



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 06:30 PM EDT

PDB ID : 3LM8
Title : Crystal Structure of Thiamine pyrophosphokinase from *Bacillus subtilis*, Northeast Structural Genomics Consortium Target SR677
Authors : Kuzin, A.; Abashidze, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Foote, E.L.; Ciccocanti, C.; Wang, H.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-01-29
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

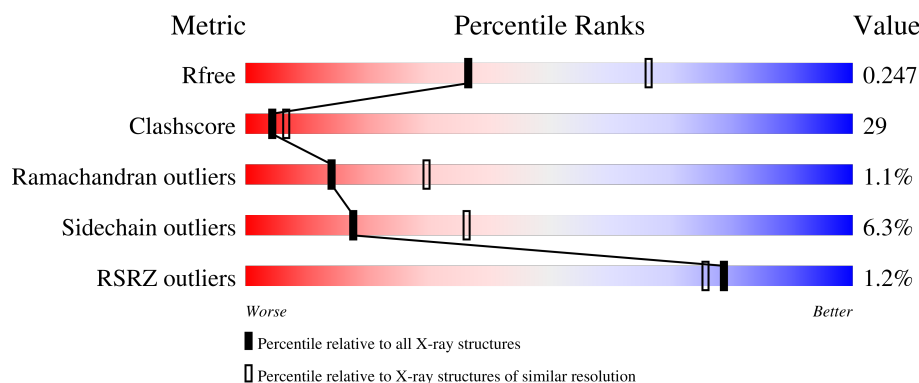
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	222	
1	B	222	
1	C	222	
1	D	222	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6941 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 Thiamine pyrophosphokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	Se	0	0	0
			1701	1091	285	321	2	2			
1	B	214	Total	C	N	O	S	Se	0	0	0
			1701	1091	285	321	2	2			
1	C	213	Total	C	N	O	S	Se	0	0	0
			1692	1086	284	318	2	2			
1	D	212	Total	C	N	O	S	Se	0	0	0
			1683	1080	282	317	2	2			

There are 36 discrepancies between the modelled and reference sequences:

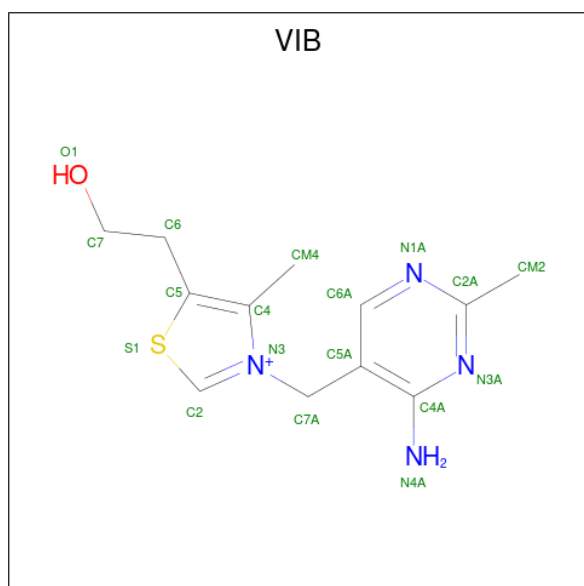
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	ALA	engineered mutation	UNP O34664
A	215	LEU	-	expression tag	UNP O34664
A	216	GLU	-	expression tag	UNP O34664
A	217	HIS	-	expression tag	UNP O34664
A	218	HIS	-	expression tag	UNP O34664
A	219	HIS	-	expression tag	UNP O34664
A	220	HIS	-	expression tag	UNP O34664
A	221	HIS	-	expression tag	UNP O34664
A	222	HIS	-	expression tag	UNP O34664
B	203	VAL	ALA	engineered mutation	UNP O34664
B	215	LEU	-	expression tag	UNP O34664
B	216	GLU	-	expression tag	UNP O34664
B	217	HIS	-	expression tag	UNP O34664
B	218	HIS	-	expression tag	UNP O34664
B	219	HIS	-	expression tag	UNP O34664
B	220	HIS	-	expression tag	UNP O34664
B	221	HIS	-	expression tag	UNP O34664
B	222	HIS	-	expression tag	UNP O34664
C	203	VAL	ALA	engineered mutation	UNP O34664
C	215	LEU	-	expression tag	UNP O34664
C	216	GLU	-	expression tag	UNP O34664

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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP O34664
C	218	HIS	-	expression tag	UNP O34664
C	219	HIS	-	expression tag	UNP O34664
C	220	HIS	-	expression tag	UNP O34664
C	221	HIS	-	expression tag	UNP O34664
C	222	HIS	-	expression tag	UNP O34664
D	203	VAL	ALA	engineered mutation	UNP O34664
D	215	LEU	-	expression tag	UNP O34664
D	216	GLU	-	expression tag	UNP O34664
D	217	HIS	-	expression tag	UNP O34664
D	218	HIS	-	expression tag	UNP O34664
D	219	HIS	-	expression tag	UNP O34664
D	220	HIS	-	expression tag	UNP O34664
D	221	HIS	-	expression tag	UNP O34664
D	222	HIS	-	expression tag	UNP O34664

- Molecule 2 is 3-(4-AMINO-2-METHYL-PYRIMIDIN-5-YLMETHYL)-5-(2-HYDROXY-ETHYL)-4-METHYL-THIAZOL-3-IUM (three-letter code: VIB) (formula: C₁₂H₁₇N₄OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	12	4	1	1		
2	B	1	Total	C	N	O	S	0	0
			18	12	4	1	1		
2	C	1	Total	C	N	O	S	0	0
			18	12	4	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			18	12	4	1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	13	Total 13	O 13	0	0
5	C	21	Total 21	O 21	0	0
5	D	13	Total 13	O 13	0	0

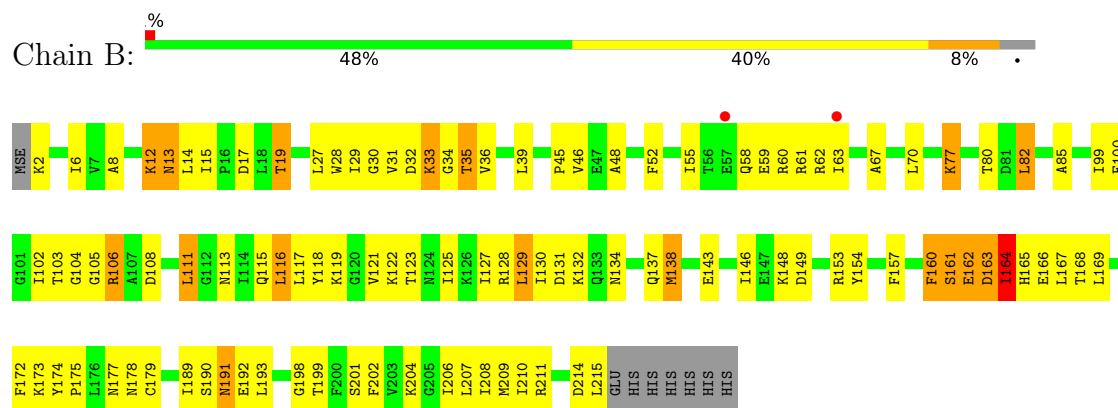
3 Residue-property plots [i](#)

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

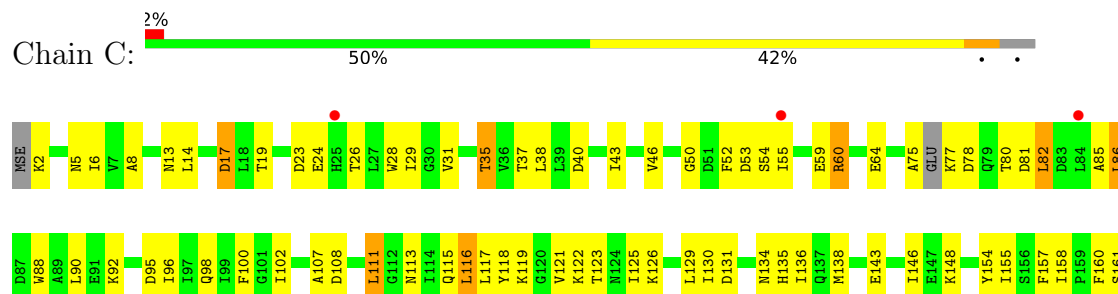
• Molecule 1: Thiamine pyrophosphokinase



