



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:51 PM UTC

PDB ID : 3PQD / pdb_00003pqd
Title : Crystal structure of L-lactate dehydrogenase from *Bacillus subtilis* complexed with FBP and NAD⁺
Authors : Zhang, Y.; Garavito, R.M.
Deposited on : 2010-11-26
Resolution : 2.38 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

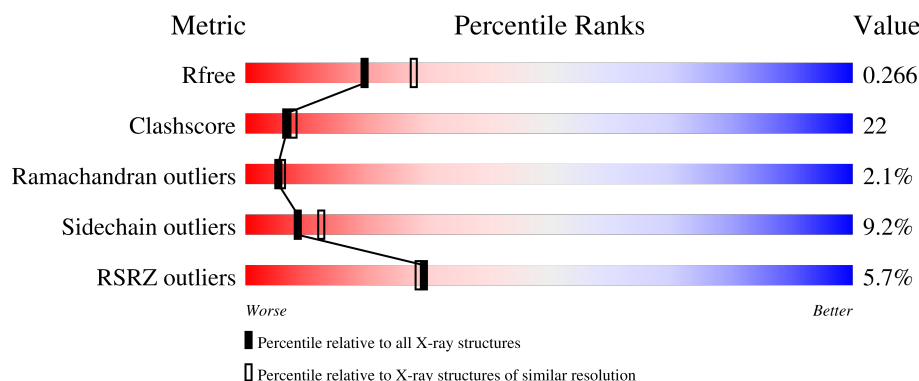
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	326	
1	B	326	
1	C	326	
1	D	326	
1	E	326	

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Mol	Chain	Length	Quality of chain
1	F	326	
1	G	326	
1	H	326	

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	FBP	C	327	-	-	X	-
2	FBP	D	328	X	-	-	-
2	FBP	F	327	X	-	-	-
2	FBP	G	327	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19005 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2367	1508	396	455	8			
1	B	312	Total	C	N	O	S	0	0	0
			2384	1520	399	457	8			
1	C	301	Total	C	N	O	S	0	0	0
			2300	1468	383	441	8			
1	D	301	Total	C	N	O	S	0	0	0
			2306	1475	382	441	8			
1	E	311	Total	C	N	O	S	0	0	0
			2379	1517	398	456	8			
1	F	311	Total	C	N	O	S	0	0	0
			2379	1517	398	456	8			
1	G	302	Total	C	N	O	S	0	0	0
			2315	1479	385	443	8			
1	H	301	Total	C	N	O	S	0	0	0
			2307	1475	383	441	8			

There are 48 discrepancies between the modelled and reference sequences:

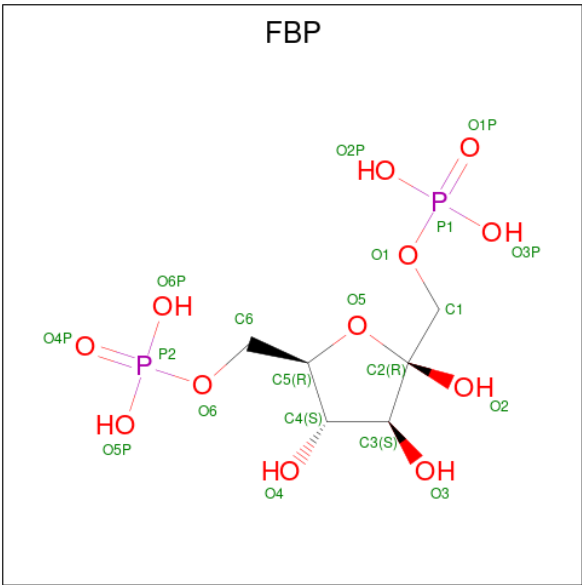
Chain	Residue	Modelled	Actual	Comment	Reference
A	321	HIS	-	expression tag	UNP P13714
A	322	HIS	-	expression tag	UNP P13714
A	323	HIS	-	expression tag	UNP P13714
A	324	HIS	-	expression tag	UNP P13714
A	325	HIS	-	expression tag	UNP P13714
A	326	HIS	-	expression tag	UNP P13714
B	321	HIS	-	expression tag	UNP P13714
B	322	HIS	-	expression tag	UNP P13714
B	323	HIS	-	expression tag	UNP P13714
B	324	HIS	-	expression tag	UNP P13714
B	325	HIS	-	expression tag	UNP P13714
B	326	HIS	-	expression tag	UNP P13714
C	321	HIS	-	expression tag	UNP P13714

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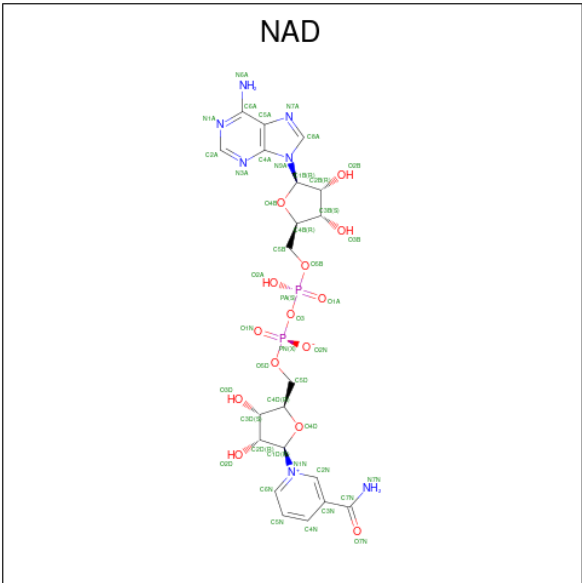
Chain	Residue	Modelled	Actual	Comment	Reference
C	322	HIS	-	expression tag	UNP P13714
C	323	HIS	-	expression tag	UNP P13714
C	324	HIS	-	expression tag	UNP P13714
C	325	HIS	-	expression tag	UNP P13714
C	326	HIS	-	expression tag	UNP P13714
D	321	HIS	-	expression tag	UNP P13714
D	322	HIS	-	expression tag	UNP P13714
D	323	HIS	-	expression tag	UNP P13714
D	324	HIS	-	expression tag	UNP P13714
D	325	HIS	-	expression tag	UNP P13714
D	326	HIS	-	expression tag	UNP P13714
E	321	HIS	-	expression tag	UNP P13714
E	322	HIS	-	expression tag	UNP P13714
E	323	HIS	-	expression tag	UNP P13714
E	324	HIS	-	expression tag	UNP P13714
E	325	HIS	-	expression tag	UNP P13714
E	326	HIS	-	expression tag	UNP P13714
F	321	HIS	-	expression tag	UNP P13714
F	322	HIS	-	expression tag	UNP P13714
F	323	HIS	-	expression tag	UNP P13714
F	324	HIS	-	expression tag	UNP P13714
F	325	HIS	-	expression tag	UNP P13714
F	326	HIS	-	expression tag	UNP P13714
G	321	HIS	-	expression tag	UNP P13714
G	322	HIS	-	expression tag	UNP P13714
G	323	HIS	-	expression tag	UNP P13714
G	324	HIS	-	expression tag	UNP P13714
G	325	HIS	-	expression tag	UNP P13714
G	326	HIS	-	expression tag	UNP P13714
H	321	HIS	-	expression tag	UNP P13714
H	322	HIS	-	expression tag	UNP P13714
H	323	HIS	-	expression tag	UNP P13714
H	324	HIS	-	expression tag	UNP P13714
H	325	HIS	-	expression tag	UNP P13714
H	326	HIS	-	expression tag	UNP P13714

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		

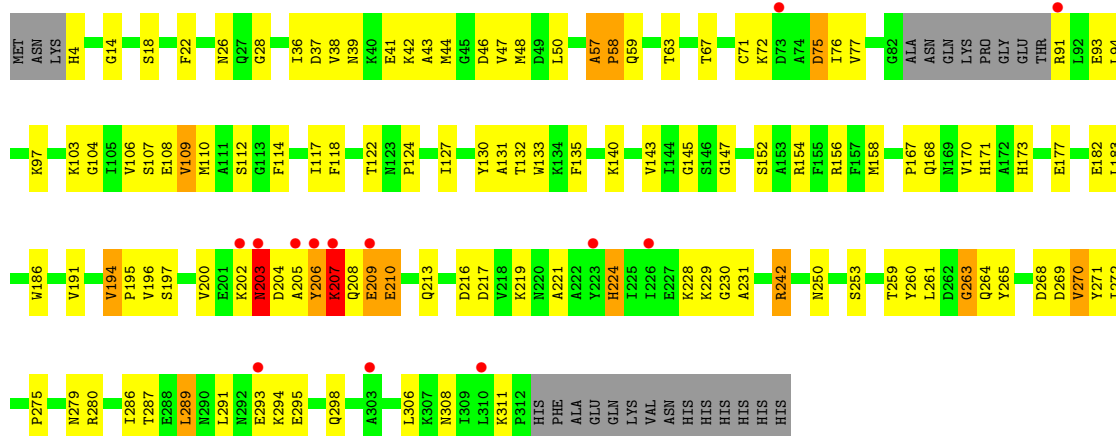
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



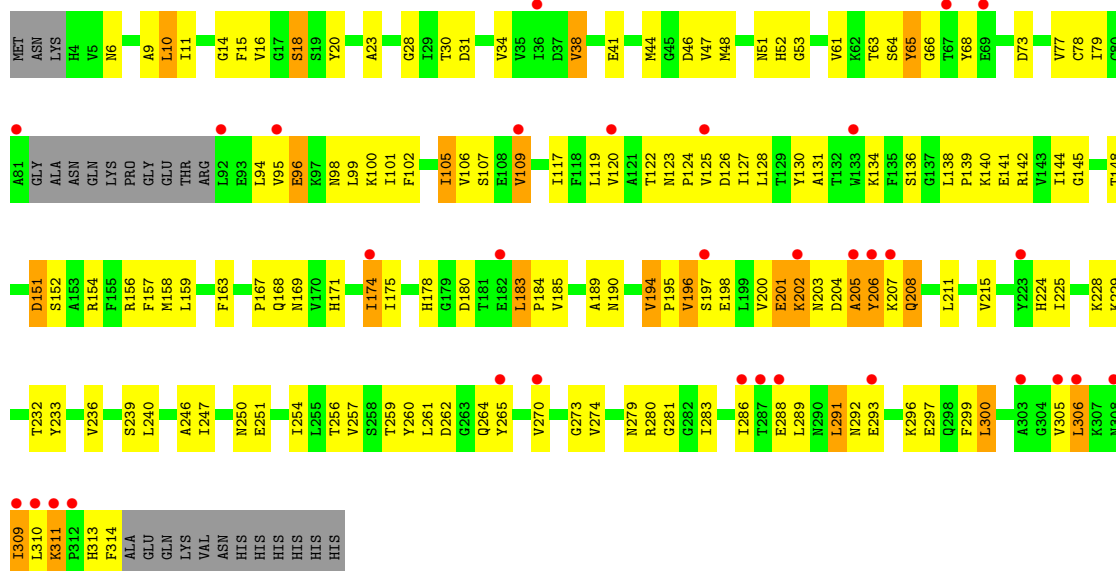
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

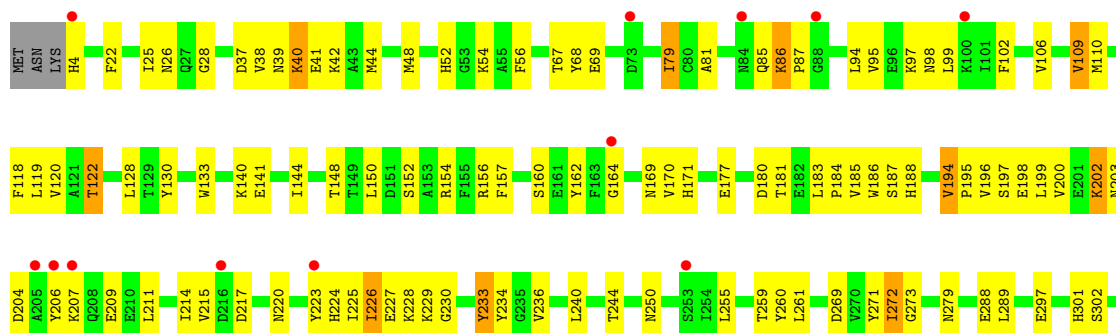
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	20	Total	O	0	0
			20	20		
4	C	24	Total	O	0	0
			24	24		
4	D	7	Total	O	0	0
			7	7		
4	E	13	Total	O	0	0
			13	13		
4	F	27	Total	O	0	0
			27	27		
4	G	20	Total	O	0	0
			20	20		
4	H	11	Total	O	0	0
			11	11		



• Molecule 1: L-lactate dehydrogenase

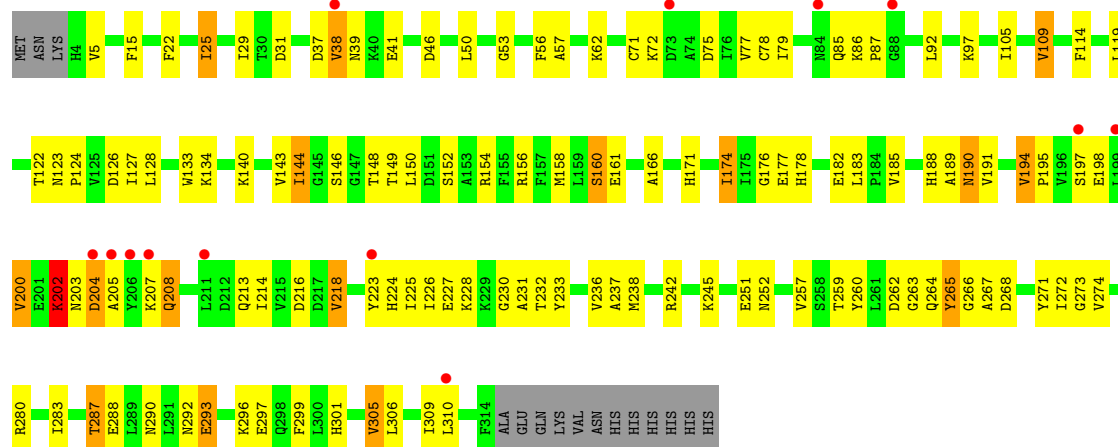


• Molecule 1: L-lactate dehydrogenase

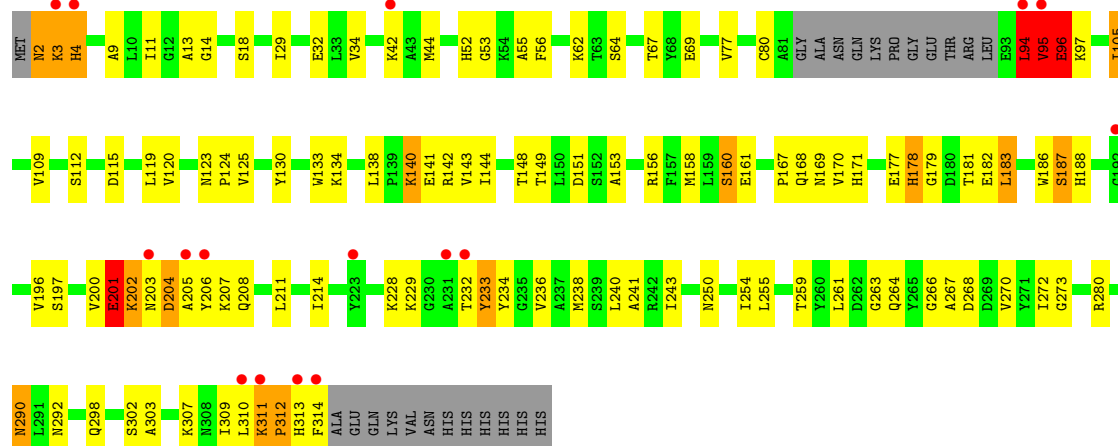




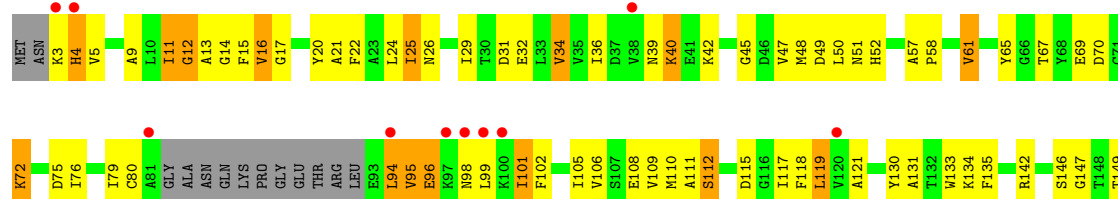
• Molecule 1: L-lactate dehydrogenase

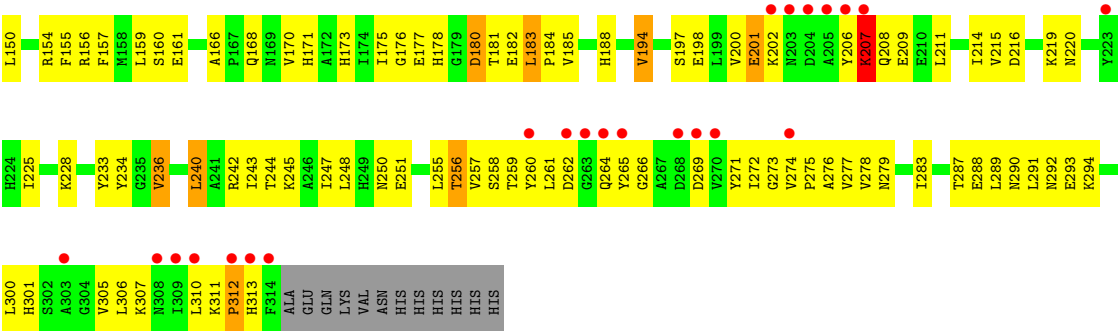


• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	171.04Å 171.04Å 96.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.45 – 2.38 29.45 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.45-2.38) 99.5 (29.45-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.214 , 0.269 0.212 , 0.266	Depositor DCC
R_{free} test set	3816 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.146 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19005	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

