



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:37 PM UTC

PDB ID : 3EX8 / pdb_00003ex8
Title : Complex structure of bacillus subtilis RibG reduction mechanism in riboflavin biosynthesis
Authors : Chen, S.C.; Lin, Y.H.; Yu, H.C.; Liaw, S.H.
Deposited on : 2008-10-16
Resolution : 2.56 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

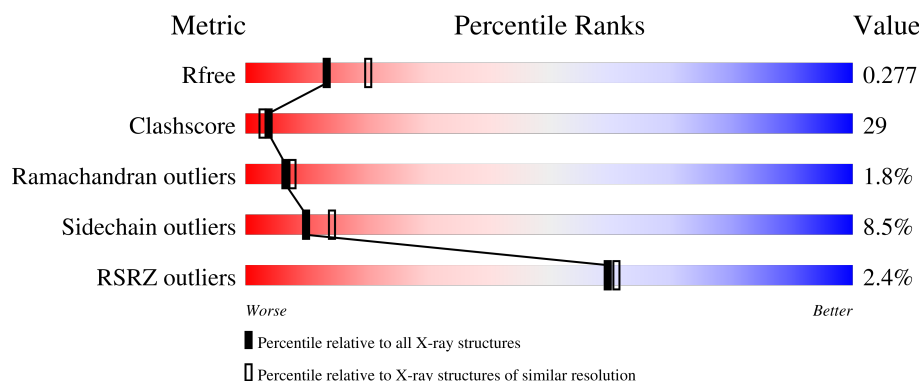
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	373	0% 57% 34% 5% .
1	B	373	3% 51% 36% 8% . .
1	C	373	2% 50% 39% 6% . .
1	D	373	4% 50% 39% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11188 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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	B	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	C	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	D	360	Total	C	N	O	S	0	0	0
			2747	1743	470	519	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P17618
A	-10	ARG	-	expression tag	UNP P17618
A	-9	GLY	-	expression tag	UNP P17618
A	-8	SER	-	expression tag	UNP P17618
A	-7	HIS	-	expression tag	UNP P17618
A	-6	HIS	-	expression tag	UNP P17618
A	-5	HIS	-	expression tag	UNP P17618
A	-4	HIS	-	expression tag	UNP P17618
A	-3	HIS	-	expression tag	UNP P17618
A	-2	HIS	-	expression tag	UNP P17618
A	-1	GLY	-	expression tag	UNP P17618
A	0	SER	-	expression tag	UNP P17618
B	-11	MET	-	expression tag	UNP P17618
B	-10	ARG	-	expression tag	UNP P17618
B	-9	GLY	-	expression tag	UNP P17618
B	-8	SER	-	expression tag	UNP P17618
B	-7	HIS	-	expression tag	UNP P17618
B	-6	HIS	-	expression tag	UNP P17618
B	-5	HIS	-	expression tag	UNP P17618
B	-4	HIS	-	expression tag	UNP P17618
B	-3	HIS	-	expression tag	UNP P17618

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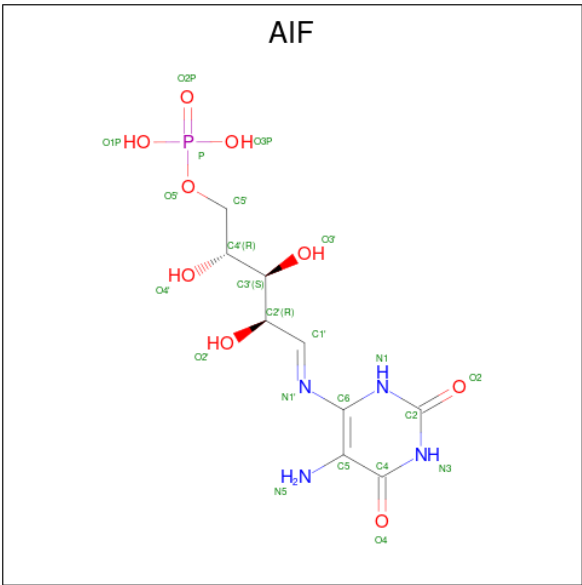
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP P17618
B	-1	GLY	-	expression tag	UNP P17618
B	0	SER	-	expression tag	UNP P17618
C	-11	MET	-	expression tag	UNP P17618
C	-10	ARG	-	expression tag	UNP P17618
C	-9	GLY	-	expression tag	UNP P17618
C	-8	SER	-	expression tag	UNP P17618
C	-7	HIS	-	expression tag	UNP P17618
C	-6	HIS	-	expression tag	UNP P17618
C	-5	HIS	-	expression tag	UNP P17618
C	-4	HIS	-	expression tag	UNP P17618
C	-3	HIS	-	expression tag	UNP P17618
C	-2	HIS	-	expression tag	UNP P17618
C	-1	GLY	-	expression tag	UNP P17618
C	0	SER	-	expression tag	UNP P17618
D	-11	MET	-	expression tag	UNP P17618
D	-10	ARG	-	expression tag	UNP P17618
D	-9	GLY	-	expression tag	UNP P17618
D	-8	SER	-	expression tag	UNP P17618
D	-7	HIS	-	expression tag	UNP P17618
D	-6	HIS	-	expression tag	UNP P17618
D	-5	HIS	-	expression tag	UNP P17618
D	-4	HIS	-	expression tag	UNP P17618
D	-3	HIS	-	expression tag	UNP P17618
D	-2	HIS	-	expression tag	UNP P17618
D	-1	GLY	-	expression tag	UNP P17618
D	0	SER	-	expression tag	UNP P17618

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

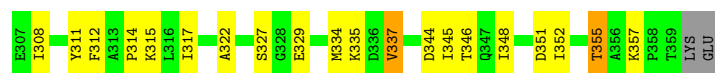
- Molecule 3 is [(2R,3S,4R,5E)-5-[(5-amino-2,6-dioxo-3H-pyrimidin-4-yl)imino]-2,3,4-trihydroxy-pentyl] dihydrogen phosphate (CCD ID: AIF) (formula: C₉H₁₅N₄O₉P).



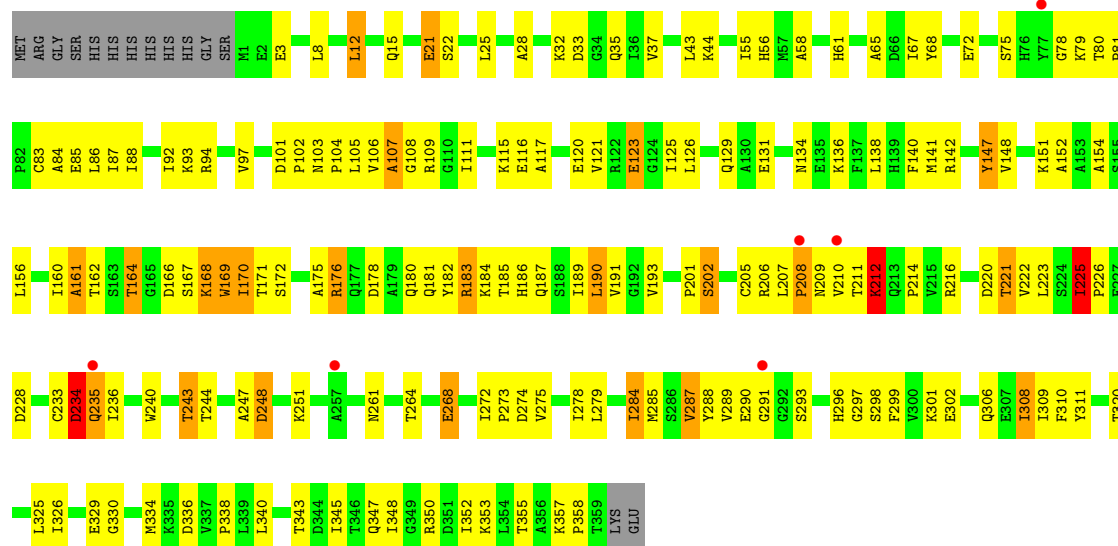
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 4 is water.

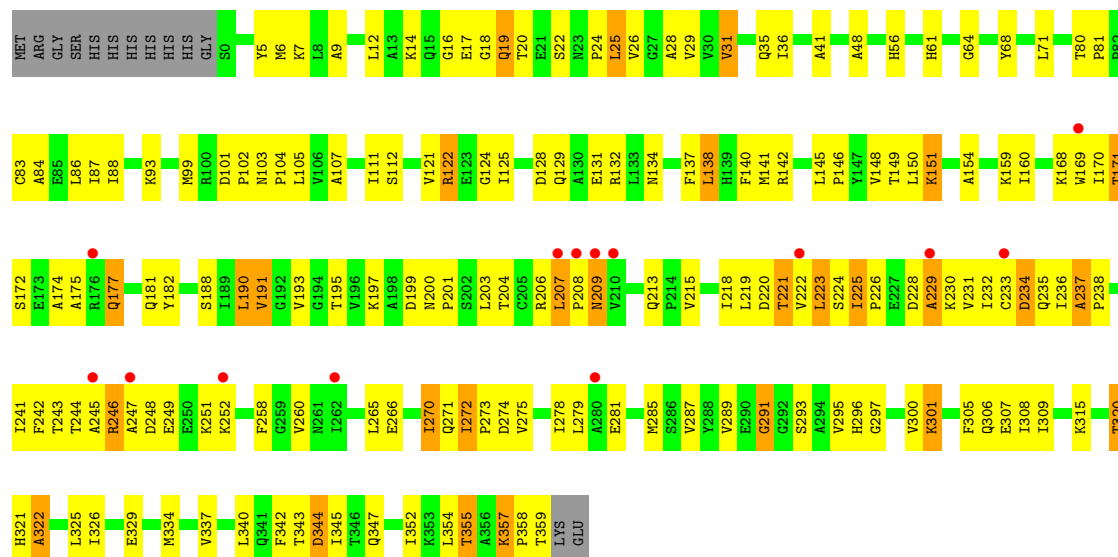
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	48	Total	O	0	0
			48	48		
4	C	37	Total	O	0	0
			37	37		
4	D	53	Total	O	0	0
			53	53		



