HE3	5:B:711:FMN:HM83	2.02	0.42
1:A:126:VAL:HG11	1:A:141:PHE:CG	2.54	0.42
1:A:54:TYR:CG	1:A:56:PRO:HD2	2.55	0.42
1:A:80:ASN:HD22	1:A:153:MET:HG2	1.84	0.42
1:C:191:GLU:OE1	1:C:191:GLU:HA	2.19	0.42
1:C:286:LEU:HD23	1:C:286:LEU:C	2.40	0.42
1:A:149:TRP:HH2	6:B:730:HOH:O	2.01	0.42
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.44	0.42
1:A:163:LEU:C	1:A:165:PRO:HD3	2.40	0.42
1:A:379:ARG:CB	1:A:381:GLU:OE2	2.67	0.42
1:B:144:ALA:HB1	1:B:147:LEU:HB2	2.02	0.42
1:B:46:LYS:CA	1:B:75:ASP:OD2	2.68	0.42
1:C:356:GLU:HG2	1:C:366:LEU:HD13	2.00	0.42
1:D:163:LEU:O	1:D:165:PRO:HD3	2.20	0.42
1:D:253:ALA:HA	1:D:397:ILE:CG2	2.50	0.42
1:A:168:ALA:O	1:A:169:PHE:HB2	2.19	0.42
1:C:37:TYR:HB2	1:C:53:VAL:HG22	2.02	0.42
1:C:50:VAL:HA	1:C:78:VAL:HB	2.02	0.42
1:A:147:LEU:HD23	1:A:154:PHE:HZ	1.84	0.42
1:A:314:ILE:HG12	1:A:319:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:511:FEO:O	4:B:612:EDO:H22	2.20	0.42
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.84	0.42
1:A:379:ARG:HG2	1:A:379:ARG:H	1.63	0.42
1:A:201:MET:N	1:A:202:PRO:CD	2.82	0.41
1:A:260:ASP:O	1:A:312:PRO:HD3	2.20	0.41
1:C:140:THR:HG23	1:C:156:TYR:HB3	2.02	0.41
1:C:81:HIS:CB	1:C:166:ASN:ND2	2.83	0.41
1:D:24:PHE:O	1:D:25:HIS:HB2	2.19	0.41
1:C:25:HIS:HB3	1:D:262:MET:CE	2.50	0.41
1:C:260:ASP:O	1:C:312:PRO:HD3	2.20	0.41
1:C:83:GLU:OE2	4:C:622:EDO:O1	2.37	0.41
1:D:375:GLN:O	1:D:376:TRP:HB2	2.19	0.41
1:D:3:GLN:HA	1:D:4:PRO:HD3	1.94	0.41
1:D:68:ILE:N	1:D:68:ILE:HD13	2.34	0.41
1:A:323:SER:HB2	1:A:324:PRO:HD3	2.02	0.41
1:B:144:ALA:N	1:B:145:PRO:CD	2.84	0.41
1:B:202:PRO:CG	1:B:332:LEU:HA	2.36	0.41
1:C:165:PRO:O	1:C:166:ASN:HB3	2.20	0.41
1:C:168:ALA:O	1:C:169:PHE:HB2	2.20	0.41
1:C:294:ARG:NH1	1:D:320:PRO:HG2	2.36	0.41
1:D:263:TRP:O	1:D:264:LEU:HB2	2.21	0.41
1:A:165:PRO:O	1:A:166:ASN:CB	2.69	0.41
1:D:286:LEU:HD23	1:D:286:LEU:C	2.41	0.41
1:A:235:ASP:OD1	1:A:238:ARG:HG3	2.20	0.41
1:A:144:ALA:N	1:A:145:PRO:HD3	2.36	0.41
1:A:217:ILE:HG22	1:A:217:ILE:O	2.19	0.41
1:B:83:GLU:CD	4:B:612:EDO:O1	2.58	0.41
1:D:188:ILE:HD11	1:D:230:ILE:CG2	2.51	0.41
1:C:290:SER:HB3	1:D:27:PRO:CG	2.51	0.41
1:A:112:LEU:HA	1:A:112:LEU:HD12	1.83	0.41
1:B:86:HIS:CE1	1:B:227:SER:HB2	2.55	0.41
1:C:259:TYR:CD1	1:C:260:ASP:N	2.89	0.41
1:C:372:PRO:CG	1:C:389:LEU:CD1	2.95	0.41
1:A:126:VAL:HG11	1:A:141:PHE:CD1	2.55	0.41
1:A:235:ASP:CG	1:A:238:ARG:HG3	2.41	0.41
1:A:269:MET:HE1	1:A:374:VAL:HB	2.02	0.41