5.1 Standard geometry

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

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	0.44	0/2412	0.88	3/3269 (0.1%)
1	B	0.48	0/2431	0.86	2/3296 (0.1%)
1	C	0.52	2/2343 (0.1%)	0.89	7/3175 (0.2%)
1	D	0.39	0/2351	0.81	1/3187 (0.0%)
1	E	0.43	0/2426	0.83	0/3289
1	F	0.47	0/2426	0.90	2/3289 (0.1%)
1	G	0.46	0/2360	0.86	4/3198 (0.1%)
1	H	0.38	0/2352	0.82	2/3187 (0.1%)
All	All	0.45	2/19101 (0.0%)	0.86	21/25890 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	LYS	C-N	9.70	1.46	1.34
1	C	206	TYR	C-N	-8.34	1.22	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	LYS	O-C-N	7.74	132.88	122.59
1	G	94	LEU	N-CA-C	7.61	121.32	109.07
1	C	206	TYR	CA-C-N	7.34	135.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	TYR	C-N-CA	7.34	135.57	121.54
1	C	57	ALA	CA-C-N	6.93	128.50	119.84
1	C	57	ALA	C-N-CA	6.93	128.50	119.84
1	A	5	VAL	N-CA-C	6.70	118.13	108.48
1	B	279	ASN	N-CA-C	6.54	117.09	108.07
1	G	95	VAL	N-CA-C	6.36	122.56	109.34
1	B	209	GLU	N-CA-C	-6.22	106.91	114.75
1	F	57	ALA	CA-C-N	6.04	126.15	119.87
1	F	57	ALA	C-N-CA	6.04	126.15	119.87
1	C	203	ASN	CB-CA-C	-5.96	108.70	115.79
1	H	208	GLN	N-CA-C	5.91	118.23	111.02
1	G	105	ILE	N-CA-C	5.90	115.96	110.42
1	D	174	ILE	N-CA-C	-5.83	100.03	108.71
1	H	75	ASP	N-CA-C	-5.63	106.57	113.50
1	A	190	ASN	N-CA-C	5.49	116.88	108.42
1	A	174	ILE	N-CA-C	-5.45	100.62	108.53
1	C	263	GLY	N-CA-C	-5.37	107.27	114.25
1	G	120	VAL	N-CA-C	5.27	115.55	108.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	207	LYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2367	0	2359	116	0
1	B	2384	0	2367	90	0
1	C	2300	0	2290	101	0
1	D	2306	0	2290	131	0
1	E	2379	0	2362	107	0
1	F	2379	0	2362	96	0
1	G	2315	0	2298	88	0
1	H	2307	0	2292	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	10	13	0
2	D	20	0	10	2	0
2	F	20	0	10	2	0
2	G	20	0	10	0	0
3	D	44	0	26	9	0
4	A	22	0	0	4	0
4	B	20	0	0	1	0
4	C	24	0	0	0	0
4	D	7	0	0	0	0
4	E	13	0	0	0	0
4	F	27	0	0	2	0
4	G	20	0	0	0	0
4	H	11	0	0	0	0
All	All	19005	0	18686	808	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 22.