• Molecule 1: Riboflavin biosynthesis protein ribD



• Molecule 1: Riboflavin biosynthesis protein ribD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.08Å 108.37Å 187.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 50.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.56) 97.3 (50.00-2.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.283 0.226 , 0.277	Depositor DCC
R_{free} test set	5746 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11188	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: ZN, AIF

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	0.56	0/2792	1.04	11/3778 (0.3%)
1	B	0.51	0/2792	1.07	22/3778 (0.6%)
1	C	0.49	0/2792	1.01	11/3778 (0.3%)
1	D	0.49	0/2798	1.04	12/3786 (0.3%)
All	All	0.51	0/11174	1.04	56/15120 (0.4%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	GLY	N-CA-C	10.32	126.20	111.14
1	D	229	ALA	N-CA-C	10.05	121.20	107.73
1	D	20	THR	N-CA-C	-9.02	100.81	114.16
1	A	2	GLU	N-CA-C	-8.93	101.62	111.36
1	A	292	GLY	N-CA-C	-8.66	92.65	113.18
1	D	320	THR	N-CA-C	-8.66	98.58	110.35
1	A	291	GLY	N-CA-C	7.48	130.91	113.18
1	B	322	ALA	CA-C-N	7.00	127.39	119.83
1	B	322	ALA	C-N-CA	7.00	127.39	119.83
1	D	322	ALA	N-CA-C	-6.92	98.52	109.04
1	D	293	SER	N-CA-C	-6.46	104.32	111.36
1	C	293	SER	N-CA-C	-6.44	104.19	111.14
1	C	147	TYR	N-CA-C	-6.43	99.54	109.76
1	A	252	LYS	N-CA-C	-6.38	104.25	111.14
1	D	291	GLY	N-CA-C	6.36	120.44	110.71
1	B	168	LYS	N-CA-C	6.33	118.19	111.28
1	D	344	ASP	N-CA-C	6.10	117.67	108.46
1	C	170	ILE	N-CA-C	-6.06	105.22	110.74
1	C	202	SER	N-CA-C	-6.01	106.08	113.41
1	D	124	GLY	N-CA-C	5.99	123.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	N-CA-C	5.84	119.50	112.38
1	B	202	SER	N-CA-C	-5.83	106.33	113.50
1	B	148	VAL	N-CA-C	5.76	116.23	108.17
1	B	103	ASN	CA-C-N	5.74	127.02	119.84
1	B	103	ASN	C-N-CA	5.74	127.02	119.84
1	A	8	LEU	N-CA-C	-5.69	105.08	111.28
1	B	290	GLU	CA-C-N	-5.67	117.06	121.82
1	B	290	GLU	C-N-CA	-5.67	117.06	121.82
1	B	2	GLU	N-CA-C	-5.65	105.64	112.54
1	C	183	ARG	N-CA-C	-5.56	106.19	112.87
1	B	357	LYS	CA-C-N	5.56	126.78	119.84
1	B	357	LYS	C-N-CA	5.56	126.78	119.84
1	B	233	CYS	N-CA-C	5.48	120.07	112.45
1	C	21	GLU	CB-CA-C	-5.47	110.28	116.63
1	D	272	ILE	CB-CA-C	-5.39	108.58	113.70
1	C	225	ILE	CA-C-N	5.34	125.60	119.83
1	C	225	ILE	C-N-CA	5.34	125.60	119.83
1	A	217	VAL	N-CA-C	5.34	115.54	107.80
1	B	213	GLN	N-CA-C	5.33	116.13	109.57
1	D	357	LYS	CA-C-N	5.32	125.22	119.85
1	D	357	LYS	C-N-CA	5.32	125.22	119.85
1	A	124	GLY	N-CA-C	5.31	122.65	115.32
1	A	123	GLU	N-CA-C	5.24	117.64	109.52
1	D	172	SER	N-CA-C	5.21	116.82	110.41
1	C	190	LEU	N-CA-C	5.20	117.55	108.76
1	B	329	GLU	N-CA-C	5.20	116.64	110.97
1	A	173	GLU	N-CA-C	-5.15	105.84	111.82
1	B	84	ALA	N-CA-C	-5.13	105.77	111.36
1	B	222	VAL	N-CA-C	5.11	117.89	112.83
1	A	155	SER	N-CA-C	-5.09	103.20	110.59
1	B	207	LEU	CA-C-N	5.09	126.21	119.84
1	B	207	LEU	C-N-CA	5.09	126.21	119.84
1	B	119	ILE	N-CA-C	5.07	115.64	109.30
1	B	147	TYR	N-CA-C	-5.07	102.36	109.96
1	C	357	LYS	CA-C-N	5.06	126.16	119.84
1	C	357	LYS	C-N-CA	5.06	126.16	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2741	0	2782	139	0
1	B	2741	0	2782	169	0
1	C	2741	0	2782	186	0
1	D	2747	0	2787	188	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	23	0	13	3	0
4	A	53	0	0	13	0
4	B	48	0	0	4	0
4	C	37	0	0	0	0
4	D	53	0	0	8	0
All	All	11188	0	11146	636	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 29.

