Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:13 PM GMT

PDB ID	:	1VCG
Title	:	Crystal Structure of IPP isomerase at P43212
Authors	:	Wada, T.; Park, S.-Y.; Tame, R.H.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-03-08
Resolution	:	3.02 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:

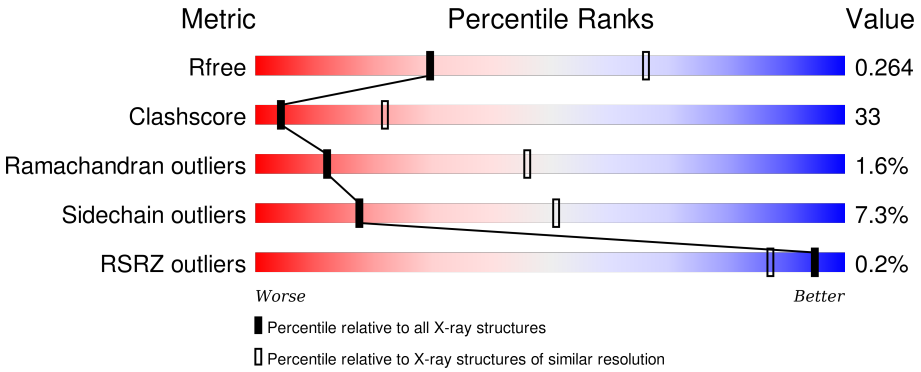
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.02 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	332	47% 40% 5% • 6%
1	B	332	48% 42% 5% • •
1	C	332	49% 40% 5% • 5%
1	D	332	48% 40% • • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	B	502	-	-	-	X
2	FMN	C	503	-	-	X	X
2	FMN	D	504	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9677 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 isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	Se	0	0	0
			2362	1505	426	424	2	5			
1	B	318	Total	C	N	O	S	Se	0	0	0
			2423	1543	439	434	2	5			
1	C	316	Total	C	N	O	S	Se	0	0	0
			2406	1531	437	431	2	5			
1	D	311	Total	C	N	O	S	Se	0	0	0
			2362	1505	426	424	2	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
C	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
D	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8

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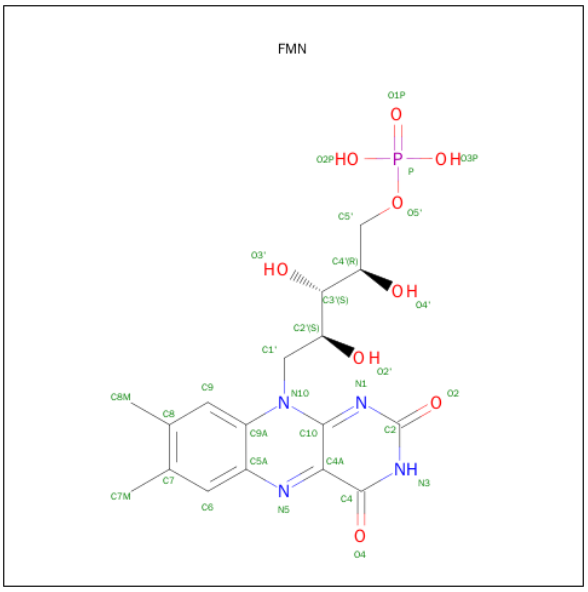
Chain	Residue	Modelled	Actual	Comment	Reference
D	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
D	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
D	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



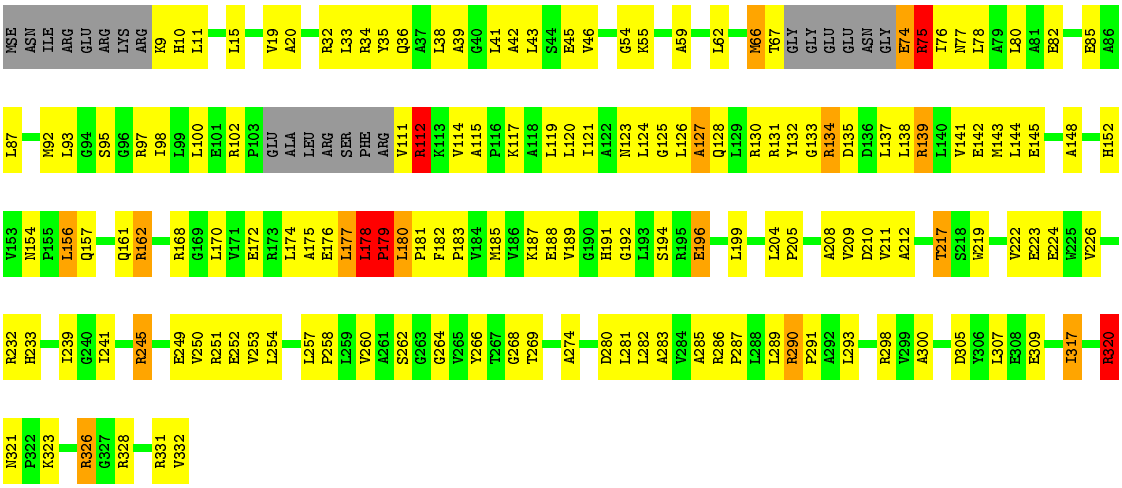
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

3 Residue-property plots (i)

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.

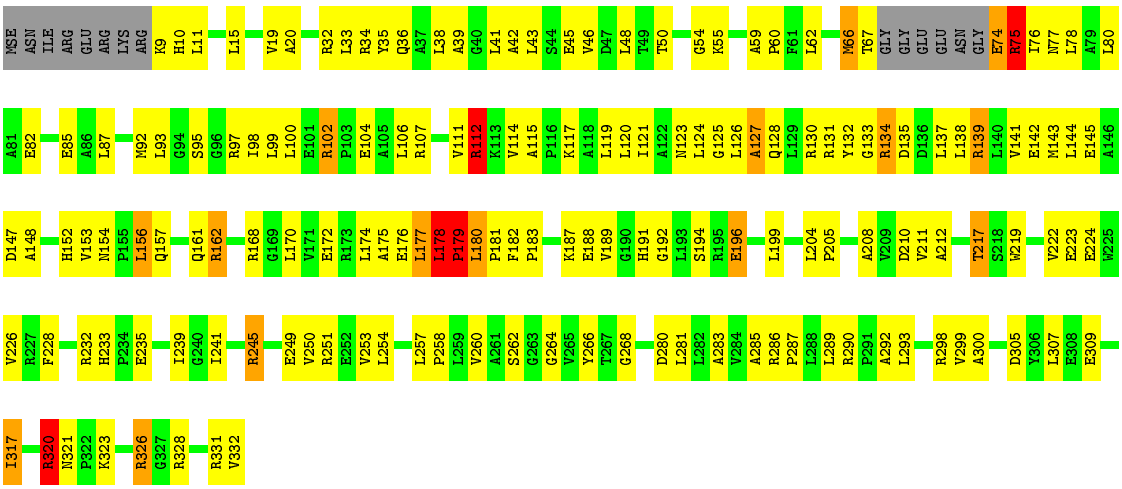
- Molecule 1: isopentenyl-diphosphate delta-isomerase

Chain A:



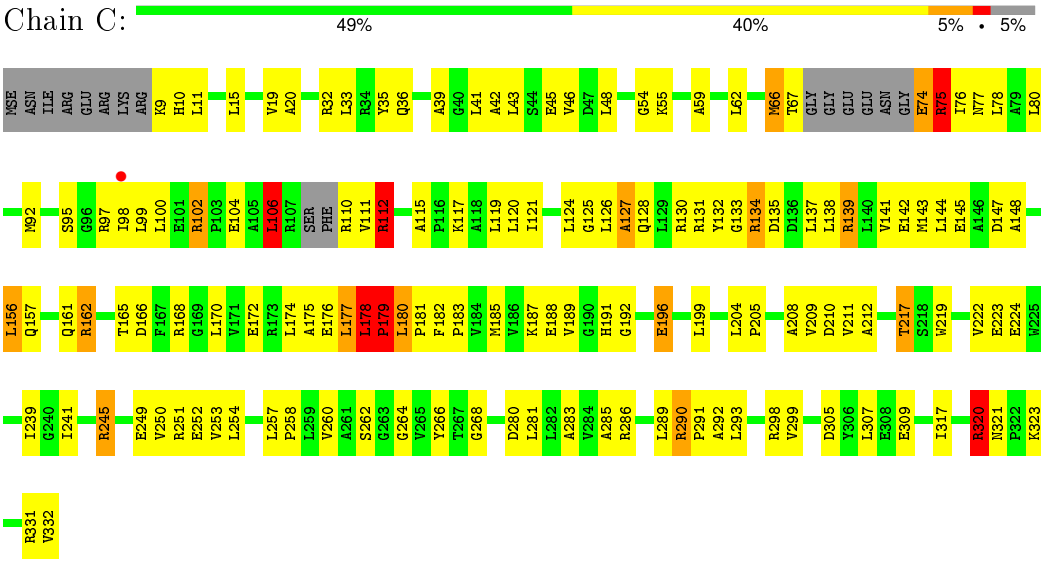
- Molecule 1: isopentenyl-diphosphate delta-isomerase

Chain B:



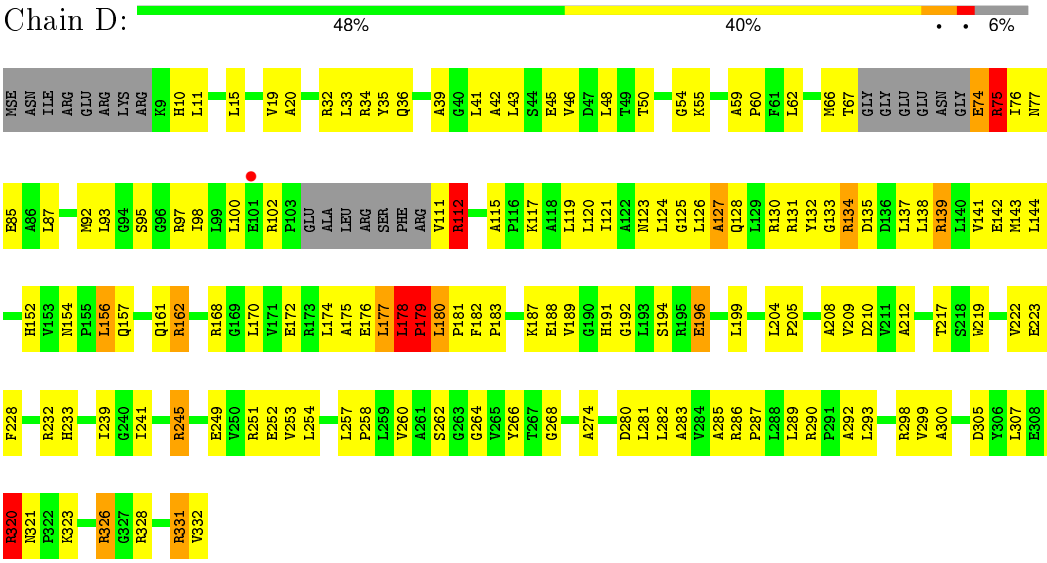
- Molecule 1: isopentenyl-diphosphate delta-isomerase