1:B:107:ARG:CB	1:B:107:ARG:HH11	2.34	0.41
1:C:177:VAL:HG22	1:C:182:GLN:CD	2.41	0.41
1:D:43:VAL:HG22	1:D:47:THR:HG21	2.02	0.41
1:D:81:HIS:HE1	1:D:149:TRP:CG	2.39	0.41
1:B:113:LYS:HD2	1:B:113:LYS:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:HD11	1:C:219:LEU:HD11	2.02	0.41
1:A:138:SER:N	1:A:159:GLU:OE1	2.49	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.95	0.41
1:C:161:ALA:HB1	1:C:220:ALA:O	2.21	0.41
1:D:195:TYR:O	1:D:199:ILE:HD12	2.21	0.41
1:B:108:ALA:CA	1:B:151:ASP:HB2	2.51	0.41
1:B:336:ASN:CG	1:B:336:ASN:O	2.59	0.41
1:C:395:ALA:O	1:C:398:ALA:HB2	2.21	0.41
1:A:81:HIS:HE1	1:A:149:TRP:CB	2.33	0.40
1:A:21:ILE:HD11	1:A:23:TYR:O	2.21	0.40
1:A:253:ALA:HB2	1:A:399:ASP:HB2	2.03	0.40
1:A:356:GLU:O	1:A:360:LYS:HD3	2.21	0.40
1:C:381:GLU:HG2	1:C:385:ARG:HH21	1.86	0.40
1:D:81:HIS:CB	1:D:166:ASN:ND2	2.84	0.40
1:A:212:ASP:O	1:A:215:GLN:HB3	2.21	0.40
1:D:40:TYR:OH	1:D:231:ILE:HD11	2.21	0.40
1:B:216:LYS:O	1:B:218:ASN:N	2.54	0.40
1:B:93:ILE:HA	1:B:93:ILE:HD13	1.89	0.40
1:C:345:TYR:HA	5:C:721:FMN:O2'	2.22	0.40
1:D:376:TRP:HA	1:D:376:TRP:CE3	2.57	0.40
1:A:25:HIS:O	1:B:262:MET:HG2	2.21	0.40
1:A:333:ARG:HD2	1:A:363:LYS:CG	2.50	0.40
1:B:397:ILE:HG22	1:B:397:ILE:O	2.21	0.40

All (3) 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)
6:C:730:HOH:O	6:C:730:HOH:O[8_663]	1.95	0.25
6:C:735:HOH:O	6:C:735:HOH:O[8_663]	2.04	0.16
6:C:740:HOH:O	6:D:745:HOH:O[3_544]	2.05	0.15

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	396/398 (100%)	360 (91%)	29 (7%)	7 (2%)	11	34
1	B	396/398 (100%)	361 (91%)	27 (7%)	8 (2%)	9	30
1	C	396/398 (100%)	364 (92%)	25 (6%)	7 (2%)	11	34
1	D	396/398 (100%)	362 (91%)	27 (7%)	7 (2%)	11	34
All	All	1584/1592 (100%)	1447 (91%)	108 (7%)	29 (2%)	11	34

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	370	PRO
1	A	398	ALA
1	B	71	PRO
1	B	83	GLU
1	B	148	HIS
1	B	370	PRO
1	B	398	ALA
1	C	71	PRO
1	C	148	HIS
1	C	370	PRO
1	C	398	ALA
1	D	71	PRO
1	D	148	HIS
1	D	370	PRO
1	D	398	ALA
1	A	74	LEU
1	C	74	LEU
1	D	117	SER
1	A	376	TRP
1	B	74	LEU
1	A	71	PRO
1	A	166	ASN
1	B	376	TRP
1	C	376	TRP
1	D	376	TRP
1	D	166	ASN
1	B	166	ASN
1	C	166	ASN

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	329/329 (100%)	297 (90%)	32 (10%)	10	29
1	B	329/329 (100%)	299 (91%)	30 (9%)	12	33
1	C	329/329 (100%)	305 (93%)	24 (7%)	17	44
1	D	329/329 (100%)	292 (89%)	37 (11%)	7	22