All (808) 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:H:98:ASN:HA	1:H:101:ILE:CD1	1.59	1.30
1:C:207:LYS:CG	1:C:208:GLN:H	1.41	1.25
1:C:207:LYS:HG3	1:C:208:GLN:N	1.49	1.16
1:H:98:ASN:CA	1:H:101:ILE:HD11	1.81	1.11
1:A:238:MET:HG3	1:D:53:GLY:HA3	1.36	1.04
1:C:171:HIS:ND1	2:C:327:FBP:H4	1.72	1.02
1:C:171:HIS:CE1	2:C:327:FBP:H4	2.00	0.97
1:B:177:GLU:HG3	1:B:306:LEU:HD21	1.47	0.96
1:H:98:ASN:CA	1:H:101:ILE:CD1	2.43	0.95
1:F:148:THR:HG21	1:F:174:ILE:O	1.66	0.95
1:C:250:ASN:OD1	1:C:279:ASN:HB2	1.68	0.94
1:A:45:GLY:HA2	1:A:48:MET:HE2	1.50	0.92
1:A:261:LEU:HD22	1:A:264:GLN:HB2	1.51	0.91
1:F:152:SER:O	1:F:156:ARG:HG3	1.70	0.90
1:C:207:LYS:HG3	1:C:208:GLN:H	0.73	0.90
1:B:280:ARG:HD2	1:B:280:ARG:O	1.72	0.90
1:F:293:GLU:CD	1:F:293:GLU:H	1.82	0.88
1:B:311:LYS:HA	1:B:314:PHE:HB2	1.55	0.87
1:D:232:THR:O	3:D:327:NAD:H5N	1.73	0.87
1:D:178:HIS:CE1	3:D:327:NAD:H72N	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:LYS:HD2	1:H:48:MET:HE1	1.56	0.87
1:G:3:LYS:O	1:G:4:HIS:HB2	1.75	0.86
1:E:44:MET:HG3	1:E:48:MET:HE2	1.58	0.86
1:H:98:ASN:HA	1:H:101:ILE:HD11	0.88	0.86
1:C:263:GLY:N	1:C:268:ASP:HB3	1.91	0.85
1:H:311:LYS:HB3	1:H:312:PRO:HD3	1.59	0.85
1:H:98:ASN:OD1	1:H:101:ILE:CD1	2.25	0.84
1:D:203:ASN:HB2	1:D:206:TYR:HD1	1.43	0.84
1:F:156:ARG:HH21	1:G:55:ALA:HB1	1.41	0.84
1:H:197:SER:O	1:H:201:GLU:HB3	1.78	0.83
1:A:48:MET:HE3	1:D:225:ILE:HG12	1.63	0.81
1:D:152:SER:O	1:D:156:ARG:HG2	1.80	0.81
1:F:223:TYR:O	1:F:227:GLU:HB2	1.80	0.81
1:H:176:GLY:HA2	1:H:272:ILE:HD11	1.63	0.80
1:A:203:ASN:HB2	1:A:207:LYS:HG3	1.63	0.80
1:H:11:ILE:HD12	1:H:79:ILE:HG12	1.64	0.79
1:A:103:LYS:HD2	1:A:135:PHE:CZ	2.17	0.79
1:B:296:LYS:O	1:B:300:LEU:HD23	1.82	0.79
1:E:225:ILE:HG12	1:H:48:MET:HE3	1.64	0.79
1:A:275:PRO:HB2	1:A:287:THR:HB	1.66	0.78
1:G:204:ASP:O	1:G:206:TYR:N	2.17	0.78
1:A:250:ASN:HB2	1:A:280:ARG:HB2	1.66	0.78
1:H:98:ASN:OD1	1:H:101:ILE:HD13	1.84	0.78
1:E:203:ASN:O	1:E:207:LYS:HG2	1.82	0.77
1:H:198:GLU:O	1:H:202:LYS:HB2	1.85	0.77
1:B:294:LYS:HG3	1:B:297:GLU:OE2	1.84	0.77
1:F:146:SER:O	1:F:149:THR:HG23	1.84	0.77
1:C:152:SER:O	1:C:156:ARG:HG3	1.84	0.77
1:B:41:GLU:O	1:C:228:LYS:HB3	1.86	0.76
1:A:203:ASN:HB3	1:A:206:TYR:HB2	1.67	0.76
1:D:130:TYR:CE1	1:D:134:LYS:HE2	2.21	0.76
1:D:122:THR:HG23	3:D:327:NAD:H4D	1.67	0.75
1:B:303:ALA:O	1:B:307:LYS:HG2	1.86	0.75
1:H:11:ILE:HA	1:H:36:ILE:O	1.87	0.75
1:B:200:VAL:HG21	1:B:208:GLN:HG2	1.68	0.75
1:B:311:LYS:HD2	1:B:314:PHE:HD1	1.49	0.74
1:H:21:ALA:O	1:H:25:ILE:HD13	1.87	0.74
1:G:105:ILE:O	1:G:109:VAL:HG23	1.88	0.74
1:C:207:LYS:CG	1:C:208:GLN:N	2.18	0.73
1:A:85:GLN:HB2	1:A:94:LEU:HD22	1.70	0.72
1:H:109:VAL:HG21	1:H:118:PHE:HZ	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:GLU:HG2	1:G:62:LYS:HB3	1.71	0.72
1:H:3:LYS:HD2	1:H:4:HIS:HD2	1.54	0.72
1:C:171:HIS:HE1	2:C:327:FBP:O6	1.72	0.71
1:A:294:LYS:O	1:A:298:GLN:HG3	1.90	0.71
1:G:270:VAL:HG23	1:G:310:LEU:HD11	1.72	0.71
1:G:280:ARG:HG2	1:H:4:HIS:HB2	1.72	0.71
1:D:200:VAL:HA	1:D:207:LYS:HG3	1.71	0.71
1:C:275:PRO:HB2	1:C:287:THR:HB	1.72	0.71
1:H:157:PHE:O	1:H:160:SER:HB3	1.90	0.71
1:E:309:ILE:O	1:E:313:HIS:HB2	1.90	0.71
1:B:37:ASP:HB3	1:B:43:ALA:HB2	1.72	0.70
1:D:261:LEU:HD22	1:D:264:GLN:HB2	1.73	0.70
1:B:96:GLU:OE2	1:B:313:HIS:HE1	1.73	0.70
1:D:96:GLU:HA	1:D:99:LEU:HD12	1.73	0.70
1:H:5:VAL:HG23	1:H:32:GLU:HG3	1.74	0.70
1:B:246:ALA:HA	1:B:251:GLU:OE1	1.91	0.70
1:H:119:LEU:HG	1:H:240:LEU:HD13	1.73	0.70
1:A:44:MET:O	1:A:48:MET:HG3	1.92	0.69
1:C:28:GLY:HA3	1:C:59:GLN:HG3	1.73	0.69
1:F:77:VAL:HG23	1:F:114:PHE:CE1	2.27	0.69
1:G:133:TRP:CD1	1:G:138:LEU:O	2.45	0.69
1:C:177:GLU:HG3	1:C:306:LEU:HD21	1.74	0.69
1:D:203:ASN:CB	1:D:206:TYR:HD1	2.05	0.69
1:F:133:TRP:CE3	1:F:134:LYS:HD3	2.28	0.69
1:E:202:LYS:HD3	1:E:203:ASN:H	1.58	0.69
1:A:171:HIS:HE1	2:C:327:FBP:H62	1.58	0.69
1:D:205:ALA:HA	1:D:208:GLN:HB2	1.74	0.69
1:E:198:GLU:OE2	1:G:290:ASN:HB2	1.92	0.69
1:E:202:LYS:HD3	1:E:203:ASN:N	2.08	0.69
1:D:197:SER:O	1:D:200:VAL:HG22	1.92	0.69
1:H:200:VAL:HG11	1:H:211:LEU:HD11	1.75	0.69
1:A:40:LYS:HD2	1:A:65:TYR:OH	1.93	0.68
1:B:229:LYS:HB2	1:C:42:LYS:HD2	1.76	0.68
1:F:177:GLU:O	1:F:182:GLU:HB3	1.94	0.67
1:F:287:THR:HG23	1:H:194:VAL:HG13	1.75	0.67
1:C:171:HIS:ND1	2:C:327:FBP:C4	2.53	0.67
1:H:275:PRO:HG2	1:H:289:LEU:HD11	1.77	0.67
1:G:167:PRO:HG2	1:G:168:GLN:NE2	2.09	0.67
1:C:261:LEU:HD11	1:C:272:ILE:HG22	1.77	0.67
1:F:171:HIS:HE1	1:H:171:HIS:CE1	2.13	0.67
1:B:156:ARG:HD3	1:B:170:VAL:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ILE:HG12	1:F:231:ALA:HA	1.77	0.67
1:C:93:GLU:O	1:C:97:LYS:HG3	1.95	0.66
1:C:263:GLY:H	1:C:268:ASP:HB3	1.58	0.66
1:F:301:HIS:O	1:F:305:VAL:HB	1.95	0.66
1:E:41:GLU:HG2	1:H:228:LYS:HA	1.76	0.66
1:G:177:GLU:O	1:G:182:GLU:HB3	1.95	0.66
1:B:207:LYS:HA	1:B:210:GLU:HG3	1.77	0.66
1:D:246:ALA:HA	1:D:251:GLU:HG3	1.77	0.66
1:F:171:HIS:CE1	1:H:171:HIS:CE1	2.83	0.66
1:A:226:ILE:HG23	1:A:230:GLY:O	1.96	0.66
1:C:261:LEU:HD11	1:C:272:ILE:CG2	2.26	0.66
1:D:265:TYR:OH	1:D:289:LEU:HB2	1.96	0.66
1:E:162:TYR:OH	1:E:207:LYS:HD2	1.95	0.66
1:F:293:GLU:CD	1:F:293:GLU:N	2.53	0.66
1:H:259:THR:HG22	1:H:274:VAL:HG22	1.78	0.65
1:G:200:VAL:O	1:G:202:LYS:N	2.30	0.65
1:D:201:GLU:O	1:D:202:LYS:HG2	1.96	0.65
1:E:312:PRO:HG2	1:E:313:HIS:CD2	2.30	0.65
1:F:29:ILE:HD13	1:F:245:LYS:HB2	1.79	0.65
1:B:155:PHE:CE2	1:B:172:ALA:HB1	2.31	0.65
1:D:148:THR:HA	1:D:151:ASP:OD1	1.97	0.65
1:F:228:LYS:HE2	1:G:44:MET:SD	2.36	0.65
1:H:98:ASN:CA	1:H:101:ILE:HD12	2.27	0.65
1:A:191:VAL:O	1:A:194:VAL:HG22	1.95	0.65
1:B:91:ARG:O	1:B:95:VAL:HG23	1.96	0.65
1:E:196:VAL:O	1:E:200:VAL:HG13	1.96	0.65
1:B:127:ILE:HD11	1:B:306:LEU:HD23	1.79	0.64
1:D:309:ILE:O	1:D:313:HIS:ND1	2.29	0.64
1:E:86:LYS:HE3	1:E:87:PRO:HD2	1.78	0.64
1:A:28:GLY:HA3	1:A:59:GLN:CB	2.27	0.64
1:G:133:TRP:HA	1:G:143:VAL:HG21	1.79	0.64
1:E:157:PHE:CE1	1:H:51:ASN:HB3	2.33	0.64
1:G:94:LEU:HG	1:G:95:VAL:HG23	1.79	0.63
1:C:43:ALA:O	1:C:47:VAL:HG23	1.97	0.63
1:G:167:PRO:HG2	1:G:168:GLN:HE21	1.62	0.63
1:B:214:ILE:O	1:B:218:VAL:HG23	1.99	0.63
1:E:67:THR:HG22	1:E:69:GLU:H	1.62	0.63
1:F:25:ILE:HD12	1:F:50:LEU:HD22	1.81	0.63
1:G:67:THR:HG23	1:G:69:GLU:HG2	1.80	0.63
1:A:261:LEU:CD2	1:A:264:GLN:HB2	2.26	0.62
1:B:41:GLU:HG3	1:C:228:LYS:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:LEU:O	1:G:268:ASP:HA	1.99	0.62
1:E:171:HIS:CE1	1:G:171:HIS:CE1	2.86	0.62
1:C:106:VAL:O	1:C:110:MET:HG2	2.00	0.62
1:C:103:LYS:O	1:C:107:SER:HB2	1.99	0.62
1:H:98:ASN:O	1:H:101:ILE:HD12	1.99	0.62
1:D:232:THR:HG22	3:D:327:NAD:H4N	1.80	0.62
1:D:44:MET:HE3	1:D:48:MET:HE2	1.81	0.61
1:D:123:ASN:HB2	3:D:327:NAD:O2D	2.00	0.61
1:D:159:LEU:HD22	1:D:163:PHE:HE2	1.65	0.61
1:H:266:GLY:O	1:H:300:LEU:HD11	2.00	0.61
1:D:134:LYS:HG3	1:D:314:PHE:HE1	1.66	0.61
1:A:171:HIS:CE1	2:C:327:FBP:H62	2.35	0.61
1:B:52:HIS:CG	1:C:154:ARG:HG2	2.35	0.61
1:E:198:GLU:CD	1:G:290:ASN:HB2	2.25	0.61
1:F:148:THR:O	1:F:148:THR:HG22	2.00	0.61
1:F:200:VAL:HG12	1:F:207:LYS:HB2	1.82	0.61
1:H:109:VAL:HG21	1:H:118:PHE:CZ	2.35	0.61
1:H:166:ALA:O	1:H:170:VAL:HG23	2.00	0.61
1:B:311:LYS:HD2	1:B:314:PHE:CD1	2.33	0.61
1:E:37:ASP:OD1	1:E:39:ASN:N	2.33	0.61
1:E:177:GLU:HB2	1:E:306:LEU:HD11	1.83	0.61
1:H:29:ILE:HD13	1:H:245:LYS:HB2	1.81	0.61
1:A:105:ILE:O	1:A:109:VAL:HG23	2.01	0.60
1:E:140:LYS:HG3	1:E:141:GLU:OE2	2.00	0.60
1:H:76:ILE:HD11	1:H:247:ILE:HG21	1.83	0.60
1:D:14:GLY:O	1:D:18:SER:HB2	2.01	0.60
1:F:37:ASP:C	1:F:39:ASN:H	2.08	0.60
1:H:256:THR:HG22	1:H:275:PRO:HD3	1.81	0.60
1:A:203:ASN:HD22	1:A:207:LYS:HG3	1.65	0.60
1:A:304:GLY:O	1:A:307:LYS:HB2	2.01	0.60
1:A:213:GLN:NE2	4:A:335:HOH:O	2.33	0.60
1:D:102:PHE:O	1:D:106:VAL:HG23	2.02	0.60
1:A:262:ASP:OD1	1:A:268:ASP:HB2	2.01	0.60
1:H:80:CYS:HA	1:H:121:ALA:HB3	1.82	0.60
1:C:44:MET:O	1:C:48:MET:HG3	2.02	0.60
1:C:275:PRO:HG2	1:C:289:LEU:HD11	1.84	0.60
1:G:197:SER:O	1:G:201:GLU:N	2.33	0.60
1:E:44:MET:HG3	1:E:48:MET:CE	2.30	0.60
1:E:86:LYS:CE	1:E:87:PRO:HD2	2.32	0.60
1:A:44:MET:HE3	1:D:228:LYS:HE3	1.84	0.59
1:C:57:ALA:HB1	1:C:58:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:N	1:C:91:ARG:HD2	2.17	0.59
1:G:178:HIS:CG	1:G:178:HIS:O	2.55	0.59
1:H:25:ILE:HA	1:H:61:VAL:HG21	1.85	0.59
1:B:297:GLU:HG2	1:B:298:GLN:N	2.15	0.59
1:E:106:VAL:O	1:E:110:MET:HG2	2.01	0.59
1:F:123:ASN:OD1	1:F:124:PRO:HA	2.02	0.59
1:A:287:THR:HG23	1:C:194:VAL:CG1	2.33	0.59
1:D:65:TYR:CG	1:D:66:GLY:N	2.71	0.59
1:F:156:ARG:O	1:F:160:SER:HB3	2.03	0.59
1:A:46:ASP:OD1	1:D:229:LYS:HE2	2.03	0.58
1:G:177:GLU:C	1:G:179:GLY:H	2.10	0.58
1:B:177:GLU:HB2	1:B:306:LEU:HD11	1.86	0.58
1:C:206:TYR:HB3	1:C:210:GLU:CD	2.29	0.58
1:E:81:ALA:O	1:E:122:THR:HG21	2.03	0.58
1:F:148:THR:HG21	1:F:174:ILE:C	2.28	0.58
1:F:166:ALA:HB2	1:H:251:GLU:O	2.03	0.58
1:H:45:GLY:HA2	1:H:48:MET:CE	2.32	0.58
1:C:46:ASP:O	1:C:50:LEU:HG	2.04	0.58
1:E:250:ASN:OD1	1:E:279:ASN:HB2	2.03	0.58
1:H:20:TYR:O	1:H:24:LEU:HG	2.04	0.58
1:C:177:GLU:HB2	1:C:306:LEU:HD11	1.85	0.58
1:G:14:GLY:HA2	1:G:42:LYS:HE3	1.84	0.58
1:E:56:PHE:CD1	1:H:242:ARG:HG3	2.38	0.58
1:G:2:ASN:N	1:H:250:ASN:HD21	2.01	0.58
1:A:243:ILE:O	1:A:247:ILE:HG13	2.04	0.58
1:C:207:LYS:NZ	1:C:208:GLN:HB2	2.17	0.58
1:E:67:THR:CG2	1:E:69:GLU:HG2	2.34	0.58
1:E:229:LYS:NZ	1:E:233:TYR:CZ	2.71	0.57
1:F:272:ILE:HG21	1:F:299:PHE:HZ	1.69	0.57
1:A:264:GLN:O	1:A:265:TYR:HB2	2.04	0.57
1:G:140:LYS:HG2	1:G:141:GLU:OE2	2.03	0.57
1:D:134:LYS:HG3	1:D:314:PHE:CE1	2.39	0.57
1:B:130:TYR:OH	1:B:314:PHE:HE2	1.88	0.57
1:C:173:HIS:CE1	2:C:327:FBP:O2P	2.57	0.57
1:D:236:VAL:O	1:D:240:LEU:HG	2.05	0.57
1:B:289:LEU:H	1:B:289:LEU:HD12	1.70	0.57
1:E:122:THR:O	1:E:128:LEU:HD12	2.05	0.57
1:A:166:ALA:O	1:A:170:VAL:HG23	2.05	0.57
1:A:194:VAL:HG12	1:C:289:LEU:HA	1.87	0.57
1:A:95:VAL:O	1:A:99:LEU:HG	2.05	0.57
1:F:177:GLU:HG2	1:F:178:HIS:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:HIS:O	1:H:305:VAL:HG23	2.05	0.57
1:B:200:VAL:HG21	1:B:208:GLN:CG	2.35	0.56
1:C:130:TYR:HE2	1:C:269:ASP:O	1.88	0.56
1:D:34:VAL:HA	1:D:64:SER:O	2.05	0.56
1:H:130:TYR:HB2	1:H:271:TYR:HB2	1.87	0.56
1:H:156:ARG:O	1:H:160:SER:HB2	2.05	0.56
1:E:224:HIS:O	1:E:228:LYS:HG3	2.05	0.56
1:G:177:GLU:HB3	1:G:181:THR:OG1	2.04	0.56
1:H:184:PRO:HG3	1:H:215:VAL:HG11	1.88	0.56
1:A:77:VAL:HG23	1:A:114:PHE:CE1	2.40	0.56
1:B:27:GLN:NE2	1:C:26:ASN:OD1	2.39	0.56
1:C:156:ARG:NH2	2:C:327:FBP:H11	2.21	0.56
1:F:156:ARG:NH2	1:G:55:ALA:HB1	2.17	0.56
1:H:175:ILE:O	1:H:183:LEU:N	2.35	0.56
1:B:56:PHE:CD1	1:C:242:ARG:HD3	2.40	0.56
1:G:123:ASN:HA	1:G:125:VAL:N	2.20	0.56
1:C:205:ALA:O	1:C:206:TYR:HB2	2.06	0.56
1:F:197:SER:O	1:F:200:VAL:HG23	2.06	0.56
1:H:260:TYR:HB2	1:H:271:TYR:CE2	2.41	0.56
1:D:178:HIS:CE1	3:D:327:NAD:N7N	2.68	0.56
1:G:9:ALA:HB3	1:G:77:VAL:HG22	1.87	0.56
1:F:25:ILE:CD1	1:F:50:LEU:HB3	2.35	0.56
1:A:157:PHE:O	1:A:160:SER:HB3	2.05	0.55
1:E:156:ARG:HD2	1:E:170:VAL:O	2.06	0.55
1:G:250:ASN:HB2	1:H:5:VAL:HG11	1.87	0.55
1:A:254:ILE:HA	1:A:276:ALA:O	2.07	0.55
1:A:261:LEU:HD13	1:A:267:ALA:HB3	1.88	0.55
1:B:169:ASN:HB3	1:D:254:ILE:HD12	1.88	0.55
1:H:3:LYS:HD2	1:H:4:HIS:CD2	2.38	0.55
1:H:265:TYR:OH	1:H:287:THR:O	2.23	0.55
1:A:171:HIS:ND1	2:C:327:FBP:O5P	2.25	0.55
1:B:95:VAL:HG12	1:B:99:LEU:CD1	2.36	0.55
1:F:188:HIS:NE2	1:F:290:ASN:HB3	2.22	0.55
1:H:12:GLY:O	1:H:17:GLY:HA3	2.05	0.55
1:B:205:ALA:HA	1:B:208:GLN:HB2	1.88	0.55
1:G:200:VAL:HG21	1:G:211:LEU:HD11	1.88	0.55
1:H:157:PHE:O	1:H:161:GLU:HG2	2.07	0.55
1:E:169:ASN:CB	1:G:254:ILE:HD12	2.36	0.55
1:G:200:VAL:C	1:G:202:LYS:N	2.65	0.55
1:H:98:ASN:OD1	1:H:101:ILE:HD11	2.03	0.55
1:E:260:TYR:HB2	1:E:271:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:ALA:O	1:G:307:LYS:HG2	2.07	0.55
1:A:305:VAL:O	1:A:308:ASN:HB2	2.07	0.55
1:B:254:ILE:N	1:D:169:ASN:OD1	2.38	0.55
1:F:262:ASP:HA	1:F:268:ASP:HA	1.87	0.55
1:C:93:GLU:HA	1:C:93:GLU:OE1	2.07	0.55
1:G:13:ALA:O	1:G:42:LYS:HE3	2.07	0.55
1:D:183:LEU:HD12	1:D:184:PRO:O	2.06	0.55
1:F:37:ASP:C	1:F:39:ASN:N	2.64	0.55
1:F:202:LYS:O	1:F:202:LYS:HG2	2.06	0.55
1:C:104:GLY:O	1:C:108:GLU:HG2	2.07	0.54
1:A:257:VAL:HG23	1:A:259:THR:HG22	1.89	0.54
1:B:52:HIS:HE1	1:C:221:ALA:HB1	1.73	0.54
1:C:291:LEU:HD22	1:C:295:GLU:HB3	1.88	0.54
1:E:186:TRP:C	1:E:188:HIS:H	2.16	0.54
1:H:69:GLU:HA	1:H:112:SER:HB3	1.87	0.54
1:E:223:TYR:CE2	1:E:227:GLU:OE1	2.60	0.54
1:D:259:THR:CG2	1:D:274:VAL:HG22	2.38	0.54
1:H:278:VAL:HG22	1:H:283:ILE:HD13	1.90	0.54
1:D:256:THR:HA	1:D:274:VAL:O	2.07	0.54
1:F:202:LYS:NZ	1:F:202:LYS:HB3	2.22	0.54
1:D:136:SER:HB2	1:D:138:LEU:HD12	1.90	0.54
1:F:287:THR:HG23	1:H:194:VAL:CG1	2.37	0.54
1:A:204:ASP:O	1:A:205:ALA:HB3	2.07	0.54
1:D:204:ASP:O	1:D:205:ALA:HB3	2.07	0.54
1:E:157:PHE:CZ	1:H:51:ASN:HB3	2.43	0.54
1:H:16:VAL:HG12	1:H:80:CYS:HB3	1.90	0.54
1:A:211:LEU:HD23	1:A:214:ILE:HD12	1.89	0.54
1:C:260:TYR:OH	1:C:269:ASP:HA	2.08	0.53
1:D:9:ALA:O	1:D:77:VAL:HA	2.08	0.53
1:C:109:VAL:CG2	1:C:118:PHE:HZ	2.21	0.53
1:E:26:ASN:HB3	1:H:26:ASN:HB3	1.90	0.53
1:F:53:GLY:HA3	1:G:238:MET:HG3	1.90	0.53
1:H:45:GLY:HA2	1:H:48:MET:HE2	1.88	0.53
1:C:182:GLU:OE2	1:C:219:LYS:HA	2.09	0.53
1:D:246:ALA:HA	1:D:251:GLU:CG	2.38	0.53
1:C:50:LEU:HD12	1:C:63:THR:HG21	1.88	0.53
1:E:228:LYS:HD2	1:H:48:MET:CE	2.32	0.53
1:A:180:ASP:HB2	4:A:331:HOH:O	2.09	0.53
2:C:327:FBP:O1P	2:C:327:FBP:H3	2.07	0.53
1:B:186:TRP:CE3	1:B:196:VAL:HG11	2.43	0.53
1:F:238:MET:HG3	1:G:53:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:THR:HG21	1:G:243:ILE:HD11	1.90	0.53
1:H:39:ASN:ND2	1:H:42:LYS:HB2	2.23	0.53
1:A:28:GLY:HA3	1:A:59:GLN:HB2	1.89	0.53
1:A:311:LYS:HB2	1:A:312:PRO:HD3	1.91	0.53
1:B:265:TYR:OH	1:B:289:LEU:HD12	2.09	0.53
1:D:206:TYR:CZ	1:D:207:LYS:NZ	2.71	0.53
1:H:260:TYR:CE1	1:H:269:ASP:HA	2.44	0.53
1:C:224:HIS:O	1:C:228:LYS:HG3	2.09	0.53
1:F:272:ILE:HG21	1:F:299:PHE:CZ	2.44	0.53
1:C:131:ALA:O	1:C:132:THR:C	2.52	0.52
1:G:309:ILE:HG23	1:G:313:HIS:ND1	2.24	0.52
1:H:150:LEU:HD22	1:H:236:VAL:HB	1.91	0.52
1:F:37:ASP:OD1	1:F:39:ASN:N	2.42	0.52
1:G:200:VAL:C	1:G:202:LYS:H	2.17	0.52
1:A:82:GLY:HA2	1:A:101:ILE:HD13	1.91	0.52
1:A:265:TYR:HD1	1:A:291:LEU:HD11	1.75	0.52
1:C:124:PRO:HG2	1:C:127:ILE:HB	1.92	0.52
1:G:34:VAL:HG12	1:G:64:SER:HB2	1.91	0.52
1:G:264:GLN:C	1:G:266:GLY:H	2.17	0.52
1:H:173:HIS:HB3	1:H:256:THR:HG21	1.90	0.52
1:A:26:ASN:ND2	1:D:23:ALA:HA	2.24	0.52
1:E:289:LEU:HD12	1:E:289:LEU:N	2.25	0.52
1:H:40:LYS:HB3	1:H:65:TYR:OH	2.09	0.52
1:E:41:GLU:O	1:H:228:LYS:HB3	2.10	0.52
1:E:152:SER:O	1:E:156:ARG:HG3	2.10	0.52
1:F:156:ARG:HH12	2:F:327:FBP:H11	1.75	0.52
1:D:117:ILE:HG23	1:D:142:ARG:HA	1.92	0.52
1:E:181:THR:HB	1:E:302:SER:HA	1.92	0.52
2:F:327:FBP:O2	1:H:168:GLN:O	2.27	0.52
1:A:156:ARG:NH2	2:C:327:FBP:O4P	2.43	0.52
1:F:257:VAL:HG21	1:F:283:ILE:HD11	1.92	0.52
1:E:67:THR:HG22	1:E:69:GLU:HG2	1.91	0.51
1:D:293:GLU:O	1:D:297:GLU:HB2	2.10	0.51
1:E:98:ASN:O	1:E:99:LEU:C	2.53	0.51
1:F:273:GLY:O	1:F:274:VAL:HG13	2.11	0.51
1:G:123:ASN:HA	1:G:124:PRO:C	2.35	0.51
1:H:147:GLY:HA2	1:H:258:SER:HB2	1.93	0.51
1:H:259:THR:HA	1:H:271:TYR:CE1	2.45	0.51
1:B:154:ARG:NH2	4:B:332:HOH:O	2.43	0.51
1:E:312:PRO:C	1:E:314:PHE:H	2.18	0.51
1:G:310:LEU:O	1:G:314:PHE:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HD22	1:D:142:ARG:NH2	2.26	0.51
1:E:38:VAL:O	1:E:40:LYS:HD3	2.11	0.51
1:E:194:VAL:HG22	1:E:199:LEU:HG	1.92	0.51
1:G:292:ASN:C	1:G:292:ASN:OD1	2.54	0.51
1:H:233:TYR:HE2	1:H:234:TYR:CZ	2.29	0.51
1:E:133:TRP:CE3	1:E:271:TYR:HE2	2.29	0.51
1:H:105:ILE:O	1:H:109:VAL:HG13	2.11	0.51
1:A:51:ASN:ND2	1:A:63:THR:O	2.44	0.51
1:A:189:ALA:C	1:A:190:ASN:HD22	2.19	0.51
1:B:254:ILE:HA	1:B:276:ALA:O	2.11	0.51
1:H:242:ARG:NH1	1:H:251:GLU:OE1	2.44	0.51
1:A:44:MET:HG3	1:D:228:LYS:HE3	1.94	0.50
1:A:133:TRP:CD1	1:A:138:LEU:O	2.64	0.50
1:C:207:LYS:HZ3	1:C:208:GLN:HB2	1.75	0.50
1:D:139:PRO:C	1:D:141:GLU:H	2.19	0.50
1:E:102:PHE:HZ	1:E:122:THR:HG23	1.77	0.50
1:G:158:MET:O	1:G:161:GLU:HB2	2.11	0.50
1:G:311:LYS:CB	1:G:312:PRO:HD3	2.40	0.50
1:H:185:VAL:CG1	1:H:188:HIS:HD2	2.23	0.50
1:F:75:ASP:OD1	1:F:280:ARG:NH2	2.44	0.50
1:D:78:CYS:HA	1:D:119:LEU:O	2.12	0.50
1:D:190:ASN:HB3	1:D:195:PRO:HA	1.92	0.50
1:E:260:TYR:CE1	1:E:269:ASP:HA	2.46	0.50
1:C:270:VAL:CG2	1:C:271:TYR:N	2.75	0.50
1:D:117:ILE:HG12	1:D:281:GLY:O	2.12	0.50
1:D:189:ALA:O	1:D:196:VAL:HG12	2.11	0.50
1:D:305:VAL:HG12	1:D:309:ILE:HD11	1.94	0.50
1:B:18:SER:OG	1:B:46:ASP:OD2	2.30	0.50
1:B:186:TRP:HE3	1:B:196:VAL:HG11	1.75	0.50
1:E:22:PHE:HD2	1:H:22:PHE:HD2	1.59	0.50
1:H:262:ASP:HB3	1:H:264:GLN:NE2	2.27	0.50
1:C:14:GLY:O	1:C:18:SER:HB3	2.12	0.50
1:C:22:PHE:O	1:C:26:ASN:ND2	2.38	0.50
1:D:68:TYR:OH	1:D:105:ILE:HG12	2.12	0.50
1:D:203:ASN:HB2	1:D:206:TYR:CD1	2.34	0.50
1:D:305:VAL:O	1:D:309:ILE:HG12	2.12	0.50
1:F:176:GLY:HA2	1:F:272:ILE:HG12	1.94	0.50
1:A:301:HIS:O	1:A:305:VAL:HG23	2.12	0.50
1:A:203:ASN:HD22	1:A:207:LYS:CG	2.24	0.50
1:A:272:ILE:HD13	1:A:299:PHE:CZ	2.47	0.49
1:D:201:GLU:O	1:D:202:LYS:CG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:GLU:O	1:H:182:GLU:HB3	2.12	0.49
1:A:303:ALA:O	1:A:307:LYS:HG2	2.11	0.49
1:D:101:ILE:O	1:D:105:ILE:HB	2.12	0.49
1:B:202:LYS:HB3	1:B:203:ASN:HD22	1.76	0.49
1:D:190:ASN:HB2	1:D:194:VAL:O	2.13	0.49
1:D:259:THR:HG21	1:D:274:VAL:HG22	1.94	0.49
1:F:5:VAL:HB	1:F:31:ASP:OD2	2.11	0.49
1:A:76:ILE:HD11	1:A:247:ILE:HG21	1.94	0.49
1:C:294:LYS:O	1:C:298:GLN:HG3	2.13	0.49
1:E:177:GLU:HB2	1:E:306:LEU:CD1	2.41	0.49
1:G:270:VAL:HG23	1:G:310:LEU:CD1	2.42	0.49
1:D:250:ASN:OD1	1:D:279:ASN:HB2	2.13	0.49
1:G:160:SER:HB2	1:G:167:PRO:HA	1.94	0.49
1:H:255:LEU:O	1:H:257:VAL:HG22	2.13	0.49
1:A:185:VAL:HB	4:A:336:HOH:O	2.13	0.49
1:D:15:PHE:HB3	1:D:233:TYR:CD1	2.47	0.49
1:D:198:GLU:HA	1:D:201:GLU:CD	2.37	0.49
1:E:67:THR:CG2	1:E:68:TYR:N	2.74	0.49
1:E:85:GLN:HB2	1:E:94:LEU:HD22	1.95	0.49