Chain C:



- Molecule 1: isopentenyl-diphosphate delta-isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.95Å 112.95Å 261.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.02 19.98 – 3.02	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.98-3.02) 94.4 (19.98-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 3.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.262 0.241 , 0.264	Depositor DCC
R_{free} test set	1593 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 32077 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9677	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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	0.49	1/2394 (0.0%)	1.34	23/3234 (0.7%)
1	B	0.47	1/2457 (0.0%)	1.08	20/3319 (0.6%)
1	C	0.45	1/2438 (0.0%)	1.09	20/3292 (0.6%)
1	D	0.48	0/2394	1.41	23/3234 (0.7%)
All	All	0.47	3/9683 (0.0%)	1.24	86/13079 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	MSE	CG-SE	-5.71	1.76	1.95
1	C	66	MSE	CG-SE	-5.55	1.76	1.95
1	A	66	MSE	CG-SE	-5.11	1.78	1.95

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ARG	NE-CZ-NH1	-26.33	107.14	120.30
1	D	331	ARG	NE-CZ-NH1	-24.27	108.16	120.30
1	A	320	ARG	NE-CZ-NH2	22.53	131.57	120.30
1	D	331	ARG	NE-CZ-NH2	22.30	131.45	120.30
1	D	112	ARG	NE-CZ-NH1	-21.18	109.71	120.30
1	A	290	ARG	NE-CZ-NH1	-20.82	109.89	120.30
1	D	112	ARG	NE-CZ-NH2	20.21	130.40	120.30
1	D	162	ARG	NE-CZ-NH1	-19.37	110.62	120.30
1	A	290	ARG	NE-CZ-NH2	19.13	129.87	120.30
1	D	162	ARG	NE-CZ-NH2	18.43	129.52	120.30
1	B	102	ARG	NE-CZ-NH1	-16.83	111.89	120.30
1	C	102	ARG	NE-CZ-NH1	-16.53	112.04	120.30
1	A	102	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	D	75	ARG	NE-CZ-NH1	16.50	128.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	102	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	A	139	ARG	NE-CZ-NH1	-16.39	112.11	120.30
1	D	75	ARG	NE-CZ-NH2	-16.37	112.11	120.30
1	B	75	ARG	NE-CZ-NH1	16.33	128.47	120.30
1	C	102	ARG	NE-CZ-NH2	16.24	128.42	120.30
1	A	75	ARG	NE-CZ-NH1	-16.18	112.21	120.30
1	C	139	ARG	NE-CZ-NH1	-16.00	112.30	120.30
1	C	75	ARG	NE-CZ-NH1	-15.98	112.31	120.30
1	D	139	ARG	NE-CZ-NH2	-15.94	112.33	120.30
1	C	75	ARG	NE-CZ-NH2	15.91	128.25	120.30
1	B	75	ARG	NE-CZ-NH2	-15.89	112.35	120.30
1	B	139	ARG	NE-CZ-NH2	-15.88	112.36	120.30
1	A	75	ARG	NE-CZ-NH2	15.83	128.21	120.30
1	A	139	ARG	NE-CZ-NH2	15.70	128.15	120.30
1	C	139	ARG	NE-CZ-NH2	15.65	128.13	120.30
1	D	102	ARG	NE-CZ-NH1	15.58	128.09	120.30
1	B	102	ARG	NE-CZ-NH2	15.54	128.07	120.30
1	D	139	ARG	NE-CZ-NH1	15.48	128.04	120.30
1	A	102	ARG	NE-CZ-NH1	15.02	127.81	120.30
1	B	139	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	D	331	ARG	CD-NE-CZ	12.11	140.55	123.60
1	A	320	ARG	CD-NE-CZ	11.99	140.39	123.60
1	B	320	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	D	112	ARG	CD-NE-CZ	9.96	137.54	123.60
1	B	75	ARG	CD-NE-CZ	9.24	136.54	123.60
1	D	75	ARG	CD-NE-CZ	9.09	136.33	123.60
1	D	320	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	C	331	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	331	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	C	102	ARG	CD-NE-CZ	8.77	135.87	123.60
1	C	75	ARG	CD-NE-CZ	8.66	135.73	123.60
1	B	102	ARG	CD-NE-CZ	8.65	135.71	123.60
1	B	331	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	290	ARG	CD-NE-CZ	8.59	135.63	123.60
1	C	320	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	A	139	ARG	CD-NE-CZ	8.49	135.49	123.60
1	C	139	ARG	CD-NE-CZ	8.42	135.39	123.60
1	D	139	ARG	CD-NE-CZ	8.41	135.37	123.60
1	B	331	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	331	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	A	75	ARG	CD-NE-CZ	8.38	135.34	123.60
1	D	102	ARG	CD-NE-CZ	8.33	135.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ARG	CD-NE-CZ	8.21	135.09	123.60
1	B	112	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	B	139	ARG	CD-NE-CZ	8.15	135.02	123.60
1	B	320	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	A	112	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	112	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	162	ARG	CD-NE-CZ	7.93	134.71	123.60
1	C	331	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	112	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	112	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	C	112	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	290	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	320	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	D	320	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	290	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	162	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	290	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	162	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	162	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	162	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	162	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	162	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	106	LEU	CA-CB-CG	5.72	128.47	115.30
1	D	162	ARG	CG-CD-NE	5.70	123.77	111.80
1	C	290	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	290	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	290	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	331	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	331	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	290	ARG	CG-CD-NE	5.02	122.34	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2362	0	2452	159	0
1	B	2423	0	2515	176	0
1	C	2406	0	2500	178	0
1	D	2362	0	2452	157	0
2	A	31	0	19	7	0
2	B	31	0	19	8	0
2	C	31	0	19	9	0
2	D	31	0	19	5	0
All	All	9677	0	9995	650	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (650) 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:257:LEU:HD12	1:C:258:PRO:HD2	1.29	1.10
1:D:257:LEU:HD12	1:D:258:PRO:HD2	1.33	1.07
1:A:257:LEU:HD12	1:A:258:PRO:HD2	1.36	1.06
1:B:257:LEU:HD12	1:B:258:PRO:HD2	1.37	1.04
1:C:106:LEU:HD22	1:C:110:ARG:HH22	1.18	1.02
1:C:33:LEU:HB3	1:C:317:ILE:HD11	1.47	0.97
1:B:33:LEU:HB3	1:B:317:ILE:HD11	1.47	0.96
1:C:127:ALA:HA	1:C:170:LEU:HD21	1.50	0.94
1:D:33:LEU:HB3	1:D:317:ILE:HD11	1.50	0.93
1:A:127:ALA:HA	1:A:170:LEU:HD21	1.50	0.92
1:B:178:LEU:HB3	1:B:179:PRO:HD3	1.52	0.92
1:D:127:ALA:HA	1:D:170:LEU:HD21	1.49	0.91
1:D:178:LEU:HB3	1:D:179:PRO:HD3	1.53	0.91
1:A:178:LEU:HB3	1:A:179:PRO:HD3	1.51	0.91
1:A:33:LEU:HB3	1:A:317:ILE:HD11	1.52	0.90
1:C:178:LEU:HB3	1:C:179:PRO:HD3	1.51	0.90
1:B:127:ALA:HA	1:B:170:LEU:HD21	1.52	0.89
1:A:326:ARG:HB2	1:A:326:ARG:HH11	1.40	0.86
1:C:268:GLY:HA3	1:C:309:GLU:HG3	1.57	0.86
1:B:188:GLU:HG3	1:B:189:VAL:N	1.88	0.86
1:D:326:ARG:HB2	1:D:326:ARG:HH11	1.41	0.86
1:D:268:GLY:HA3	1:D:309:GLU:HG3	1.57	0.86
1:C:188:GLU:HG3	1:C:189:VAL:N	1.92	0.85
1:A:188:GLU:HG3	1:A:189:VAL:N	1.90	0.85
1:D:188:GLU:HG3	1:D:189:VAL:N	1.89	0.84
1:C:326:ARG:HH11	1:C:326:ARG:HB2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:HA3	1:A:309:GLU:HG3	1.60	0.83
1:B:326:ARG:HB2	1:B:326:ARG:HH11	1.42	0.83
1:C:106:LEU:HD22	1:C:110:ARG:NH2	1.93	0.83
1:D:85:GLU:HG3	1:D:115:ALA:HA	1.62	0.82
1:A:85:GLU:HG3	1:A:115:ALA:HA	1.61	0.82
1:B:268:GLY:HA3	1:B:309:GLU:HG3	1.58	0.81
1:B:99:LEU:HD11	1:B:106:LEU:HA	1.61	0.81
1:C:85:GLU:HG3	1:C:115:ALA:HA	1.61	0.81
1:A:178:LEU:HB3	1:A:179:PRO:CD	2.11	0.81
1:B:85:GLU:HG3	1:B:115:ALA:HA	1.62	0.80
1:D:178:LEU:HB3	1:D:179:PRO:CD	2.12	0.80
1:C:178:LEU:HB3	1:C:179:PRO:CD	2.11	0.79
1:B:178:LEU:HB3	1:B:179:PRO:CD	2.10	0.78
1:D:174:LEU:HG	1:D:178:LEU:HD23	1.66	0.78
1:B:174:LEU:HG	1:B:178:LEU:HD23	1.66	0.78
1:C:174:LEU:HG	1:C:178:LEU:HD23	1.67	0.77
1:C:78:LEU:HD23	1:C:111:VAL:HG23	1.67	0.77
1:D:43:LEU:O	1:D:46:VAL:HG12	1.84	0.77
1:A:43:LEU:O	1:A:46:VAL:HG12	1.86	0.76
1:C:43:LEU:O	1:C:46:VAL:HG12	1.85	0.76
1:D:78:LEU:HD23	1:D:111:VAL:HG23	1.64	0.76
1:A:78:LEU:HD23	1:A:111:VAL:HG23	1.68	0.76
1:C:98:ILE:HD12	1:C:98:ILE:H	1.52	0.75
1:A:174:LEU:HG	1:A:178:LEU:HD23	1.67	0.75
1:B:188:GLU:HG3	1:B:189:VAL:H	1.49	0.75
1:B:78:LEU:HD23	1:B:111:VAL:HG23	1.68	0.74
1:B:43:LEU:O	1:B:46:VAL:HG12	1.87	0.74
1:C:125:GLY:HA2	1:C:152:HIS:H	1.52	0.74
1:D:125:GLY:HA2	1:D:152:HIS:H	1.52	0.74
1:A:98:ILE:H	1:A:98:ILE:HD12	1.51	0.73
1:C:99:LEU:HD11	1:C:106:LEU:HA	1.69	0.73
1:A:125:GLY:HA2	1:A:152:HIS:H	1.52	0.73
1:A:188:GLU:HG3	1:A:189:VAL:H	1.51	0.73
1:D:326:ARG:HB2	1:D:326:ARG:NH1	2.04	0.73
1:A:41:LEU:HD22	1:A:320:ARG:HD2	1.71	0.72
1:A:67:THR:H	2:A:501:FMN:H6	1.54	0.72
1:A:326:ARG:HB2	1:A:326:ARG:NH1	2.03	0.72
1:D:188:GLU:HG3	1:D:189:VAL:H	1.52	0.72