All	All	1316/1316 (100%)	1193 (91%)	123 (9%)	11	32

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	73	LYS
1	A	77	LEU
1	A	112	LEU
1	A	124	THR
1	A	130	THR
1	A	139	LEU
1	A	140	THR
1	A	153	MET
1	A	162	LEU
1	A	171	GLN
1	A	204	SER
1	A	218	ASN
1	A	222	LYS
1	A	230	ILE
1	A	233	ARG
1	A	234	LYS
1	A	239	ILE
1	A	260	ASP
1	A	291	VAL
1	A	308	LEU
1	A	313	THR
1	A	314	ILE
1	A	325	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	358	ARG
1	A	360	LYS
1	A	363	LYS
1	A	364	ILE
1	A	367	ILE
1	A	373	THR
1	A	379	ARG
1	A	381	GLU
1	B	71	PRO
1	B	73	LYS
1	B	96	LEU
1	B	107	ARG
1	B	124	THR
1	B	130	THR
1	B	131	SER
1	B	139	LEU
1	B	140	THR
1	B	147	LEU
1	B	162	LEU
1	B	171	GLN
1	B	177	VAL
1	B	210	LYS
1	B	218	ASN
1	B	230	ILE
1	B	233	ARG
1	B	239	ILE
1	B	261	THR
1	B	308	LEU
1	B	314	ILE
1	B	321	VAL
1	B	325	LEU
1	B	358	ARG
1	B	366	LEU
1	B	370	PRO
1	B	374	VAL
1	B	377	VAL
1	B	379	ARG
1	B	381	GLU
1	C	24	PHE
1	C	53	VAL
1	C	73	LYS
1	C	94	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	96	LEU
1	C	107	ARG
1	C	112	LEU
1	C	127	LYS
1	C	147	LEU
1	C	148	HIS
1	C	162	LEU
1	C	171	GLN
1	C	208	THR
1	C	218	ASN
1	C	230	ILE
1	C	234	LYS
1	C	239	ILE
1	C	260	ASP
1	C	282	CYS
1	C	291	VAL
1	C	317	ASP
1	C	325	LEU
1	C	358	ARG
1	C	370	PRO
1	D	9	ASP
1	D	21	ILE
1	D	24	PHE
1	D	43	VAL
1	D	50	VAL
1	D	53	VAL
1	D	73	LYS
1	D	74	LEU
1	D	77	LEU
1	D	82	THR
1	D	97	CYS
1	D	112	LEU
1	D	125	ILE
1	D	130	THR
1	D	139	LEU
1	D	140	THR
1	D	147	LEU
1	D	148	HIS
1	D	153	MET
1	D	162	LEU
1	D	171	GLN
1	D	173	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	177	VAL
1	D	218	ASN
1	D	224	ILE
1	D	230	ILE
1	D	233	ARG
1	D	234	LYS
1	D	239	ILE
1	D	291	VAL
1	D	308	LEU
1	D	313	THR
1	D	318	ILE
1	D	325	LEU
1	D	358	ARG
1	D	369	GLU
1	D	370	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	122	ASN
1	A	166	ASN
1	A	171	GLN
1	A	218	ASN
1	A	295	ASN
1	A	352	GLN
1	A	375	GLN
1	B	80	ASN
1	B	118	HIS
1	B	166	ASN
1	B	171	GLN
1	B	352	GLN
1	B	375	GLN
1	C	3	GLN
1	C	67	GLN
1	C	80	ASN
1	C	101	HIS
1	C	122	ASN
1	C	166	ASN
1	C	218	ASN
1	C	250	GLN
1	C	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	315	ASN
1	C	375	GLN
1	D	3	GLN
1	D	67	GLN
1	D	80	ASN
1	D	101	HIS
1	D	122	ASN
1	D	166	ASN
1	D	171	GLN
1	D	218	ASN
1	D	295	ASN
1	D	375	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 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	$\# Z > 2$