All (636) 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:D:270:ILE:HD13	1:D:270:ILE:H	1.13	1.11
1:D:223:LEU:HD22	1:D:251:LYS:HE3	1.29	1.06
1:B:213:GLN:HA	1:B:213:GLN:HE21	1.24	1.00
1:A:25:LEU:H	1:A:134:ASN:HD21	1.03	0.96
1:B:220:ASP:O	1:B:243:THR:HG22	1.66	0.95
1:C:148:VAL:H	1:C:306:GLN:HE21	1.11	0.92
1:D:230:LYS:O	1:D:234:ASP:HB3	1.70	0.91
1:D:243:THR:HG22	1:D:244:THR:H	1.35	0.91
1:D:148:VAL:H	1:D:306:GLN:NE2	1.67	0.90
1:A:25:LEU:H	1:A:134:ASN:ND2	1.67	0.90
1:B:223:LEU:HG	1:B:243:THR:HG21	1.54	0.90
1:A:69:VAL:HB	4:A:411:HOH:O	1.73	0.86
1:D:270:ILE:H	1:D:270:ILE:CD1	1.88	0.86
1:C:111:ILE:HG23	1:C:121:VAL:HG11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HB2	1:C:206:ARG:HH11	1.42	0.85
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.01	0.84
1:C:206:ARG:HB2	1:C:206:ARG:NH1	1.92	0.84
1:A:213:GLN:HE21	1:A:214:PRO:HD2	1.43	0.82
1:C:148:VAL:HG22	1:C:287:VAL:HG13	1.61	0.82
1:D:221:THR:HG23	1:D:270:ILE:HD12	1.61	0.81
1:D:301:LYS:HE2	1:D:301:LYS:O	1.81	0.81
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.62	0.80
1:D:271:GLN:HG2	1:D:273:PRO:HD2	1.63	0.80
1:A:243:THR:HG21	1:A:247:ALA:HB2	1.61	0.80
1:A:355:THR:HG22	4:A:367:HOH:O	1.80	0.80
1:A:220:ASP:O	1:A:243:THR:HG23	1.82	0.79
1:D:132:ARG:HD2	4:D:388:HOH:O	1.81	0.79
1:C:32:LYS:HD3	1:C:61:HIS:O	1.81	0.79
1:C:171:THR:OG1	3:C:381:AIF:N3	2.15	0.79
1:D:344:ASP:HB3	1:D:355:THR:HG23	1.65	0.78
1:D:270:ILE:HD13	1:D:270:ILE:N	1.96	0.78
1:C:220:ASP:O	1:C:243:THR:HG23	1.83	0.78
1:C:55:ILE:HG21	1:C:86:LEU:HD11	1.66	0.78
1:D:160:ILE:HD11	1:D:325:LEU:HD23	1.66	0.78
1:B:32:LYS:HD3	1:B:65:ALA:HB2	1.65	0.77
1:B:37:VAL:HG22	1:B:58:ALA:HA	1.66	0.77
1:C:184:LYS:HE2	1:C:205:CYS:SG	2.24	0.77
1:C:171:THR:HG1	3:C:381:AIF:HN3	1.33	0.77
1:D:64:GLY:HA2	1:D:93:LYS:HG2	1.67	0.77
1:B:181:GLN:HG3	1:B:182:TYR:N	1.99	0.77
1:B:37:VAL:HG21	1:B:61:HIS:HB2	1.67	0.76
1:A:170:ILE:HG12	1:C:334:MET:HE2	1.65	0.76
1:C:166:ASP:OD1	1:C:168:LYS:HB2	1.84	0.76
1:C:25:LEU:H	1:C:134:ASN:HD21	1.33	0.76
1:D:359:THR:HG23	4:D:409:HOH:O	1.86	0.76
1:A:23:ASN:HD22	1:A:42:HIS:HE1	1.34	0.75
1:D:343:THR:HG21	1:D:357:LYS:HD2	1.66	0.75
1:A:64:GLY:HA2	1:A:93:LYS:HG2	1.67	0.75
1:D:193:VAL:HG13	1:D:219:LEU:O	1.87	0.74
1:A:32:LYS:HB3	4:A:366:HOH:O	1.88	0.73
1:C:167:SER:C	1:C:169:TRP:H	1.96	0.73
1:C:176:ARG:HG2	1:C:176:ARG:HH11	1.53	0.73
1:A:171:THR:HG23	4:A:381:HOH:O	1.87	0.73
1:A:309:ILE:HG12	1:A:355:THR:HB	1.69	0.72
1:D:193:VAL:HG11	1:D:220:ASP:CG	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HB3	1:C:208:PRO:CD	2.19	0.72
1:A:33:ASP:N	4:A:366:HOH:O	2.23	0.71
1:C:125:ILE:HD12	1:C:125:ILE:H	1.54	0.71
1:D:99:MET:HE1	1:D:138:LEU:HD21	1.70	0.71
1:C:172:SER:HB3	1:C:350:ARG:NH1	2.05	0.71
1:D:266:GLU:H	1:D:266:GLU:CD	1.99	0.71
1:A:8:LEU:HD21	1:A:39:MET:HE3	1.72	0.71
1:A:106:VAL:O	1:A:109:ARG:HB2	1.90	0.71
1:D:207:LEU:HD23	1:D:208:PRO:HD2	1.71	0.71
1:C:151:LYS:HD2	1:C:151:LYS:C	2.16	0.70
1:A:25:LEU:N	1:A:134:ASN:HD21	1.84	0.70
1:C:167:SER:O	1:C:169:TRP:N	2.21	0.70
1:B:193:VAL:CG2	1:B:220:ASP:HA	2.22	0.70
1:B:166:ASP:OD2	1:B:168:LYS:HE2	1.92	0.70
1:B:213:GLN:HE21	1:B:213:GLN:CA	2.02	0.70
1:A:84:ALA:O	1:A:88:ILE:HG12	1.91	0.70
1:C:151:LYS:HD2	1:C:152:ALA:N	2.07	0.70
1:D:274:ASP:O	1:D:278:ILE:HG12	1.92	0.69
1:D:320:THR:O	1:D:321:HIS:HB2	1.91	0.69
1:A:223:LEU:HD13	1:A:251:LYS:HD3	1.74	0.69
1:C:106:VAL:HG22	1:C:109:ARG:NH2	2.08	0.69
1:A:12:LEU:HD11	1:A:39:MET:HE2	1.73	0.69
1:D:140:PHE:CD2	1:D:141:MET:HE2	2.28	0.68
1:B:240:TRP:CD1	1:B:261:ASN:HB2	2.29	0.68
1:C:243:THR:HG22	1:C:244:THR:H	1.59	0.68
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.76	0.68
1:C:207:LEU:HB3	1:C:208:PRO:HD2	1.75	0.68
1:B:190:LEU:HD11	1:B:219:LEU:HG	1.76	0.68
1:B:213:GLN:HA	1:B:213:GLN:NE2	2.06	0.68
1:D:159:LYS:HE3	1:D:322:ALA:HB3	1.75	0.68
1:D:140:PHE:HD2	1:D:141:MET:HE2	1.58	0.67
1:D:229:ALA:HA	1:D:233:CYS:SG	2.34	0.67
1:A:311:TYR:CE1	1:A:353:LYS:HG3	2.29	0.67
1:A:334:MET:HB2	1:C:168:LYS:HB3	1.76	0.67
1:C:148:VAL:H	1:C:306:GLN:NE2	1.89	0.67
1:D:258:PHE:HB2	1:D:260:VAL:HG23	1.76	0.67
1:A:347:GLN:HG2	1:A:352:ILE:HG12	1.75	0.67
1:A:344:ASP:HB3	1:A:355:THR:HG23	1.76	0.67
1:B:162:THR:HG23	1:D:334:MET:HE2	1.77	0.67
1:B:344:ASP:OD2	1:B:346:THR:HG23	1.94	0.66
1:A:308:ILE:HG22	1:A:356:ALA:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASN:HD22	1:A:42:HIS:CE1	2.14	0.66
1:A:42:HIS:HD2	1:A:48:ALA:O	1.79	0.66
1:B:31:VAL:HG13	1:B:66:ASP:HB2	1.77	0.66
1:A:277:LYS:HE2	1:A:281:GLU:OE2	1.95	0.66
1:B:97:VAL:O	1:B:123:GLU:HA	1.95	0.66
1:B:345:ILE:O	1:B:345:ILE:HG13	1.95	0.66
1:A:205:CYS:H	1:A:213:GLN:HE22	1.44	0.66
1:D:308:ILE:C	1:D:309:ILE:HD12	2.21	0.66
1:A:82:PRO:HG2	1:A:85:GLU:HB2	1.78	0.66
1:D:148:VAL:HB	1:D:305:PHE:HA	1.79	0.64
1:A:213:GLN:NE2	1:A:214:PRO:HD2	2.10	0.64
1:C:79:LYS:O	1:C:80:THR:HG23	1.97	0.64
1:D:191:VAL:HG22	1:D:291:GLY:HA3	1.79	0.64
1:C:37:VAL:HG12	1:C:58:ALA:HA	1.78	0.64
1:B:312:PHE:O	1:B:351:ASP:HB3	1.98	0.63
1:C:222:VAL:HG12	1:C:222:VAL:O	1.99	0.63
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.78	0.63
1:B:167:SER:HA	1:D:334:MET:HE3	1.80	0.63
1:D:208:PRO:O	1:D:209:ASN:HB2	1.98	0.63
1:A:342:PHE:CE2	1:C:352:ILE:HG12	2.34	0.63
1:B:157:ASP:HA	1:D:325:LEU:HD12	1.80	0.63
1:B:84:ALA:HB3	1:B:113:MET:HE2	1.80	0.63
1:C:240:TRP:CD1	1:C:261:ASN:HB2	2.34	0.63
1:A:88:ILE:HD12	1:A:117:ALA:HB2	1.79	0.62
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.80	0.62
1:D:103:ASN:OD1	1:D:105:LEU:HB3	1.99	0.62
1:B:69:VAL:CG2	1:B:97:VAL:HG22	2.28	0.62
1:B:191:VAL:HG21	1:B:195:THR:HG21	1.81	0.62
1:A:44:LYS:HB2	1:A:47:GLU:HB2	1.82	0.62
1:B:344:ASP:HB3	1:B:355:THR:CG2	2.29	0.62
1:C:55:ILE:HG13	1:C:86:LEU:CD1	2.30	0.62
1:C:221:THR:HG22	1:C:222:VAL:HG23	1.81	0.62
1:D:221:THR:CG2	1:D:270:ILE:HD12	2.29	0.62
1:C:180:GLN:HE22	1:C:206:ARG:HH22	1.47	0.62
1:D:148:VAL:H	1:D:306:GLN:HE21	1.42	0.62
1:A:22:SER:HA	1:A:285:MET:HE2	1.82	0.62
1:D:201:PRO:HG2	1:D:203:LEU:HD21	1.81	0.62
1:C:268:GLU:CD	1:C:268:GLU:H	2.06	0.61
1:D:190:LEU:HD11	1:D:219:LEU:HG	1.81	0.61
1:C:168:LYS:O	1:C:169:TRP:HB2	1.99	0.61
1:D:237:ALA:HB1	1:D:238:PRO:CD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:O	1:A:243:THR:HG22	2.01	0.61
1:B:190:LEU:HD12	1:B:191:VAL:N	2.16	0.61
1:A:88:ILE:HD12	1:A:117:ALA:CB	2.31	0.61
1:A:84:ALA:HB3	1:A:113:MET:HE2	1.82	0.60
1:B:227:GLU:HG2	1:B:255:LEU:HD21	1.81	0.60
1:B:95:VAL:HG13	1:B:121:VAL:HG13	1.83	0.60
1:B:190:LEU:HD12	1:B:191:VAL:H	1.66	0.60
1:C:176:ARG:HG2	1:C:176:ARG:NH1	2.14	0.60
1:D:25:LEU:H	1:D:134:ASN:HD21	1.50	0.60
1:A:8:LEU:HD11	1:A:39:MET:CE	2.31	0.60
1:C:55:ILE:HD11	1:C:92:ILE:HD11	1.84	0.60
1:B:71:LEU:HD12	1:B:99:MET:HG3	1.84	0.60
1:C:97:VAL:O	1:C:123:GLU:HA	2.02	0.60
1:D:218:ILE:N	1:D:218:ILE:HD12	2.16	0.59
1:A:36:ILE:HD12	1:B:15:GLN:HG3	1.83	0.59
1:A:53:HIS:CD2	1:B:57:MET:HG3	2.36	0.59
1:C:43:LEU:HD22	1:C:43:LEU:N	2.17	0.59
1:D:99:MET:HE1	1:D:138:LEU:CD2	2.32	0.59
1:C:86:LEU:C	1:C:86:LEU:HD13	2.27	0.59
1:C:243:THR:HG21	1:C:247:ALA:HB2	1.84	0.59