1:E:203:ASN:HB3	1:E:207:LYS:HE2	1.94	0.49
1:F:154:ARG:O	1:F:158:MET:HG3	2.12	0.49
1:F:86:LYS:HB3	1:F:87:PRO:HD2	1.93	0.49
1:G:115:ASP:O	1:G:142:ARG:NH2	2.45	0.49
1:H:180:ASP:OD1	1:H:180:ASP:N	2.43	0.49
1:A:265:TYR:CE2	1:A:288:GLU:OE1	2.66	0.49
1:E:130:TYR:O	1:E:133:TRP:HB3	2.13	0.49
1:A:203:ASN:ND2	1:A:207:LYS:HG3	2.27	0.49
1:D:51:ASN:OD1	1:D:63:THR:HB	2.13	0.49
1:E:229:LYS:NZ	1:E:233:TYR:CE1	2.81	0.49
1:F:41:GLU:HG3	1:G:228:LYS:HG2	1.94	0.49
1:F:191:VAL:HG12	1:F:191:VAL:O	2.12	0.49
1:C:75:ASP:HB3	1:C:280:ARG:NH2	2.27	0.48
1:D:124:PRO:HB2	1:D:127:ILE:HG12	1.95	0.48
1:E:52:HIS:CE1	1:H:225:ILE:HD11	2.47	0.48
1:A:54:LYS:HD3	1:D:167:PRO:HG2	1.94	0.48
1:F:297:GLU:OE1	4:F:352:HOH:O	2.20	0.48
1:H:147:GLY:CA	1:H:258:SER:HB2	2.43	0.48
1:A:51:ASN:O	1:A:54:LYS:HB2	2.13	0.48
1:C:264:GLN:O	1:C:265:TYR:HB2	2.12	0.48
1:E:79:ILE:HD12	1:E:120:VAL:HG22	1.95	0.48
1:H:95:VAL:HG12	1:H:96:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:GLU:HB2	4:F:352:HOH:O	2.13	0.48
1:H:5:VAL:CG2	1:H:32:GLU:HG3	2.42	0.48
1:H:70:ASP:C	1:H:72:LYS:H	2.20	0.48
1:B:52:HIS:CE1	1:C:221:ALA:HB1	2.49	0.48
1:C:260:TYR:CZ	1:C:269:ASP:HA	2.48	0.48
1:D:148:THR:OG1	1:D:174:ILE:O	2.31	0.48
1:G:119:LEU:HA	1:G:144:ILE:O	2.13	0.48
1:H:76:ILE:HD11	1:H:247:ILE:CG2	2.44	0.48
1:H:177:GLU:HB3	1:H:181:THR:OG1	2.13	0.48
1:D:203:ASN:CB	1:D:206:TYR:CD1	2.92	0.48
1:E:25:ILE:HG22	1:E:25:ILE:O	2.12	0.48
1:E:67:THR:HG22	1:E:68:TYR:N	2.28	0.48
1:H:211:LEU:O	1:H:214:ILE:HB	2.13	0.48
1:B:95:VAL:HG12	1:B:99:LEU:HD11	1.95	0.48
1:C:109:VAL:HG21	1:C:118:PHE:CZ	2.49	0.48
1:G:95:VAL:O	1:G:97:LYS:N	2.46	0.48
1:H:178:HIS:O	1:H:178:HIS:CG	2.66	0.48
1:C:191:VAL:O	1:C:194:VAL:HG13	2.13	0.48
1:H:109:VAL:CG2	1:H:118:PHE:HZ	2.25	0.48
1:B:54:LYS:HG2	1:C:167:PRO:HG2	1.96	0.48
1:D:232:THR:CG2	3:D:327:NAD:H4N	2.44	0.48
1:F:148:THR:O	1:F:148:THR:CG2	2.62	0.48
1:H:257:VAL:O	1:H:273:GLY:HA2	2.14	0.48
1:A:228:LYS:HG2	1:D:41:GLU:HG3	1.95	0.47
1:A:229:LYS:HE2	1:D:46:ASP:HA	1.95	0.47
1:C:156:ARG:HD2	1:C:170:VAL:O	2.14	0.47
1:D:106:VAL:O	1:D:109:VAL:HG13	2.14	0.47
1:D:154:ARG:O	1:D:158:MET:HG3	2.14	0.47
1:D:310:LEU:O	1:D:314:PHE:HD2	1.96	0.47
1:E:311:LYS:O	1:E:314:PHE:CE2	2.67	0.47
1:A:250:ASN:OD1	1:A:250:ASN:O	2.32	0.47
1:C:197:SER:O	1:C:200:VAL:HG22	2.14	0.47
1:D:94:LEU:HD23	1:D:94:LEU:N	2.29	0.47
1:D:257:VAL:O	1:D:273:GLY:HA2	2.14	0.47
1:F:140:LYS:HD2	1:F:260:TYR:CD2	2.49	0.47
1:F:185:VAL:O	1:F:189:ALA:HB2	2.14	0.47
1:B:171:HIS:CE1	1:D:171:HIS:CE1	3.02	0.47
1:C:213:GLN:O	1:C:217:ASP:OD1	2.31	0.47
1:E:309:ILE:O	1:E:309:ILE:HG22	2.14	0.47
1:H:106:VAL:O	1:H:110:MET:HG2	2.14	0.47
1:A:203:ASN:CB	1:A:207:LYS:HG3	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:LYS:NZ	1:G:233:TYR:CZ	2.83	0.47
1:C:109:VAL:CG2	1:C:118:PHE:CZ	2.97	0.47
1:C:229:LYS:O	1:C:231:ALA:N	2.44	0.47
1:F:292:ASN:O	1:F:296:LYS:HE2	2.14	0.47
1:A:122:THR:HB	1:A:128:LEU:HD13	1.97	0.47
1:D:211:LEU:O	1:D:215:VAL:HG23	2.14	0.47
1:E:102:PHE:CZ	1:E:122:THR:HG23	2.50	0.47
1:F:79:ILE:HD13	1:F:105:ILE:HG21	1.97	0.47
1:G:169:ASN:O	1:G:171:HIS:CD2	2.67	0.47
1:H:133:TRP:CZ3	1:H:134:LYS:HE2	2.50	0.47
1:H:12:GLY:C	1:H:14:GLY:H	2.22	0.47
1:H:76:ILE:HD12	1:H:248:LEU:HD21	1.96	0.47
1:A:228:LYS:HE2	1:D:44:MET:HG2	1.96	0.47
1:A:250:ASN:OD1	1:A:250:ASN:C	2.56	0.47
1:A:268:ASP:O	1:A:269:ASP:C	2.57	0.47
1:E:169:ASN:HB3	1:G:254:ILE:HD12	1.97	0.47
1:A:246:ALA:HA	1:A:251:GLU:CD	2.39	0.47
1:D:47:VAL:HG12	1:D:47:VAL:O	2.15	0.47
1:E:186:TRP:O	1:E:188:HIS:N	2.48	0.47
1:A:265:TYR:CD1	1:A:291:LEU:HD11	2.50	0.46
1:C:106:VAL:HG11	1:C:135:PHE:HB2	1.96	0.46
1:D:247:ILE:O	1:D:280:ARG:HA	2.15	0.46
1:E:236:VAL:HG22	1:E:240:LEU:HD11	1.96	0.46
1:F:25:ILE:HD13	1:F:50:LEU:HB3	1.97	0.46
1:A:225:ILE:HG22	1:A:231:ALA:O	2.16	0.46
1:B:106:VAL:HA	1:B:109:VAL:HG12	1.96	0.46
1:B:117:ILE:HG23	1:B:142:ARG:O	2.16	0.46
1:E:204:ASP:O	1:E:206:TYR:N	2.46	0.46
1:H:261:LEU:HG	1:H:272:ILE:HG22	1.96	0.46
1:D:203:ASN:OD1	1:D:207:LYS:HG2	2.16	0.46
1:D:296:LYS:O	1:D:300:LEU:HD12	2.14	0.46
1:E:272:ILE:HG12	1:E:273:GLY:N	2.30	0.46
1:H:180:ASP:HA	1:H:219:LYS:HD2	1.98	0.46
1:B:202:LYS:HB3	1:B:203:ASN:ND2	2.30	0.46
1:C:26:ASN:O	1:C:58:PRO:HG3	2.15	0.46
1:C:270:VAL:HG22	1:C:271:TYR:N	2.30	0.46
1:D:120:VAL:O	1:D:145:GLY:HA2	2.16	0.46
1:F:85:GLN:HE21	1:F:86:LYS:N	2.13	0.46
1:F:105:ILE:O	1:F:109:VAL:HG13	2.15	0.46
1:G:134:LYS:HA	1:G:134:LYS:HD3	1.82	0.46
1:H:274:VAL:O	1:H:275:PRO:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HA	1:B:144:ILE:O	2.16	0.46
1:D:117:ILE:N	1:D:117:ILE:HD12	2.29	0.46
1:B:117:ILE:HG12	1:B:142:ARG:HB3	1.98	0.46
1:D:16:VAL:HG13	1:D:236:VAL:HG13	1.97	0.46
1:A:311:LYS:CB	1:A:312:PRO:HD3	2.46	0.46
1:C:145:GLY:C	1:C:147:GLY:H	2.23	0.46
1:E:37:ASP:OD1	1:E:38:VAL:N	2.49	0.46
1:F:122:THR:C	1:F:128:LEU:HD12	2.40	0.46
1:H:206:TYR:O	1:H:207:LYS:O	2.34	0.46
1:B:40:LYS:HE2	1:B:41:GLU:OE2	2.15	0.45
1:B:105:ILE:O	1:B:109:VAL:HG12	2.15	0.45
1:H:311:LYS:HB3	1:H:312:PRO:CD	2.38	0.45
1:E:312:PRO:O	1:E:314:PHE:N	2.49	0.45
1:F:190:ASN:HB2	1:F:194:VAL:O	2.15	0.45
1:G:11:ILE:O	1:G:80:CYS:N	2.48	0.45
1:G:186:TRP:C	1:G:188:HIS:H	2.24	0.45
1:B:12:GLY:O	1:B:17:GLY:HA3	2.16	0.45
1:D:204:ASP:O	1:D:205:ALA:CB	2.64	0.45
1:E:240:LEU:O	1:E:244:THR:OG1	2.34	0.45
1:F:127:ILE:HD13	1:F:310:LEU:HG	1.98	0.45
1:F:264:GLN:C	1:F:266:GLY:H	2.24	0.45
1:F:287:THR:O	1:F:287:THR:HG22	2.15	0.45
1:C:133:TRP:HB2	1:C:143:VAL:HG11	1.99	0.45
1:E:157:PHE:O	1:E:160:SER:HB3	2.16	0.45
1:E:313:HIS:O	1:E:314:PHE:O	2.35	0.45
1:F:260:TYR:HB2	1:F:271:TYR:CE2	2.51	0.45
1:H:255:LEU:O	1:H:257:VAL:N	2.46	0.45
1:A:91:ARG:O	1:A:95:VAL:HG23	2.17	0.45
1:E:39:ASN:ND2	1:E:42:LYS:HB2	2.31	0.45
1:E:119:LEU:HA	1:E:144:ILE:O	2.15	0.45
1:A:36:ILE:HG12	1:A:66:GLY:O	2.17	0.45
1:D:168:GLN:O	2:D:328:FBP:O2	2.31	0.45
1:E:214:ILE:HA	1:E:217:ASP:OD2	2.16	0.45
1:F:154:ARG:HB3	1:F:218:VAL:HG22	1.98	0.45
1:A:203:ASN:CB	1:A:206:TYR:HB2	2.42	0.45
1:D:175:ILE:HG22	1:D:274:VAL:HA	1.98	0.45
1:H:155:PHE:CE1	1:H:159:LEU:HD11	2.51	0.45
1:A:76:ILE:HD11	1:A:247:ILE:CG2	2.47	0.45
1:A:202:LYS:N	1:A:202:LYS:HD3	2.32	0.45
1:F:204:ASP:CG	1:F:205:ALA:H	2.25	0.45
1:H:188:HIS:CE1	1:H:290:ASN:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASP:HB3	1:C:205:ALA:H	1.64	0.45
1:D:296:LYS:HG2	1:D:300:LEU:HD12	1.99	0.45
1:E:52:HIS:CG	1:H:154:ARG:HG2	2.52	0.45
1:E:202:LYS:CD	1:E:203:ASN:N	2.79	0.45
1:G:264:GLN:C	1:G:266:GLY:N	2.74	0.45
1:H:146:SER:HB3	1:H:240:LEU:HD21	1.99	0.45
1:H:219:LYS:HE3	1:H:220:ASN:OD1	2.17	0.45
1:E:196:VAL:HG13	1:E:197:SER:N	2.32	0.44
1:F:15:PHE:HB3	1:F:233:TYR:CD1	2.53	0.44
1:F:213:GLN:O	1:F:216:ASP:HB3	2.17	0.44
1:G:3:LYS:O	1:G:4:HIS:CB	2.53	0.44
1:G:183:LEU:HD22	1:G:298:GLN:HB3	1.99	0.44
1:A:190:ASN:HD22	1:A:190:ASN:N	2.15	0.44
1:B:16:VAL:HG13	1:B:236:VAL:HG13	2.00	0.44
1:C:77:VAL:HG23	1:C:114:PHE:CE1	2.52	0.44
1:C:194:VAL:HA	1:C:195:PRO:HD3	1.85	0.44
1:D:175:ILE:HG12	1:D:185:VAL:CG2	2.47	0.44
1:D:236:VAL:HG22	1:D:240:LEU:HD21	1.99	0.44
1:A:201:GLU:HB3	1:A:202:LYS:HZ2	1.83	0.44
1:D:265:TYR:HB3	1:D:299:PHE:CD2	2.52	0.44
1:A:156:ARG:NH1	1:A:167:PRO:O	2.50	0.44
1:A:280:ARG:O	1:A:280:ARG:NH1	2.50	0.44
1:C:71:CYS:O	1:C:72:LYS:C	2.61	0.44
1:E:186:TRP:CZ2	1:E:215:VAL:CG2	3.01	0.44
1:F:204:ASP:O	1:F:205:ALA:HB3	2.18	0.44
1:C:37:ASP:C	1:C:39:ASN:H	2.25	0.44
1:C:171:HIS:CE1	2:C:327:FBP:O6	2.61	0.44
1:E:260:TYR:HB2	1:E:271:TYR:CE2	2.52	0.44
1:E:260:TYR:OH	1:E:269:ASP:HA	2.18	0.44
1:H:117:ILE:HD12	1:H:117:ILE:N	2.33	0.44
1:A:190:ASN:N	1:A:190:ASN:ND2	2.66	0.44
1:D:105:ILE:HD11	3:D:327:NAD:C2A	2.47	0.44
1:G:141:GLU:CD	1:G:141:GLU:H	2.26	0.44
1:A:149:THR:HG21	1:A:243:ILE:HD11	1.99	0.44
1:B:206:TYR:OH	1:E:41:GLU:HB3	2.18	0.44
1:C:264:GLN:CD	1:C:286:ILE:HD12	2.43	0.44
1:D:94:LEU:HD23	1:D:94:LEU:H	1.83	0.44
1:D:310:LEU:O	1:D:311:LYS:C	2.60	0.44
1:D:127:ILE:HD13	1:D:306:LEU:HD21	2.00	0.44
1:D:309:ILE:HG12	1:D:309:ILE:H	1.40	0.44
1:E:220:ASN:HB3	1:E:224:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:ILE:CD1	1:G:241:ALA:HB1	2.47	0.44
1:H:188:HIS:NE2	1:H:289:LEU:HB3	2.33	0.44
1:B:106:VAL:HA	1:B:109:VAL:CG1	2.48	0.44
1:B:261:LEU:HD21	1:B:274:VAL:HG21	1.99	0.44
1:B:268:ASP:OD1	1:B:268:ASP:C	2.60	0.44
1:D:6:ASN:O	1:D:30:THR:OG1	2.35	0.44
1:E:202:LYS:HE3	1:E:202:LYS:HB2	1.63	0.44
1:E:260:TYR:CE2	1:E:261:LEU:O	2.71	0.44
1:F:143:VAL:C	1:F:144:ILE:HG12	2.39	0.44
1:B:203:ASN:HB2	1:B:207:LYS:HG3	2.00	0.43
1:C:168:GLN:OE1	1:C:168:GLN:N	2.51	0.43
1:D:96:GLU:O	1:D:96:GLU:HG3	2.18	0.43
1:D:159:LEU:O	1:D:163:PHE:HD2	2.01	0.43
1:F:92:LEU:HD23	1:F:309:ILE:HG23	2.00	0.43
1:G:133:TRP:HD1	1:G:138:LEU:O	1.99	0.43
1:G:272:ILE:HG12	1:G:273:GLY:N	2.32	0.43
1:H:14:GLY:O	1:H:15:PHE:C	2.61	0.43
1:A:172:ALA:HB2	1:A:189:ALA:HB1	1.98	0.43
1:A:200:VAL:O	1:A:201:GLU:C	2.61	0.43
1:A:232:THR:O	1:A:232:THR:HG23	2.17	0.43
1:A:261:LEU:HD11	1:A:272:ILE:HG21	2.00	0.43
1:B:16:VAL:HG13	1:B:236:VAL:CG1	2.48	0.43
1:B:133:TRP:HA	1:B:143:VAL:HG21	1.99	0.43
1:C:219:LYS:HE2	1:C:219:LYS:HB3	1.77	0.43
1:E:39:ASN:CG	1:E:42:LYS:HB2	2.43	0.43
1:E:186:TRP:HZ2	1:E:215:VAL:HG23	1.83	0.43
1:E:308:ASN:O	1:E:313:HIS:CE1	2.71	0.43
1:H:16:VAL:CG1	1:H:80:CYS:HB3	2.49	0.43
1:A:287:THR:HG23	1:C:194:VAL:HG12	1.98	0.43
1:B:130:TYR:CZ	1:B:314:PHE:HE2	2.36	0.43
1:H:276:ALA:HB1	1:H:283:ILE:HD12	1.99	0.43
1:C:72:LYS:HG3	1:C:112:SER:O	2.17	0.43
1:F:56:PHE:CE2	1:G:153:ALA:HB2	2.54	0.43
1:F:133:TRP:CZ3	1:F:134:LYS:HD3	2.54	0.43
1:G:96:GLU:HG3	1:G:96:GLU:O	2.18	0.43
1:G:130:TYR:CD1	1:G:310:LEU:HD22	2.54	0.43
1:G:187:SER:OG	1:G:188:HIS:CD2	2.72	0.43
1:C:36:ILE:HG23	1:C:67:THR:HA	2.01	0.43
1:D:10:LEU:HD22	1:D:20:TYR:HD2	1.84	0.43
1:E:307:LYS:HA	1:E:310:LEU:HB2	2.01	0.43
1:G:203:ASN:OD1	1:G:207:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:LEU:N	1:H:94:LEU:CD1	2.81	0.43
1:H:98:ASN:C	1:H:101:ILE:HD12	2.42	0.43
1:A:154:ARG:HG2	1:D:52:HIS:CG	2.54	0.43
1:B:275:PRO:HB2	1:B:287:THR:HB	2.01	0.43
1:B:183:LEU:HD12	1:B:184:PRO:O	2.18	0.43
1:G:156:ARG:HD3	1:G:170:VAL:O	2.19	0.43
1:G:254:ILE:C	1:G:255:LEU:HG	2.43	0.43
1:H:149:THR:HG21	1:H:243:ILE:HD11	2.00	0.43
1:H:277:VAL:O	1:H:277:VAL:HG12	2.18	0.43
1:A:201:GLU:HB2	1:A:202:LYS:HZ3	1.84	0.43
1:A:233:TYR:HA	1:A:236:VAL:CG1	2.49	0.43
1:B:191:VAL:O	1:B:194:VAL:HG13	2.19	0.43
1:D:206:TYR:O	1:D:206:TYR:CD2	2.72	0.43
1:E:186:TRP:C	1:E:188:HIS:N	2.76	0.43
1:F:29:ILE:CD1	1:F:245:LYS:HB2	2.47	0.43
1:F:177:GLU:HG2	1:F:178:HIS:O	2.19	0.43
1:H:50:LEU:HD23	1:H:50:LEU:HA	1.80	0.43
1:H:98:ASN:CB	1:H:101:ILE:CD1	2.97	0.43
1:A:20:TYR:O	1:A:24:LEU:HG	2.19	0.43
1:A:29:ILE:HG23	1:A:245:LYS:HA	2.00	0.43
1:B:95:VAL:O	1:B:96:GLU:C	2.61	0.43
1:B:313:HIS:CD2	1:B:313:HIS:N	2.87	0.43
1:A:58:PRO:HG2	1:A:59:GLN:H	1.83	0.43
1:A:85:GLN:CB	1:A:94:LEU:HD22	2.45	0.43
1:B:134:LYS:HD2	1:B:134:LYS:HA	1.77	0.43
1:B:255:LEU:O	1:B:257:VAL:N	2.48	0.43
1:E:140:LYS:HD3	1:E:260:TYR:CD2	2.53	0.43
1:E:150:LEU:O	1:E:150:LEU:HD12	2.19	0.43
1:G:263:GLY:CA	1:G:267:ALA:O	2.67	0.43
1:H:131:ALA:HB1	1:H:135:PHE:CE2	2.54	0.43
1:B:178:HIS:O	1:B:178:HIS:CG	2.72	0.42
1:B:207:LYS:C	1:B:209:GLU:H	2.27	0.42
1:C:37:ASP:C	1:C:39:ASN:N	2.77	0.42
1:G:14:GLY:HA2	1:G:42:LYS:CE	2.47	0.42
1:H:101:ILE:H	1:H:101:ILE:HG13	1.22	0.42
1:A:24:LEU:HD23	1:A:29:ILE:HD12	2.01	0.42
1:C:200:VAL:HB	1:C:207:LYS:HD2	2.00	0.42
1:D:128:LEU:HA	1:D:131:ALA:HB3	2.01	0.42
1:D:239:SER:O	1:D:240:LEU:C	2.61	0.42
1:D:261:LEU:HD13	1:D:264:GLN:O	2.20	0.42
1:E:234:TYR:HB2	1:H:49:ASP:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:CYS:HA	1:F:119:LEU:O	2.19	0.42
1:G:148:THR:HB	1:G:151:ASP:HB2	2.00	0.42
1:H:9:ALA:HA	1:H:34:VAL:HG12	2.00	0.42
1:H:289:LEU:HD12	1:H:289:LEU:H	1.84	0.42
1:B:138:LEU:HB3	1:B:139:PRO:HD2	2.01	0.42
1:D:38:VAL:HG12	3:D:327:NAD:C2A	2.48	0.42
1:D:94:LEU:H	1:D:94:LEU:CD2	2.33	0.42
1:E:313:HIS:CD2	1:E:313:HIS:N	2.86	0.42
1:F:260:TYR:HB2	1:F:271:TYR:CZ	2.54	0.42
1:G:187:SER:OG	1:G:188:HIS:HD2	2.02	0.42
1:A:200:VAL:HA	1:A:207:LYS:HD3	2.01	0.42
1:C:145:GLY:C	1:C:147:GLY:N	2.78	0.42
1:F:198:GLU:OE1	1:H:290:ASN:HB2	2.19	0.42
1:F:264:GLN:H	1:F:264:GLN:CD	2.28	0.42
1:G:148:THR:O	1:G:149:THR:C	2.61	0.42
1:H:40:LYS:CB	1:H:65:TYR:OH	2.68	0.42
1:A:261:LEU:O	1:A:268:ASP:HA	2.19	0.42
1:C:57:ALA:CB	1:C:58:PRO:HD2	2.46	0.42
1:D:305:VAL:O	1:D:309:ILE:CG1	2.67	0.42
1:E:25:ILE:O	1:E:25:ILE:CG2	2.66	0.42
1:E:301:HIS:O	1:E:302:SER:C	2.63	0.42
1:E:311:LYS:HD2	1:E:311:LYS:HA	1.86	0.42
1:H:31:ASP:O	1:H:32:GLU:HG2	2.19	0.42
1:H:264:GLN:O	1:H:265:TYR:HB2	2.20	0.42
1:A:263:GLY:N	1:A:267:ALA:O	2.48	0.42
1:C:229:LYS:C	1:C:231:ALA:H	2.26	0.42
1:F:150:LEU:HD22	1:F:236:VAL:HB	2.01	0.42
1:H:292:ASN:OD1	1:H:292:ASN:C	2.63	0.42
1:H:307:LYS:HA	1:H:310:LEU:HD12	2.01	0.42
1:B:229:LYS:NZ	1:B:231:ALA:O	2.40	0.42
1:E:206:TYR:O	1:E:209:GLU:HG2	2.20	0.42
1:H:25:ILE:N	1:H:25:ILE:CD1	2.83	0.42
1:H:57:ALA:HA	1:H:58:PRO:HD3	1.94	0.42
1:A:156:ARG:HD3	1:A:170:VAL:O	2.20	0.42
1:A:234:TYR:O	1:A:238:MET:HG2	2.20	0.42
1:B:138:LEU:HB3	1:B:139:PRO:CD	2.50	0.42
1:C:268:ASP:O	1:C:269:ASP:HB3	2.20	0.42
1:D:98:ASN:O	1:D:102:PHE:HD1	2.03	0.42
1:H:3:LYS:O	1:H:5:VAL:HG13	2.19	0.42
1:H:25:ILE:O	1:H:25:ILE:HG22	2.19	0.42
1:H:244:THR:O	1:H:248:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ASP:O	1:D:61:VAL:HG13	2.20	0.42
1:D:139:PRO:O	1:D:141:GLU:N	2.53	0.42
1:E:154:ARG:HG2	1:H:52:HIS:CG	2.55	0.42
1:B:251:GLU:O	1:B:252:ASN:HB2	2.20	0.42
1:F:200:VAL:O	1:F:204:ASP:HB2	2.19	0.42
1:F:236:VAL:HG13	1:F:237:ALA:N	2.35	0.42
1:A:69:GLU:HA	1:A:112:SER:HB2	2.01	0.41
1:B:103:LYS:O	1:B:107:SER:HB2	2.20	0.41
1:D:127:ILE:HD13	1:D:306:LEU:CD2	2.50	0.41
1:D:130:TYR:HE2	1:D:260:TYR:HE1	1.68	0.41
1:E:109:VAL:HG21	1:E:118:PHE:CZ	2.55	0.41
1:F:154:ARG:HH22	1:F:232:THR:HG21	1.84	0.41
1:A:257:VAL:O	1:A:273:GLY:HA2	2.20	0.41
1:B:296:LYS:O	1:B:300:LEU:CD2	2.61	0.41
1:D:296:LYS:HG2	1:D:300:LEU:CD1	2.51	0.41
1:F:71:CYS:O	1:F:72:LYS:C	2.63	0.41
1:F:251:GLU:O	1:F:252:ASN:HB2	2.21	0.41
1:B:272:ILE:HG12	1:B:273:GLY:H	1.85	0.41
1:D:123:ASN:HA	1:D:125:VAL:N	2.35	0.41
1:E:94:LEU:HD12	1:E:94:LEU:O	2.20	0.41
1:E:226:ILE:O	1:E:230:GLY:N	2.51	0.41
1:G:206:TYR:C	1:G:208:GLN:N	2.77	0.41
1:G:236:VAL:O	1:G:240:LEU:HG	2.20	0.41
1:H:279:ASN:OD1	1:H:279:ASN:C	2.63	0.41
1:C:76:ILE:HA	1:C:117:ILE:O	2.19	0.41
1:D:73:ASP:OD1	1:D:73:ASP:N	2.45	0.41
1:D:291:LEU:HB3	1:D:292:ASN:H	1.45	0.41
1:G:234:TYR:O	1:G:238:MET:HG2	2.20	0.41
1:H:272:ILE:HG13	1:H:306:LEU:HD11	2.02	0.41
1:H:289:LEU:HD12	1:H:289:LEU:N	2.36	0.41
1:A:51:ASN:HB3	1:D:157:PHE:CZ	2.56	0.41
1:A:238:MET:HG3	1:D:53:GLY:CA	2.27	0.41
1:B:125:VAL:HG21	1:B:146:SER:H	1.85	0.41
1:C:264:GLN:OE1	1:C:286:ILE:HD12	2.20	0.41
1:D:10:LEU:HD12	1:D:11:ILE:N	2.35	0.41
1:D:126:ASP:HB3	1:D:306:LEU:HD11	2.01	0.41
1:D:134:LYS:CG	1:D:314:PHE:HE1	2.32	0.41
1:F:225:ILE:HD11	1:G:52:HIS:CE1	2.55	0.41
1:F:265:TYR:CE2	1:F:274:VAL:HG11	2.55	0.41
1:G:200:VAL:HA	1:G:203:ASN:CG	2.45	0.41
1:H:259:THR:HA	1:H:271:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HE2	1:A:86:LYS:HB3	1.83	0.41
1:C:75:ASP:O	1:C:76:ILE:HG13	2.19	0.41
1:H:70:ASP:C	1:H:72:LYS:N	2.79	0.41
1:B:203:ASN:HD22	1:B:203:ASN:N	2.19	0.41
1:D:79:ILE:HB	1:D:120:VAL:HG13	2.03	0.41
1:F:144:ILE:HD13	1:F:283:ILE:HG12	2.03	0.41
1:H:94:LEU:HD22	1:H:95:VAL:N	2.36	0.41
1:H:108:GLU:O	1:H:111:ALA:HB3	2.21	0.41
1:A:3:LYS:N	4:A:337:HOH:O	2.53	0.41
1:D:20:TYR:CD1	1:D:240:LEU:HB3	2.56	0.41
1:D:292:ASN:O	1:D:293:GLU:C	2.64	0.41
1:G:187:SER:HB3	1:G:292:ASN:ND2	2.36	0.41
1:A:118:PHE:CE2	1:A:138:LEU:HD12	2.56	0.41
1:A:209:GLU:HA	1:A:212:ASP:OD2	2.21	0.41
1:B:9:ALA:HB3	1:B:77:VAL:HG22	2.02	0.41
1:B:280:ARG:HD2	1:B:280:ARG:C	2.36	0.41
1:B:311:LYS:HB3	1:B:312:PRO:HD3	2.02	0.41
1:C:156:ARG:NH1	2:C:327:FBP:O4	2.54	0.41
1:D:309:ILE:O	1:D:313:HIS:CE1	2.73	0.41
1:F:224:HIS:O	1:F:227:GLU:HB3	2.21	0.41
1:F:263:GLY:N	1:F:267:ALA:O	2.54	0.41
1:H:115:ASP:OD1	1:H:142:ARG:NH2	2.53	0.41
1:A:108:GLU:O	1:A:109:VAL:C	2.64	0.41
1:A:204:ASP:O	1:A:205:ALA:CB	2.69	0.41
1:B:54:LYS:HE3	1:B:61:VAL:O	2.20	0.41
1:B:243:ILE:O	1:B:247:ILE:HG13	2.21	0.41
1:C:202:LYS:HA	1:C:202:LYS:HD2	1.85	0.41
1:A:226:ILE:HG12	1:A:231:ALA:HA	2.02	0.40
1:A:232:THR:O	1:A:232:THR:CG2	2.69	0.40
1:B:300:LEU:O	1:B:303:ALA:HB3	2.21	0.40
1:A:262:ASP:HA	1:A:268:ASP:HB2	2.02	0.40
1:D:10:LEU:HD12	1:D:10:LEU:C	2.46	0.40
1:E:184:PRO:HG3	1:E:215:VAL:HG11	2.04	0.40
1:F:242:ARG:HG2	1:G:56:PHE:CD1	2.57	0.40
1:B:168:GLN:HB3	2:D:328:FBP:H4	2.04	0.40
1:C:202:LYS:O	1:C:203:ASN:C	2.64	0.40
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.96	0.40
1:E:194:VAL:HA	1:E:195:PRO:HD3	1.88	0.40
1:E:305:VAL:O	1:E:305:VAL:CG1	2.69	0.40
1:B:141:GLU:O	1:B:282:GLY:HA3	2.21	0.40
1:B:275:PRO:HG2	1:B:289:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD11	1:C:272:ILE:HG21	2.02	0.40
1:F:22:PHE:CD1	1:G:234:TYR:CD1	3.09	0.40
1:F:194:VAL:HA	1:F:195:PRO:HD3	1.85	0.40
1:G:238:MET:HG2	1:G:238:MET:H	1.71	0.40
1:B:85:GLN:HB2	1:B:94:LEU:HD22	2.04	0.40
1:C:186:TRP:CE3	1:C:196:VAL:HG11	2.56	0.40
1:C:209:GLU:H	1:C:209:GLU:HG2	1.50	0.40
1:F:226:ILE:HG23	1:F:230:GLY:O	2.22	0.40
1:H:260:TYR:CZ	1:H:269:ASP:HA	2.57	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	308/326 (94%)	281 (91%)	26 (8%)	1 (0%)	36	48
1	B	310/326 (95%)	276 (89%)	27 (9%)	7 (2%)	5	5
1	C	297/326 (91%)	258 (87%)	37 (12%)	2 (1%)	18	26
1	D	297/326 (91%)	251 (84%)	36 (12%)	10 (3%)	3	2
1	E	309/326 (95%)	273 (88%)	30 (10%)	6 (2%)	6	7
1	F	309/326 (95%)	271 (88%)	32 (10%)	6 (2%)	6	7
1	G	298/326 (91%)	266 (89%)	23 (8%)	9 (3%)	3	3
1	H	297/326 (91%)	255 (86%)	32 (11%)	10 (3%)	3	2
All	All	2425/2608 (93%)	2131 (88%)	243 (10%)	51 (2%)	5	6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	ASP