3	FEO	A	501	1	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	A	602	1	3,3,3	0.36	0	2,2,2	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMN	A	701	-	32,33,33	3.29	13 (40%)	34,50,50	3.35	10 (29%)
3	FEO	B	511	1	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	612	-	3,3,3	0.60	0	2,2,2	0.27	0
5	FMN	B	711	-	32,33,33	3.26	13 (40%)	34,50,50	3.32	11 (32%)
3	FEO	C	521	1	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	C	622	1	3,3,3	0.45	0	2,2,2	0.38	0
5	FMN	C	721	-	32,33,33	3.18	15 (46%)	34,50,50	3.34	10 (29%)
3	FEO	D	531	1	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	D	632	1	3,3,3	0.56	0	2,2,2	0.28	0
5	FMN	D	731	-	32,33,33	3.21	13 (40%)	34,50,50	3.29	11 (32%)

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
3	FEO	A	501	1	-	0/0/0/0	0/0/0/0
4	EDO	A	602	1	-	0/1/1/1	0/0/0/0
5	FMN	A	701	-	-	0/18/18/18	0/3/3/3
3	FEO	B	511	1	-	0/0/0/0	0/0/0/0
4	EDO	B	612	-	-	0/1/1/1	0/0/0/0
5	FMN	B	711	-	-	0/18/18/18	0/3/3/3
3	FEO	C	521	1	-	0/0/0/0	0/0/0/0
4	EDO	C	622	1	-	0/1/1/1	0/0/0/0
5	FMN	C	721	-	-	0/18/18/18	0/3/3/3
3	FEO	D	531	1	-	0/0/0/0	0/0/0/0
4	EDO	D	632	1	-	0/1/1/1	0/0/0/0
5	FMN	D	731	-	-	0/18/18/18	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	FMN	C2'-C3'	-2.67	1.48	1.53
5	C	721	FMN	C2'-C3'	-2.34	1.48	1.53
5	C	721	FMN	P-O2P	-2.20	1.47	1.54
5	B	711	FMN	P-O2P	-2.11	1.47	1.54
5	A	701	FMN	C9A-N10	2.04	1.41	1.38
5	D	731	FMN	C9A-N10	2.09	1.41	1.38
5	C	721	FMN	O3'-C3'	2.14	1.48	1.43
5	D	731	FMN	C10-N10	2.17	1.41	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	731	FMN	C6-C5A	2.21	1.45	1.41
5	C	721	FMN	C10-N10	2.27	1.41	1.39
5	C	721	FMN	C9A-N10	2.47	1.42	1.38
5	C	721	FMN	C6-C5A	2.63	1.45	1.41
5	B	711	FMN	C6-C5A	2.63	1.45	1.41
5	B	711	FMN	C10-N10	2.64	1.42	1.39
5	D	731	FMN	O3'-C3'	2.66	1.49	1.43
5	B	711	FMN	C5'-C4'	2.69	1.55	1.51
5	A	701	FMN	O3'-C3'	2.74	1.49	1.43
5	A	701	FMN	C6-C5A	2.75	1.46	1.41
5	C	721	FMN	C8-C7	2.78	1.48	1.41
5	A	701	FMN	C8-C7	2.78	1.48	1.41
5	B	711	FMN	C8-C7	2.83	1.48	1.41
5	D	731	FMN	C8-C7	2.83	1.48	1.41
5	C	721	FMN	C5'-C4'	2.91	1.56	1.51
5	D	731	FMN	C5'-C4'	2.91	1.56	1.51
5	A	701	FMN	C5'-C4'	3.13	1.56	1.51
5	B	711	FMN	C9A-N10	3.18	1.43	1.38
5	C	721	FMN	C6-C7	3.24	1.46	1.37
5	B	711	FMN	C6-C7	3.95	1.48	1.37
5	D	731	FMN	C6-C7	3.95	1.48	1.37
5	A	701	FMN	C6-C7	4.11	1.49	1.37
5	C	721	FMN	C9-C9A	4.56	1.50	1.40
5	B	711	FMN	C9A-C5A	4.63	1.52	1.42
5	A	701	FMN	C9A-C5A	4.64	1.52	1.42