1:B:67:THR:H	2:B:502:FMN:H6	1.53	0.71
1:C:188:GLU:HG3	1:C:189:VAL:H	1.52	0.71
1:D:98:ILE:HD12	1:D:98:ILE:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HB2	1:B:326:ARG:NH1	2.04	0.71
1:C:326:ARG:NH1	1:C:326:ARG:HB2	2.04	0.70
1:B:98:ILE:HD12	1:B:98:ILE:H	1.54	0.70
1:C:67:THR:H	2:C:503:FMN:H6	1.57	0.69
1:B:125:GLY:HA2	1:B:152:HIS:H	1.57	0.69
1:C:260:VAL:HG22	1:C:281:LEU:HB2	1.75	0.69
1:D:260:VAL:HG22	1:D:281:LEU:HB2	1.75	0.68
1:D:257:LEU:HD12	1:D:258:PRO:CD	2.20	0.68
1:C:317:ILE:CG2	1:C:328:ARG:HD2	2.24	0.67
1:B:178:LEU:O	1:B:179:PRO:C	2.32	0.67
1:C:257:LEU:HD12	1:C:258:PRO:CD	2.17	0.67
1:B:317:ILE:CG2	1:B:328:ARG:HD2	2.24	0.67
1:C:41:LEU:HD22	1:C:320:ARG:HD3	1.77	0.67
1:D:317:ILE:CG2	1:D:328:ARG:HD2	2.24	0.67
1:C:85:GLU:CG	1:C:115:ALA:HA	2.23	0.67
1:D:178:LEU:O	1:D:179:PRO:C	2.32	0.67
1:C:161:GLN:HB2	1:C:223:GLU:HG2	1.77	0.67
1:A:178:LEU:O	1:A:179:PRO:C	2.33	0.66
1:B:99:LEU:HD11	1:B:106:LEU:CA	2.25	0.66
1:D:41:LEU:HD22	1:D:320:ARG:HD3	1.78	0.66
1:D:180:LEU:HD23	1:D:182:PHE:CE1	2.30	0.66
1:A:180:LEU:HD23	1:A:182:PHE:CE1	2.31	0.66
1:D:85:GLU:CG	1:D:115:ALA:HA	2.25	0.66
1:A:98:ILE:N	1:A:98:ILE:HD12	2.10	0.66
1:B:161:GLN:HB2	1:B:223:GLU:HG2	1.78	0.66
1:B:85:GLU:CG	1:B:115:ALA:HA	2.25	0.66
1:A:260:VAL:HG22	1:A:281:LEU:HB2	1.76	0.65
1:D:161:GLN:HB2	1:D:223:GLU:HG2	1.79	0.65
1:A:257:LEU:HD12	1:A:258:PRO:CD	2.22	0.65
1:B:260:VAL:HG22	1:B:281:LEU:HB2	1.79	0.65
1:A:317:ILE:CG2	1:A:328:ARG:HD2	2.27	0.65
1:A:85:GLU:CG	1:A:115:ALA:HA	2.26	0.64
1:B:217:THR:CG2	2:B:502:FMN:O3P	2.45	0.64
1:C:98:ILE:HD12	1:C:98:ILE:N	2.10	0.64
1:B:98:ILE:HD12	1:B:98:ILE:N	2.12	0.64
1:C:178:LEU:O	1:C:179:PRO:C	2.34	0.64
1:D:98:ILE:HD12	1:D:98:ILE:N	2.12	0.64
1:B:188:GLU:CG	1:B:189:VAL:N	2.61	0.63
1:C:99:LEU:HD11	1:C:106:LEU:HB3	1.80	0.63
1:B:217:THR:HG22	2:B:502:FMN:O3P	1.99	0.63
1:B:41:LEU:HD22	1:B:320:ARG:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD12	1:C:205:PRO:HG2	1.81	0.63
1:B:178:LEU:HD12	1:B:205:PRO:HG2	1.81	0.63
1:A:285:ALA:HB3	2:A:501:FMN:O5'	1.99	0.63
1:C:251:ARG:NH2	1:C:257:LEU:O	2.32	0.62
1:A:177:LEU:O	1:A:177:LEU:HD12	1.99	0.62
1:C:180:LEU:HD23	1:C:182:PHE:CE1	2.34	0.62
1:C:62:LEU:CD1	1:C:92:MSE:HE2	2.29	0.62
1:B:180:LEU:HD23	1:B:182:PHE:CE1	2.34	0.62
1:C:62:LEU:HD12	1:C:92:MSE:HE2	1.81	0.62
1:A:161:GLN:HB2	1:A:223:GLU:HG2	1.80	0.62
1:C:66:MSE:HA	2:C:503:FMN:C5A	2.29	0.62
1:C:110:ARG:HB3	1:C:110:ARG:CZ	2.28	0.61
1:B:188:GLU:CG	1:B:189:VAL:H	2.13	0.61
1:B:106:LEU:HD11	1:B:143:MSE:HB3	1.82	0.61
1:B:11:LEU:HD21	1:B:289:LEU:HD11	1.83	0.61
1:D:177:LEU:HD12	1:D:177:LEU:O	2.00	0.61
1:A:253:VAL:HG12	1:A:254:LEU:HD23	1.83	0.61
1:C:42:ALA:O	1:C:45:GLU:HG2	2.00	0.60
1:A:188:GLU:CG	1:A:189:VAL:N	2.63	0.60
1:B:251:ARG:NH2	1:B:257:LEU:O	2.34	0.60
1:D:11:LEU:HD21	1:D:289:LEU:HD11	1.83	0.60
1:D:67:THR:H	2:D:504:FMN:H6	1.65	0.60
1:C:19:VAL:HB	1:C:222:VAL:HG22	1.84	0.60
1:D:251:ARG:NH2	1:D:257:LEU:O	2.34	0.60
1:B:42:ALA:O	1:B:45:GLU:HG2	2.02	0.60
1:D:112:ARG:HD2	1:D:115:ALA:O	2.02	0.60
1:D:178:LEU:HD12	1:D:205:PRO:HG2	1.83	0.60
1:B:177:LEU:HD12	1:B:177:LEU:O	2.02	0.59
1:A:251:ARG:NH2	1:A:257:LEU:O	2.34	0.59
1:C:20:ALA:HB2	1:C:286:ARG:NH2	2.16	0.59
1:A:178:LEU:HD12	1:A:205:PRO:HG2	1.84	0.59
1:A:42:ALA:O	1:A:45:GLU:HG2	2.02	0.59
1:A:188:GLU:CG	1:A:189:VAL:H	2.15	0.59
1:B:19:VAL:HB	1:B:222:VAL:HG22	1.85	0.59
1:C:99:LEU:HD11	1:C:106:LEU:CA	2.31	0.59
1:C:188:GLU:CG	1:C:189:VAL:H	2.15	0.59
1:D:188:GLU:CG	1:D:189:VAL:N	2.63	0.59
1:C:11:LEU:HD21	1:C:289:LEU:HD11	1.84	0.59
1:D:188:GLU:CG	1:D:189:VAL:H	2.15	0.59
1:D:285:ALA:HB3	2:D:504:FMN:O5'	2.03	0.59
1:D:62:LEU:HD12	1:D:92:MSE:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:VAL:HG12	1:D:254:LEU:HD23	1.84	0.59
1:D:148:ALA:HB2	1:D:183:PRO:HG2	1.82	0.59
1:B:161:GLN:HB2	1:B:223:GLU:CG	2.33	0.58
1:D:62:LEU:CD1	1:D:92:MSE:HE2	2.33	0.58
1:C:99:LEU:HD11	1:C:106:LEU:CB	2.34	0.58
1:C:127:ALA:CA	1:C:170:LEU:HD21	2.30	0.58
1:D:42:ALA:O	1:D:45:GLU:HG2	2.03	0.58
1:C:110:ARG:HB2	1:C:110:ARG:NH2	2.18	0.58
1:A:180:LEU:HG	1:A:181:PRO:HD2	1.86	0.58
1:C:177:LEU:HD12	1:C:177:LEU:O	2.03	0.58
1:C:161:GLN:HB2	1:C:223:GLU:CG	2.32	0.58
1:C:178:LEU:O	1:C:180:LEU:HD13	2.02	0.58
1:C:285:ALA:HB3	2:C:503:FMN:O5'	2.03	0.58
1:D:156:LEU:HD12	1:D:191:HIS:CD2	2.39	0.58
1:A:62:LEU:HD12	1:A:92:MSE:HE2	1.86	0.58
1:D:180:LEU:HG	1:D:181:PRO:HD2	1.86	0.58
1:D:245:ARG:HH11	1:D:245:ARG:HG2	1.68	0.58
1:A:305:ASP:OD2	1:B:233:HIS:HE1	1.85	0.58
1:B:20:ALA:HB2	1:B:286:ARG:NH2	2.19	0.58
1:A:233:HIS:HE1	1:D:305:ASP:OD2	1.87	0.57
1:A:11:LEU:HD21	1:A:289:LEU:HD11	1.85	0.57
1:D:127:ALA:CA	1:D:170:LEU:HD21	2.30	0.57
1:C:188:GLU:HG2	1:C:192:GLY:H	1.68	0.57
1:D:154:ASN:HD22	1:D:157:GLN:HB3	1.69	0.57
1:D:178:LEU:O	1:D:180:LEU:HD13	2.04	0.57
1:C:188:GLU:CG	1:C:189:VAL:N	2.64	0.57
1:B:172:GLU:H	1:B:172:GLU:CD	2.07	0.57
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.68	0.57
1:A:245:ARG:HH11	1:A:245:ARG:HG2	1.69	0.57
1:A:191:HIS:HD2	1:A:239:ILE:O	1.87	0.57
1:A:148:ALA:HB2	1:A:183:PRO:HG2	1.85	0.57
1:A:224:GLU:OE1	1:A:233:HIS:HD2	1.88	0.57
1:C:156:LEU:HD12	1:C:191:HIS:CD2	2.38	0.57
1:A:20:ALA:HB2	1:A:286:ARG:NH2	2.20	0.57
1:B:178:LEU:O	1:B:180:LEU:HD13	2.03	0.57
1:C:253:VAL:HG12	1:C:254:LEU:HD23	1.86	0.57
1:C:245:ARG:HG2	1:C:245:ARG:HH11	1.70	0.57
1:B:224:GLU:OE1	1:B:233:HIS:HD2	1.88	0.57
1:D:161:GLN:HB2	1:D:223:GLU:CG	2.34	0.56
1:A:87:LEU:N	1:A:87:LEU:HD12	2.20	0.56
1:D:224:GLU:OE1	1:D:233:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:HIS:HD2	1:A:219:TRP:HZ3	1.53	0.56
1:A:172:GLU:CD	1:A:172:GLU:H	2.09	0.56
1:D:19:VAL:HB	1:D:222:VAL:HG22	1.85	0.56
1:B:130:ARG:HG3	1:B:130:ARG:HH11	1.70	0.56
1:D:124:LEU:CD1	1:D:128:GLN:HB2	2.34	0.56
1:B:222:VAL:O	1:B:226:VAL:HG23	2.05	0.56
1:C:121:ILE:HD12	1:C:121:ILE:N	2.21	0.56
1:D:172:GLU:H	1:D:172:GLU:CD	2.07	0.56
1:A:178:LEU:O	1:A:180:LEU:HD13	2.04	0.56
1:A:222:VAL:O	1:A:226:VAL:HG23	2.05	0.56
1:B:156:LEU:HD12	1:B:191:HIS:CD2	2.41	0.56
1:A:62:LEU:CD1	1:A:92:MSE:HE2	2.36	0.56
1:A:156:LEU:HD12	1:A:191:HIS:CD2	2.40	0.56
1:C:148:ALA:HB2	1:C:183:PRO:HG2	1.86	0.56
1:A:232:ARG:HH21	1:A:232:ARG:HG2	1.71	0.56
1:B:127:ALA:CA	1:B:170:LEU:HD21	2.32	0.56
1:A:161:GLN:HB2	1:A:223:GLU:CG	2.36	0.56
1:C:138:LEU:O	1:C:142:GLU:HB2	2.06	0.56
1:B:188:GLU:HG2	1:B:192:GLY:H	1.70	0.56
1:D:10:HIS:HD2	1:D:219:TRP:HZ3	1.54	0.56
1:B:62:LEU:CD1	1:B:92:MSE:HE2	2.36	0.56
1:B:62:LEU:HD12	1:B:92:MSE:HE2	1.88	0.56
1:D:20:ALA:HB2	1:D:286:ARG:NH2	2.21	0.56
1:C:10:HIS:HD2	1:C:219:TRP:HZ3	1.53	0.56
1:B:124:LEU:CD1	1:B:128:GLN:HB2	2.36	0.55
1:B:10:HIS:HD2	1:B:219:TRP:HZ3	1.54	0.55
1:A:19:VAL:HB	1:A:222:VAL:HG22	1.87	0.55
1:A:124:LEU:CD1	1:A:128:GLN:HB2	2.37	0.55
1:A:66:MSE:HA	2:A:501:FMN:C5A	2.35	0.55
1:C:222:VAL:O	1:C:226:VAL:HG23	2.06	0.55
1:B:305:ASP:OD2	1:C:233:HIS:HE1	1.90	0.55
1:D:121:ILE:N	1:D:121:ILE:HD12	2.22	0.55
1:B:191:HIS:HD2	1:B:239:ILE:O	1.89	0.55
1:C:139:ARG:O	1:C:142:GLU:HB3	2.07	0.55
1:A:154:ASN:HD22	1:A:157:GLN:HB3	1.72	0.55
1:C:172:GLU:CD	1:C:172:GLU:H	2.09	0.55
1:B:232:ARG:HH21	1:B:232:ARG:HG2	1.71	0.55
1:C:110:ARG:CB	1:C:110:ARG:CZ	2.85	0.55
1:D:138:LEU:O	1:D:142:GLU:HB2	2.07	0.55
1:A:188:GLU:HG2	1:A:192:GLY:H	1.72	0.55
1:B:253:VAL:HG12	1:B:254:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:OE1	1:C:233:HIS:HD2	1.90	0.55
1:C:99:LEU:CD1	1:C:106:LEU:HA	2.37	0.54
1:C:124:LEU:CD1	1:C:128:GLN:HB2	2.37	0.54
1:C:98:ILE:CD1	1:C:98:ILE:H	2.19	0.54
1:D:176:GLU:C	1:D:178:LEU:H	2.11	0.54
1:B:285:ALA:HB3	2:B:502:FMN:O5'	2.08	0.54
1:B:148:ALA:HB2	1:B:183:PRO:HG2	1.89	0.54
1:C:188:GLU:HG2	1:C:192:GLY:N	2.22	0.54
1:D:222:VAL:O	1:D:226:VAL:HG23	2.08	0.54
1:C:180:LEU:HG	1:C:181:PRO:HD2	1.89	0.54
1:B:178:LEU:O	1:B:180:LEU:N	2.40	0.54
1:D:126:LEU:HB3	1:D:170:LEU:HD23	1.90	0.54
1:C:176:GLU:C	1:C:178:LEU:H	2.11	0.54
1:C:187:LYS:CB	1:C:210:ASP:HB3	2.37	0.54
1:B:245:ARG:NH1	1:B:245:ARG:HG2	2.23	0.54
1:D:139:ARG:O	1:D:142:GLU:HB3	2.08	0.54
1:D:191:HIS:HD2	1:D:239:ILE:O	1.91	0.54
1:D:245:ARG:HG2	1:D:245:ARG:NH1	2.23	0.54
1:A:176:GLU:C	1:A:178:LEU:H	2.11	0.54
1:B:187:LYS:CB	1:B:210:ASP:HB3	2.38	0.54
1:B:257:LEU:HD12	1:B:258:PRO:CD	2.24	0.53
1:D:178:LEU:O	1:D:180:LEU:N	2.40	0.53
1:A:245:ARG:HG2	1:A:245:ARG:NH1	2.24	0.53
1:B:87:LEU:N	1:B:87:LEU:HD12	2.22	0.53
1:C:232:ARG:HG2	1:C:232:ARG:HH21	1.73	0.53
1:B:176:GLU:C	1:B:178:LEU:H	2.12	0.53
1:C:178:LEU:O	1:C:180:LEU:N	2.41	0.53
1:D:232:ARG:HH21	1:D:232:ARG:HG2	1.72	0.53
1:B:121:ILE:HD12	1:B:121:ILE:N	2.23	0.53
1:C:154:ASN:HD22	1:C:157:GLN:HB3	1.73	0.53
1:C:191:HIS:HD2	1:C:239:ILE:O	1.90	0.53