• Molecule 1: Thiamine pyrophosphokinase

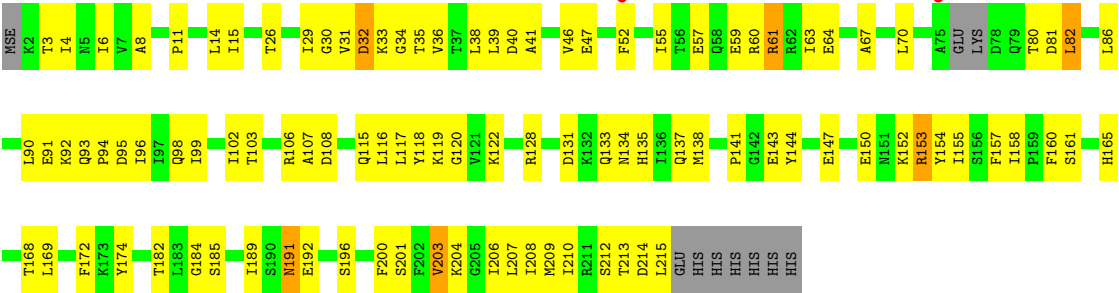


• Molecule 1: Thiamine pyrophosphokinase





● Molecule 1: Thiamine pyrophosphokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.94Å 62.15Å 84.16Å 82.89° 82.02° 87.61°	Depositor
Resolution (Å)	20.00 – 2.60 41.38 – 2.56	Depositor EDS
% Data completeness (in resolution range)	82.4 (20.00-2.60) 91.9 (41.38-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2, REFMAC	Depositor
R, R_{free}	0.213 , 0.253 0.218 , 0.247	Depositor DCC
R_{free} test set	2734 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6941	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: MG, PO4, VIB