5	C	721	FMN	C9A-C5A	4.66	1.52	1.42
5	D	731	FMN	C9-C9A	4.94	1.51	1.40
5	D	731	FMN	C9A-C5A	5.03	1.53	1.42
5	B	711	FMN	C9-C9A	5.12	1.51	1.40
5	A	701	FMN	C9-C9A	5.23	1.52	1.40
5	C	721	FMN	C2-N3	5.33	1.49	1.38
5	D	731	FMN	C2-N3	5.72	1.50	1.38
5	A	701	FMN	C2-N3	5.77	1.50	1.38
5	B	711	FMN	C2-N3	6.08	1.50	1.38
5	B	711	FMN	C5A-N5	6.30	1.45	1.35
5	D	731	FMN	C5A-N5	6.55	1.45	1.35
5	C	721	FMN	C5A-N5	6.99	1.46	1.35
5	A	701	FMN	C5A-N5	7.03	1.46	1.35
5	D	731	FMN	C4-N3	7.09	1.45	1.33
5	A	701	FMN	C4-N3	7.17	1.46	1.33
5	B	711	FMN	C4-N3	7.48	1.46	1.33
5	C	721	FMN	C4-N3	7.48	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	721	FMN	C4A-C10	8.68	1.56	1.40
5	A	701	FMN	C4A-C10	8.74	1.57	1.40
5	D	731	FMN	C4A-C10	8.82	1.57	1.40
5	B	711	FMN	C4A-C10	9.15	1.57	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	FMN	N3-C2-N1	-6.45	116.83	127.69
5	C	721	FMN	N3-C2-N1	-6.24	117.18	127.69
5	D	731	FMN	N3-C2-N1	-6.21	117.23	127.69
5	B	711	FMN	N3-C2-N1	-6.17	117.30	127.69
5	C	721	FMN	C4A-C4-N3	-5.47	116.38	123.52
5	B	711	FMN	C4A-C4-N3	-5.45	116.40	123.52
5	A	701	FMN	C4A-C4-N3	-5.16	116.78	123.52
5	D	731	FMN	C4A-C4-N3	-5.15	116.79	123.52
5	C	721	FMN	C7M-C7-C6	-4.22	108.41	120.33
5	A	701	FMN	C7M-C7-C6	-4.09	108.77	120.33
5	B	711	FMN	C7M-C7-C6	-4.03	108.95	120.33
5	D	731	FMN	C7M-C7-C6	-4.03	108.95	120.33
5	A	701	FMN	C9A-C5A-N5	-3.51	116.46	122.18
5	C	721	FMN	C9A-C5A-N5	-3.41	116.62	122.18
5	B	711	FMN	C9A-C5A-N5	-3.39	116.66	122.18
5	D	731	FMN	C9A-C5A-N5	-3.30	116.81	122.18
5	D	731	FMN	O3'-C3'-C4'	-2.33	102.69	108.73
5	B	711	FMN	O3'-C3'-C4'	-2.26	102.87	108.73
5	B	711	FMN	C6-C5A-N5	3.60	123.40	118.92
5	D	731	FMN	C6-C5A-N5	3.66	123.48	118.92
5	C	721	FMN	C6-C5A-N5	3.75	123.58	118.92
5	D	731	FMN	C4A-N5-C5A	3.82	121.22	116.72
5	A	701	FMN	C4A-N5-C5A	3.88	121.30	116.72
5	C	721	FMN	C4A-N5-C5A	4.03	121.47	116.72
5	A	701	FMN	C6-C5A-N5	4.21	124.17	118.92
5	B	711	FMN	C4A-N5-C5A	4.34	121.84	116.72
5	D	731	FMN	C7M-C7-C8	4.65	130.73	120.73
5	B	711	FMN	C7M-C7-C8	4.76	130.97	120.73
5	A	701	FMN	C7M-C7-C8	4.76	130.97	120.73
5	C	721	FMN	C7M-C7-C8	4.89	131.25	120.73
5	A	701	FMN	C1'-N10-C9A	6.36	126.21	118.83
5	B	711	FMN	C1'-N10-C9A	6.38	126.23	118.83
5	D	731	FMN	C1'-N10-C9A	6.70	126.60	118.83
5	C	721	FMN	C1'-N10-C9A	6.73	126.64	118.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	731	FMN	C5A-C9A-N10	8.73	124.12	117.58
5	C	721	FMN	C5A-C9A-N10	8.85	124.21	117.58