1:C:126:LEU:HB3	1:C:170:LEU:HD23	1.90	0.53
1:A:66:MSE:HE3	1:A:80:LEU:HD11	1.90	0.53
1:C:268:GLY:H	1:C:309:GLU:CD	2.12	0.53
1:A:178:LEU:O	1:A:180:LEU:N	2.42	0.53
1:B:317:ILE:HG22	1:B:328:ARG:HD2	1.91	0.53
1:B:66:MSE:HE3	1:B:80:LEU:HD11	1.91	0.53
1:A:67:THR:H	2:A:501:FMN:C6	2.20	0.52
1:A:121:ILE:N	1:A:121:ILE:HD12	2.25	0.52
1:B:138:LEU:O	1:B:142:GLU:HB2	2.09	0.52
1:B:126:LEU:HB3	1:B:170:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.73	0.52
1:D:268:GLY:H	1:D:309:GLU:CD	2.13	0.52
1:D:157:GLN:NE2	1:D:189:VAL:HG21	2.25	0.52
1:D:172:GLU:HA	1:D:175:ALA:HB3	1.92	0.52
1:A:85:GLU:OE1	1:A:117:LYS:N	2.43	0.52
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.73	0.52
1:A:126:LEU:HB3	1:A:170:LEU:HD23	1.92	0.52
1:B:180:LEU:HG	1:B:181:PRO:HD2	1.92	0.52
1:D:187:LYS:CB	1:D:210:ASP:HB3	2.40	0.52
1:A:98:ILE:H	1:A:98:ILE:CD1	2.19	0.52
1:B:76:ILE:HG13	1:B:77:ASN:N	2.25	0.52
1:A:188:GLU:HG2	1:A:192:GLY:N	2.25	0.52
1:B:85:GLU:OE1	1:B:117:LYS:N	2.43	0.51
1:A:187:LYS:CB	1:A:210:ASP:HB3	2.40	0.51
1:C:66:MSE:HA	2:C:503:FMN:C6	2.40	0.51
1:A:138:LEU:O	1:A:142:GLU:HB2	2.10	0.51
1:B:188:GLU:HG2	1:B:192:GLY:N	2.25	0.51
1:A:127:ALA:CA	1:A:170:LEU:HD21	2.31	0.51
1:B:157:GLN:NE2	1:B:189:VAL:HG21	2.25	0.51
1:C:67:THR:H	2:C:503:FMN:C6	2.24	0.51
1:C:119:LEU:O	1:C:120:LEU:HD23	2.10	0.51
1:D:188:GLU:HG2	1:D:192:GLY:H	1.75	0.51
1:B:266:TYR:HE1	2:B:502:FMN:O1P	1.94	0.51
1:A:76:ILE:HG13	1:A:77:ASN:N	2.26	0.51
1:C:104:GLU:O	1:C:106:LEU:HD12	2.10	0.51
1:A:41:LEU:CD2	1:A:320:ARG:HD2	2.41	0.51
1:C:110:ARG:CB	1:C:110:ARG:NH2	2.73	0.51
1:D:130:ARG:HH11	1:D:130:ARG:HG3	1.76	0.51
1:D:66:MSE:HE3	1:D:80:LEU:HD11	1.92	0.51
1:C:112:ARG:NH1	1:C:145:GLU:O	2.42	0.51
1:B:139:ARG:O	1:B:142:GLU:HB3	2.11	0.51
1:C:157:GLN:NE2	1:C:189:VAL:HG21	2.26	0.51
1:B:98:ILE:CD1	1:B:98:ILE:H	2.22	0.51
1:C:87:LEU:N	1:C:87:LEU:HD12	2.25	0.51
1:C:317:ILE:HG22	1:C:328:ARG:HD2	1.91	0.51
1:D:87:LEU:N	1:D:87:LEU:HD12	2.25	0.51
1:C:245:ARG:NH1	1:C:245:ARG:HG2	2.25	0.50
1:D:76:ILE:HG13	1:D:77:ASN:N	2.26	0.50
1:C:212:ALA:HA	1:C:262:SER:O	2.11	0.50
1:D:317:ILE:HG22	1:D:328:ARG:HD2	1.93	0.50
1:D:188:GLU:HG2	1:D:192:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLN:HE21	1:D:189:VAL:HG21	1.76	0.50
1:B:172:GLU:HA	1:B:175:ALA:HB3	1.94	0.50
1:A:144:LEU:O	1:A:145:GLU:HB2	2.12	0.50
1:D:85:GLU:OE1	1:D:117:LYS:N	2.43	0.50
1:D:98:ILE:CD1	1:D:98:ILE:H	2.22	0.50
1:C:66:MSE:HE3	1:C:80:LEU:HD11	1.93	0.50
1:C:172:GLU:HA	1:C:175:ALA:HB3	1.94	0.50
1:C:85:GLU:OE1	1:C:117:LYS:N	2.45	0.50
1:A:36:GLN:HB2	1:A:39:ALA:HB2	1.93	0.50
1:C:76:ILE:HG13	1:C:77:ASN:N	2.26	0.50
1:C:100:LEU:HD13	1:C:132:TYR:CD1	2.47	0.49
1:A:317:ILE:HG22	1:A:328:ARG:HD2	1.92	0.49
1:A:139:ARG:O	1:A:142:GLU:HB3	2.12	0.49
1:B:157:GLN:HE21	1:B:189:VAL:HG21	1.77	0.49
1:A:172:GLU:HA	1:A:175:ALA:HB3	1.94	0.49
1:D:317:ILE:HG23	1:D:328:ARG:HD2	1.94	0.49
1:C:36:GLN:CB	1:C:39:ALA:HB2	2.43	0.49
1:B:144:LEU:O	1:B:145:GLU:HB2	2.13	0.49
1:B:66:MSE:HA	2:B:502:FMN:C5A	2.42	0.49
1:C:95:SER:OG	1:C:97:ARG:HB2	2.12	0.49
1:C:144:LEU:O	1:C:145:GLU:HB2	2.13	0.49
1:C:36:GLN:HB2	1:C:39:ALA:HB2	1.95	0.49
1:D:59:ALA:HB1	1:D:307:LEU:HD22	1.95	0.49
1:A:268:GLY:H	1:A:309:GLU:CD	2.16	0.48
1:A:100:LEU:HD13	1:A:132:TYR:CD1	2.48	0.48
1:B:66:MSE:HA	2:B:502:FMN:C6	2.42	0.48
1:A:112:ARG:NH1	1:A:145:GLU:O	2.42	0.48
1:B:212:ALA:HA	1:B:262:SER:O	2.12	0.48
1:A:95:SER:OG	1:A:97:ARG:HB2	2.13	0.48
1:C:102:ARG:HB3	1:C:104:GLU:OE2	2.13	0.48
1:C:134:ARG:O	1:C:138:LEU:HG	2.13	0.48
1:A:35:TYR:HB3	1:B:241:ILE:CD1	2.43	0.48
1:C:106:LEU:HD12	1:C:106:LEU:H	1.78	0.48
1:C:176:GLU:CG	1:C:177:LEU:H	2.26	0.48
1:B:36:GLN:HB2	1:B:39:ALA:HB2	1.95	0.48
1:D:36:GLN:HB2	1:D:39:ALA:HB2	1.94	0.48
1:C:135:ASP:HA	1:C:138:LEU:HD12	1.96	0.48
1:B:126:LEU:O	1:B:128:GLN:N	2.47	0.48
1:A:157:GLN:NE2	1:A:189:VAL:HG21	2.28	0.48
1:D:212:ALA:HA	1:D:262:SER:O	2.13	0.48
1:A:66:MSE:HA	2:A:501:FMN:C6	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD23	1:B:153:VAL:HG21	1.96	0.48
1:A:326:ARG:HH11	1:A:326:ARG:CB	2.21	0.48
1:B:100:LEU:HD13	1:B:132:TYR:CD1	2.48	0.48
1:C:110:ARG:HB2	1:C:110:ARG:HH21	1.79	0.48
1:C:41:LEU:HD22	1:C:320:ARG:CD	2.42	0.48
1:A:204:LEU:HD12	1:A:204:LEU:N	2.28	0.48
1:A:241:ILE:CD1	1:D:35:TYR:HB3	2.44	0.48
1:B:268:GLY:H	1:B:309:GLU:CD	2.17	0.48
1:B:38:LEU:HD23	1:C:153:VAL:HG21	1.94	0.48
1:D:196:GLU:HA	1:D:199:LEU:HD12	1.96	0.48
1:B:95:SER:OG	1:B:97:ARG:HB2	2.13	0.48
1:A:126:LEU:O	1:A:128:GLN:N	2.47	0.48
1:B:67:THR:H	2:B:502:FMN:C6	2.23	0.48
1:D:141:VAL:HG21	1:D:182:PHE:CE2	2.48	0.47
1:C:126:LEU:O	1:C:128:GLN:N	2.48	0.47
1:B:176:GLU:CG	1:B:177:LEU:H	2.27	0.47
1:A:36:GLN:CB	1:A:39:ALA:HB2	2.44	0.47
1:B:262:SER:HB3	1:B:283:ALA:HB3	1.95	0.47
1:C:305:ASP:OD2	1:D:233:HIS:HE1	1.97	0.47
1:C:119:LEU:C	1:C:120:LEU:HD23	2.34	0.47
1:D:144:LEU:O	1:D:145:GLU:HB2	2.14	0.47
1:C:208:ALA:HB2	1:C:258:PRO:HG2	1.95	0.47
1:D:176:GLU:CG	1:D:177:LEU:H	2.28	0.47
1:C:157:GLN:HE21	1:C:189:VAL:HG21	1.79	0.47
1:B:36:GLN:CB	1:B:39:ALA:HB2	2.43	0.47
1:B:119:LEU:O	1:B:120:LEU:HD23	2.14	0.47
1:D:100:LEU:HD13	1:D:132:TYR:CD1	2.49	0.47
1:C:264:GLY:HA2	1:C:266:TYR:CE1	2.50	0.47
1:D:161:GLN:O	1:D:162:ARG:HB2	2.14	0.47
1:D:36:GLN:CB	1:D:39:ALA:HB2	2.45	0.47
1:D:119:LEU:O	1:D:120:LEU:HD23	2.13	0.47
1:D:204:LEU:HD12	1:D:204:LEU:N	2.30	0.47
1:B:317:ILE:HA	1:B:317:ILE:HD13	1.70	0.47
1:A:157:GLN:HE21	1:A:189:VAL:HG21	1.80	0.47
1:C:266:TYR:HE1	2:C:503:FMN:O1P	1.98	0.47
1:A:262:SER:HB3	1:A:283:ALA:HB3	1.97	0.47
1:C:204:LEU:N	1:C:204:LEU:HD12	2.30	0.47
1:B:317:ILE:HG23	1:B:328:ARG:HD2	1.96	0.47
1:C:217:THR:CG2	2:C:503:FMN:O3P	2.63	0.47
1:B:19:VAL:HB	1:B:222:VAL:CG2	2.45	0.47
1:D:208:ALA:HA	1:D:257:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:VAL:HG21	1:C:182:PHE:CE2	2.50	0.47
1:B:280:ASP:C	1:B:281:LEU:HD22	2.35	0.47
1:A:119:LEU:O	1:A:120:LEU:HD23	2.15	0.47
1:B:59:ALA:HB1	1:B:307:LEU:HD22	1.97	0.47
1:A:176:GLU:CG	1:A:177:LEU:H	2.28	0.46
1:B:154:ASN:HD22	1:B:157:GLN:HB3	1.79	0.46
1:A:217:THR:CG2	2:A:501:FMN:O3P	2.62	0.46
1:A:253:VAL:HG12	1:A:254:LEU:CD2	2.45	0.46
1:C:76:ILE:HG22	1:C:293:LEU:HD23	1.97	0.46
1:D:95:SER:OG	1:D:97:ARG:HB2	2.15	0.46
1:C:138:LEU:CD2	1:C:181:PRO:HG3	2.45	0.46
1:A:130:ARG:C	1:A:131:ARG:HG3	2.35	0.46
1:B:204:LEU:HD12	1:B:204:LEU:N	2.30	0.46
1:B:141:VAL:HG21	1:B:182:PHE:CE2	2.50	0.46
1:B:112:ARG:NH1	1:B:145:GLU:O	2.43	0.46
1:C:280:ASP:C	1:C:281:LEU:HD22	2.36	0.46
1:B:11:LEU:HD13	1:B:11:LEU:O	2.15	0.46
1:C:196:GLU:HA	1:C:199:LEU:HD12	1.98	0.46
1:D:135:ASP:HA	1:D:138:LEU:HD12	1.97	0.46
1:C:217:THR:HG22	2:C:503:FMN:O3P	2.16	0.46
1:B:34:ARG:NH1	1:C:196:GLU:OE2	2.49	0.46
1:A:59:ALA:HB1	1:A:307:LEU:HD22	1.97	0.46
1:D:168:ARG:O	1:D:170:LEU:HD12	2.16	0.46
1:C:264:GLY:HA2	1:C:266:TYR:CZ	2.50	0.46
1:A:332:VAL:HG12	1:A:332:VAL:OXT	2.15	0.46
1:B:99:LEU:CD1	1:B:106:LEU:HA	2.40	0.46
1:C:119:LEU:HD12	1:C:147:ASP:HB2	1.97	0.46
1:A:209:VAL:HG23	1:A:257:LEU:HD21	1.97	0.46
1:D:138:LEU:CD2	1:D:181:PRO:HG3	2.46	0.46
1:B:41:LEU:HD22	1:B:320:ARG:CD	2.45	0.46
1:D:119:LEU:HD12	1:D:147:ASP:HB2	1.98	0.46
1:B:196:GLU:HA	1:B:199:LEU:HD12	1.97	0.46
1:D:208:ALA:HB2	1:D:258:PRO:HG2	1.98	0.46
1:D:126:LEU:O	1:D:128:GLN:N	2.49	0.46
1:A:133:GLY:O	1:A:135:ASP:N	2.49	0.46
1:B:35:TYR:HB3	1:C:241:ILE:CD1	2.45	0.46
1:A:269:THR:HG21	1:B:235:GLU:HG2	1.98	0.46
1:C:187:LYS:HB3	1:C:210:ASP:HB3	1.98	0.45
1:B:187:LYS:HB3	1:B:210:ASP:HB3	1.98	0.45
1:C:19:VAL:HB	1:C:222:VAL:CG2	2.45	0.45
1:D:224:GLU:OE1	1:D:233:HIS:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ASN:OD1	1:C:323:LYS:HB2	2.16	0.45
1:A:75:ARG:CD	1:A:75:ARG:C	2.84	0.45
1:A:141:VAL:HG21	1:A:182:PHE:CE2	2.51	0.45
1:D:152:HIS:HA	1:D:187:LYS:O	2.16	0.45
1:D:134:ARG:O	1:D:138:LEU:HG	2.16	0.45
1:A:135:ASP:HA	1:A:138:LEU:HD12	1.98	0.45
1:A:138:LEU:CD2	1:A:181:PRO:HG3	2.46	0.45
1:C:152:HIS:HA	1:C:187:LYS:O	2.15	0.45
1:D:19:VAL:HB	1:D:222:VAL:CG2	2.46	0.45
1:C:208:ALA:HA	1:C:257:LEU:HD11	1.97	0.45
1:B:138:LEU:CD2	1:B:181:PRO:HG3	2.47	0.45
1:B:137:LEU:HD23	1:B:180:LEU:HD21	1.98	0.45
1:D:249:GLU:O	1:D:252:GLU:HB3	2.17	0.45
1:B:130:ARG:HG3	1:B:130:ARG:NH1	2.32	0.45
1:C:262:SER:HB3	1:C:283:ALA:HB3	1.96	0.45
1:C:317:ILE:HG23	1:C:328:ARG:HD2	1.96	0.45
1:D:41:LEU:HD22	1:D:320:ARG:CD	2.44	0.45
1:A:196:GLU:HA	1:A:199:LEU:HD12	1.98	0.45
1:A:217:THR:HG22	2:A:501:FMN:O3P	2.15	0.45
1:D:66:MSE:HA	2:D:504:FMN:C6	2.47	0.45
1:B:42:ALA:HB2	1:C:166:ASP:OD1	2.16	0.45
1:B:43:LEU:HB3	1:C:165:THR:CG2	2.47	0.45
1:D:253:VAL:HG12	1:D:254:LEU:CD2	2.47	0.45
1:A:19:VAL:HB	1:A:222:VAL:CG2	2.47	0.45
1:C:11:LEU:O	1:C:11:LEU:HD13	2.17	0.45