1:C:184:LYS:NZ	1:C:210:VAL:HA	2.17	0.59
1:B:111:ILE:HG22	1:B:115:LYS:HE2	1.85	0.59
1:C:234:ASP:C	1:C:234:ASP:OD2	2.44	0.59
1:C:67:ILE:HB	1:C:92:ILE:HD13	1.83	0.59
1:A:106:VAL:HG13	1:A:109:ARG:NH1	2.18	0.59
1:B:196:VAL:HA	1:B:201:PRO:HD2	1.85	0.59
1:B:148:VAL:HG22	1:B:287:VAL:CG1	2.32	0.59
1:C:103:ASN:HD21	1:C:105:LEU:HD13	1.66	0.59
1:C:181:GLN:HA	1:C:207:LEU:HD11	1.85	0.59
1:B:148:VAL:HG22	1:B:287:VAL:HG13	1.84	0.59
1:C:347:GLN:O	1:C:348:ILE:HD13	2.02	0.58
1:A:347:GLN:C	1:A:348:ILE:HD12	2.28	0.58
1:B:85:GLU:HG2	1:B:89:ASN:HD21	1.68	0.58
1:C:140:PHE:CD2	1:C:285:MET:HG2	2.39	0.58
1:A:125:ILE:HD12	1:A:125:ILE:H	1.67	0.58
1:B:102:PRO:HB2	1:B:141:MET:HB3	1.85	0.58
1:D:80:THR:HB	1:D:81:PRO:HD2	1.84	0.58
1:D:99:MET:HE1	1:D:138:LEU:CG	2.33	0.58
1:B:105:LEU:HG	1:B:106:VAL:H	1.68	0.58
1:C:35:GLN:NE2	1:D:19:GLN:HB3	2.19	0.58
1:B:213:GLN:NE2	1:B:214:PRO:HD2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LEU:HD11	1:D:219:LEU:CD1	2.33	0.58
1:B:178:ASP:O	1:B:181:GLN:HG2	2.03	0.57
1:B:6:MET:HB3	1:B:126:LEU:HD12	1.87	0.57
1:D:170:ILE:HG23	1:D:171:THR:N	2.19	0.57
1:D:191:VAL:HG13	1:D:195:THR:HB	1.85	0.57
1:A:132:ARG:HG3	4:A:405:HOH:O	2.04	0.57
1:C:172:SER:HB3	1:C:350:ARG:HH12	1.67	0.57
1:B:103:ASN:CA	1:B:141:MET:HG3	2.34	0.57
1:C:35:GLN:NE2	1:D:19:GLN:CB	2.68	0.57
1:C:67:ILE:HD13	1:C:87:ILE:CD1	2.34	0.57
1:C:162:THR:C	1:C:164:THR:H	2.12	0.57
1:D:222:VAL:HG23	1:D:246:ARG:HG2	1.85	0.57
1:A:47:GLU:OE2	1:B:61:HIS:HE1	1.88	0.57
1:B:213:GLN:HE21	1:B:214:PRO:HD2	1.69	0.57
1:D:169:TRP:O	1:D:315:LYS:NZ	2.32	0.57
1:D:265:LEU:HD12	1:D:265:LEU:N	2.20	0.57
1:C:83:CYS:O	1:C:87:ILE:HG12	2.04	0.56
1:C:223:LEU:HB2	1:C:243:THR:HG21	1.86	0.56
1:D:128:ASP:O	1:D:132:ARG:HG3	2.05	0.56
1:C:142:ARG:HG3	1:C:142:ARG:HH11	1.68	0.56
1:A:26:VAL:O	1:A:41:ALA:HA	2.06	0.56
1:B:126:LEU:HB3	1:B:129:GLN:HE22	1.71	0.56
1:D:28:ALA:HA	1:D:68:TYR:O	2.06	0.56
1:B:211:THR:O	1:B:212:LYS:HB2	2.06	0.56
1:A:21:GLU:HB2	1:A:45:TYR:CD1	2.41	0.56
1:B:72:GLU:OE2	1:B:111:ILE:HG12	2.06	0.56
1:C:8:LEU:O	1:C:12:LEU:HD22	2.06	0.56
1:C:302:GLU:OE2	1:C:302:GLU:HA	2.04	0.56
1:D:271:GLN:CG	1:D:273:PRO:HD2	2.33	0.56
1:B:75:SER:HA	1:B:82:PRO:HB3	1.88	0.56
1:B:103:ASN:HA	1:B:141:MET:HG3	1.87	0.55
1:A:4:TYR:OH	1:B:15:GLN:NE2	2.38	0.55
1:B:23:ASN:ND2	1:B:45:TYR:CD2	2.74	0.55
1:B:223:LEU:CG	1:B:243:THR:HG21	2.33	0.55
1:C:169:TRP:HA	1:C:169:TRP:CE3	2.41	0.55
1:D:5:TYR:CE1	1:D:36:ILE:HD11	2.41	0.55
1:C:189:ILE:HD11	1:C:214:PRO:HG2	1.89	0.55
1:D:248:ASP:O	1:D:252:LYS:HB2	2.05	0.55
1:C:181:GLN:O	1:C:184:LYS:HB3	2.05	0.55
1:C:182:TYR:C	1:C:184:LYS:H	2.13	0.55
1:B:134:ASN:O	1:B:138:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LEU:HB3	1:D:289:VAL:HG22	1.88	0.55
1:C:106:VAL:HG22	1:C:109:ARG:HH22	1.70	0.55
1:C:233:CYS:O	1:C:235:GLN:N	2.40	0.55
1:D:222:VAL:O	1:D:223:LEU:C	2.50	0.55
1:B:6:MET:HE1	1:B:70:THR:HG22	1.88	0.55
1:C:201:PRO:HB3	3:C:381:AIF:H5'	1.89	0.55
1:D:278:ILE:O	1:D:281:GLU:HB2	2.06	0.55
1:D:24:PRO:HD3	1:D:137:PHE:CE2	2.42	0.55
1:C:272:ILE:O	1:C:275:VAL:HG22	2.07	0.54
1:D:160:ILE:HD11	1:D:325:LEU:HA	1.89	0.54
1:D:246:ARG:HG3	1:D:246:ARG:HH11	1.72	0.54
1:B:23:ASN:HD22	1:B:45:TYR:HA	1.72	0.54
1:D:122:ARG:HH11	1:D:122:ARG:HA	1.73	0.54
1:B:103:ASN:HB3	1:B:106:VAL:HB	1.90	0.54
1:D:243:THR:HG22	1:D:244:THR:N	2.15	0.54
1:A:348:ILE:HD12	1:A:348:ILE:N	2.23	0.54
1:A:352:ILE:HD13	1:C:345:ILE:HG12	1.89	0.54
1:A:32:LYS:HD2	1:A:61:HIS:O	2.08	0.54
1:B:184:LYS:HZ2	1:B:207:LEU:HD12	1.72	0.54
1:C:301:LYS:HD2	1:C:329:GLU:HB2	1.88	0.54
1:C:191:VAL:HG12	1:C:291:GLY:HA3	1.90	0.54
1:D:6:MET:HG2	1:D:125:ILE:HG22	1.90	0.54
1:B:293:SER:OG	1:B:327:SER:HB2	2.07	0.53
1:B:311:TYR:HE1	1:B:348:ILE:HD12	1.72	0.53
1:B:173:GLU:O	1:B:177:GLN:HB2	2.08	0.53
1:D:171:THR:HG23	1:D:175:ALA:HB3	1.91	0.53
1:D:222:VAL:O	1:D:222:VAL:HG22	2.07	0.53
1:B:168:LYS:HE3	1:B:169:TRP:CZ3	2.42	0.53
1:B:151:LYS:C	1:B:151:LYS:HD2	2.34	0.53
1:B:352:ILE:HD13	1:D:345:ILE:CD1	2.37	0.53
1:C:160:ILE:O	1:C:161:ALA:HB2	2.08	0.53
1:C:308:ILE:HD11	1:C:310:PHE:CE2	2.44	0.53
1:D:344:ASP:HB3	1:D:355:THR:CG2	2.36	0.53
1:A:88:ILE:HD11	1:A:114:MET:HA	1.90	0.53
1:B:105:LEU:HG	1:B:106:VAL:N	2.23	0.53
1:C:206:ARG:HH11	1:C:206:ARG:CB	2.18	0.53
1:B:8:LEU:HD22	1:B:12:LEU:HD22	1.91	0.53
1:C:44:LYS:NZ	1:D:35:GLN:OE1	2.38	0.53
1:C:148:VAL:N	1:C:306:GLN:HE21	1.94	0.53
1:D:151:LYS:HA	1:D:309:ILE:O	2.09	0.53
1:D:245:ALA:O	1:D:247:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ALA:HB2	1:C:325:LEU:HD21	1.91	0.52
1:D:320:THR:O	1:D:321:HIS:CB	2.53	0.52
1:A:235:GLN:NE2	4:A:363:HOH:O	2.42	0.52
1:D:159:LYS:CE	1:D:322:ALA:HB3	2.39	0.52
1:D:220:ASP:O	1:D:270:ILE:HG21	2.10	0.52
1:B:181:GLN:HG3	1:B:182:TYR:H	1.72	0.52
1:B:111:ILE:CG2	1:B:115:LYS:HE2	2.39	0.52
1:D:7:LYS:NZ	1:D:129:GLN:HE22	2.06	0.52
1:D:223:LEU:HD23	1:D:225:ILE:HG22	1.92	0.52
1:B:315:LYS:HD3	1:D:337:VAL:HG11	1.92	0.52
1:A:42:HIS:CD2	1:A:48:ALA:O	2.62	0.52
1:A:242:PHE:CD2	1:A:275:VAL:HG12	2.44	0.52
1:C:298:SER:O	1:C:302:GLU:HG2	2.10	0.52
1:D:291:GLY:O	1:D:295:VAL:HB	2.10	0.52
1:A:22:SER:HA	1:A:285:MET:CE	2.40	0.51
1:C:86:LEU:HD13	1:C:86:LEU:O	2.11	0.51
1:C:223:LEU:HD23	1:C:247:ALA:HB1	1.92	0.51
1:A:53:HIS:HB3	1:B:57:MET:HE2	1.90	0.51
1:A:222:VAL:CG1	1:A:222:VAL:O	2.57	0.51
1:B:235:GLN:NE2	4:B:367:HOH:O	2.43	0.51
1:C:75:SER:OG	1:C:109:ARG:HD2	2.09	0.51
1:D:242:PHE:CE2	1:D:275:VAL:HG13	2.45	0.51
1:B:193:VAL:HG22	1:B:220:ASP:HA	1.92	0.51
1:D:347:GLN:HG3	1:D:352:ILE:HD13	1.91	0.51
1:C:22:SER:HB3	1:C:187:GLN:HE22	1.76	0.51
1:B:87:ILE:O	1:B:92:ILE:HG12	2.11	0.51
1:B:272:ILE:HB	1:B:273:PRO:HD3	1.91	0.51
1:A:35:GLN:HB2	4:A:366:HOH:O	2.11	0.51
1:D:84:ALA:O	1:D:88:ILE:HG13	2.10	0.51
1:C:279:LEU:O	1:C:284:ILE:HB	2.11	0.51
1:C:72:GLU:HG3	1:C:111:ILE:CD1	2.41	0.51
1:C:126:LEU:HG	1:C:129:GLN:HE21	1.76	0.51
1:D:150:LEU:HB2	1:D:308:ILE:HD13	1.93	0.51
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.93	0.51
1:B:352:ILE:HD11	1:D:342:PHE:CG	2.46	0.51
1:C:151:LYS:HA	1:C:309:ILE:O	2.11	0.50
1:C:189:ILE:HD11	1:C:214:PRO:CG	2.40	0.50
1:B:182:TYR:O	1:B:186:HIS:HD2	1.95	0.50
1:C:151:LYS:HE3	1:C:290:GLU:HB2	1.94	0.50
1:D:19:GLN:OE1	1:D:19:GLN:O	2.28	0.50
1:A:140:PHE:CE2	1:A:285:MET:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ILE:HD12	1:C:125:ILE:N	2.24	0.50
1:A:154:ALA:HB2	1:A:325:LEU:HD21	1.93	0.50
1:C:94:ARG:HG2	1:C:120:GLU:HB3	1.93	0.50
1:C:178:ASP:O	1:C:181:GLN:HG2	2.12	0.50
1:D:83:CYS:O	1:D:87:ILE:HG13	2.12	0.50
1:A:1:MET:HE3	1:A:1:MET:HA	1.94	0.50
1:B:334:MET:HA	1:B:337:VAL:HG13	1.93	0.50
1:A:308:ILE:HG23	1:A:308:ILE:O	2.11	0.50
1:B:37:VAL:HG21	1:B:61:HIS:CB	2.39	0.50
1:C:182:TYR:C	1:C:184:LYS:N	2.64	0.50
1:B:150:LEU:CD2	1:B:289:VAL:HB	2.42	0.50
1:B:191:VAL:HG23	1:B:291:GLY:CA	2.42	0.50
1:B:344:ASP:HB3	1:B:355:THR:HG23	1.94	0.50
1:C:142:ARG:HG3	1:C:142:ARG:NH1	2.26	0.50
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.94	0.50
1:D:301:LYS:HE2	1:D:301:LYS:C	2.36	0.50
1:C:115:LYS:C	1:C:117:ALA:H	2.19	0.50
1:C:181:GLN:O	1:C:185:THR:HG23	2.12	0.50