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	0.37	0/1734	0.64	0/2346
1	B	0.96	20/1734 (1.2%)	0.76	1/2346 (0.0%)
1	C	0.38	0/1724	0.65	0/2331
1	D	0.37	0/1715	0.63	0/2320
All	All	0.58	20/6907 (0.3%)	0.67	1/9343 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	ASP	C-O	-12.21	1.00	1.23
1	B	166	GLU	C-O	-10.88	1.02	1.23
1	B	167	LEU	C-O	-8.98	1.06	1.23
1	B	164	ILE	C-O	-7.97	1.08	1.23
1	B	166	GLU	CD-OE1	-7.91	1.17	1.25
1	B	161	SER	C-O	-7.49	1.09	1.23
1	B	165	HIS	C-O	-7.46	1.09	1.23
1	B	163	ASP	CG-OD1	-7.22	1.08	1.25
1	B	163	ASP	CB-CG	-7.19	1.36	1.51
1	B	161	SER	CB-OG	-6.90	1.33	1.42
1	B	165	HIS	CA-C	-6.38	1.36	1.52
1	B	163	ASP	N-CA	-5.54	1.35	1.46
1	B	162	GLU	C-O	-5.48	1.12	1.23
1	B	166	GLU	CB-CG	-5.42	1.41	1.52
1	B	164	ILE	CB-CG1	-5.37	1.39	1.54
1	B	161	SER	CA-CB	-5.29	1.45	1.52
1	B	166	GLU	N-CA	-5.19	1.35	1.46
1	B	163	ASP	CG-OD2	-5.10	1.13	1.25
1	B	164	ILE	CA-CB	-5.09	1.43	1.54
1	B	164	ILE	CB-CG2	-5.03	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASP	CB-CG-OD2	9.20	126.58	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1701	0	1708	107	0
1	B	1701	0	1708	99	0
1	C	1692	0	1701	107	0
1	D	1683	0	1688	99	0
2	A	18	0	17	2	0
2	B	18	0	17	3	0
2	C	18	0	17	2	0
2	D	18	0	17	1	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	20	0	0	0	0
5	B	13	0	0	0	0
5	C	21	0	0	0	0
5	D	13	0	0	0	0
All	All	6941	0	6873	397	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 (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:H	1:B:77:LYS:HD3	1.08	1.18
1:A:113:ASN:HA	1:A:116:LEU:HD23	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG23	1:A:47:GLU:HG2	1.47	0.95
1:A:6:ILE:HG12	1:A:29:ILE:HD11	1.48	0.94
1:C:160:PHE:HB3	1:C:206:ILE:HD13	1.53	0.91
1:B:138:MSE:HE3	1:B:206:ILE:HG21	1.55	0.89
1:D:138:MSE:HE1	1:D:160:PHE:HB2	1.57	0.86
1:B:77:LYS:HD3	1:B:77:LYS:N	1.90	0.85
1:B:134:ASN:ND2	1:D:107:ALA:H	1.74	0.85
1:A:191:ASN:HD22	1:A:192:GLU:H	1.22	0.85
1:C:206:ILE:HD12	1:C:206:ILE:H	1.37	0.85
1:D:138:MSE:HE1	1:D:160:PHE:CB	2.08	0.84
1:B:191:ASN:HD22	1:B:192:GLU:H	1.24	0.84
1:D:138:MSE:HE3	1:D:208:ILE:CG1	2.08	0.84
1:B:13:ASN:HD22	1:B:13:ASN:H	1.25	0.84
1:B:17:ASP:OD2	1:B:19:THR:HG22	1.77	0.83
1:A:113:ASN:CA	1:A:116:LEU:HD23	2.08	0.83
1:C:138:MSE:HG2	1:C:208:ILE:HG12	1.60	0.81
1:B:12:LYS:H	1:B:12:LYS:HD2	1.44	0.81
1:C:161:SER:H	1:C:206:ILE:HD11	1.46	0.81
1:D:138:MSE:HE2	1:D:206:ILE:HG22	1.64	0.80
1:B:119:LYS:HA	1:B:122:LYS:HE2	1.64	0.80
1:A:79:GLN:HG3	1:A:83:ASP:OD2	1.82	0.80
1:D:30:GLY:HA3	1:D:35:THR:HG22	1.62	0.79
1:D:138:MSE:HE3	1:D:208:ILE:HG13	1.66	0.77
1:C:143:GLU:HG3	1:C:201:SER:HB3	1.65	0.77
1:C:75:ALA:HB1	1:C:77:LYS:N	2.00	0.76
1:C:146:ILE:HD13	1:C:209:MSE:HE1	1.66	0.76
1:C:157:PHE:CZ	1:C:209:MSE:HE3	2.21	0.76
1:A:120:GLY:HA3	1:A:127:ILE:HD12	1.66	0.75
1:B:102:ILE:HG13	1:B:113:ASN:ND2	2.02	0.74
1:C:35:THR:HA	1:C:38:LEU:HD12	1.68	0.74
1:D:134:ASN:ND2	1:D:212:SER:HB3	2.02	0.74
1:C:161:SER:H	1:C:206:ILE:CD1	2.00	0.74
1:D:191:ASN:HD22	1:D:192:GLU:H	1.36	0.74
1:B:13:ASN:HD22	1:B:13:ASN:N	1.83	0.73
1:D:95:ASP:C	1:D:96:ILE:HD12	2.09	0.73
1:B:12:LYS:H	1:B:12:LYS:CD	1.99	0.72
1:C:60:ARG:O	1:C:64:GLU:HG3	1.89	0.72
1:B:111:LEU:HD23	1:D:210:ILE:HD11	1.69	0.72
1:A:56:THR:HG23	1:A:57:GLU:HG2	1.70	0.72
1:B:2:LYS:HE3	1:B:27:LEU:HD23	1.72	0.71
1:C:165:HIS:HB2	1:C:204:LYS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HD2	1:A:208:ILE:HD11	1.56	0.70
1:B:102:ILE:HG13	1:B:113:ASN:HD22	1.57	0.69
1:B:160:PHE:HD2	1:B:208:ILE:HD11	1.57	0.69
1:D:174:TYR:H	1:D:191:ASN:HD21	1.37	0.69
1:A:32:ASP:CG	1:A:33:LYS:H	1.95	0.69
1:B:14:LEU:HD23	1:B:103:THR:HG22	1.75	0.69
1:B:161:SER:OG	1:D:161:SER:O	2.10	0.69
1:D:138:MSE:HE3	1:D:208:ILE:HG12	1.75	0.69
1:D:138:MSE:CE	1:D:206:ILE:HG22	2.23	0.68
1:D:117:LEU:HB3	1:D:138:MSE:HG3	1.75	0.68
1:D:157:PHE:HE1	1:D:209:MSE:HE2	1.59	0.68
1:A:174:TYR:H	1:A:191:ASN:HD21	1.42	0.67
1:A:38:LEU:HD13	1:A:45:PRO:HG3	1.77	0.67
1:A:106:ARG:HB3	1:A:108:ASP:OD2	1.94	0.67
1:C:82:LEU:HD11	1:C:102:ILE:HD11	1.77	0.67
1:B:123:THR:O	1:B:125:ILE:HG13	1.95	0.67
1:A:132:LYS:HE3	1:A:215:LEU:HD21	1.75	0.67
1:B:115:GLN:HG3	1:D:184:GLY:HA2	1.77	0.66
1:C:111:LEU:O	1:C:115:GLN:HG2	1.95	0.66
1:D:55:ILE:O	1:D:55:ILE:HD12	1.95	0.66
1:A:115:GLN:HB3	1:C:184:GLY:HA2	1.79	0.65
1:A:11:PRO:HG2	1:A:14:LEU:HD23	1.78	0.65
1:A:134:ASN:ND2	1:C:107:ALA:H	1.94	0.65
1:C:13:ASN:OD1	1:C:14:LEU:HD13	1.97	0.65
1:A:186:THR:HB	1:A:189:ILE:HD12	1.78	0.65
1:B:134:ASN:HD21	1:D:107:ALA:H	1.44	0.65
1:C:123:THR:O	1:C:125:ILE:HG13	1.97	0.65
1:C:191:ASN:HD22	1:C:192:GLU:H	1.43	0.64
1:A:38:LEU:CD1	1:A:45:PRO:HG3	2.28	0.63
1:C:148:LYS:HA	1:C:193:LEU:HD23	1.79	0.63
1:A:109:HIS:CE1	1:A:113:ASN:HD21	2.17	0.63
1:D:138:MSE:CE	1:D:160:PHE:HB2	2.28	0.63
1:B:191:ASN:HD22	1:B:192:GLU:N	1.95	0.63
1:C:174:TYR:H	1:C:191:ASN:HD21	1.45	0.63
1:A:168:THR:O	1:A:200:PHE:HA	1.99	0.63
1:C:88:TRP:CZ2	1:C:92:LYS:HE2	2.34	0.62
1:A:119:LYS:HA	1:A:122:LYS:HE2	1.80	0.62
1:C:136:ILE:HD12	1:C:136:ILE:N	2.15	0.62
1:A:146:ILE:HG21	1:A:209:MSE:HE1	1.82	0.62
1:C:134:ASN:HB3	1:C:136:ILE:HD11	1.82	0.62
1:A:56:THR:HG22	1:A:59:GLU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASP:HA	1:D:210:ILE:HD12	1.81	0.61
1:C:23:ASP:HB3	1:C:26:THR:OG1	2.00	0.61
1:A:191:ASN:ND2	1:A:192:GLU:H	1.96	0.61
1:B:12:LYS:HD2	1:B:12:LYS:N	2.15	0.61
1:C:117:LEU:HD21	1:C:129:LEU:HG	1.82	0.61
1:C:169:LEU:HD12	1:C:176:LEU:HB2	1.83	0.60
1:D:31:VAL:HG13	1:D:81:ASP:HB3	1.81	0.60
1:A:102:ILE:CD1	1:A:129:LEU:HD22	2.30	0.60
1:B:191:ASN:ND2	1:B:192:GLU:H	1.95	0.60
1:A:134:ASN:HD21	1:C:107:ALA:H	1.49	0.60
1:A:134:ASN:ND2	1:A:212:SER:HB3	2.16	0.60
1:D:191:ASN:ND2	1:D:192:GLU:H	1.99	0.60
1:B:117:LEU:HD21	1:B:129:LEU:HD13	1.83	0.59
1:D:155:ILE:N	1:D:155:ILE:HD12	2.17	0.59
1:B:39:LEU:HB3	1:B:62:ARG:NH2	2.17	0.59
1:A:111:LEU:HB3	1:C:158:ILE:HD13	1.85	0.59
1:D:14:LEU:HD23	1:D:103:THR:HG21	1.84	0.59
1:D:134:ASN:HD22	1:D:212:SER:HB3	1.65	0.59
1:A:113:ASN:HA	1:A:116:LEU:CD2	2.26	0.59
1:B:14:LEU:HD23	1:B:103:THR:CG2	2.32	0.59
1:B:2:LYS:HE3	1:B:27:LEU:CD2	2.33	0.59
1:C:82:LEU:HD13	1:C:116:LEU:CD2	2.33	0.59
1:A:113:ASN:O	1:A:116:LEU:HB2	2.03	0.58
1:C:86:LEU:HD22	1:C:90:LEU:HD11	1.85	0.58
1:D:154:TYR:C	1:D:155:ILE:HD12	2.24	0.58
1:B:138:MSE:CE	1:B:206:ILE:HG21	2.30	0.58
1:D:144:TYR:HB2	1:D:200:PHE:CE1	2.38	0.58