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Mol	Chain	Res	Type
1	D	202	LYS
1	D	208	GLN
1	F	204	ASP
1	G	205	ALA
1	H	72	LYS
1	H	95	VAL
1	H	207	LYS
1	B	256	THR
1	D	201	GLU
1	D	291	LEU
1	F	38	VAL
1	F	202	LYS
1	F	203	ASN
1	G	96	GLU
1	H	312	PRO
1	B	208	GLN
1	B	233	TYR
1	D	205	ALA
1	E	187	SER
1	E	312	PRO
1	F	265	TYR
1	G	187	SER
1	G	201	GLU
1	G	204	ASP
1	G	312	PRO
1	H	13	ALA
1	A	58	PRO
1	C	230	GLY
1	D	140	LYS
1	E	28	GLY
1	E	233	TYR
1	G	3	LYS
1	G	178	HIS
1	H	4	HIS
1	H	96	GLU
1	H	313	HIS
1	B	222	ALA
1	E	313	HIS
1	F	208	GLN
1	H	256	THR
1	D	28	GLY
1	E	164	GLY

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Mol	Chain	Res	Type
1	D	270	VAL
1	G	95	VAL
1	H	12	GLY
1	B	28	GLY
1	D	95	VAL
1	B	38	VAL
1	C	58	PRO
1	D	311	LYS