1:A:212:ALA:HA	1:A:262:SER:O	2.17	0.45
1:D:93:LEU:O	1:D:123:ASN:CB	2.65	0.45
1:D:264:GLY:HA2	1:D:266:TYR:CZ	2.52	0.44
1:C:59:ALA:HB1	1:C:307:LEU:HD22	1.99	0.44
1:C:54:GLY:O	1:C:55:LYS:CG	2.65	0.44
1:D:137:LEU:HD23	1:D:180:LEU:HD21	1.98	0.44
1:A:11:LEU:HD13	1:A:11:LEU:O	2.17	0.44
1:C:75:ARG:C	1:C:75:ARG:CD	2.84	0.44
1:D:133:GLY:O	1:D:135:ASP:N	2.51	0.44
1:D:11:LEU:O	1:D:11:LEU:HD13	2.17	0.44
1:B:326:ARG:CB	1:B:326:ARG:HH11	2.24	0.44
1:D:209:VAL:HG23	1:D:257:LEU:HD21	1.99	0.44
1:B:134:ARG:O	1:B:138:LEU:HG	2.17	0.44
1:B:139:ARG:O	1:B:143:MSE:HG3	2.18	0.44
1:A:134:ARG:O	1:A:138:LEU:HG	2.18	0.44
1:C:253:VAL:HG12	1:C:254:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:SER:HB3	1:D:283:ALA:HB3	1.98	0.44
1:A:194:SER:OG	1:A:196:GLU:HG2	2.18	0.44
1:D:321:ASN:OD1	1:D:323:LYS:HB2	2.18	0.44
1:B:99:LEU:HD21	1:B:106:LEU:HG	1.98	0.44
1:C:138:LEU:HD22	1:C:181:PRO:HG3	2.00	0.44
1:C:161:GLN:O	1:C:162:ARG:HB2	2.17	0.44
1:D:280:ASP:C	1:D:281:LEU:HD22	2.37	0.44
1:A:224:GLU:OE1	1:A:233:HIS:CD2	2.70	0.44
1:A:74:GLU:HG2	1:A:75:ARG:N	2.33	0.44
1:D:76:ILE:HG22	1:D:293:LEU:HD23	1.99	0.44
1:B:119:LEU:HD12	1:B:147:ASP:HB2	1.99	0.44
1:D:74:GLU:HG2	1:D:75:ARG:N	2.33	0.44
1:A:208:ALA:HA	1:A:257:LEU:HD11	2.00	0.43
1:D:139:ARG:O	1:D:143:MSE:HG3	2.18	0.43
1:D:130:ARG:C	1:D:131:ARG:HG3	2.38	0.43
1:D:187:LYS:HB3	1:D:210:ASP:HB3	2.01	0.43
1:B:48:LEU:O	1:B:50:THR:HG23	2.18	0.43
1:A:280:ASP:C	1:A:281:LEU:HD22	2.38	0.43
1:D:119:LEU:C	1:D:120:LEU:HD23	2.38	0.43
1:A:76:ILE:HG22	1:A:293:LEU:HD23	1.99	0.43
1:B:292:ALA:HA	1:B:299:VAL:CG2	2.49	0.43
1:C:128:GLN:C	1:C:130:ARG:H	2.21	0.43
1:B:106:LEU:CD1	1:B:143:MSE:SE	3.16	0.43
1:B:176:GLU:CG	1:B:177:LEU:N	2.82	0.43
1:C:95:SER:C	1:C:97:ARG:H	2.22	0.43
1:A:321:ASN:OD1	1:A:323:LYS:HB2	2.18	0.43
1:A:249:GLU:O	1:A:252:GLU:HB3	2.19	0.43
1:C:209:VAL:HG23	1:C:257:LEU:HD21	2.00	0.43
1:C:137:LEU:HD23	1:C:180:LEU:HD21	2.00	0.43
1:B:168:ARG:O	1:B:170:LEU:HD12	2.19	0.43
1:C:224:GLU:OE1	1:C:233:HIS:CD2	2.72	0.43
1:B:161:GLN:O	1:B:162:ARG:HB2	2.18	0.43
1:D:228:PHE:CD2	1:D:232:ARG:NE	2.86	0.43
1:B:133:GLY:O	1:B:135:ASP:N	2.52	0.43
1:A:161:GLN:O	1:A:162:ARG:HB2	2.19	0.43
1:A:264:GLY:HA2	1:A:266:TYR:CZ	2.53	0.43
1:D:54:GLY:O	1:D:55:LYS:CG	2.67	0.43
1:B:45:GLU:OE2	1:C:168:ARG:HD3	2.19	0.43
1:A:168:ARG:O	1:A:170:LEU:HD12	2.18	0.43
1:D:274:ALA:HB3	1:D:282:LEU:HD11	2.01	0.43
1:B:74:GLU:HG2	1:B:75:ARG:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG23	1:A:257:LEU:CD2	2.49	0.42
1:D:266:TYR:CD1	1:D:287:PRO:HG2	2.53	0.42
1:B:102:ARG:O	1:B:104:GLU:N	2.52	0.42
1:A:138:LEU:HD22	1:A:181:PRO:HG3	2.01	0.42
1:B:152:HIS:HA	1:B:187:LYS:O	2.19	0.42
1:B:208:ALA:HB2	1:B:258:PRO:HG2	2.01	0.42
1:D:66:MSE:HA	2:D:504:FMN:C5A	2.49	0.42
1:B:194:SER:OG	1:B:196:GLU:HG2	2.19	0.42
1:C:35:TYR:HB3	1:D:241:ILE:CD1	2.50	0.42
1:C:292:ALA:HA	1:C:299:VAL:CG2	2.49	0.42
1:D:292:ALA:HA	1:D:299:VAL:CG2	2.49	0.42
1:B:135:ASP:HA	1:B:138:LEU:HD12	2.00	0.42
1:D:138:LEU:HD22	1:D:181:PRO:HG3	2.01	0.42
1:B:111:VAL:O	1:B:111:VAL:HG22	2.20	0.42
1:B:172:GLU:N	1:B:172:GLU:CD	2.71	0.42
1:D:124:LEU:HD11	1:D:128:GLN:HB2	2.01	0.42
1:A:187:LYS:HB3	1:A:210:ASP:HB3	2.01	0.42
1:A:124:LEU:HD11	1:A:128:GLN:HB2	2.02	0.42
1:A:317:ILE:HG23	1:A:328:ARG:HD2	2.00	0.42
1:A:95:SER:C	1:A:97:ARG:H	2.22	0.42
1:C:249:GLU:O	1:C:252:GLU:HB3	2.20	0.42
1:C:74:GLU:HG2	1:C:75:ARG:N	2.33	0.42
1:B:93:LEU:O	1:B:123:ASN:CB	2.68	0.42
1:B:119:LEU:C	1:B:120:LEU:HD23	2.39	0.42
1:A:119:LEU:C	1:A:120:LEU:HD23	2.40	0.42
1:A:290:ARG:N	1:A:291:PRO:HD2	2.35	0.42
1:A:54:GLY:O	1:A:55:LYS:CG	2.68	0.42
1:D:332:VAL:OXT	1:D:332:VAL:HG12	2.19	0.42
1:C:130:ARG:NH1	1:C:130:ARG:HG3	2.34	0.42
1:B:138:LEU:HD22	1:B:181:PRO:HG3	2.02	0.42
1:D:126:LEU:CD2	1:D:170:LEU:HB3	2.50	0.42
1:C:176:GLU:CG	1:C:177:LEU:N	2.82	0.42
1:B:217:THR:HB	1:B:286:ARG:NH1	2.35	0.42
1:D:264:GLY:HA2	1:D:266:TYR:CE1	2.55	0.42
1:B:106:LEU:HD11	1:B:143:MSE:CG	2.50	0.42
1:B:19:VAL:CB	1:B:222:VAL:HG22	2.49	0.42
1:B:228:PHE:CD2	1:B:232:ARG:NE	2.88	0.42
1:A:35:TYR:HB3	1:B:241:ILE:HD12	2.02	0.42
1:A:139:ARG:O	1:A:143:MSE:HG3	2.19	0.42
1:C:41:LEU:CD2	1:C:320:ARG:HD3	2.47	0.42
1:B:130:ARG:C	1:B:131:ARG:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HG22	1:B:293:LEU:HD23	2.00	0.42
1:C:185:MSE:HB2	1:C:208:ALA:O	2.20	0.41
1:C:130:ARG:C	1:C:131:ARG:HG3	2.39	0.41
1:C:168:ARG:O	1:C:170:LEU:HD12	2.19	0.41
1:B:219:TRP:O	1:B:223:GLU:HB2	2.19	0.41
1:C:332:VAL:OXT	1:C:332:VAL:HG12	2.20	0.41
1:B:211:VAL:HG12	1:B:250:VAL:HG21	2.01	0.41
1:C:326:ARG:CB	1:C:326:ARG:HH11	2.23	0.41
1:C:11:LEU:HD13	1:C:11:LEU:C	2.41	0.41
1:A:196:GLU:OE2	1:D:34:ARG:NH1	2.54	0.41
1:A:211:VAL:HG12	1:A:250:VAL:HG21	2.01	0.41
1:D:176:GLU:CG	1:D:177:LEU:N	2.82	0.41
1:D:194:SER:OG	1:D:196:GLU:HG2	2.20	0.41
1:A:137:LEU:HD23	1:A:180:LEU:HD21	2.01	0.41
1:C:217:THR:HG23	2:C:503:FMN:H5'1	2.02	0.41
1:A:100:LEU:HB3	1:A:132:TYR:HE1	1.86	0.41
1:A:82:GLU:HB2	1:A:114:VAL:HG11	2.03	0.41
1:C:317:ILE:HD13	1:C:317:ILE:HA	1.71	0.41
1:D:317:ILE:HG23	1:D:328:ARG:HB3	2.03	0.41
1:D:128:GLN:C	1:D:130:ARG:H	2.24	0.41
1:D:112:ARG:HD3	1:D:112:ARG:HA	1.60	0.41
1:B:264:GLY:HA2	1:B:266:TYR:CZ	2.56	0.41
1:C:161:GLN:HA	1:C:223:GLU:HG3	2.02	0.41
1:C:19:VAL:CB	1:C:222:VAL:HG22	2.49	0.41
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.34	0.41
1:B:100:LEU:HB3	1:B:132:TYR:HE1	1.85	0.41
1:B:95:SER:C	1:B:97:ARG:H	2.23	0.41
1:A:196:GLU:H	1:A:196:GLU:CD	2.23	0.41
1:C:48:LEU:HB3	1:C:59:ALA:HA	2.03	0.41
1:B:54:GLY:O	1:B:55:LYS:CG	2.68	0.41
1:D:48:LEU:O	1:D:50:THR:HG23	2.19	0.41
1:B:208:ALA:HA	1:B:257:LEU:HD11	2.02	0.41
1:A:98:ILE:O	1:A:98:ILE:HG22	2.20	0.41
1:B:266:TYR:CD1	1:B:287:PRO:HG2	2.56	0.41
1:D:60:PRO:HA	1:D:281:LEU:HD13	2.03	0.41
1:D:266:TYR:HE1	2:D:504:FMN:O1P	2.04	0.41
1:B:224:GLU:OE1	1:B:233:HIS:CD2	2.70	0.41
1:A:93:LEU:O	1:A:123:ASN:CB	2.69	0.41
1:A:111:VAL:O	1:A:111:VAL:HG22	2.20	0.41
1:B:82:GLU:HB2	1:B:114:VAL:HG11	2.01	0.41
1:A:152:HIS:HA	1:A:187:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLY:HA2	1:A:266:TYR:CE1	2.55	0.41
1:C:211:VAL:HG12	1:C:250:VAL:HG21	2.01	0.41
1:D:209:VAL:HG23	1:D:257:LEU:CD2	2.51	0.41
1:B:317:ILE:HG23	1:B:328:ARG:HB3	2.02	0.41
1:C:133:GLY:O	1:C:135:ASP:N	2.53	0.41
1:D:11:LEU:C	1:D:11:LEU:HD13	2.41	0.41
1:D:172:GLU:N	1:D:172:GLU:CD	2.72	0.41
1:D:87:LEU:HD11	1:D:300:ALA:HB1	2.02	0.41
1:D:317:ILE:HD13	1:D:317:ILE:HA	1.70	0.41
1:A:176:GLU:CG	1:A:177:LEU:N	2.83	0.41
1:D:19:VAL:CB	1:D:222:VAL:HG22	2.50	0.41
1:D:95:SER:C	1:D:97:ARG:H	2.23	0.41
1:A:266:TYR:CD1	1:A:287:PRO:HG2	2.56	0.41
1:B:332:VAL:HG12	1:B:332:VAL:OXT	2.21	0.41
1:B:321:ASN:OD1	1:B:323:LYS:HB2	2.21	0.41
1:A:34:ARG:HH22	1:B:249:GLU:CD	2.24	0.41
1:B:106:LEU:HD11	1:B:143:MSE:CB	2.49	0.40
1:D:187:LYS:HB2	1:D:210:ASP:HB3	2.03	0.40
1:B:187:LYS:HB2	1:B:210:ASP:HB3	2.02	0.40
1:D:161:GLN:HA	1:D:223:GLU:HG3	2.03	0.40
1:B:11:LEU:HD13	1:B:11:LEU:C	2.41	0.40
1:C:126:LEU:CD2	1:C:170:LEU:HB3	2.51	0.40
1:B:106:LEU:HD11	1:B:143:MSE:SE	2.71	0.40
1:A:133:GLY:O	1:A:134:ARG:C	2.59	0.40
1:C:139:ARG:O	1:C:143:MSE:HG3	2.21	0.40
1:B:126:LEU:CD2	1:B:170:LEU:HB3	2.51	0.40
1:D:326:ARG:CB	1:D:326:ARG:HH11	2.22	0.40
1:C:111:VAL:HG22	1:C:111:VAL:O	2.21	0.40
1:C:187:LYS:HB2	1:C:210:ASP:HB3	2.01	0.40
1:A:219:TRP:O	1:A:223:GLU:HB2	2.20	0.40
1:C:172:GLU:CD	1:C:172:GLU:N	2.73	0.40
1:D:196:GLU:CD	1:D:196:GLU:H	2.25	0.40
1:B:102:ARG:C	1:B:104:GLU:N	2.74	0.40
1:C:290:ARG:N	1:C:291:PRO:HD2	2.36	0.40
1:A:185:MSE:HB2	1:A:208:ALA:O	2.20	0.40
1:C:124:LEU:HD11	1:C:128:GLN:HB2	2.03	0.40
1:A:126:LEU:CD2	1:A:170:LEU:HB3	2.51	0.40
1:C:219:TRP:O	1:C:223:GLU:HB2	2.22	0.40
1:B:87:LEU:HD11	1:B:300:ALA:HB1	2.03	0.40
1:B:34:ARG:HH22	1:C:249:GLU:CD	2.23	0.40
1:C:317:ILE:HG23	1:C:328:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:GLU:C	1:D:178:LEU:N	2.75	0.40
1:C:217:THR:HB	1:C:286:ARG:NH1	2.36	0.40
1:A:87:LEU:HD11	1:A:300:ALA:HB1	2.03	0.40
1:B:48:LEU:HB3	1:B:59:ALA:HA	2.04	0.40
1:A:274:ALA:HB3	1:A:282:LEU:HD11	2.04	0.40
1:A:317:ILE:HG23	1:A:328:ARG:HB3	2.04	0.40
1:B:60:PRO:HA	1:B:281:LEU:HD13	2.04	0.40
1:D:93:LEU:O	1:D:123:ASN:HB2	2.22	0.40
1:A:34:ARG:NH2	1:B:249:GLU:OE2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/332 (92%)	281 (92%)	19 (6%)	5 (2%)	12	46
1	B	314/332 (95%)	288 (92%)	21 (7%)	5 (2%)	12	46
1	C	310/332 (93%)	283 (91%)	22 (7%)	5 (2%)	12	46
1	D	305/332 (92%)	278 (91%)	22 (7%)	5 (2%)	12	46
All	All	1234/1328 (93%)	1130 (92%)	84 (7%)	20 (2%)	12	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	A	178	LEU
1	A	179	PRO
1	B	134	ARG
1	B	178	LEU
1	B	179	PRO