1:B:157:PHE:CE1	1:B:209:MSE:HE3	2.39	0.58
1:C:60:ARG:HH21	1:C:60:ARG:HG3	1.68	0.58
1:D:55:ILE:HD13	1:D:60:ARG:HB2	1.86	0.58
1:C:193:LEU:HD11	1:C:198:GLY:HA3	1.86	0.58
1:B:67:ALA:HB1	1:B:70:LEU:HB2	1.86	0.57
1:A:6:ILE:HG12	1:A:29:ILE:CD1	2.28	0.57
1:A:143:GLU:HA	1:A:201:SER:HB3	1.87	0.57
1:A:191:ASN:HD22	1:A:192:GLU:N	1.96	0.57
1:B:169:LEU:HB3	1:B:172:PHE:CD2	2.39	0.57
1:C:208:ILE:HG22	1:C:210:ILE:CD1	2.34	0.57
1:C:210:ILE:N	1:C:210:ILE:HD12	2.19	0.57
1:D:33:LYS:HE3	1:D:59:GLU:OE1	2.04	0.57
1:A:190:SER:HB3	2:A:223:VIB:HM43	1.84	0.57
1:B:39:LEU:HD23	1:B:62:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HD12	1:A:210:ILE:N	2.19	0.57
1:A:123:THR:O	1:A:125:ILE:HG13	2.04	0.57
1:A:194:ILE:HG13	1:A:195:HIS:ND1	2.19	0.57
1:D:93:GLN:N	1:D:94:PRO:HD3	2.19	0.56
1:A:157:PHE:CE1	1:A:209:MSE:HE3	2.40	0.56
1:C:28:TRP:O	1:C:46:VAL:HG12	2.05	0.56
1:C:113:ASN:HA	1:C:116:LEU:HD22	1.87	0.56
1:C:118:TYR:CE2	1:C:122:LYS:HE3	2.41	0.56
1:C:191:ASN:ND2	1:C:192:GLU:H	2.01	0.56
1:A:33:LYS:O	1:A:36:VAL:HB	2.05	0.56
1:B:13:ASN:H	1:B:13:ASN:ND2	1.98	0.56
1:B:27:LEU:N	1:B:27:LEU:HD22	2.20	0.56
1:B:118:TYR:O	1:B:121:VAL:HG22	2.06	0.56
1:D:135:HIS:CD2	1:D:152:LYS:HE3	2.41	0.56
1:A:52:PHE:HD2	1:A:55:ILE:HG12	1.69	0.56
1:B:163:ASP:OD1	1:B:163:ASP:N	2.30	0.56
1:D:200:PHE:CE1	1:D:209:MSE:HE1	2.41	0.56
1:A:118:TYR:HA	1:A:138:MSE:HE1	1.87	0.56
1:D:6:ILE:HG12	1:D:29:ILE:HD11	1.88	0.56
1:C:134:ASN:ND2	1:C:212:SER:HB3	2.21	0.55
1:D:182:THR:HG23	1:D:185:SER:HB2	1.87	0.55
1:A:76:GLU:O	1:A:77:LYS:HG2	2.06	0.55
1:A:118:TYR:O	1:A:121:VAL:HG22	2.05	0.55
1:A:138:MSE:HE3	1:A:206:ILE:CG2	2.37	0.55
1:A:214:ASP:O	1:A:215:LEU:HB2	2.07	0.55
1:B:30:GLY:O	1:B:48:ALA:HA	2.06	0.55
1:C:138:MSE:CE	1:C:206:ILE:HB	2.35	0.55
1:D:4:ILE:HD12	1:D:94:PRO:CG	2.36	0.55
1:C:187:LEU:O	2:C:223:VIB:HC2	2.07	0.55
1:B:146:ILE:HG21	1:B:209:MSE:HE1	1.89	0.55
1:B:214:ASP:O	1:B:215:LEU:HB3	2.06	0.54
1:C:155:ILE:CG2	1:C:209:MSE:HE2	2.37	0.54
1:D:35:THR:HA	1:D:38:LEU:HD12	1.89	0.54
1:B:146:ILE:HD12	1:B:198:GLY:H	1.72	0.54
1:C:157:PHE:HZ	1:C:209:MSE:HE3	1.72	0.54
1:B:128:ARG:HD2	1:B:130:ILE:HD11	1.90	0.54
1:A:133:GLN:HB2	1:A:213:THR:HG22	1.89	0.54
1:D:31:VAL:HG13	1:D:81:ASP:CB	2.38	0.54
1:B:103:THR:HG22	1:B:104:GLY:N	2.23	0.54
1:B:17:ASP:CG	1:B:19:THR:HG22	2.28	0.53
1:B:118:TYR:HD1	1:B:138:MSE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:TYR:O	1:C:121:VAL:HG22	2.08	0.53
2:A:223:VIB:HC72	1:C:80:THR:HA	1.89	0.53
1:C:86:LEU:HD12	1:C:116:LEU:HG	1.90	0.53
1:A:160:PHE:HB3	1:A:206:ILE:HB	1.90	0.53
1:B:8:ALA:HA	1:B:31:VAL:HB	1.91	0.53
1:D:157:PHE:CE1	1:D:209:MSE:HE2	2.42	0.53
1:A:13:ASN:OD1	1:A:14:LEU:HD22	2.09	0.53
1:A:144:TYR:HB2	1:A:200:PHE:CE1	2.44	0.53
1:C:2:LYS:HG2	1:C:95:ASP:OD1	2.08	0.53
1:B:157:PHE:HB3	1:B:207:LEU:HD11	1.89	0.53
2:B:223:VIB:HC71	1:D:80:THR:HG22	1.91	0.53
1:D:191:ASN:HD22	1:D:192:GLU:N	2.04	0.53
1:D:52:PHE:O	1:D:55:ILE:HG13	2.09	0.53
1:D:86:LEU:CD2	1:D:116:LEU:HG	2.39	0.53
1:A:55:ILE:C	1:A:55:ILE:HD12	2.29	0.52
1:D:135:HIS:NE2	1:D:152:LYS:HE3	2.23	0.52
1:A:52:PHE:CD2	1:A:55:ILE:HG12	2.44	0.52
1:B:174:TYR:H	1:B:191:ASN:HD21	1.56	0.52
1:C:148:LYS:CA	1:C:193:LEU:HD23	2.39	0.52
1:C:208:ILE:HG22	1:C:210:ILE:HD11	1.89	0.52
1:D:143:GLU:HA	1:D:201:SER:HB3	1.91	0.52
1:A:13:ASN:H	1:A:13:ASN:ND2	2.07	0.52
1:A:131:ASP:OD1	1:A:134:ASN:HB2	2.09	0.52
1:A:17:ASP:OD2	1:A:19:THR:HB	2.10	0.52
1:B:214:ASP:O	1:B:215:LEU:CB	2.57	0.52
1:C:6:ILE:HG12	1:C:29:ILE:HG12	1.90	0.52
1:B:157:PHE:HE1	1:B:209:MSE:HE3	1.74	0.52
1:C:172:PHE:HD1	1:C:192:GLU:O	1.93	0.52
1:A:88:TRP:CZ2	1:A:92:LYS:HE2	2.45	0.51
1:D:63:ILE:HG22	1:D:64:GLU:N	2.24	0.51
1:B:58:GLN:OE1	1:B:61:ARG:NH2	2.44	0.51
1:D:153:ARG:HD3	1:D:154:TYR:CE2	2.44	0.51
1:B:189:ILE:HG22	1:B:190:SER:N	2.26	0.51
2:B:223:VIB:HC71	1:D:80:THR:CG2	2.40	0.51
1:C:213:THR:OG1	1:C:214:ASP:N	2.44	0.51
1:D:138:MSE:HE1	1:D:160:PHE:CG	2.46	0.51
1:B:32:ASP:O	1:B:35:THR:HG22	2.11	0.51
1:D:91:GLU:C	1:D:93:GLN:H	2.14	0.51
1:A:108:ASP:OD2	1:A:108:ASP:N	2.42	0.51
1:B:134:ASN:HD21	1:D:106:ARG:HA	1.75	0.51
1:C:82:LEU:HD13	1:C:116:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:CD1	1:C:102:ILE:HD11	2.39	0.51
1:B:106:ARG:NH1	1:B:108:ASP:OD1	2.44	0.51
1:C:60:ARG:HG3	1:C:60:ARG:NH2	2.26	0.51
1:C:119:LYS:O	1:C:122:LYS:HB2	2.11	0.50
1:C:173:LYS:O	1:C:175:PRO:HD3	2.11	0.50
1:B:6:ILE:O	1:B:99:ILE:HA	2.11	0.50
1:D:99:ILE:HG21	1:D:102:ILE:HD12	1.94	0.50
1:C:6:ILE:HG23	1:C:29:ILE:HG13	1.92	0.50
1:A:164:ILE:HB	1:A:181:ILE:HB	1.93	0.50
1:C:37:THR:O	1:C:40:ASP:HB2	2.12	0.50
1:D:206:ILE:HD12	1:D:206:ILE:N	2.27	0.50
1:A:118:TYR:HE1	1:A:206:ILE:CD1	2.24	0.49
1:D:46:VAL:O	1:D:47:GLU:HG2	2.13	0.49
1:D:118:TYR:C	1:D:120:GLY:H	2.16	0.49
1:A:56:THR:HG23	1:A:57:GLU:N	2.27	0.49
1:B:39:LEU:HD22	1:B:63:ILE:HD12	1.93	0.49
1:B:148:LYS:CA	1:B:193:LEU:HD23	2.43	0.49
1:A:197:ARG:NH2	1:A:197:ARG:HB2	2.28	0.49
1:A:90:LEU:HD22	1:A:125:ILE:HD12	1.94	0.49
1:A:102:ILE:HD13	1:A:129:LEU:HD22	1.94	0.49
1:A:157:PHE:CZ	1:A:209:MSE:HE3	2.47	0.49
1:C:206:ILE:HD12	1:C:206:ILE:N	2.14	0.49
1:D:165:HIS:HB2	1:D:204:LYS:HB3	1.95	0.49
1:C:102:ILE:HG23	1:C:102:ILE:O	2.13	0.49
1:D:4:ILE:HD12	1:D:94:PRO:HG2	1.95	0.49
1:D:11:PRO:O	1:D:15:ILE:HG13	2.13	0.49
1:B:148:LYS:HA	1:B:193:LEU:HD23	1.95	0.48
1:C:102:ILE:HG13	1:C:113:ASN:CG	2.34	0.48
1:D:57:GLU:HB3	1:D:61:ARG:NH1	2.29	0.48
1:D:141:PRO:HB3	1:D:203:VAL:HA	1.95	0.48
1:D:133:GLN:O	1:D:212:SER:HA	2.14	0.48
1:A:161:SER:HB3	1:A:206:ILE:HD12	1.95	0.48
1:B:80:THR:HG22	1:B:82:LEU:H	1.78	0.48
1:A:84:LEU:HD12	1:A:84:LEU:O	2.14	0.48
1:B:52:PHE:CD2	1:B:60:ARG:NH1	2.82	0.48
1:B:99:ILE:HG22	1:B:102:ILE:HD13	1.95	0.48
1:D:172:PHE:HA	1:D:192:GLU:O	2.13	0.48
1:A:52:PHE:CD2	1:A:60:ARG:HG3	2.48	0.48
1:C:6:ILE:HG12	1:C:29:ILE:CG1	2.44	0.48
1:B:99:ILE:CG2	1:B:102:ILE:HD13	2.43	0.48
1:D:8:ALA:HA	1:D:31:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ASN:OD1	1:C:98:GLN:HB2	2.13	0.47
1:C:8:ALA:HA	1:C:31:VAL:HB	1.96	0.47
1:C:23:ASP:CG	1:C:24:GLU:N	2.67	0.47
1:C:191:ASN:HD22	1:C:192:GLU:N	2.10	0.47
1:A:161:SER:CB	1:A:206:ILE:HD12	2.44	0.47
1:D:174:TYR:CE2	2:D:223:VIB:H7A2	2.49	0.47
1:A:150:GLU:HG3	1:A:151:ASN:OD1	2.15	0.47
1:A:76:GLU:C	1:A:78:ASP:H	2.17	0.47
1:B:118:TYR:CD1	1:B:138:MSE:HE1	2.50	0.47
1:D:131:ASP:OD2	1:D:134:ASN:HB2	2.15	0.47