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	252/267 (94%)	233 (92%)	19 (8%)	12	19
1	B	253/267 (95%)	230 (91%)	23 (9%)	9	13
1	C	245/267 (92%)	221 (90%)	24 (10%)	7	10
1	D	246/267 (92%)	222 (90%)	24 (10%)	7	10
1	E	253/267 (95%)	231 (91%)	22 (9%)	9	14
1	F	253/267 (95%)	228 (90%)	25 (10%)	7	10
1	G	247/267 (92%)	228 (92%)	19 (8%)	12	18
1	H	246/267 (92%)	219 (89%)	27 (11%)	6	8
All	All	1995/2136 (93%)	1812 (91%)	183 (9%)	8	12

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	HIS
1	A	25	ILE
1	A	40	LYS
1	A	41	GLU
1	A	69	GLU
1	A	103	LYS

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Mol	Chain	Res	Type
1	A	107	SER
1	A	122	THR
1	A	125	VAL
1	A	146	SER
1	A	190	ASN
1	A	201	GLU
1	A	236	VAL
1	A	239	SER
1	A	243	ILE
1	A	247	ILE
1	A	253	SER
1	A	259	THR
1	B	4	HIS
1	B	25	ILE
1	B	40	LYS
1	B	41	GLU
1	B	96	GLU
1	B	103	LYS
1	B	183	LEU
1	B	194	VAL
1	B	201	GLU
1	B	203	ASN
1	B	204	ASP
1	B	210	GLU
1	B	216	ASP
1	B	239	SER
1	B	251	GLU
1	B	257	VAL
1	B	259	THR
1	B	277	VAL
1	B	280	ARG
1	B	289	LEU
1	B	297	GLU
1	B	313	HIS
1	B	314	PHE
1	C	4	HIS
1	C	38	VAL
1	C	41	GLU
1	C	75	ASP
1	C	94	LEU
1	C	109	VAL
1	C	122	THR

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Mol	Chain	Res	Type
1	C	140	LYS
1	C	158	MET
1	C	183	LEU
1	C	194	VAL
1	C	203	ASN
1	C	209	GLU
1	C	210	GLU
1	C	216	ASP
1	C	224	HIS
1	C	242	ARG
1	C	253	SER
1	C	259	THR
1	C	270	VAL
1	C	289	LEU
1	C	293	GLU
1	C	308	ASN
1	C	311	LYS
1	D	10	LEU
1	D	18	SER
1	D	38	VAL
1	D	65	TYR
1	D	96	GLU
1	D	100	LYS
1	D	105	ILE
1	D	107	SER
1	D	109	VAL
1	D	144	ILE
1	D	151	ASP
1	D	180	ASP
1	D	183	LEU
1	D	194	VAL
1	D	196	VAL
1	D	206	TYR
1	D	224	HIS
1	D	262	ASP
1	D	283	ILE
1	D	286	ILE
1	D	288	GLU
1	D	300	LEU
1	D	306	LEU
1	D	309	ILE
1	E	4	HIS

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Mol	Chain	Res	Type
1	E	40	LYS
1	E	54	LYS
1	E	79	ILE
1	E	86	LYS
1	E	95	VAL
1	E	97	LYS
1	E	109	VAL
1	E	122	THR
1	E	148	THR
1	E	180	ASP
1	E	183	LEU
1	E	185	VAL
1	E	194	VAL
1	E	202	LYS
1	E	211	LEU
1	E	226	ILE
1	E	255	LEU
1	E	259	THR
1	E	272	ILE
1	E	288	GLU
1	E	297	GLU
1	F	25	ILE
1	F	38	VAL
1	F	46	ASP
1	F	62	LYS
1	F	97	LYS
1	F	109	VAL
1	F	126	ASP
1	F	144	ILE
1	F	160	SER
1	F	161	GLU
1	F	174	ILE
1	F	183	LEU
1	F	190	ASN
1	F	194	VAL
1	F	200	VAL
1	F	202	LYS
1	F	208	GLN
1	F	214	ILE
1	F	218	VAL
1	F	259	THR
1	F	287	THR

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Mol	Chain	Res	Type
1	F	288	GLU
1	F	293	GLU
1	F	305	VAL
1	F	306	LEU
1	G	2	ASN
1	G	4	HIS
1	G	18	SER
1	G	94	LEU
1	G	96	GLU
1	G	112	SER
1	G	140	LYS
1	G	160	SER
1	G	183	LEU
1	G	196	VAL
1	G	201	GLU
1	G	202	LYS
1	G	214	ILE
1	G	232	THR
1	G	233	TYR
1	G	259	THR
1	G	290	ASN
1	G	302	SER
1	G	311	LYS
1	H	11	ILE
1	H	16	VAL
1	H	25	ILE
1	H	34	VAL
1	H	40	LYS
1	H	47	VAL
1	H	61	VAL
1	H	67	THR
1	H	94	LEU
1	H	99	LEU
1	H	101	ILE
1	H	102	PHE
1	H	112	SER
1	H	119	LEU
1	H	180	ASP
1	H	183	LEU
1	H	194	VAL
1	H	201	GLU
1	H	207	LYS

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Mol	Chain	Res	Type
1	H	209	GLU
1	H	216	ASP
1	H	236	VAL
1	H	240	LEU
1	H	288	GLU
1	H	291	LEU
1	H	293	GLU
1	H	294	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	26	ASN
1	B	203	ASN
1	B	224	HIS
1	B	313	HIS
1	C	27	GLN
1	C	98	ASN
1	C	123	ASN
1	C	178	HIS
1	D	39	ASN
1	D	178	HIS
1	E	52	HIS
1	E	59	GLN
1	E	84	ASN
1	E	188	HIS
1	E	203	ASN
1	E	213	GLN
1	E	224	HIS
1	E	252	ASN
1	F	85	GLN
1	F	169	ASN
1	F	173	HIS
1	F	313	HIS
1	G	2	ASN
1	G	6	ASN
1	G	39	ASN
1	G	168	GLN
1	G	290	ASN
1	G	308	ASN
1	H	4	HIS

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Mol	Chain	Res	Type
1	H	188	HIS
1	H	190	ASN
1	H	213	GLN
1	H	252	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	FBP	D	328	-	18,20,20	0.94	1 (5%)	21,32,32	0.87	0
2	FBP	F	327	-	18,20,20	0.98	2 (11%)	21,32,32	1.13	2 (9%)
3	NAD	D	327	-	46,48,48	1.79	5 (10%)	64,73,73	1.61	11 (17%)
2	FBP	C	327	-	18,20,20	1.07	1 (5%)	21,32,32	1.71	5 (23%)
2	FBP	G	327	-	18,20,20	1.03	2 (11%)	21,32,32	1.08	3 (14%)

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	FBP	D	328	-	1/1/6/6	7/13/32/32	0/1/1/1
2	FBP	F	327	-	1/1/6/6	6/13/32/32	0/1/1/1
3	NAD	D	327	-	-	7/30/62/62	0/5/5/5
2	FBP	C	327	-	-	2/13/32/32	0/1/1/1
2	FBP	G	327	-	1/1/6/6	3/13/32/32	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	327	NAD	O7N-C7N	9.67	1.42	1.24
2	C	327	FBP	O2-C2	2.86	1.45	1.40
2	G	327	FBP	O2-C2	2.77	1.45	1.40
3	D	327	NAD	C2A-N1A	2.66	1.38	1.33
3	D	327	NAD	C2A-N3A	2.64	1.38	1.33
2	D	328	FBP	O2-C2	2.63	1.45	1.40
3	D	327	NAD	C2N-N1N	2.47	1.37	1.35
2	F	327	FBP	O5-C2	-2.35	1.39	1.43
3	D	327	NAD	C8A-N7A	2.21	1.35	1.31
2	G	327	FBP	O5-C2	-2.12	1.40	1.43
2	F	327	FBP	O2-C2	2.09	1.44	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	327	NAD	N3A-C2A-N1A	-5.53	120.21	128.58
3	D	327	NAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	C	327	FBP	O6P-P2-O6	4.45	118.26	106.67
3	D	327	NAD	N9A-C8A-N7A	-4.03	108.22	113.94
3	D	327	NAD	C5A-N7A-C8A	3.45	108.88	103.45
3	D	327	NAD	C2A-N3A-C4A	3.40	120.13	111.83
2	F	327	FBP	O2-C2-O5	-3.10	103.37	109.33
3	D	327	NAD	N3A-C4A-N9A	3.05	132.36	127.17
2	C	327	FBP	O5-C5-C6	2.95	116.44	109.50
2	C	327	FBP	O6-C6-C5	2.69	118.16	108.99
2	G	327	FBP	O2-C2-O5	-2.62	104.29	109.33
2	G	327	FBP	O3P-P1-O1	2.38	112.88	106.67
3	D	327	NAD	C4A-C5A-N7A	-2.32	107.94	110.58
2	F	327	FBP	O1-P1-O1P	2.30	112.65	106.44
2	C	327	FBP	O3P-P1-O1	2.27	112.59	106.67
3	D	327	NAD	O5B-C5B-C4B	-2.20	101.52	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	327	NAD	C6N-N1N-C2N	-2.18	120.02	121.88
3	D	327	NAD	O2A-PA-O3	2.17	113.13	107.27
2	G	327	FBP	O6P-P2-O6	2.08	112.10	106.67
3	D	327	NAD	C4A-N9A-C8A	2.04	107.89	105.74
2	C	327	FBP	C5-C4-C3	2.00	108.29	102.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	328	FBP	C2
2	F	327	FBP	C2
2	G	327	FBP	C2

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	327	FBP	C6-O6-P2-O6P
2	D	328	FBP	C1-O1-P1-O2P
2	D	328	FBP	O1-C1-C2-C3
2	F	327	FBP	O1-C1-C2-O2
2	F	327	FBP	O1-C1-C2-C3
2	F	327	FBP	O1-C1-C2-O5
2	G	327	FBP	C1-O1-P1-O2P
2	G	327	FBP	C1-O1-P1-O3P
3	D	327	NAD	C5B-O5B-PA-O1A
3	D	327	NAD	PN-O3-PA-O5B
3	D	327	NAD	C2N-C3N-C7N-O7N
3	D	327	NAD	C2N-C3N-C7N-N7N
2	F	327	FBP	C4-C5-C6-O6
2	D	328	FBP	C4-C5-C6-O6
2	F	327	FBP	O5-C5-C6-O6
2	D	328	FBP	C1-O1-P1-O1P
2	G	327	FBP	C1-O1-P1-O1P
2	C	327	FBP	O5-C5-C6-O6
2	D	328	FBP	O5-C5-C6-O6
2	F	327	FBP	C1-O1-P1-O2P
2	D	328	FBP	O1-C1-C2-O2
3	D	327	NAD	C5B-O5B-PA-O2A
2	D	328	FBP	C1-O1-P1-O3P
3	D	327	NAD	PA-O3-PN-O2N
3	D	327	NAD	C4B-C5B-O5B-PA

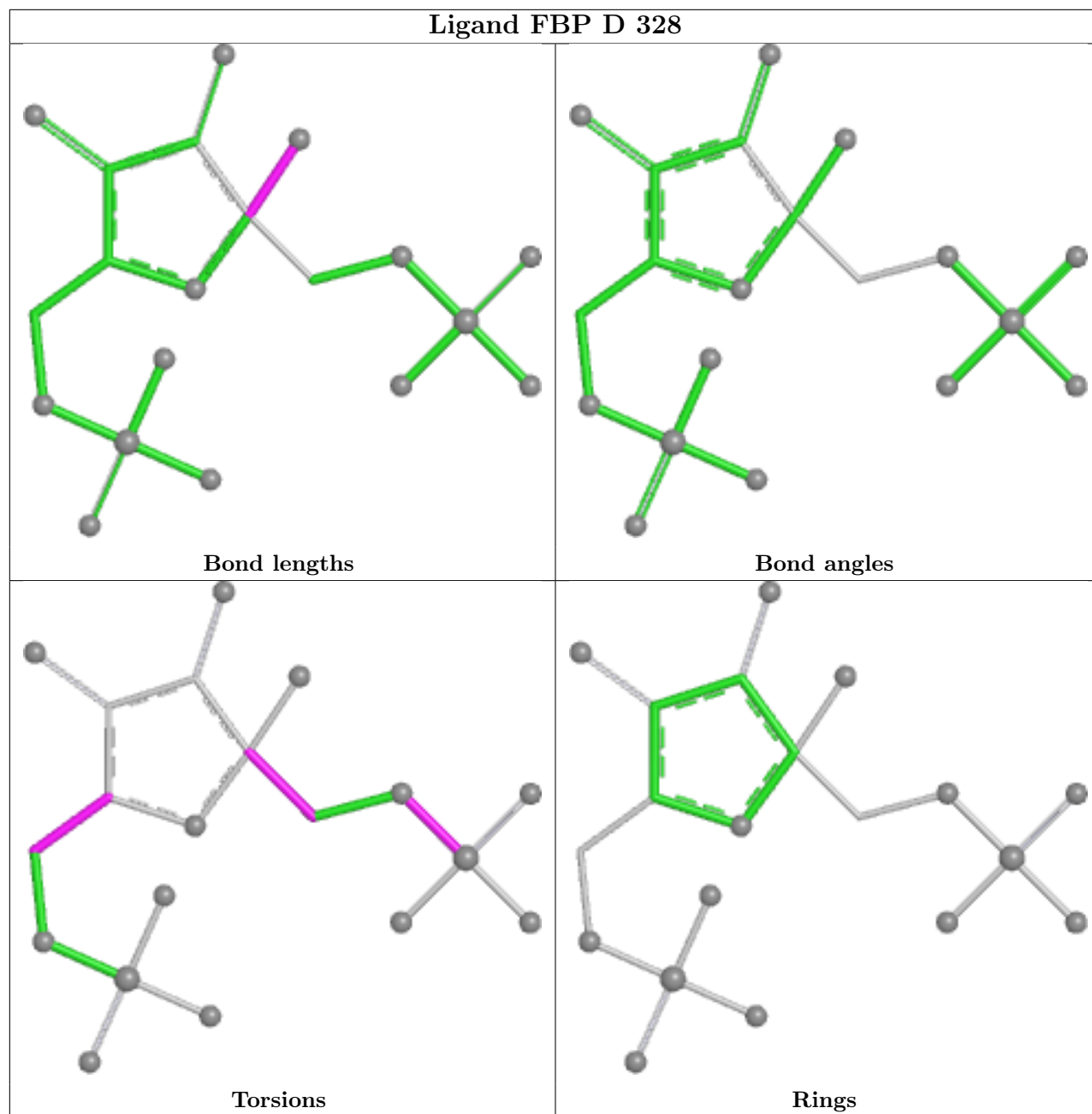
There are no ring outliers.