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Mol	Chain	Res	Type
1	C	134	ARG
1	C	178	LEU
1	C	179	PRO
1	D	134	ARG
1	D	178	LEU
1	D	179	PRO
1	A	127	ALA
1	A	177	LEU
1	B	127	ALA
1	B	177	LEU
1	C	127	ALA
1	C	177	LEU
1	D	127	ALA
1	D	177	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/246 (96%)	218 (93%)	17 (7%)	18	52
1	B	241/246 (98%)	223 (92%)	18 (8%)	17	50
1	C	239/246 (97%)	222 (93%)	17 (7%)	18	53
1	D	235/246 (96%)	218 (93%)	17 (7%)	18	52
All	All	950/984 (96%)	881 (93%)	69 (7%)	17	51

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	15	LEU
1	A	32	ARG
1	A	74	GLU
1	A	75	ARG
1	A	112	ARG
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	178	LEU
1	A	179	PRO
1	A	180	LEU
1	A	196	GLU
1	A	217	THR
1	A	245	ARG
1	A	298	ARG
1	A	317	ILE
1	A	320	ARG
1	A	326	ARG
1	B	9	LYS
1	B	15	LEU
1	B	32	ARG
1	B	74	GLU
1	B	75	ARG
1	B	107	ARG
1	B	112	ARG
1	B	156	LEU
1	B	178	LEU
1	B	179	PRO
1	B	180	LEU
1	B	196	GLU
1	B	217	THR
1	B	245	ARG
1	B	298	ARG
1	B	317	ILE
1	B	320	ARG
1	B	326	ARG
1	C	9	LYS
1	C	15	LEU
1	C	32	ARG
1	C	74	GLU
1	C	75	ARG
1	C	106	LEU
1	C	112	ARG
1	C	156	LEU
1	C	178	LEU
1	C	179	PRO
1	C	180	LEU
1	C	196	GLU
1	C	217	THR
1	C	245	ARG