1:A:48:ALA:O	1:A:72:VAL:HA	2.15	0.47
1:B:153:ARG:HD2	1:B:154:TYR:CZ	2.50	0.47
1:A:118:TYR:HE1	1:A:206:ILE:HD13	1.80	0.47
1:C:135:HIS:C	1:C:136:ILE:HD12	2.36	0.47
1:C:157:PHE:HB3	1:C:207:LEU:HD11	1.97	0.47
1:D:86:LEU:HG	1:D:90:LEU:HD11	1.96	0.47
1:B:13:ASN:N	1:B:13:ASN:ND2	2.56	0.46
1:C:157:PHE:CD1	1:C:207:LEU:HD21	2.50	0.46
1:C:173:LYS:C	1:C:175:PRO:HD3	2.35	0.46
1:A:125:ILE:O	1:A:127:ILE:HG13	2.15	0.46
1:B:77:LYS:H	1:B:77:LYS:CD	1.99	0.46
1:B:149:ASP:HB2	1:B:211:ARG:NH2	2.30	0.46
1:C:146:ILE:HD13	1:C:209:MSE:CE	2.40	0.46
1:D:157:PHE:HE1	1:D:209:MSE:CE	2.28	0.46
1:B:146:ILE:HD12	1:B:146:ILE:O	2.14	0.46
1:C:100:PHE:N	1:C:100:PHE:CD2	2.84	0.46
1:D:95:ASP:HB3	1:D:96:ILE:HD12	1.98	0.46
1:A:120:GLY:HA3	1:A:127:ILE:CD1	2.40	0.46
1:B:55:ILE:CG2	1:B:59:GLU:HB3	2.45	0.46
1:D:31:VAL:CG1	1:D:81:ASP:HB2	2.46	0.46
1:D:119:LYS:HG2	1:D:119:LYS:O	2.15	0.46
1:B:210:ILE:HD12	1:B:210:ILE:N	2.31	0.46
1:B:164:ILE:HA	1:B:204:LYS:O	2.16	0.46
1:C:174:TYR:HD2	1:C:191:ASN:ND2	2.14	0.46
1:D:86:LEU:HG	1:D:90:LEU:CD1	2.46	0.46
1:D:106:ARG:HB3	1:D:108:ASP:OD2	2.15	0.46
1:A:80:THR:HG22	1:A:81:ASP:N	2.30	0.46
1:D:96:ILE:HD12	1:D:96:ILE:N	2.31	0.46
1:B:6:ILE:HG12	1:B:29:ILE:HD11	1.96	0.45
1:C:28:TRP:CD1	1:C:43:ILE:HG21	2.51	0.45
1:D:168:THR:O	1:D:200:PHE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:HD23	1:B:62:ARG:HH21	1.81	0.45
1:C:157:PHE:CE1	1:C:209:MSE:HE3	2.51	0.45
1:D:158:ILE:HG12	1:D:189:ILE:HD11	1.97	0.45
1:B:202:PHE:CD1	1:B:202:PHE:N	2.84	0.45
1:A:60:ARG:HG2	1:A:60:ARG:HH21	1.81	0.45
1:A:144:TYR:HB2	1:A:200:PHE:CZ	2.52	0.45
1:B:118:TYR:O	1:B:122:LYS:HG3	2.17	0.45
1:C:164:ILE:HB	1:C:181:ILE:HB	1.98	0.45
1:A:32:ASP:CG	1:A:33:LYS:N	2.65	0.45
1:C:162:GLU:OE2	1:C:204:LYS:HG2	2.16	0.45
1:D:153:ARG:HH21	1:D:153:ARG:HB2	1.82	0.45
1:B:82:LEU:O	1:B:85:ALA:N	2.50	0.45
1:C:96:ILE:HG22	1:C:126:LYS:HB2	1.99	0.45
1:D:32:ASP:C	1:D:34:GLY:H	2.19	0.44
1:B:33:LYS:O	1:B:36:VAL:HB	2.17	0.44
1:D:55:ILE:HD12	1:D:55:ILE:C	2.38	0.44
1:A:112:GLY:O	1:A:115:GLN:N	2.50	0.44
1:B:32:ASP:O	1:B:34:GLY:N	2.50	0.44
1:C:167:LEU:HD12	1:C:201:SER:O	2.17	0.44
1:B:6:ILE:HG21	1:B:82:LEU:CD2	2.48	0.44
1:B:39:LEU:HB3	1:B:62:ARG:HH22	1.81	0.44
1:B:106:ARG:NE	1:D:214:ASP:OD2	2.44	0.44
1:A:52:PHE:O	1:A:55:ILE:HG13	2.18	0.44
1:B:52:PHE:CD2	1:B:60:ARG:CZ	3.01	0.44
1:B:127:ILE:O	1:B:137:GLN:HG2	2.17	0.44
1:B:189:ILE:CG2	1:B:190:SER:N	2.81	0.44
1:D:98:GLN:OE1	1:D:128:ARG:NH1	2.51	0.44
1:D:200:PHE:CZ	1:D:209:MSE:HE3	2.53	0.44
1:A:119:LYS:O	1:A:123:THR:HG23	2.17	0.44
1:B:28:TRP:O	1:B:45:PRO:HA	2.18	0.44
1:C:155:ILE:HG21	1:C:209:MSE:HE2	1.99	0.44
1:D:36:VAL:O	1:D:40:ASP:OD2	2.36	0.44
1:D:38:LEU:O	1:D:41:ALA:HB3	2.17	0.44
1:D:32:ASP:C	1:D:34:GLY:N	2.71	0.44
1:A:173:LYS:O	1:A:175:PRO:HD3	2.18	0.43
1:B:12:LYS:HA	1:B:15:ILE:HD12	1.99	0.43
1:B:100:PHE:N	1:B:100:PHE:CD2	2.85	0.43
1:D:30:GLY:CA	1:D:35:THR:HG22	2.41	0.43
1:A:161:SER:OG	1:A:206:ILE:HD12	2.18	0.43
1:C:86:LEU:HD22	1:C:90:LEU:CD1	2.48	0.43
1:A:39:LEU:CD2	1:A:63:ILE:HG12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASP:OD2	1:D:40:ASP:N	2.51	0.43
1:A:46:VAL:HG23	1:A:47:GLU:N	2.34	0.43
1:A:202:PHE:CD1	1:A:202:PHE:N	2.86	0.43
1:C:118:TYR:O	1:C:122:LYS:HG2	2.19	0.43
1:C:154:TYR:C	1:C:155:ILE:HG13	2.39	0.43
1:D:3:THR:O	1:D:26:THR:HA	2.19	0.43
1:A:102:ILE:HG23	1:A:102:ILE:O	2.19	0.43
1:A:143:GLU:HG3	1:A:201:SER:HB3	2.00	0.43
1:B:161:SER:OG	1:B:161:SER:O	2.29	0.42
1:B:173:LYS:O	1:B:175:PRO:HD3	2.19	0.42
1:C:6:ILE:HG12	1:C:29:ILE:HD11	2.01	0.42
1:C:86:LEU:O	1:C:90:LEU:HG	2.18	0.42
1:A:141:PRO:HD3	1:A:205:GLY:O	2.18	0.42
1:C:102:ILE:HA	1:C:102:ILE:HD12	1.77	0.42
1:A:47:GLU:HG3	1:A:88:TRP:CZ2	2.54	0.42
1:B:143:GLU:HG3	1:B:201:SER:HB3	2.01	0.42
1:C:209:MSE:C	1:C:210:ILE:HD12	2.40	0.42
1:D:157:PHE:HB3	1:D:207:LEU:HD11	2.00	0.42
1:C:17:ASP:OD1	1:C:19:THR:HB	2.19	0.42
1:C:176:LEU:HD13	2:C:223:VIB:HM23	2.01	0.42
1:D:214:ASP:O	1:D:215:LEU:HB3	2.20	0.42
1:A:13:ASN:H	1:A:13:ASN:HD22	1.67	0.42
2:B:223:VIB:C7	1:D:80:THR:HG23	2.50	0.42
1:A:15:ILE:HA	1:A:16:PRO:HD3	1.82	0.42
1:A:71:HIS:ND1	1:A:73:TYR:CE1	2.88	0.42
1:A:167:LEU:HA	1:A:201:SER:O	2.20	0.42
1:B:59:GLU:O	1:B:63:ILE:HD13	2.20	0.42
1:C:29:ILE:HD12	1:C:85:ALA:HB1	2.01	0.42
1:C:52:PHE:C	1:C:54:SER:H	2.23	0.42
1:C:52:PHE:O	1:C:54:SER:N	2.53	0.41
1:A:157:PHE:CD1	1:A:207:LEU:HD21	2.55	0.41
1:D:4:ILE:HD12	1:D:94:PRO:HG3	2.02	0.41
1:D:32:ASP:O	1:D:34:GLY:N	2.53	0.41
1:D:67:ALA:HB1	1:D:70:LEU:HB2	2.02	0.41
1:B:168:THR:HG23	1:B:177:ASN:HA	2.02	0.41
1:C:130:ILE:HG12	1:C:135:HIS:CD2	2.56	0.41
1:D:82:LEU:HD11	1:D:99:ILE:HD13	2.01	0.41
1:B:168:THR:OG1	1:B:178:ASN:ND2	2.53	0.41
1:C:134:ASN:HB3	1:C:136:ILE:CD1	2.49	0.41
1:B:82:LEU:HD13	1:B:116:LEU:HD23	2.02	0.41
1:D:46:VAL:C	1:D:47:GLU:HG2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:O	1:A:135:HIS:HD2	2.03	0.41
1:B:29:ILE:HG22	1:B:46:VAL:HG13	2.02	0.41
1:C:208:ILE:HG22	1:C:210:ILE:HD12	2.01	0.41
1:A:95:ASP:C	1:A:96:ILE:HG13	2.41	0.41
1:A:130:ILE:HG23	1:A:135:HIS:CD2	2.56	0.41
1:A:210:ILE:HB	1:C:108:ASP:HB3	2.03	0.41
1:C:50:GLY:HA2	1:C:81:ASP:OD1	2.21	0.41
1:C:136:ILE:N	1:C:136:ILE:CD1	2.83	0.41
1:A:33:LYS:HE3	1:A:33:LYS:HB3	1.92	0.40
1:B:39:LEU:HD22	1:B:63:ILE:CD1	2.51	0.40
1:B:111:LEU:O	1:B:115:GLN:OE1	2.39	0.40
1:D:118:TYR:C	1:D:120:GLY:N	2.74	0.40
1:D:147:GLU:HG3	1:D:196:SER:O	2.21	0.40
1:A:18:LEU:O	1:A:21:TYR:HB2	2.21	0.40
1:A:132:LYS:HE3	1:A:215:LEU:HD11	2.02	0.40
1:C:55:ILE:HG23	1:C:59:GLU:HB3	2.02	0.40
1:D:169:LEU:HB3	1:D:172:PHE:CD2	2.56	0.40
1:A:56:THR:CG2	1:A:57:GLU:N	2.81	0.40
1:A:187:LEU:HD13	1:C:78:ASP:HB3	2.02	0.40
1:A:55:ILE:CD1	1:A:60:ARG:HB2	2.52	0.40
1:A:76:GLU:O	1:A:78:ASP:N	2.55	0.40
1:C:202:PHE:HE2	1:C:205:GLY:O	2.04	0.40
1:A:183:LEU:HD23	1:C:118:TYR:CZ	2.57	0.40
1:C:35:THR:O	1:C:38:LEU:HB2	2.21	0.40
1:C:52:PHE:C	1:C:54:SER:N	2.75	0.40
1:C:172:PHE:CE1	1:C:193:LEU:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/222 (96%)	199 (94%)	12 (6%)	1 (0%)	29	52
1	B	212/222 (96%)	193 (91%)	15 (7%)	4 (2%)	8	15
1	C	209/222 (94%)	190 (91%)	18 (9%)	1 (0%)	29	52
1	D	208/222 (94%)	193 (93%)	12 (6%)	3 (1%)	11	22
All	All	841/888 (95%)	775 (92%)	57 (7%)	9 (1%)	14	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	GLY
1	B	132	LYS
1	A	77	LYS
1	B	160	PHE
1	D	92	LYS
1	B	33	LYS
1	D	39	LEU
1	D	150	GLU
1	C	53	ASP