1:D:203:LEU:HD22	1:D:203:LEU:N	2.27	0.50
1:D:225:ILE:HG23	1:D:225:ILE:O	2.12	0.50
1:D:230:LYS:O	1:D:232:ILE:N	2.45	0.50
1:A:134:ASN:C	1:A:138:LEU:HD22	2.37	0.49
1:C:209:ASN:CG	1:C:209:ASN:O	2.54	0.49
1:D:174:ALA:O	1:D:177:GLN:HB3	2.11	0.49
1:B:166:ASP:CG	1:B:168:LYS:HE2	2.37	0.49
1:C:225:ILE:HD13	1:C:226:PRO:N	2.28	0.49
1:D:234:ASP:O	1:D:234:ASP:OD1	2.29	0.49
1:D:243:THR:HG21	1:D:247:ALA:HB2	1.94	0.49
1:A:170:ILE:HG12	1:C:334:MET:CE	2.38	0.49
1:C:148:VAL:HG22	1:C:287:VAL:CG1	2.39	0.49
1:C:151:LYS:O	1:C:290:GLU:HA	2.12	0.49
1:D:241:ILE:HG21	4:D:422:HOH:O	2.13	0.49
1:D:355:THR:CG2	4:D:380:HOH:O	2.60	0.49
1:A:339:LEU:C	1:A:340:LEU:HD23	2.37	0.49
1:B:154:ALA:HB1	1:B:159:LYS:O	2.13	0.49
1:C:210:VAL:HG23	1:C:211:THR:N	2.28	0.49
1:D:5:TYR:CD1	1:D:36:ILE:HD11	2.47	0.49
1:D:181:GLN:HG2	1:D:182:TYR:N	2.26	0.49
1:C:3:GLU:HB2	1:C:126:LEU:HD11	1.95	0.49
1:C:180:GLN:HE22	1:C:206:ARG:NH2	2.11	0.49
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLN:NE2	1:A:213:GLN:HA	2.27	0.49
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.95	0.49
1:D:223:LEU:HD23	4:D:422:HOH:O	2.13	0.49
1:B:21:GLU:HG3	1:B:22:SER:H	1.77	0.48
1:C:193:VAL:HG11	1:C:220:ASP:OD2	2.13	0.48
1:D:204:THR:HB	1:D:213:GLN:NE2	2.28	0.48
1:A:190:LEU:HD12	1:A:191:VAL:N	2.28	0.48
1:C:181:GLN:HG3	1:C:182:TYR:N	2.26	0.48
1:D:232:ILE:HG22	1:D:233:CYS:N	2.29	0.48
1:B:82:PRO:HB2	1:B:113:MET:HE1	1.96	0.48
1:B:151:LYS:HE3	1:B:290:GLU:HG2	1.95	0.48
1:B:187:GLN:OE1	1:B:285:MET:N	2.43	0.48
1:B:269:ARG:HG3	1:B:269:ARG:NH1	2.28	0.48
1:C:184:LYS:HB2	1:C:205:CYS:SG	2.54	0.48
1:C:103:ASN:ND2	1:C:105:LEU:HD13	2.28	0.48
1:C:140:PHE:CG	1:C:285:MET:HG2	2.47	0.48
1:C:172:SER:O	1:C:175:ALA:HB3	2.13	0.48
1:C:180:GLN:NE2	1:C:206:ARG:HH22	2.10	0.48
1:D:128:ASP:HB2	4:D:394:HOH:O	2.12	0.48
1:A:56:HIS:CE1	1:B:56:HIS:CE1	3.02	0.48
1:B:82:PRO:HD2	1:B:85:GLU:OE1	2.14	0.48
1:A:193:VAL:HG22	1:A:219:LEU:O	2.14	0.48
1:A:355:THR:CG2	4:A:367:HOH:O	2.48	0.48
1:B:6:MET:HG3	1:B:125:ILE:HB	1.95	0.48
1:B:157:ASP:HA	1:D:325:LEU:CD1	2.43	0.48
1:D:236:ILE:O	1:D:237:ALA:HB2	2.13	0.48
1:A:312:PHE:CE2	1:A:354:LEU:HD12	2.49	0.48
1:B:25:LEU:H	1:B:134:ASN:HD21	1.60	0.48
1:C:162:THR:C	1:C:164:THR:N	2.71	0.48
1:D:160:ILE:O	1:D:160:ILE:HG22	2.13	0.48
1:C:93:LYS:HG3	1:C:94:ARG:N	2.28	0.48
1:C:169:TRP:HA	1:C:169:TRP:HE3	1.79	0.48
1:C:310:PHE:CE2	1:C:325:LEU:HD13	2.48	0.48
1:A:171:THR:HA	4:A:381:HOH:O	2.14	0.48
1:A:190:LEU:CD1	1:A:219:LEU:HG	2.44	0.48
1:C:168:LYS:O	1:C:169:TRP:CB	2.62	0.48
1:A:151:LYS:HD2	1:A:288:TYR:OH	2.14	0.47
1:C:37:VAL:HG12	1:C:37:VAL:O	2.12	0.47
1:C:234:ASP:O	1:C:236:ILE:HG12	2.14	0.47
1:A:312:PHE:HE2	1:A:354:LEU:HD12	1.79	0.47
1:D:104:PRO:HB3	4:D:418:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ALA:C	1:D:247:ALA:H	2.21	0.47
1:D:296:HIS:O	1:D:300:VAL:HG23	2.14	0.47
1:A:21:GLU:HG3	1:A:45:TYR:CG	2.48	0.47
1:A:336:ASP:O	1:A:338:PRO:HD3	2.15	0.47
1:B:90:SER:OG	1:B:92:ILE:HG12	2.14	0.47
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.79	0.47
1:A:213:GLN:HE21	1:A:213:GLN:HA	1.79	0.47
1:B:37:VAL:HG22	1:B:37:VAL:O	2.13	0.47
1:A:345:ILE:CD1	1:C:352:ILE:HD12	2.44	0.47
1:B:137:PHE:HD1	1:B:138:LEU:HD12	1.80	0.47
1:C:220:ASP:OD2	1:C:225:ILE:HB	2.15	0.47
1:D:14:LYS:O	1:D:17:GLU:HB2	2.14	0.47
1:D:122:ARG:HA	1:D:122:ARG:NH1	2.29	0.47
1:B:25:LEU:H	1:B:134:ASN:ND2	2.13	0.47
1:D:190:LEU:O	1:D:191:VAL:HG23	2.15	0.47
1:B:83:CYS:O	1:B:87:ILE:HG13	2.15	0.47
1:B:216:ARG:HD2	1:B:237:ALA:HB3	1.96	0.47
1:B:306:GLN:N	1:B:306:GLN:CD	2.72	0.47
1:B:315:LYS:HD3	1:D:337:VAL:CG1	2.44	0.47
1:C:125:ILE:H	1:C:125:ILE:CD1	2.23	0.47
1:D:190:LEU:CB	1:D:289:VAL:HG22	2.43	0.47
1:B:234:ASP:OD2	1:B:234:ASP:C	2.58	0.47
1:B:237:ALA:HB1	1:B:238:PRO:CD	2.44	0.47
1:B:277:LYS:NZ	1:B:281:GLU:OE2	2.46	0.47
1:C:28:ALA:HA	1:C:68:TYR:O	2.14	0.47
1:C:37:VAL:HG11	1:C:61:HIS:HB2	1.97	0.47
1:D:193:VAL:O	1:D:197:LYS:HG2	2.15	0.47
1:A:97:VAL:HA	4:A:411:HOH:O	2.15	0.47
1:B:105:LEU:HD23	1:B:105:LEU:H	1.79	0.47
1:B:69:VAL:HG23	1:B:97:VAL:HG22	1.95	0.47
1:D:230:LYS:C	1:D:232:ILE:N	2.71	0.47
1:D:243:THR:CG2	1:D:247:ALA:HB2	2.45	0.47
1:B:151:LYS:HE2	1:B:288:TYR:OH	2.15	0.46
1:B:184:LYS:HD3	1:B:210:VAL:HG12	1.97	0.46
1:A:88:ILE:HG23	1:A:117:ALA:HB1	1.97	0.46
1:D:26:VAL:O	1:D:41:ALA:HA	2.14	0.46
1:D:101:ASP:OD2	1:D:102:PRO:HD2	2.16	0.46
1:D:131:GLU:OE1	1:D:142:ARG:NH1	2.41	0.46
1:D:193:VAL:HG12	1:D:218:ILE:HG22	1.97	0.46
1:D:200:ASN:OD1	1:D:230:LYS:CG	2.63	0.46
1:D:245:ALA:C	1:D:247:ALA:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD13	1:D:105:LEU:O	2.15	0.46
1:A:64:GLY:HA2	1:A:93:LYS:CG	2.42	0.46
1:C:184:LYS:HB2	1:C:207:LEU:HD12	1.98	0.46
1:C:202:SER:O	1:C:216:ARG:HD3	2.16	0.46
1:A:111:ILE:HG23	1:A:121:VAL:HG11	1.98	0.46
1:D:358:PRO:O	1:D:359:THR:C	2.58	0.46
1:A:188:SER:C	1:A:189:ILE:HD13	2.41	0.46
1:B:82:PRO:O	1:B:85:GLU:HB3	2.16	0.46
1:B:223:LEU:HD12	1:B:247:ALA:HB1	1.98	0.46
1:C:297:GLY:HA2	1:C:326:ILE:HG23	1.98	0.46
1:A:150:LEU:HB2	1:A:308:ILE:HD12	1.97	0.46
1:C:25:LEU:H	1:C:134:ASN:ND2	2.07	0.46
1:C:222:VAL:O	1:C:222:VAL:CG1	2.63	0.46
1:A:28:ALA:HA	1:A:68:TYR:O	2.16	0.45
1:A:66:ASP:OD2	1:A:94:ARG:HB2	2.16	0.45
1:A:75:SER:OG	1:A:109:ARG:NH1	2.35	0.45
1:B:184:LYS:NZ	1:B:207:LEU:HD12	2.32	0.45
1:C:80:THR:HB	1:C:81:PRO:HD2	1.98	0.45
1:C:272:ILE:HB	1:C:273:PRO:HD3	1.98	0.45
1:D:16:GLY:O	1:D:17:GLU:C	2.59	0.45
1:A:19:GLN:HG2	1:B:35:GLN:OE1	2.16	0.45
1:A:180:GLN:HE21	1:A:180:GLN:HB2	1.63	0.45
1:C:207:LEU:O	1:C:208:PRO:O	2.35	0.45
1:C:210:VAL:C	1:C:212:LYS:H	2.24	0.45
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.51	0.45
1:D:190:LEU:HD11	1:D:219:LEU:CG	2.44	0.45
1:D:190:LEU:HD13	1:D:191:VAL:H	1.81	0.45
1:D:236:ILE:O	1:D:236:ILE:HG22	2.17	0.45
1:A:1:MET:HE3	1:A:4:TYR:HB3	1.98	0.45
1:B:317:ILE:HD13	1:D:337:VAL:HG21	1.98	0.45
1:C:169:TRP:CH2	1:C:176:ARG:NH1	2.85	0.45
1:C:234:ASP:O	1:C:236:ILE:N	2.50	0.45
1:D:300:VAL:HG21	1:D:326:ILE:CD1	2.45	0.45
1:A:122:ARG:HB3	4:A:378:HOH:O	2.17	0.45
1:C:193:VAL:CG1	1:C:220:ASP:CG	2.84	0.45
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.82	0.45
1:C:84:ALA:O	1:C:88:ILE:HG13	2.15	0.45
1:B:159:LYS:HE2	4:B:372:HOH:O	2.17	0.45
1:C:44:LYS:HD3	1:D:61:HIS:NE2	2.32	0.45
1:A:75:SER:OG	1:A:109:ARG:HD2	2.17	0.45
1:A:311:TYR:OH	1:A:353:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG21	1:B:220:ASP:HA	1.96	0.45
1:A:129:GLN:HE21	1:A:129:GLN:HB3	1.62	0.45
1:B:128:ASP:OD1	1:B:129:GLN:NE2	2.50	0.45
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.77	0.45
1:D:275:VAL:O	1:D:279:LEU:HG	2.17	0.45
1:A:1:MET:HE3	1:A:4:TYR:CB	2.47	0.45
1:A:334:MET:HA	1:A:337:VAL:CG1	2.47	0.45
1:B:6:MET:HE1	1:B:70:THR:HA	1.99	0.45
1:B:131:GLU:OE1	1:B:142:ARG:NH2	2.51	0.45
1:C:85:GLU:O	1:C:88:ILE:HB	2.17	0.45
1:A:21:GLU:HG3	1:A:45:TYR:CB	2.47	0.44
1:A:72:GLU:OE1	1:A:111:ILE:HG12	2.17	0.44
1:D:111:ILE:HD12	1:D:121:VAL:HG11	1.98	0.44
1:A:272:ILE:HA	1:A:275:VAL:HG22	1.99	0.44
1:A:345:ILE:HD11	1:C:352:ILE:HD12	1.98	0.44