5	B	711	FMN	C5A-C9A-N10	8.89	124.24	117.58
5	A	701	FMN	C5A-C9A-N10	8.89	124.24	117.58
5	D	731	FMN	C4-N3-C2	9.24	122.87	115.16
5	C	721	FMN	C4-N3-C2	9.27	122.89	115.16
5	B	711	FMN	C4-N3-C2	9.30	122.92	115.16
5	A	701	FMN	C4-N3-C2	9.52	123.10	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	FEO	4	0
4	A	602	EDO	8	0
3	B	511	FEO	5	0
4	B	612	EDO	12	0
5	B	711	FMN	2	0
3	C	521	FEO	1	0
4	C	622	EDO	9	0
5	C	721	FMN	2	0
3	D	531	FEO	2	0
4	D	632	EDO	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	398/398 (100%)	-0.14	6 (1%) 76 68	37, 58, 77, 90	0
1	B	398/398 (100%)	-0.02	8 (2%) 68 58	39, 60, 84, 96	0
1	C	398/398 (100%)	-0.35	0 100 100	36, 50, 70, 85	0
1	D	398/398 (100%)	-0.31	0 100 100	37, 50, 71, 87	0
All	All	1592/1592 (100%)	-0.20	14 (0%) 85 79	36, 54, 77, 96	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ASP	3.5
1	B	74	LEU	3.4
1	A	45	ASP	3.0
1	B	103	LEU	2.9
1	B	76	TYR	2.7
1	A	238	ARG	2.3
1	B	369	GLU	2.3
1	A	139	LEU	2.3
1	B	100	ALA	2.3
1	A	365	GLU	2.3
1	A	219	LEU	2.2
1	B	44	ASP	2.1
1	B	46	LYS	2.1
1	B	134	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
4	EDO	C	622	4/4	0.75	0.42	8.80	40,45,48,59	0
4	EDO	A	602	4/4	0.87	0.33	6.43	52,56,58,63	0
4	EDO	D	632	4/4	0.64	0.38	5.93	58,61,61,63	0
4	EDO	B	612	4/4	0.85	0.30	5.09	57,62,63,65	0
5	FMN	D	731	31/31	0.96	0.18	0.71	41,43,47,47	0
3	FEO	A	501	3/3	0.92	0.16	0.03	52,52,56,56	0
5	FMN	C	721	31/31	0.97	0.15	-0.06	39,43,46,47	0
5	FMN	A	701	31/31	0.97	0.15	-0.17	50,60,63,64	0
3	FEO	C	521	3/3	0.93	0.13	-0.45	43,43,45,46	0
5	FMN	B	711	31/31	0.98	0.14	-0.57	45,59,63,64	0
3	FEO	D	531	3/3	0.94	0.13	-0.75	42,42,46,46	0
3	FEO	B	511	3/3	0.92	0.13	-0.85	54,54,55,56	0
2	ZN	C	422	1/1	0.99	0.06	-1.91	96,96,96,96	0
2	ZN	D	432	1/1	0.99	0.09	-2.03	97,97,97,97	0
2	ZN	A	402	1/1	0.98	0.06	-2.83	87,87,87,87	0
2	ZN	A	403	1/1	0.87	0.06	-	106,106,106,106	0
2	ZN	B	412	1/1	0.99	0.07	-	91,91,91,91	0
2	ZN	D	431	1/1	0.99	0.04	-	78,78,78,78	0
2	ZN	B	411	1/1	0.98	0.08	-	92,92,92,92	0
2	ZN	B	414	1/1	0.77	0.09	-	130,130,130,130	0
2	ZN	A	401	1/1	0.98	0.06	-	81,81,81,81	0
2	ZN	C	421	1/1	0.98	0.05	-	77,77,77,77	0
2	ZN	D	433	1/1	0.91	0.10	-	199,199,199,199	0
2	ZN	B	413	1/1	0.43	0.12	-	200,200,200,200	0
2	ZN	A	404	1/1	0.87	0.09	-	161,161,161,161	0
2	ZN	C	423	1/1	0.93	0.16	-	200,200,200,200	0

6.5 Other polymers ⓘ

There are no such residues in this entry.