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	187/192 (97%)	177 (95%)	10 (5%)	22	45
1	B	187/192 (97%)	170 (91%)	17 (9%)	9	18
1	C	186/192 (97%)	176 (95%)	10 (5%)	22	44
1	D	185/192 (96%)	175 (95%)	10 (5%)	22	44
All	All	745/768 (97%)	698 (94%)	47 (6%)	18	36

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	35	THR

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Mol	Chain	Res	Type
1	A	56	THR
1	A	57	GLU
1	A	74	GLN
1	A	102	ILE
1	A	111	LEU
1	A	191	ASN
1	A	193	LEU
1	A	195	HIS
1	B	12	LYS
1	B	13	ASN
1	B	19	THR
1	B	35	THR
1	B	77	LYS
1	B	82	LEU
1	B	106	ARG
1	B	111	LEU
1	B	116	LEU
1	B	129	LEU
1	B	131	ASP
1	B	138	MSE
1	B	162	GLU
1	B	164	ILE
1	B	179	CYS
1	B	191	ASN
1	B	199	THR
1	C	17	ASP
1	C	35	THR
1	C	60	ARG
1	C	82	LEU
1	C	86	LEU
1	C	111	LEU
1	C	116	LEU
1	C	131	ASP
1	C	191	ASN
1	C	206	ILE
1	D	32	ASP
1	D	61	ARG
1	D	82	LEU
1	D	115	GLN
1	D	122	LYS
1	D	137	GLN
1	D	153	ARG

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Mol	Chain	Res	Type
1	D	191	ASN
1	D	203	VAL
1	D	213	THR

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	109	HIS
1	A	113	ASN
1	A	124	ASN
1	A	133	GLN
1	A	134	ASN
1	A	135	HIS
1	A	178	ASN
1	A	180	HIS
1	A	191	ASN
1	B	13	ASN
1	B	79	GLN
1	B	98	GLN
1	B	113	ASN
1	B	115	GLN
1	B	134	ASN
1	B	151	ASN
1	B	178	ASN
1	B	180	HIS
1	B	191	ASN
1	C	98	GLN
1	C	115	GLN
1	C	124	ASN
1	C	134	ASN
1	C	151	ASN
1	C	178	ASN
1	C	191	ASN
1	D	58	GLN
1	D	74	GLN
1	D	115	GLN
1	D	124	ASN
1	D	134	ASN
1	D	137	GLN
1	D	178	ASN
1	D	191	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	PO4	C	224	-	4,4,4	1.59	0	6,6,6	0.42	0
2	VIB	B	223	-	16,19,19	2.33	3 (18%)	20,26,26	2.03	8 (40%)
3	PO4	B	224	-	4,4,4	1.61	0	6,6,6	0.44	0
2	VIB	A	223	-	16,19,19	2.34	3 (18%)	20,26,26	2.02	7 (35%)
2	VIB	C	223	-	16,19,19	2.35	3 (18%)	20,26,26	2.10	9 (45%)
3	PO4	B	225	-	4,4,4	1.60	0	6,6,6	0.43	0
3	PO4	A	224	-	4,4,4	1.57	0	6,6,6	0.44	0
2	VIB	D	223	-	16,19,19	2.44	2 (12%)	20,26,26	1.94	6 (30%)

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	VIB	D	223	-	-	4/6/7/7	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VIB	A	223	-	-	2/6/7/7	0/2/2/2
2	VIB	B	223	-	-	1/6/7/7	0/2/2/2
2	VIB	C	223	-	-	0/6/7/7	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	VIB	C4-N3	-6.69	1.33	1.39
2	A	223	VIB	C4-N3	-6.57	1.34	1.39
2	C	223	VIB	C4-N3	-6.56	1.34	1.39
2	D	223	VIB	C4-N3	-6.42	1.34	1.39
2	D	223	VIB	C6-C5	6.33	1.53	1.50
2	C	223	VIB	C6-C5	5.67	1.53	1.50
2	A	223	VIB	C6-C5	5.56	1.53	1.50
2	B	223	VIB	C6-C5	5.29	1.53	1.50
2	B	223	VIB	C5A-C4A	-2.10	1.39	1.42
2	A	223	VIB	C5A-C4A	-2.07	1.39	1.42
2	C	223	VIB	C5A-C4A	-2.03	1.39	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	VIB	C5-C4-N3	4.17	115.91	107.57
2	A	223	VIB	C5-C4-N3	3.96	115.50	107.57
2	C	223	VIB	C5-C4-N3	3.91	115.39	107.57
2	B	223	VIB	C5-C4-N3	3.84	115.25	107.57
2	C	223	VIB	C6-C5-C4	3.30	130.08	127.43
2	D	223	VIB	C6A-N1A-C2A	3.18	121.37	115.96
2	D	223	VIB	N1A-C2A-N3A	-3.15	120.13	125.54
2	B	223	VIB	C6A-N1A-C2A	3.10	121.24	115.96
2	A	223	VIB	N1A-C2A-N3A	-3.03	120.32	125.54
2	B	223	VIB	N1A-C2A-N3A	-3.01	120.36	125.54
2	A	223	VIB	C6A-N1A-C2A	3.00	121.06	115.96
2	C	223	VIB	C6A-N1A-C2A	2.96	121.00	115.96
2	C	223	VIB	N1A-C2A-N3A	-2.95	120.46	125.54
2	B	223	VIB	C6-C5-C4	2.74	129.63	127.43
2	A	223	VIB	CM2-C2A-N1A	2.70	120.10	117.14
2	D	223	VIB	CM4-C4-C5	-2.68	121.75	127.60
2	A	223	VIB	CM4-C4-C5	-2.61	121.90	127.60
2	B	223	VIB	CM2-C2A-N1A	2.61	120.00	117.14
2	A	223	VIB	C6-C5-C4	2.57	129.50	127.43
2	D	223	VIB	CM2-C2A-N1A	2.52	119.91	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	223	VIB	N4A-C4A-N3A	2.52	120.59	117.03
2	C	223	VIB	CM4-C4-C5	-2.49	122.17	127.60
2	B	223	VIB	CM4-C4-C5	-2.48	122.17	127.60
2	A	223	VIB	N4A-C4A-N3A	2.39	120.41	117.03
2	C	223	VIB	CM2-C2A-N1A	2.36	119.73	117.14
2	B	223	VIB	N4A-C4A-N3A	2.23	120.18	117.03
2	B	223	VIB	C5A-C6A-N1A	-2.10	120.32	123.82
2	C	223	VIB	C7A-N3-C2	-2.06	121.62	125.35
2	D	223	VIB	C6-C5-C4	2.06	129.09	127.43
2	C	223	VIB	C5A-C6A-N1A	-2.00	120.49	123.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	223	VIB	C4-C5-C6-C7
2	D	223	VIB	C4A-C5A-C7A-N3
2	D	223	VIB	C6A-C5A-C7A-N3
2	A	223	VIB	C5A-C7A-N3-C2
2	A	223	VIB	C5A-C7A-N3-C4
2	B	223	VIB	C5A-C7A-N3-C4
2	D	223	VIB	C5A-C7A-N3-C4