1:B:67:ILE:HG23	1:B:95:VAL:HG23	1.99	0.44
1:B:222:VAL:O	1:B:222:VAL:HG13	2.17	0.44
1:C:56:HIS:CE1	1:D:56:HIS:CE1	3.06	0.44
1:C:102:PRO:O	1:C:104:PRO:HD3	2.17	0.44
1:D:221:THR:O	1:D:244:THR:OG1	2.35	0.44
1:B:184:LYS:NZ	1:B:184:LYS:CB	2.80	0.44
1:C:72:GLU:HG3	1:C:111:ILE:HD11	1.98	0.44
1:C:167:SER:C	1:C:169:TRP:N	2.66	0.44
1:C:306:GLN:N	1:C:306:GLN:CD	2.76	0.44
1:C:106:VAL:HG13	1:C:109:ARG:NH1	2.32	0.44
1:C:272:ILE:HA	1:C:275:VAL:HG22	1.98	0.44
1:D:190:LEU:HD13	1:D:191:VAL:N	2.33	0.44
1:D:201:PRO:HG2	1:D:203:LEU:CD2	2.47	0.44
1:B:191:VAL:HG23	1:B:291:GLY:N	2.33	0.44
1:D:190:LEU:CD1	1:D:219:LEU:HG	2.47	0.44
1:B:8:LEU:HD23	1:B:12:LEU:HD13	2.00	0.44
1:B:93:LYS:NZ	1:B:93:LYS:HB3	2.32	0.44
1:A:345:ILE:HD11	1:C:352:ILE:CD1	2.48	0.44
1:C:140:PHE:HD2	1:C:141:MET:HE2	1.82	0.44
1:D:7:LYS:HZ3	1:D:129:GLN:HE22	1.66	0.44
1:D:193:VAL:HG11	1:D:220:ASP:OD2	2.18	0.44
1:D:230:LYS:C	1:D:232:ILE:H	2.25	0.44
1:A:319:GLY:N	1:C:330:GLY:HA3	2.33	0.43
1:A:334:MET:HA	1:A:337:VAL:HG12	1.99	0.43
1:B:87:ILE:HG23	1:B:92:ILE:HG13	2.00	0.43
1:C:101:ASP:O	1:C:107:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HB3	1:A:208:PRO:HD2	2.00	0.43
1:C:101:ASP:HB3	1:C:107:ALA:HA	2.00	0.43
1:C:311:TYR:OH	1:C:353:LYS:HE3	2.19	0.43
1:D:347:GLN:HG3	1:D:352:ILE:CD1	2.48	0.43
1:A:87:ILE:HG23	1:A:92:ILE:HG13	1.99	0.43
1:C:131:GLU:OE1	1:C:142:ARG:NH2	2.44	0.43
1:C:136:LYS:HG2	1:C:147:TYR:CD2	2.54	0.43
1:D:246:ARG:HG3	1:D:246:ARG:NH1	2.33	0.43
1:B:72:GLU:HA	1:B:73:PRO:HD3	1.89	0.43
1:B:314:PRO:HG3	1:D:342:PHE:CD2	2.53	0.43
1:D:181:GLN:CG	1:D:182:TYR:N	2.80	0.43
1:B:162:THR:HG23	1:D:334:MET:CE	2.45	0.43
1:B:334:MET:HE3	1:D:169:TRP:O	2.18	0.43
1:C:180:GLN:O	1:C:183:ARG:N	2.52	0.43
1:D:22:SER:HA	1:D:285:MET:HE1	2.00	0.43
1:B:31:VAL:CG1	1:B:66:ASP:HB2	2.46	0.43
1:B:166:ASP:OD1	1:B:168:LYS:HG3	2.18	0.43
1:B:188:SER:C	1:B:189:ILE:HD13	2.44	0.43
1:D:222:VAL:HG13	1:D:224:SER:HB2	2.01	0.43
1:A:9:ALA:O	1:A:27:GLY:HA3	2.19	0.43
1:A:140:PHE:CD2	1:A:285:MET:HG2	2.54	0.43
1:A:275:VAL:HG23	1:A:276:LEU:N	2.33	0.43
1:A:344:ASP:HB3	1:A:355:THR:CG2	2.46	0.43
1:B:206:ARG:HB2	4:B:384:HOH:O	2.19	0.43
1:B:207:LEU:N	4:B:384:HOH:O	2.52	0.43
1:D:208:PRO:O	1:D:209:ASN:CB	2.66	0.43
1:D:230:LYS:C	1:D:234:ASP:HB3	2.39	0.43
1:C:55:ILE:CD1	1:C:92:ILE:HD11	2.48	0.43
1:A:125:ILE:HD12	1:A:125:ILE:N	2.33	0.42
1:B:181:GLN:CG	1:B:182:TYR:N	2.77	0.42
1:C:136:LYS:HG2	1:C:147:TYR:CG	2.53	0.42
1:C:296:HIS:HB3	1:C:326:ILE:HD12	2.00	0.42
1:D:307:GLU:HB3	1:D:309:ILE:CD1	2.49	0.42
1:D:320:THR:O	4:D:404:HOH:O	2.21	0.42
1:D:343:THR:HG21	1:D:357:LYS:CD	2.43	0.42
1:B:191:VAL:HG23	1:B:291:GLY:H	1.84	0.42
1:C:32:LYS:O	1:C:33:ASP:C	2.62	0.42
1:D:99:MET:HE1	1:D:138:LEU:HG	2.01	0.42
1:C:12:LEU:O	1:C:15:GLN:HG2	2.20	0.42
1:D:101:ASP:HB3	1:D:107:ALA:HA	2.00	0.42
1:D:234:ASP:O	1:D:236:ILE:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:O	1:B:222:VAL:CG1	2.67	0.42
1:D:248:ASP:OD1	1:D:249:GLU:N	2.52	0.42
1:B:200:ASN:N	1:B:201:PRO:CD	2.82	0.42
1:C:289:VAL:HG21	1:C:299:PHE:CZ	2.54	0.42
1:D:31:VAL:HA	1:D:35:GLN:O	2.20	0.42
1:A:156:LEU:O	1:A:156:LEU:HD12	2.19	0.42
1:A:310:PHE:CD2	1:C:156:LEU:HG	2.54	0.42
1:A:345:ILE:HG23	1:A:354:LEU:HD23	2.02	0.42
1:B:9:ALA:O	1:B:27:GLY:HA3	2.20	0.42
1:D:340:LEU:CD2	1:D:358:PRO:HA	2.49	0.42
1:A:318:GLY:C	1:C:330:GLY:HA3	2.44	0.42
1:B:169:TRP:H	1:D:334:MET:HG2	1.85	0.42
1:D:170:ILE:CG2	1:D:171:THR:N	2.82	0.42
1:B:80:THR:HG23	1:B:81:PRO:HD2	2.01	0.42
1:B:126:LEU:HB3	1:B:129:GLN:NE2	2.32	0.42
1:C:108:GLY:O	1:C:109:ARG:C	2.61	0.42
1:D:181:GLN:HA	1:D:207:LEU:HD12	2.02	0.42
1:A:223:LEU:HB2	1:A:243:THR:HG21	2.02	0.42
1:A:342:PHE:CD2	1:C:352:ILE:HG12	2.55	0.41
1:B:162:THR:CG2	1:D:334:MET:HE2	2.46	0.41
1:B:207:LEU:HA	1:B:208:PRO:HD3	1.82	0.41
1:C:55:ILE:HG13	1:C:86:LEU:HD11	2.01	0.41
1:D:309:ILE:HD12	1:D:309:ILE:N	2.35	0.41
1:B:131:GLU:CD	1:B:142:ARG:HH22	2.29	0.41
1:B:257:ALA:C	1:B:259:GLY:H	2.28	0.41
1:C:106:VAL:O	1:C:107:ALA:C	2.63	0.41
1:A:136:LYS:HG2	1:A:147:TYR:CG	2.55	0.41
1:B:184:LYS:HZ3	1:B:184:LYS:HB3	1.85	0.41
1:B:177:GLN:O	1:B:180:GLN:HB2	2.20	0.41
1:B:337:VAL:O	1:B:337:VAL:CG2	2.67	0.41
1:D:145:LEU:HA	1:D:146:PRO:HD3	1.85	0.41
1:D:149:THR:HG23	1:D:309:ILE:HD13	2.02	0.41
1:A:95:VAL:HG23	1:A:119:ILE:HG21	2.03	0.41
1:B:352:ILE:HD12	1:D:354:LEU:HD13	2.02	0.41
1:C:210:VAL:C	1:C:212:LYS:N	2.78	0.41
1:C:211:THR:O	1:C:212:LYS:HB2	2.20	0.41
1:D:188:SER:HA	1:D:215:VAL:O	2.19	0.41
1:A:51:GLU:O	1:A:55:ILE:HG12	2.21	0.41
1:A:190:LEU:HD11	1:A:219:LEU:HG	2.02	0.41
1:A:353:LYS:HD2	4:A:367:HOH:O	2.20	0.41
1:B:32:LYS:CD	1:B:65:ALA:HB2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASP:HA	1:B:102:PRO:HD2	1.95	0.41
1:C:336:ASP:O	1:C:338:PRO:HD3	2.19	0.41
1:D:154:ALA:HB1	1:D:159:LYS:O	2.21	0.41
1:D:226:PRO:C	1:D:228:ASP:N	2.78	0.41
1:A:103:ASN:HA	1:A:104:PRO:HD3	1.93	0.41
1:A:134:ASN:HB2	1:A:138:LEU:HD22	2.02	0.41
1:B:17:GLU:HA	1:B:25:LEU:HD21	2.02	0.41
1:B:51:GLU:O	1:B:55:ILE:HG13	2.20	0.41
1:B:352:ILE:CD1	1:D:345:ILE:HD11	2.51	0.41
1:C:35:GLN:NE2	1:D:19:GLN:HB2	2.35	0.41
1:C:190:LEU:HD23	1:C:190:LEU:C	2.46	0.41
1:C:212:LYS:HD3	1:C:212:LYS:C	2.46	0.41
1:A:36:ILE:CD1	1:B:15:GLN:HG3	2.49	0.41
1:A:66:ASP:OD1	1:A:94:ARG:NH2	2.50	0.41
1:A:188:SER:O	1:A:189:ILE:HD13	2.21	0.41
1:B:85:GLU:O	1:B:89:ASN:ND2	2.54	0.41
1:B:253:LYS:HE3	1:B:253:LYS:HB2	1.87	0.41
1:C:190:LEU:HD22	1:C:289:VAL:HG22	2.03	0.41
1:A:223:LEU:HB2	1:A:247:ALA:CB	2.50	0.41
1:B:6:MET:O	1:B:10:LEU:HG	2.21	0.41
1:C:186:HIS:CD2	1:C:288:TYR:HB2	2.55	0.41
1:A:269:ARG:HH11	1:A:269:ARG:HG2	1.86	0.40
1:A:279:LEU:HB3	1:A:284:ILE:HB	2.03	0.40
1:B:37:VAL:O	1:B:37:VAL:CG2	2.68	0.40
1:B:334:MET:CE	1:D:170:ILE:HA	2.51	0.40
1:B:335:LYS:HB3	1:D:169:TRP:HZ3	1.85	0.40
1:C:248:ASP:OD2	1:C:251:LYS:HB2	2.21	0.40
1:D:9:ALA:HA	1:D:12:LEU:HD12	2.03	0.40
1:A:48:ALA:HB3	1:A:53:HIS:CE1	2.56	0.40
1:C:55:ILE:HD13	1:C:55:ILE:HA	1.86	0.40
1:A:29:VAL:O	1:A:67:ILE:HA	2.21	0.40
1:A:240:TRP:HA	1:A:261:ASN:O	2.21	0.40
1:B:8:LEU:HD11	1:B:36:ILE:HD13	2.02	0.40
1:C:102:PRO:HB2	1:C:141:MET:CB	2.51	0.40
1:C:182:TYR:CZ	1:C:309:ILE:HD13	2.57	0.40
1:C:234:ASP:CG	1:C:236:ILE:HG12	2.46	0.40
1:D:150:LEU:HD12	1:D:308:ILE:HD11	2.03	0.40
1:D:225:ILE:O	1:D:225:ILE:CG2	2.69	0.40
1:A:21:GLU:HG3	1:A:45:TYR:HB2	2.03	0.40
1:A:334:MET:HE2	1:C:170:ILE:HA	2.03	0.40
1:B:311:TYR:CE1	1:B:348:ILE:HD12	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:SER:OG	1:D:287:VAL:HG22	2.21	0.40
1:A:318:GLY:HA3	1:C:330:GLY:CA	2.51	0.40
1:C:21:GLU:HB3	1:C:22:SER:H	1.60	0.40
1:C:65:ALA:O	1:C:92:ILE:HG23	2.21	0.40
1:C:274:ASP:O	1:C:278:ILE:HG12	2.22	0.40
1:D:191:VAL:O	1:D:218:ILE:HA	2.21	0.40
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.36	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	357/373 (96%)	339 (95%)	16 (4%)	2 (1%)	21	28
1	B	357/373 (96%)	327 (92%)	25 (7%)	5 (1%)	9	11
1	C	357/373 (96%)	322 (90%)	25 (7%)	10 (3%)	4	3
1	D	358/373 (96%)	311 (87%)	38 (11%)	9 (2%)	4	4
All	All	1429/1492 (96%)	1299 (91%)	104 (7%)	26 (2%)	6	8