4 monomers are involved in 26 short contacts:

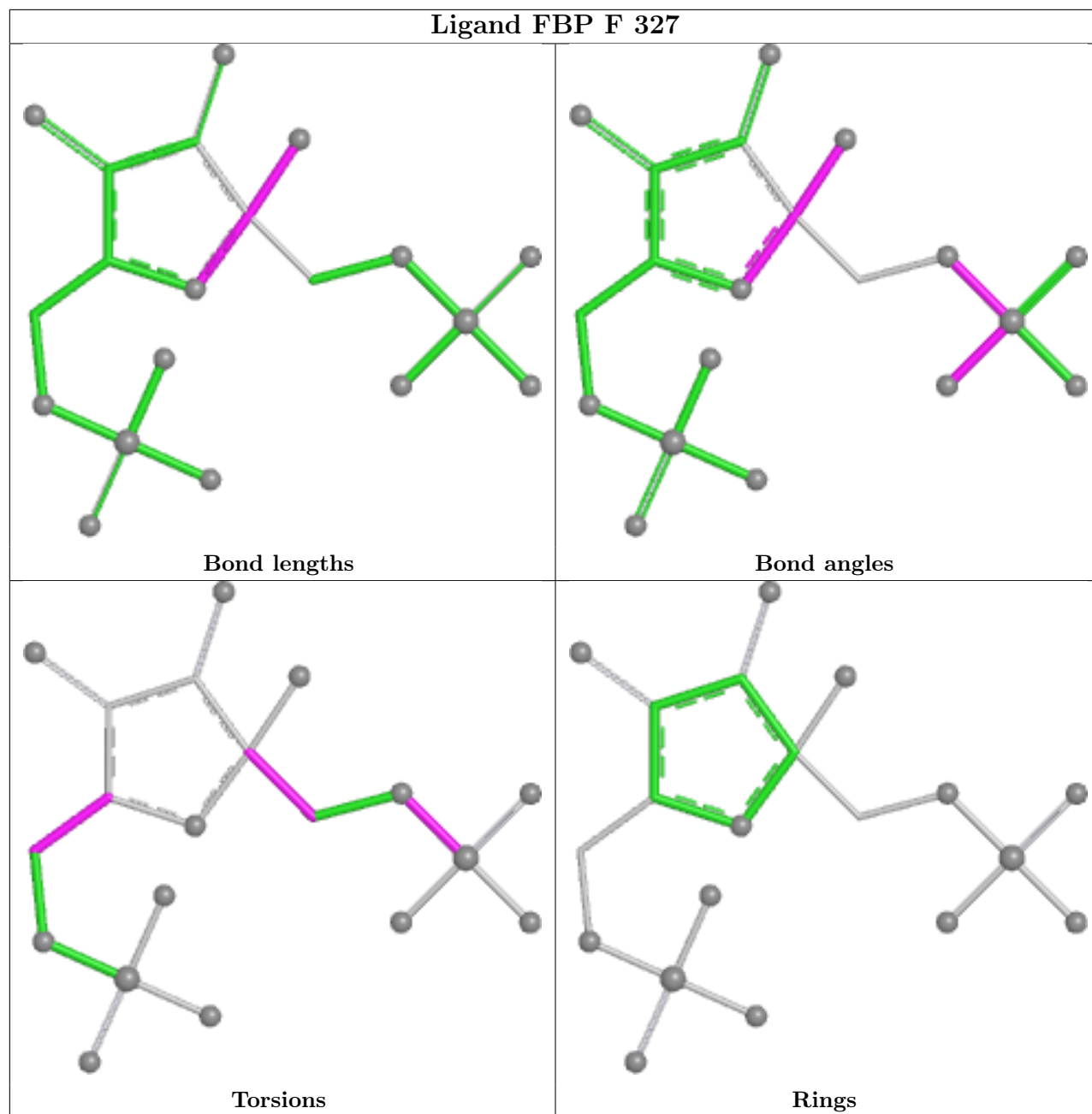
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	328	FBP	2	0
2	F	327	FBP	2	0
3	D	327	NAD	9	0
2	C	327	FBP	13	0

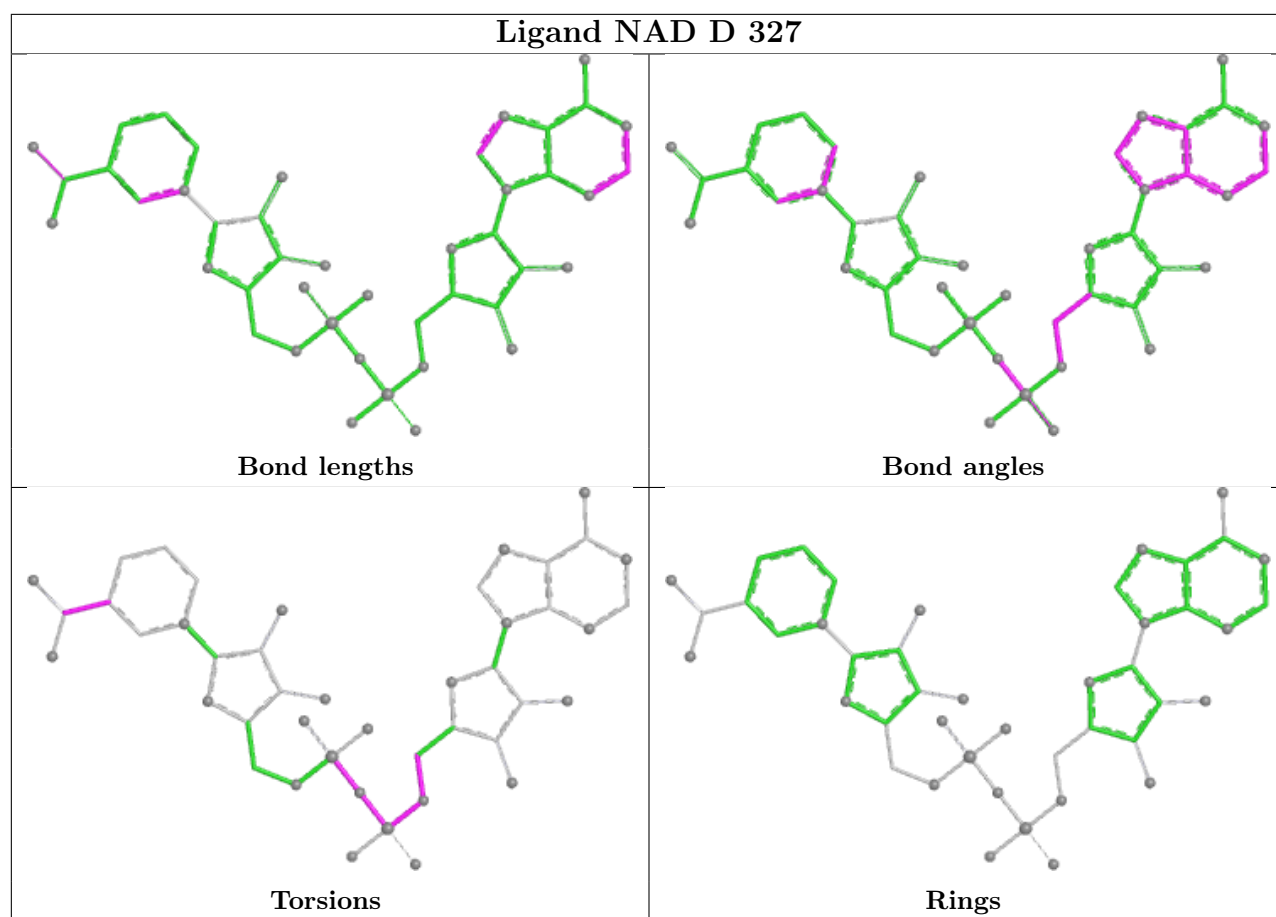
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FBP D 328