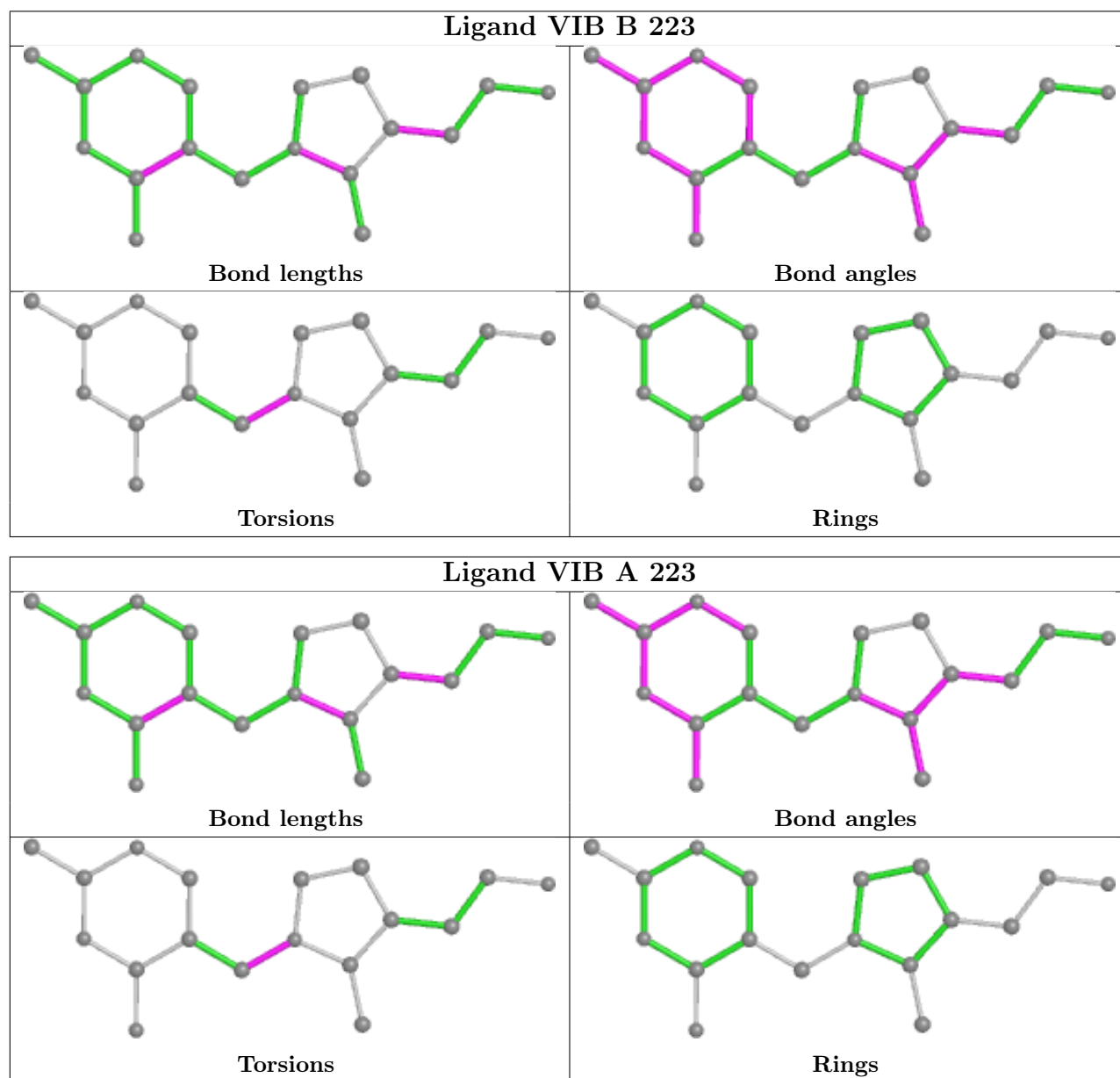
There are no ring outliers.

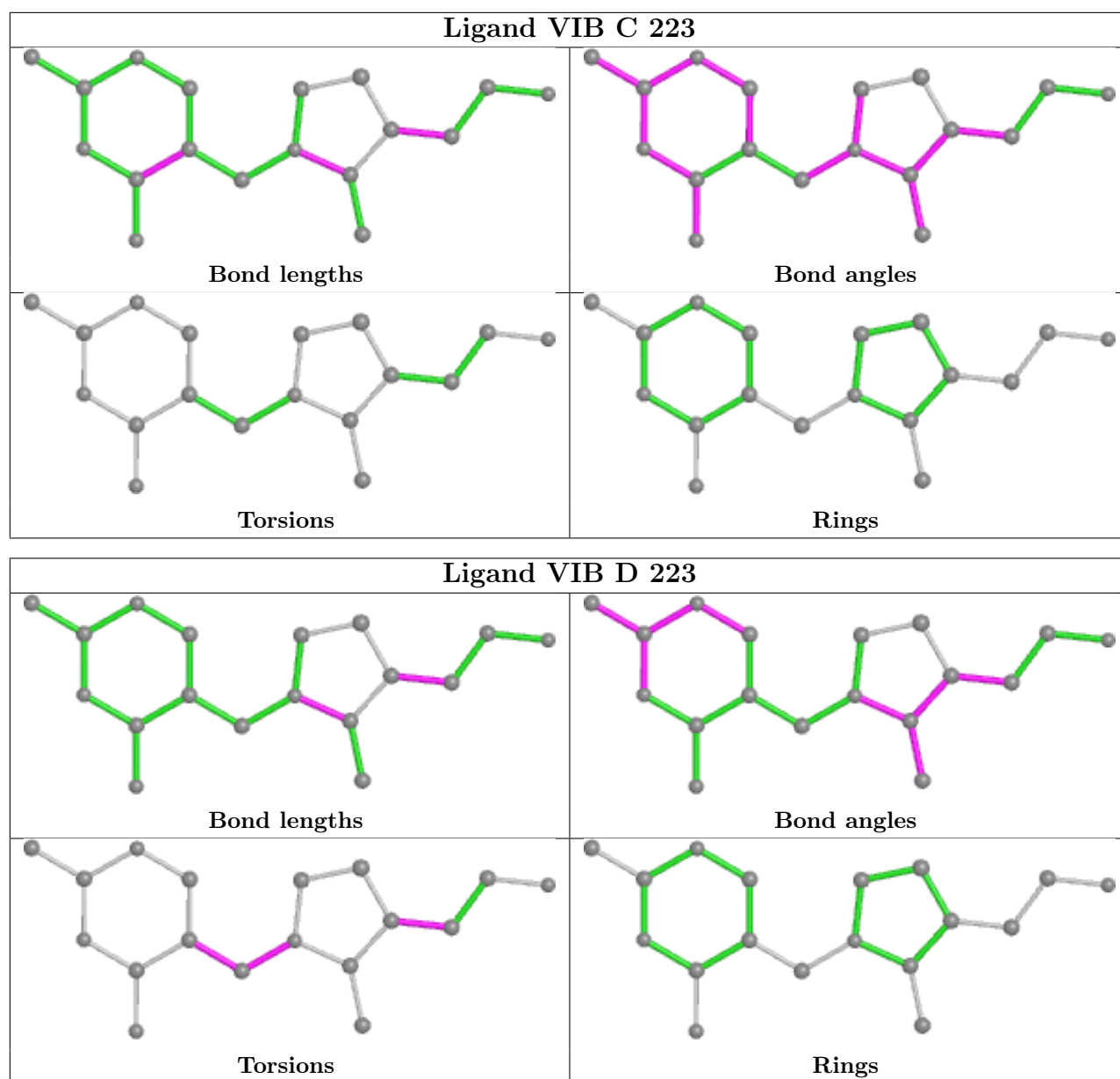
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	223	VIB	3	0
2	A	223	VIB	2	0
2	C	223	VIB	2	0
2	D	223	VIB	1	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	212/222 (95%)	0.04	1 (0%) 91 89	16, 34, 64, 95	0
1	B	212/222 (95%)	-0.00	2 (0%) 84 82	16, 36, 63, 74	0
1	C	211/222 (95%)	0.16	5 (2%) 59 53	16, 35, 66, 98	0
1	D	210/222 (94%)	0.12	2 (0%) 82 80	16, 36, 72, 100	0
All	All	845/888 (95%)	0.08	10 (1%) 79 76	16, 35, 65, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	PHE	3.0
1	C	214	ASP	3.0
1	B	63	ILE	2.8
1	A	77	LYS	2.8
1	C	84	LEU	2.5
1	C	55	ILE	2.3
1	D	75	ALA	2.3
1	C	25	HIS	2.2
1	C	215	LEU	2.1
1	B	57	GLU	2.1

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 monosaccharides in this entry.