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
1	B	212	LYS
1	C	168	LYS
1	C	208	PRO
1	C	234	ASP
1	C	235	GLN
1	C	78	GLY
1	C	169	TRP

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Mol	Chain	Res	Type
1	C	284	ILE
1	D	18	GLY
1	D	246	ARG
1	D	329	GLU
1	A	48	ALA
1	B	17	GLU
1	C	107	ALA
1	C	212	LYS
1	D	48	ALA
1	D	209	ASN
1	B	76	HIS
1	C	161	ALA
1	D	235	GLN
1	B	235	GLN
1	D	168	LYS
1	D	231	VAL
1	D	237	ALA
1	B	170	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/305 (96%)	266 (91%)	27 (9%)	8	11
1	B	293/305 (96%)	265 (90%)	28 (10%)	8	10
1	C	293/305 (96%)	271 (92%)	22 (8%)	12	18
1	D	294/305 (96%)	271 (92%)	23 (8%)	11	17
All	All	1173/1220 (96%)	1073 (92%)	100 (8%)	10	14

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	23	ASN
1	A	29	VAL

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Mol	Chain	Res	Type
1	A	71	LEU
1	A	86	LEU
1	A	109	ARG
1	A	128	ASP
1	A	129	GLN
1	A	138	LEU
1	A	171	THR
1	A	180	GLN
1	A	181	GLN
1	A	190	LEU
1	A	193	VAL
1	A	208	PRO
1	A	222	VAL
1	A	223	LEU
1	A	231	VAL
1	A	243	THR
1	A	267	THR
1	A	281	GLU
1	A	301	LYS
1	A	337	VAL
1	A	343	THR
1	A	347	GLN
1	A	350	ARG
1	A	355	THR
1	B	3	GLU
1	B	8	LEU
1	B	12	LEU
1	B	15	GLN
1	B	17	GLU
1	B	22	SER
1	B	25	LEU
1	B	29	VAL
1	B	35	GLN
1	B	37	VAL
1	B	76	HIS
1	B	88	ILE
1	B	93	LYS
1	B	125	ILE
1	B	128	ASP
1	B	129	GLN
1	B	138	LEU
1	B	173	GLU

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Mol	Chain	Res	Type
1	B	184	LYS
1	B	193	VAL
1	B	213	GLN
1	B	222	VAL
1	B	223	LEU
1	B	231	VAL
1	B	287	VAL
1	B	308	ILE
1	B	337	VAL
1	B	355	THR
1	C	12	LEU
1	C	116	GLU
1	C	123	GLU
1	C	138	LEU
1	C	164	THR
1	C	176	ARG
1	C	212	LYS
1	C	221	THR
1	C	225	ILE
1	C	228	ASP
1	C	234	ASP
1	C	243	THR
1	C	248	ASP
1	C	264	THR
1	C	268	GLU
1	C	287	VAL
1	C	308	ILE
1	C	320	THR
1	C	340	LEU
1	C	343	THR
1	C	355	THR
1	C	358	PRO
1	D	19	GLN
1	D	25	LEU
1	D	29	VAL
1	D	31	VAL
1	D	71	LEU
1	D	86	LEU
1	D	112	SER
1	D	122	ARG
1	D	138	LEU
1	D	151	LYS