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Mol	Chain	Res	Type
1	C	298	ARG
1	C	320	ARG
1	C	326	ARG
1	D	15	LEU
1	D	32	ARG
1	D	74	GLU
1	D	75	ARG
1	D	112	ARG
1	D	156	LEU
1	D	178	LEU
1	D	179	PRO
1	D	180	LEU
1	D	196	GLU
1	D	217	THR
1	D	245	ARG
1	D	298	ARG
1	D	317	ILE
1	D	320	ARG
1	D	326	ARG
1	D	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	154	ASN
1	A	157	GLN
1	A	191	HIS
1	A	233	HIS
1	B	77	ASN
1	B	154	ASN
1	B	157	GLN
1	B	191	HIS
1	B	233	HIS
1	C	77	ASN
1	C	154	ASN
1	C	157	GLN
1	C	191	HIS
1	C	233	HIS
1	D	77	ASN
1	D	154	ASN
1	D	157	GLN

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Mol	Chain	Res	Type
1	D	191	HIS
1	D	233	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	501	-	32,33,33	2.78	10 (31%)	34,50,50	4.36	17 (50%)
2	FMN	B	502	-	32,33,33	2.69	10 (31%)	34,50,50	4.34	17 (50%)
2	FMN	C	503	-	32,33,33	2.70	9 (28%)	34,50,50	4.38	17 (50%)
2	FMN	D	504	-	32,33,33	2.68	9 (28%)	34,50,50	4.33	17 (50%)