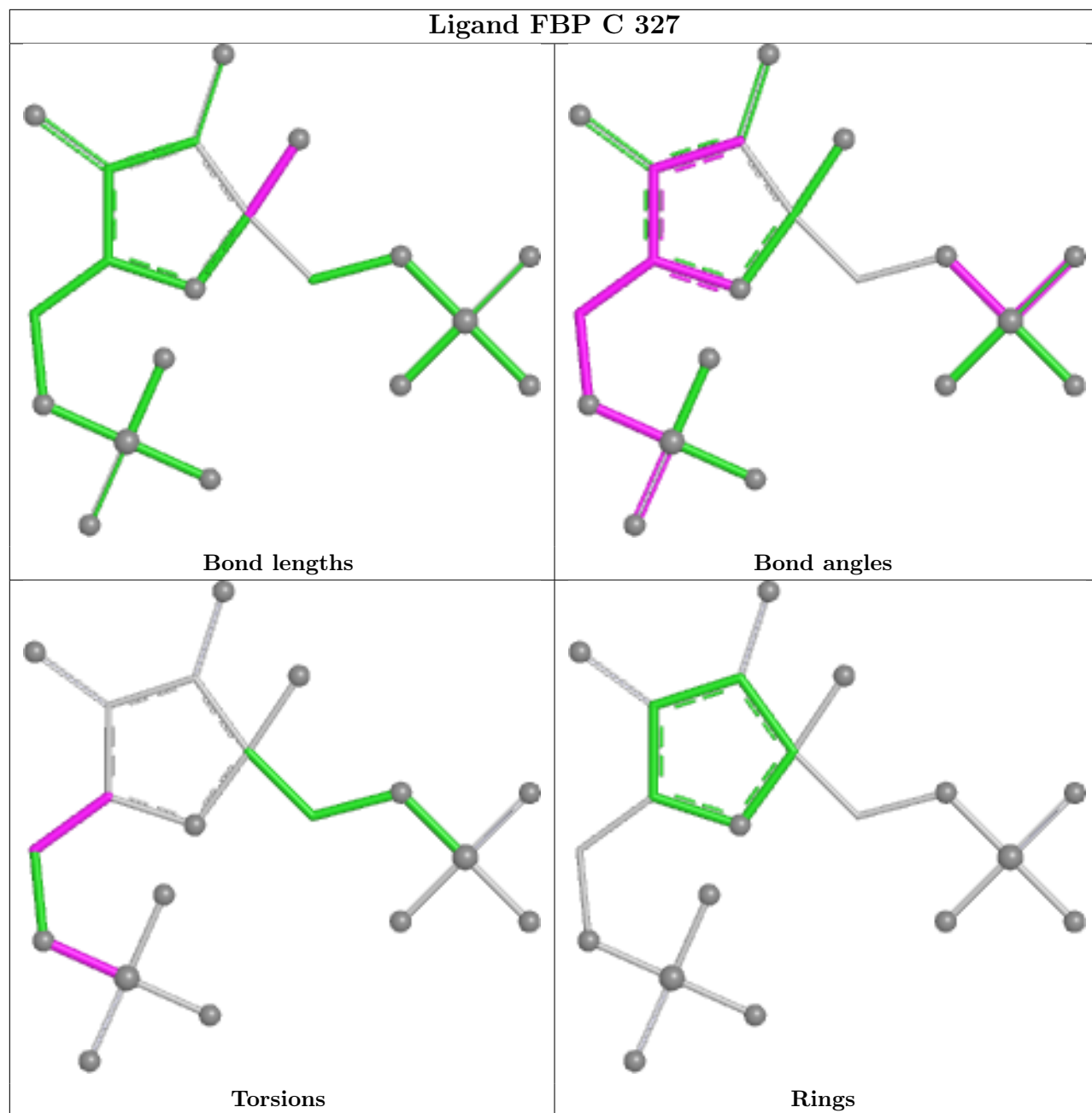


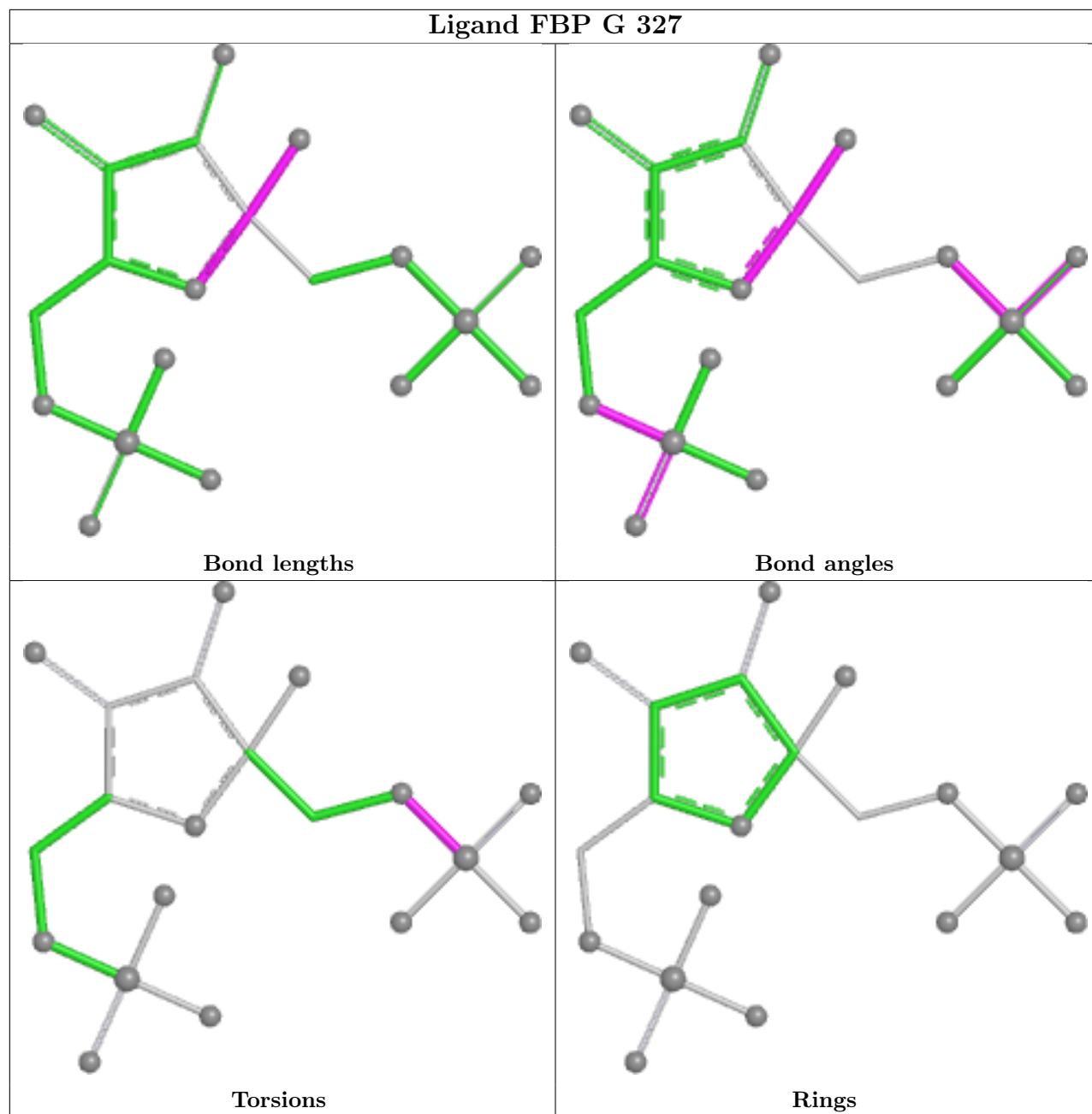
Ligand FBP F 327





Ligand FBP C 327





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	310/326 (95%)	0.36	7 (2%) 61 60	30, 50, 71, 90	0
1	B	312/326 (95%)	0.32	11 (3%) 47 47	28, 46, 70, 80	0
1	C	301/326 (92%)	0.39	13 (4%) 40 39	30, 50, 72, 89	0
1	D	301/326 (92%)	0.96	32 (10%) 11 10	45, 67, 89, 103	0
1	E	311/326 (95%)	0.35	14 (4%) 38 37	33, 50, 69, 89	0
1	F	311/326 (95%)	0.39	13 (4%) 40 40	30, 50, 71, 90	0
1	G	302/326 (92%)	0.40	16 (5%) 32 31	31, 51, 73, 90	0
1	H	301/326 (92%)	0.94	33 (10%) 10 9	45, 65, 95, 116	0
All	All	2449/2608 (93%)	0.51	139 (5%) 29 28	28, 53, 81, 116	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	8.7
1	C	223	TYR	5.6
1	D	287	THR	5.5
1	D	308	ASN	4.9
1	H	206	TYR	4.6
1	G	206	TYR	4.2
1	F	73	ASP	4.1
1	G	95	VAL	4.1
1	G	205	ALA	4.0
1	D	206	TYR	4.0
1	B	4	HIS	3.9
1	H	3	LYS	3.9
1	C	207	LYS	3.9
1	A	223	TYR	3.8
1	D	205	ALA	3.8
1	D	92	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	206	TYR	3.7
1	H	204	ASP	3.6
1	F	38	VAL	3.5
1	E	223	TYR	3.5
1	G	231	ALA	3.4
1	D	306	LEU	3.4
1	F	84	ASN	3.4
1	H	207	LYS	3.4
1	H	4	HIS	3.3
1	F	205	ALA	3.2
1	H	309	ILE	3.2
1	H	270	VAL	3.2
1	G	223	TYR	3.1
1	H	223	TYR	3.1
1	G	311	LYS	3.1
1	E	205	ALA	3.1
1	A	196	VAL	3.1
1	H	313	HIS	3.1
1	H	262	ASP	3.1
1	D	310	LEU	3.1
1	C	73	ASP	3.0
1	E	84	ASN	3.0
1	D	311	LYS	3.0
1	B	197	SER	3.0
1	D	270	VAL	2.9
1	H	263	GLY	2.9
1	H	100	LYS	2.9
1	A	205	ALA	2.9
1	H	203	ASN	2.9
1	B	202	LYS	2.8
1	H	312	PRO	2.8
1	E	73	ASP	2.8
1	E	313	HIS	2.8
1	E	206	TYR	2.8
1	C	209	GLU	2.8
1	H	264	GLN	2.8
1	H	205	ALA	2.8
1	D	312	PRO	2.8
1	G	203	ASN	2.7
1	F	206	TYR	2.7
1	D	95	VAL	2.7
1	H	99	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	81	ALA	2.6
1	G	94	LEU	2.6
1	D	202	LYS	2.6
1	E	314	PHE	2.6
1	H	38	VAL	2.6
1	B	205	ALA	2.6
1	B	193	GLY	2.6
1	E	216	ASP	2.6
1	H	98	ASN	2.6
1	D	125	VAL	2.6
1	G	232	THR	2.5
1	F	197	SER	2.5
1	D	223	TYR	2.5
1	H	94	LEU	2.5
1	C	205	ALA	2.5
1	E	4	HIS	2.5
1	D	305	VAL	2.5
1	G	192	GLY	2.5
1	D	69	GLU	2.5
1	H	314	PHE	2.5
1	D	174	ILE	2.5
1	H	260	TYR	2.5
1	F	211	LEU	2.5
1	G	3	LYS	2.5
1	B	308	ASN	2.5
1	E	253	SER	2.4
1	D	286	ILE	2.4
1	F	310	LEU	2.4
1	C	202	LYS	2.4
1	H	303	ALA	2.4
1	D	182	GLU	2.4
1	B	253	SER	2.4
1	G	313	HIS	2.4
1	C	303	ALA	2.4
1	H	265	TYR	2.4
1	C	203	ASN	2.4
1	F	88	GLY	2.4
1	D	109	VAL	2.4
1	D	309	ILE	2.4
1	B	164	GLY	2.3
1	G	314	PHE	2.3
1	H	120	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	4	HIS	2.3
1	H	308	ASN	2.3
1	F	207	LYS	2.3
1	B	196	VAL	2.3
1	D	120	VAL	2.3
1	F	199	LEU	2.3
1	H	268	ASP	2.3
1	B	206	TYR	2.3
1	D	133	TRP	2.3
1	C	310	LEU	2.3
1	H	97	LYS	2.3
1	E	88	GLY	2.3
1	H	81	ALA	2.3
1	D	67	THR	2.3
1	A	207	LYS	2.3
1	H	202	LYS	2.3
1	H	274	VAL	2.3
1	A	204	ASP	2.2
1	D	288	GLU	2.2
1	D	303	ALA	2.2
1	C	226	ILE	2.2
1	D	36	ILE	2.2
1	E	207	LYS	2.2
1	A	180	ASP	2.2
1	E	164	GLY	2.2
1	D	197	SER	2.2
1	G	42	LYS	2.1
1	D	265	TYR	2.1
1	D	207	LYS	2.1
1	E	100	LYS	2.1
1	A	4	HIS	2.1
1	G	310	LEU	2.1
1	H	310	LEU	2.1
1	F	223	TYR	2.1
1	C	91	ARG	2.1
1	C	293	GLU	2.0
1	F	204	ASP	2.0
1	H	269	ASP	2.0
1	D	293	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

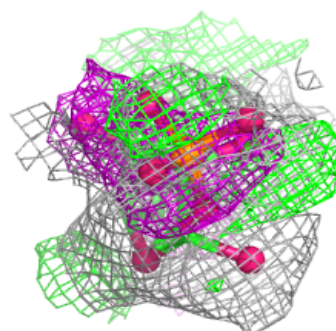
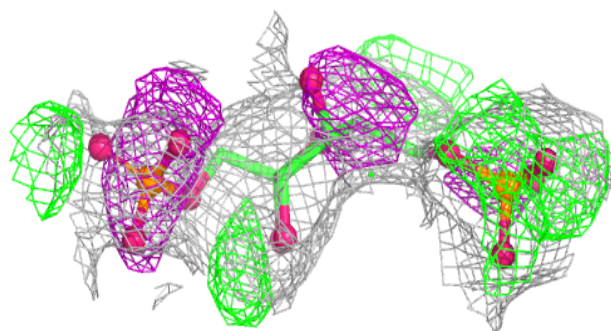
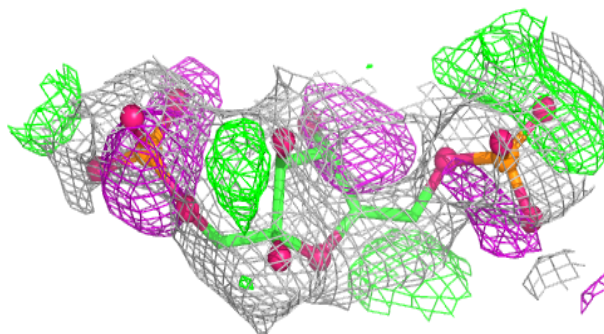
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	C	327	20/20	0.69	0.20	38,67,79,87	0
2	FBP	D	328	20/20	0.88	0.11	46,59,65,79	0
3	NAD	D	327	44/44	0.88	0.12	66,74,81,83	0
2	FBP	F	327	20/20	0.91	0.09	43,53,60,65	0
2	FBP	G	327	20/20	0.95	0.09	36,42,52,60	0

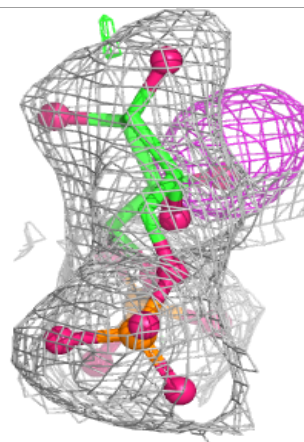
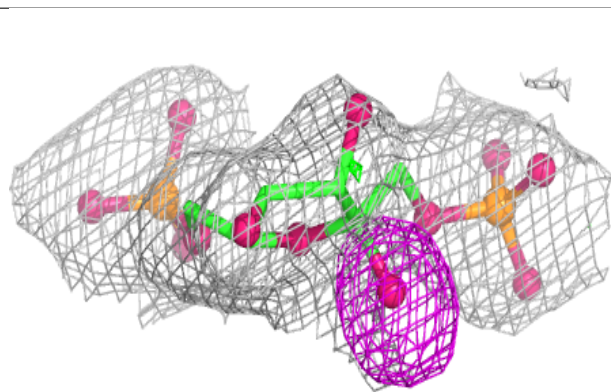
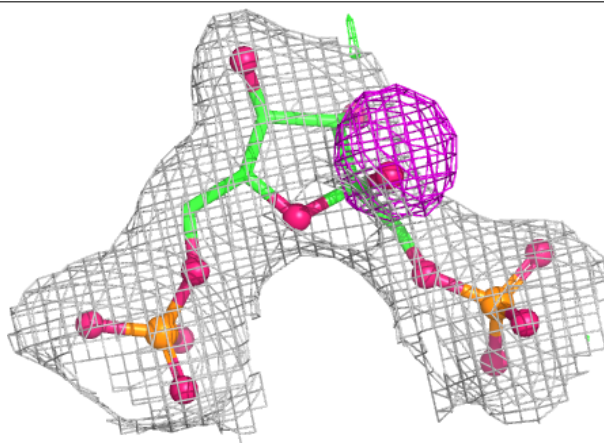
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FBP C 327:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

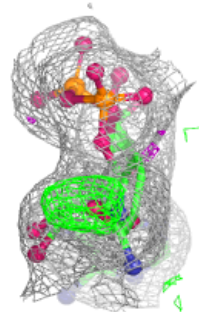
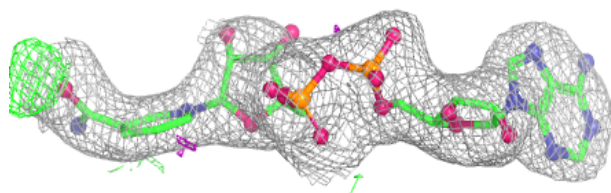
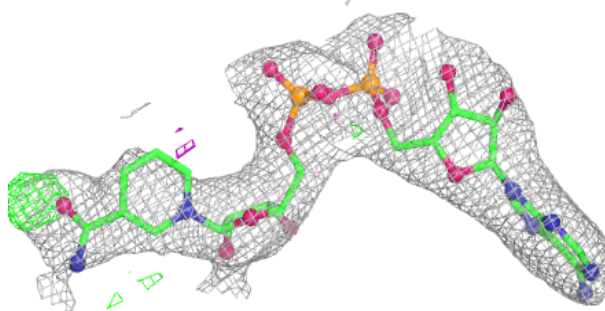
**Electron density around FBP D 328:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

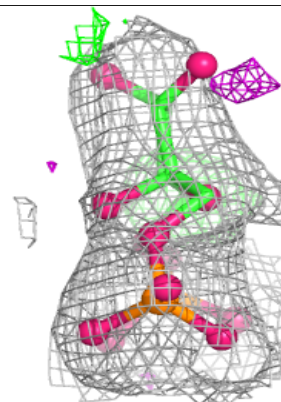
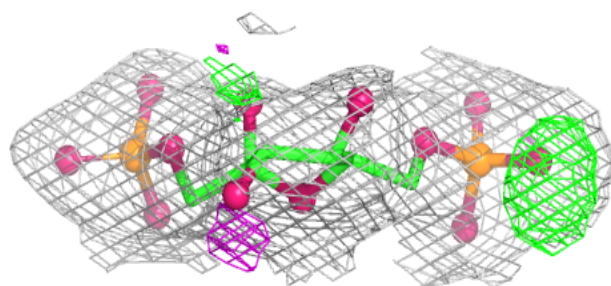
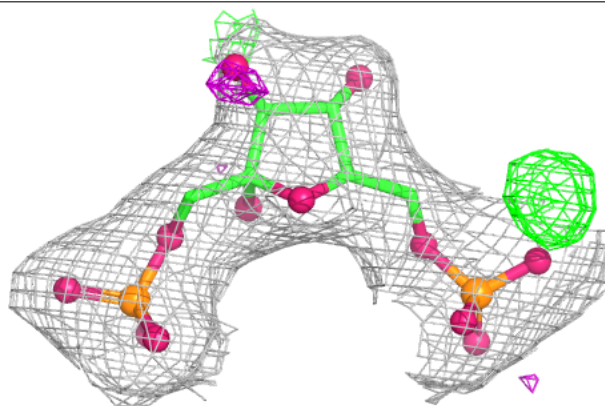


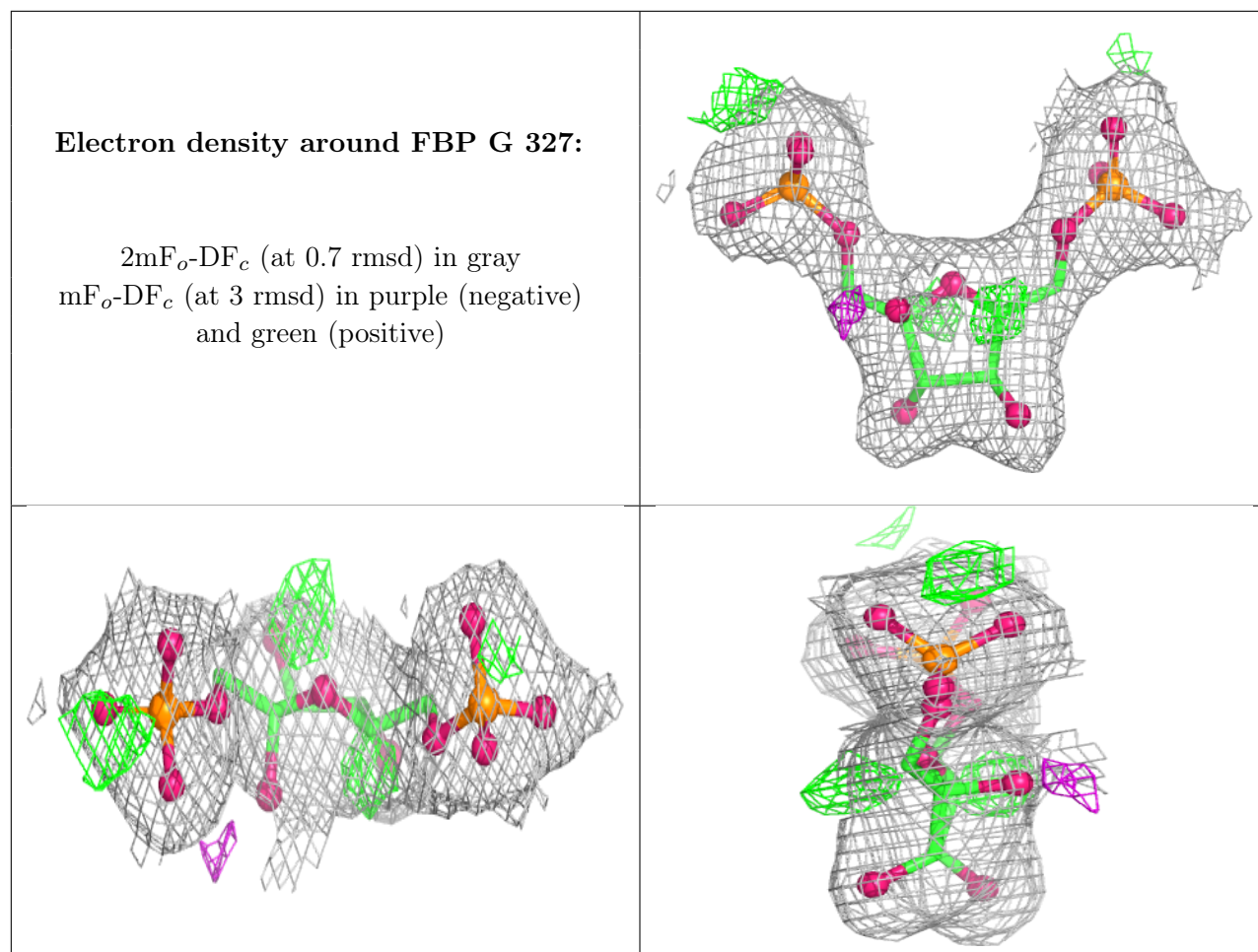
Electron density around NAD D 327:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FBP F 327:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.