6.4 Ligands

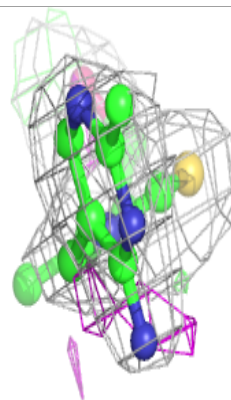
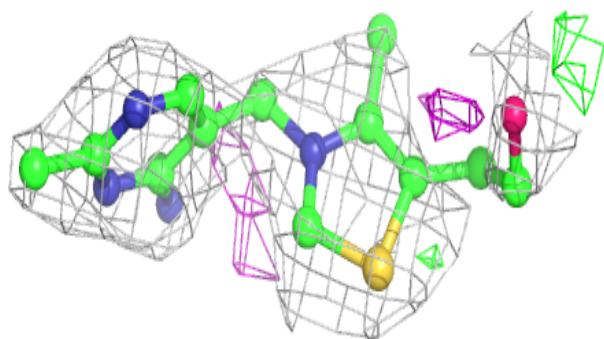
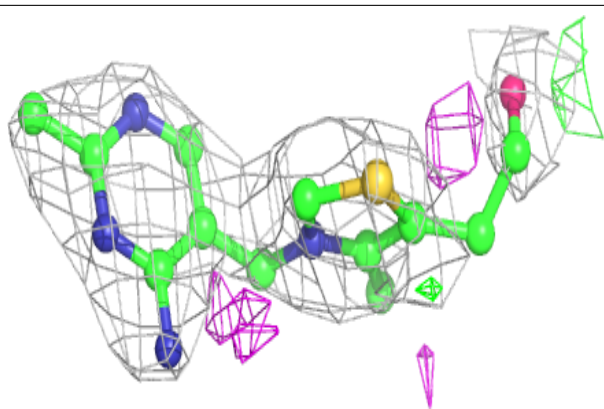
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	226	1/1	0.79	0.26	46,46,46,46	0
4	MG	B	228	1/1	0.79	0.25	40,40,40,40	0
4	MG	A	226	1/1	0.81	0.27	43,43,43,43	0
3	PO4	A	224	5/5	0.88	0.19	63,68,86,89	0
3	PO4	B	225	5/5	0.89	0.26	81,82,85,87	0
2	VIB	D	223	18/18	0.90	0.28	12,36,52,58	0
2	VIB	B	223	18/18	0.91	0.22	18,37,78,81	0
4	MG	B	227	1/1	0.92	0.16	40,40,40,40	0
2	VIB	A	223	18/18	0.93	0.20	14,32,72,72	0
4	MG	A	225	1/1	0.93	0.32	52,52,52,52	0
3	PO4	B	224	5/5	0.93	0.22	70,72,75,79	0
2	VIB	C	223	18/18	0.94	0.18	5,28,53,57	0
3	PO4	C	224	5/5	0.95	0.13	63,68,73,80	0

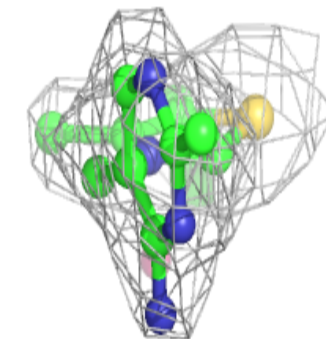
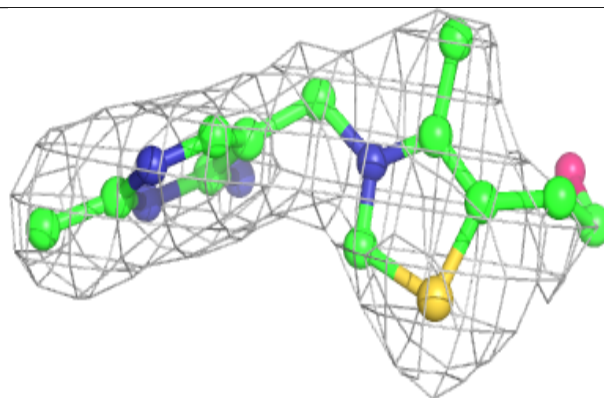
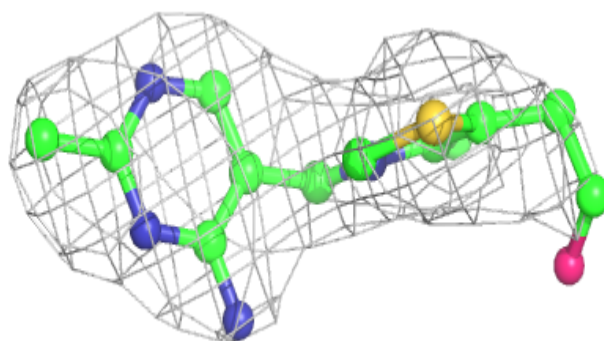
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VIB D 223:

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

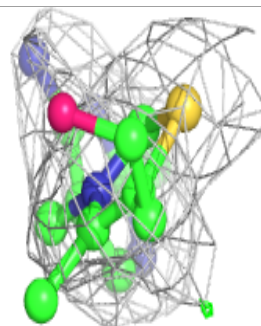
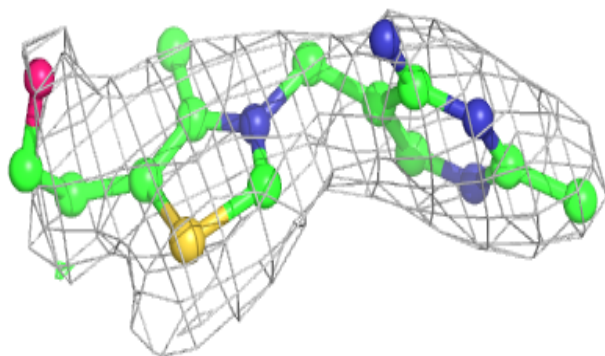
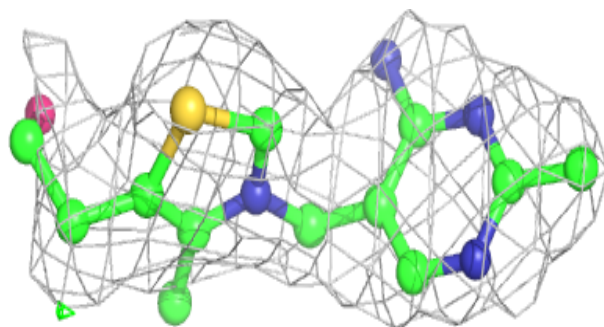
**Electron density around VIB B 223:**

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

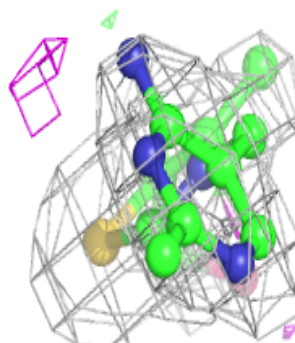
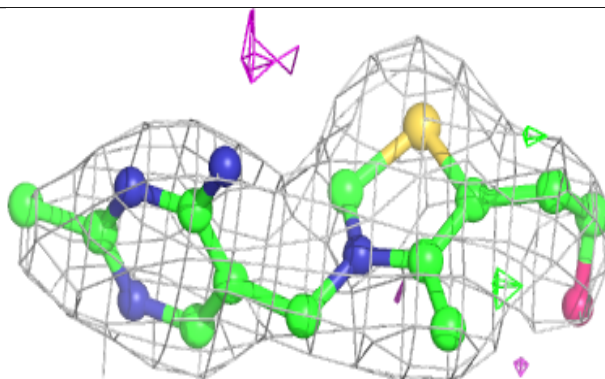
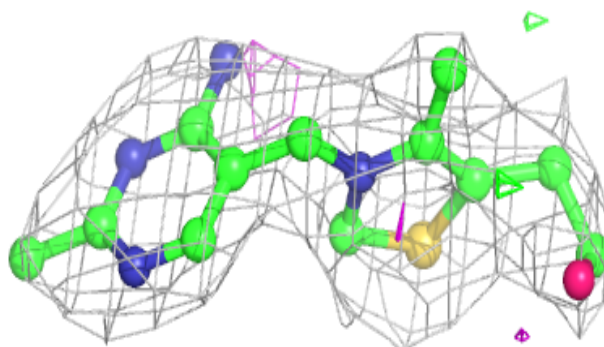


Electron density around VIB A 223:

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

**Electron density around VIB C 223:**

$2mF_o-DF_c$ (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.