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	501	-	-	0/18/18/18	0/3/3/3
2	FMN	B	502	-	-	0/18/18/18	0/3/3/3
2	FMN	C	503	-	-	0/18/18/18	0/3/3/3
2	FMN	D	504	-	-	0/18/18/18	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FMN	C4A-N5	-2.00	1.30	1.33
2	A	501	FMN	C9A-N10	2.07	1.41	1.38
2	A	501	FMN	C8-C7	2.48	1.47	1.41
2	B	502	FMN	C8-C7	2.53	1.47	1.41
2	D	504	FMN	C8-C7	2.61	1.48	1.41
2	C	503	FMN	C8-C7	2.63	1.48	1.41
2	A	501	FMN	C6-C7	2.68	1.45	1.37
2	C	503	FMN	C6-C7	2.75	1.45	1.37
2	C	503	FMN	C5'-C4'	2.79	1.56	1.51
2	B	502	FMN	C6-C7	2.80	1.45	1.37
2	B	502	FMN	C5'-C4'	2.84	1.56	1.51
2	D	504	FMN	C6-C7	2.94	1.46	1.37
2	D	504	FMN	C5'-C4'	3.13	1.56	1.51
2	A	501	FMN	C5'-C4'	3.38	1.56	1.51
2	B	502	FMN	C9A-C5A	3.84	1.50	1.42
2	D	504	FMN	C9A-C5A	3.93	1.50	1.42
2	C	503	FMN	C9A-C5A	3.95	1.50	1.42
2	A	501	FMN	C9A-C5A	3.95	1.50	1.42
2	C	503	FMN	C9-C9A	4.67	1.50	1.40
2	B	502	FMN	C2-N3	4.69	1.47	1.38
2	D	504	FMN	C9-C9A	4.71	1.51	1.40
2	D	504	FMN	C2-N3	4.74	1.48	1.38
2	D	504	FMN	C5A-N5	4.76	1.42	1.35
2	B	502	FMN	C9-C9A	4.78	1.51	1.40
2	A	501	FMN	C9-C9A	4.80	1.51	1.40
2	C	503	FMN	C5A-N5	4.86	1.43	1.35
2	C	503	FMN	C2-N3	4.97	1.48	1.38
2	A	501	FMN	C2-N3	4.97	1.48	1.38
2	A	501	FMN	C5A-N5	4.98	1.43	1.35
2	B	502	FMN	C5A-N5	5.02	1.43	1.35
2	B	502	FMN	C4-N3	5.89	1.43	1.33
2	C	503	FMN	C4-N3	6.08	1.44	1.33
2	D	504	FMN	C4-N3	6.19	1.44	1.33
2	A	501	FMN	C4-N3	6.41	1.44	1.33
2	D	504	FMN	C4A-C10	7.34	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FMN	C4A-C10	7.38	1.54	1.40
2	C	503	FMN	C4A-C10	7.52	1.54	1.40
2	A	501	FMN	C4A-C10	7.64	1.55	1.40

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FMN	O3P-P-O1P	-9.39	79.99	110.63
2	B	502	FMN	O3P-P-O1P	-9.15	80.77	110.63
2	C	503	FMN	O3P-P-O5'	-9.13	80.08	106.72
2	B	502	FMN	O3P-P-O5'	-9.09	80.18	106.72
2	C	503	FMN	O3P-P-O1P	-9.07	81.03	110.63
2	D	504	FMN	O3P-P-O5'	-8.98	80.53	106.72
2	D	504	FMN	O3P-P-O1P	-8.96	81.38	110.63
2	A	501	FMN	O3P-P-O5'	-8.92	80.68	106.72
2	C	503	FMN	N3-C2-N1	-5.92	117.72	127.69
2	D	504	FMN	N3-C2-N1	-5.88	117.80	127.69
2	A	501	FMN	N3-C2-N1	-5.79	117.94	127.69
2	C	503	FMN	C4A-C4-N3	-5.74	116.02	123.52
2	A	501	FMN	C4A-C4-N3	-5.74	116.02	123.52
2	B	502	FMN	C4A-C4-N3	-5.72	116.05	123.52
2	B	502	FMN	N3-C2-N1	-5.67	118.15	127.69
2	D	504	FMN	C4A-C4-N3	-5.63	116.16	123.52
2	D	504	FMN	O3P-P-O2P	-5.42	87.55	107.44
2	B	502	FMN	O3P-P-O2P	-5.26	88.14	107.44
2	C	503	FMN	O3P-P-O2P	-5.17	88.47	107.44
2	A	501	FMN	O3P-P-O2P	-5.14	88.57	107.44
2	A	501	FMN	C7M-C7-C6	-4.36	108.00	120.33
2	B	502	FMN	C7M-C7-C6	-4.35	108.04	120.33
2	C	503	FMN	C7M-C7-C6	-4.32	108.13	120.33
2	D	504	FMN	C7M-C7-C6	-4.30	108.17	120.33
2	A	501	FMN	C9A-C5A-N5	-3.19	116.99	122.18
2	B	502	FMN	C9A-C5A-N5	-3.18	117.01	122.18
2	C	503	FMN	C9A-C5A-N5	-3.11	117.11	122.18
2	D	504	FMN	C9A-C5A-N5	-3.09	117.15	122.18
2	B	502	FMN	O3'-C3'-C4'	-2.75	101.60	108.73
2	D	504	FMN	O3'-C3'-C4'	-2.67	101.80	108.73
2	C	503	FMN	O3'-C3'-C4'	-2.60	101.99	108.73
2	A	501	FMN	O3'-C3'-C4'	-2.51	102.21	108.73
2	C	503	FMN	O2P-P-O1P	2.15	117.64	110.63
2	B	502	FMN	O2P-P-O1P	2.16	117.67	110.63
2	D	504	FMN	O2P-P-O1P	2.47	118.70	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FMN	O2P-P-O1P	2.49	118.75	110.63
2	D	504	FMN	C6-C5A-N5	2.86	122.49	118.92
2	C	503	FMN	C6-C5A-N5	2.93	122.56	118.92
2	B	502	FMN	C6-C5A-N5	2.97	122.61	118.92
2	A	501	FMN	C6-C5A-N5	3.00	122.66	118.92
2	C	503	FMN	O2P-P-O5'	3.23	116.15	106.72
2	D	504	FMN	O2P-P-O5'	3.25	116.22	106.72
2	B	502	FMN	O2P-P-O5'	3.27	116.27	106.72
2	A	501	FMN	O2P-P-O5'	3.35	116.49	106.72
2	D	504	FMN	C4A-N5-C5A	3.38	120.71	116.72
2	C	503	FMN	C4A-N5-C5A	3.41	120.74	116.72
2	B	502	FMN	C4A-N5-C5A	3.42	120.75	116.72
2	A	501	FMN	C4A-N5-C5A	3.46	120.80	116.72
2	C	503	FMN	C7M-C7-C8	4.96	131.39	120.73
2	A	501	FMN	C7M-C7-C8	4.97	131.41	120.73
2	D	504	FMN	C7M-C7-C8	4.98	131.44	120.73
2	B	502	FMN	C7M-C7-C8	4.99	131.46	120.73
2	A	501	FMN	O5'-P-O1P	5.28	120.37	107.08
2	D	504	FMN	O5'-P-O1P	5.46	120.81	107.08
2	B	502	FMN	O5'-P-O1P	5.77	121.58	107.08
2	C	503	FMN	O5'-P-O1P	5.90	121.92	107.08
2	D	504	FMN	C5A-C9A-N10	8.25	123.76	117.58
2	B	502	FMN	C5A-C9A-N10	8.33	123.82	117.58
2	A	501	FMN	C5A-C9A-N10	8.42	123.89	117.58
2	C	503	FMN	C5A-C9A-N10	8.45	123.91	117.58
2	B	502	FMN	C4-N3-C2	8.91	122.59	115.16
2	A	501	FMN	C4-N3-C2	9.05	122.71	115.16
2	D	504	FMN	C4-N3-C2	9.08	122.74	115.16
2	C	503	FMN	C4-N3-C2	9.30	122.92	115.16
2	B	502	FMN	C1'-N10-C9A	9.30	129.62	118.83
2	D	504	FMN	C1'-N10-C9A	9.46	129.80	118.83
2	C	503	FMN	C1'-N10-C9A	9.50	129.84	118.83
2	A	501	FMN	C1'-N10-C9A	9.65	130.02	118.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	FMN	8	0
2	C	503	FMN	9	0
2	D	504	FMN	5	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	306/332 (92%)	-0.38	0	100	100	28, 50, 78, 97	0
1	B	313/332 (94%)	-0.46	0	100	100	29, 50, 80, 96	0
1	C	311/332 (93%)	-0.38	1 (0%)	94	84	31, 52, 81, 97	0
1	D	306/332 (92%)	-0.34	1 (0%)	94	84	33, 53, 79, 98	0
All	All	1236/1328 (93%)	-0.39	2 (0%)	95	87	28, 51, 80, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ILE	2.5
1	D	101	GLU	2.1

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FMN	B	502	31/31	0.89	0.28	4.35	60,89,93,94	0
2	FMN	C	503	31/31	0.84	0.33	2.97	60,91,94,94	0
2	FMN	D	504	31/31	0.86	0.28	2.31	61,91,93,93	0
2	FMN	A	501	31/31	0.89	0.26	1.72	56,91,93,94	0

6.5 Other polymers (i)

There are no such residues in this entry.