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Mol	Chain	Res	Type
1	D	171	THR
1	D	177	GLN
1	D	190	LEU
1	D	191	VAL
1	D	199	ASP
1	D	207	LEU
1	D	221	THR
1	D	223	LEU
1	D	225	ILE
1	D	234	ASP
1	D	270	ILE
1	D	301	LYS
1	D	355	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	42	HIS
1	A	53	HIS
1	A	56	HIS
1	A	129	GLN
1	A	134	ASN
1	A	180	GLN
1	A	186	HIS
1	A	209	ASN
1	A	213	GLN
1	A	235	GLN
1	A	296	HIS
1	A	341	GLN
1	B	15	GLN
1	B	23	ASN
1	B	35	GLN
1	B	56	HIS
1	B	61	HIS
1	B	89	ASN
1	B	129	GLN
1	B	186	HIS
1	B	209	ASN
1	B	213	GLN
1	B	271	GLN
1	B	332	GLN

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Mol	Chain	Res	Type
1	B	341	GLN
1	C	23	ASN
1	C	42	HIS
1	C	103	ASN
1	C	134	ASN
1	C	180	GLN
1	C	186	HIS
1	C	306	GLN
1	C	341	GLN
1	C	347	GLN
1	D	53	HIS
1	D	89	ASN
1	D	129	GLN
1	D	177	GLN
1	D	180	GLN
1	D	181	GLN
1	D	186	HIS
1	D	271	GLN
1	D	306	GLN
1	D	332	GLN
1	D	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AIF	C	381	-	20,23,23	1.08	2 (10%)	25,33,33	1.78	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AIF	C	381	-	-	3/15/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	381	AIF	C2-N3	2.03	1.40	1.37
3	C	381	AIF	C2-N1	2.03	1.40	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	381	AIF	C5-C4-N3	4.97	120.59	111.10
3	C	381	AIF	C4-N3-C2	-4.71	119.88	126.37
3	C	381	AIF	O4-C4-C5	-2.89	120.18	127.48
3	C	381	AIF	N3-C2-N1	2.66	119.92	115.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

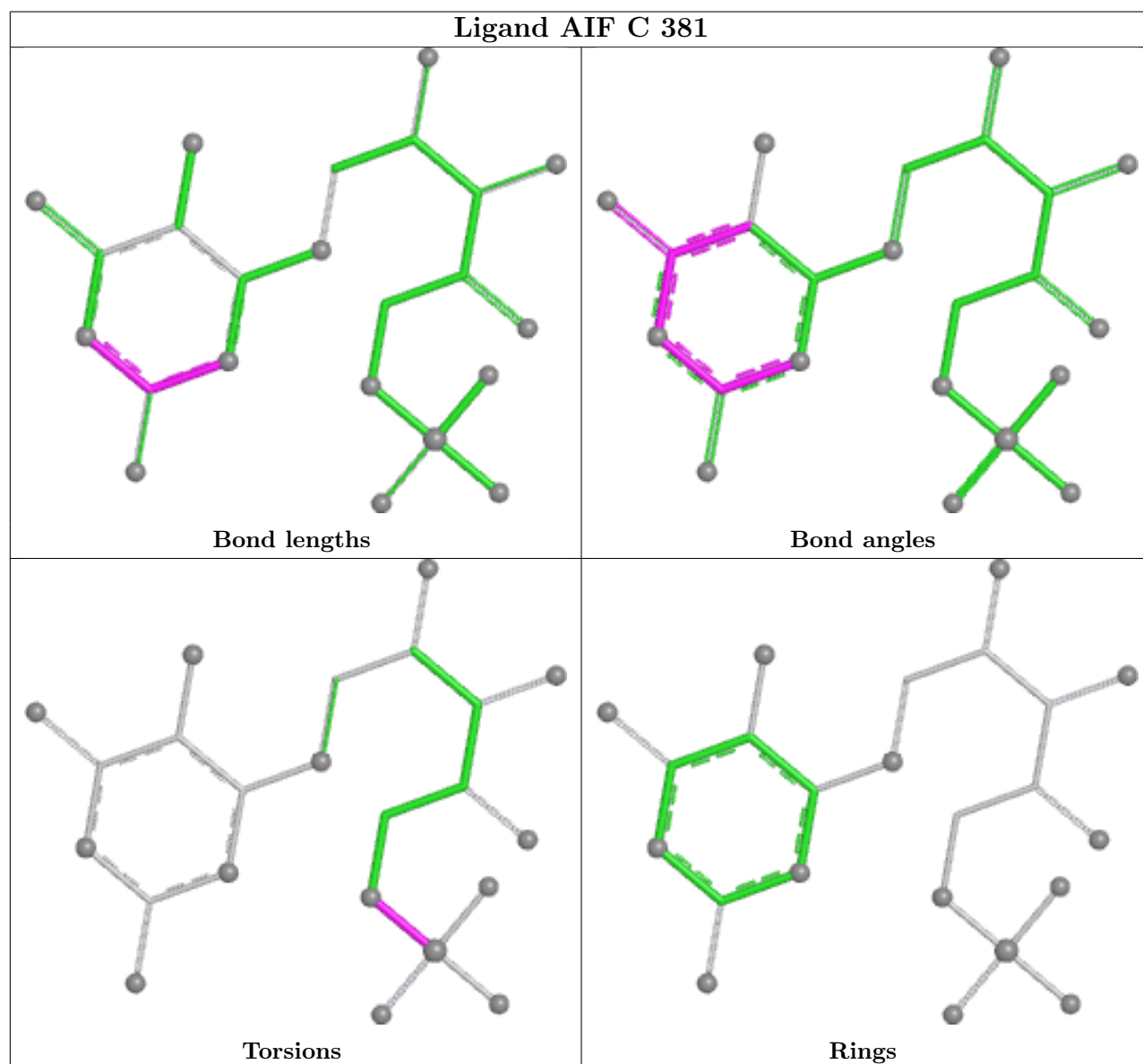
Mol	Chain	Res	Type	Atoms
3	C	381	AIF	C5'-O5'-P-O1P
3	C	381	AIF	C5'-O5'-P-O3P
3	C	381	AIF	C5'-O5'-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	381	AIF	3	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/373 (96%)	-0.19	3 (0%) 82 85	28, 45, 65, 79	0
1	B	359/373 (96%)	0.19	12 (3%) 49 50	37, 55, 81, 107	0
1	C	359/373 (96%)	0.10	6 (1%) 69 70	37, 54, 79, 102	0
1	D	360/373 (96%)	0.26	14 (3%) 43 44	37, 58, 100, 112	0
All	All	1437/1492 (96%)	0.09	35 (2%) 59 61	28, 52, 88, 112	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	PRO	4.1
1	D	209	ASN	3.8
1	D	229	ALA	3.6
1	D	207	LEU	3.5
1	B	169	TRP	3.4
1	B	76	HIS	3.1
1	B	211	THR	3.0
1	B	77	TYR	2.9
1	B	209	ASN	2.9
1	D	169	TRP	2.8
1	C	210	VAL	2.8
1	D	233	CYS	2.8
1	D	252	LYS	2.6
1	C	77	TYR	2.6
1	D	176	ARG	2.5
1	D	280	ALA	2.5
1	B	210	VAL	2.4
1	B	87	ILE	2.4
1	B	81	PRO	2.3
1	A	211	THR	2.3
1	D	247	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	2.2
1	D	262	ILE	2.2
1	D	245	ALA	2.2
1	C	291	GLY	2.2
1	B	208	PRO	2.2
1	D	222	VAL	2.2
1	B	80	THR	2.1
1	C	208	PRO	2.1
1	D	210	VAL	2.1
1	C	257	ALA	2.1
1	A	209	ASN	2.0
1	C	235	GLN	2.0
1	B	130	ALA	2.0
1	A	333	SER	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](#)

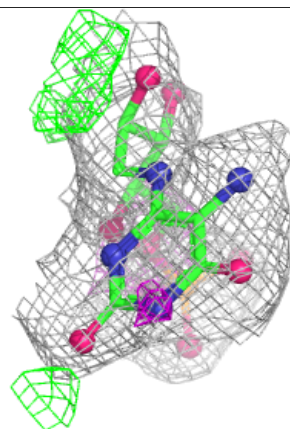
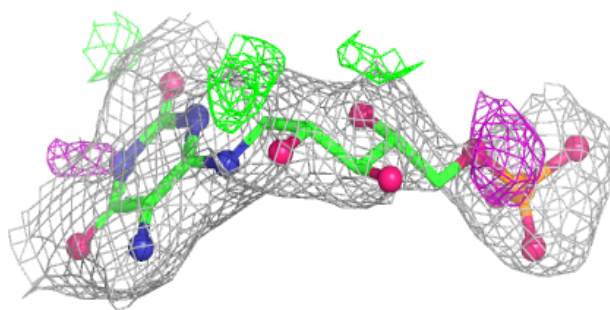
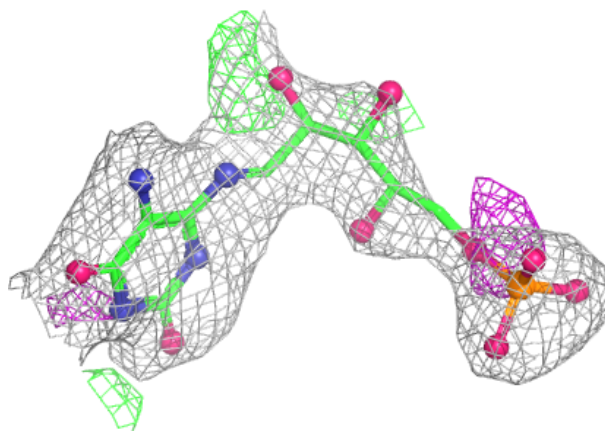
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	AIF	C	381	23/23	0.83	0.12	64,66,69,71	0
2	ZN	A	362	1/1	0.98	0.08	49,49,49,49	0
2	ZN	C	362	1/1	0.99	0.05	55,55,55,55	0
2	ZN	D	362	1/1	0.99	0.06	52,52,52,52	0
2	ZN	B	362	1/1	0.99	0.02	60,60,60,60	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 AIF C 381:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.