



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2ISL  
Title : BluB bound to reduced flavin (FMNH<sub>2</sub>) and molecular oxygen. (clear crystal form)  
Authors : Larsen, N.A.; Taga, M.E.; Howard-Jones, A.R.; Walsh, C.T.; Walker, G.C.  
Deposited on : 2006-10-17  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

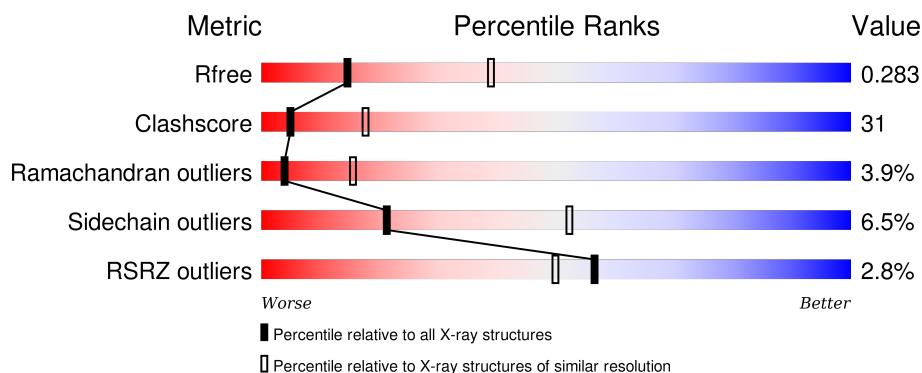
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



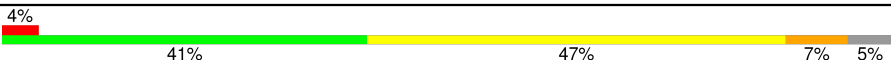


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXY	A	606	-	-	X	-
3	OXY	C	605	-	-	-	X
3	OXY	G	603	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14255 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 BluB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	B	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	C	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	D	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	E	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	F	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	G	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	H	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			

There are 24 discrepancies between the modelled and reference sequences:

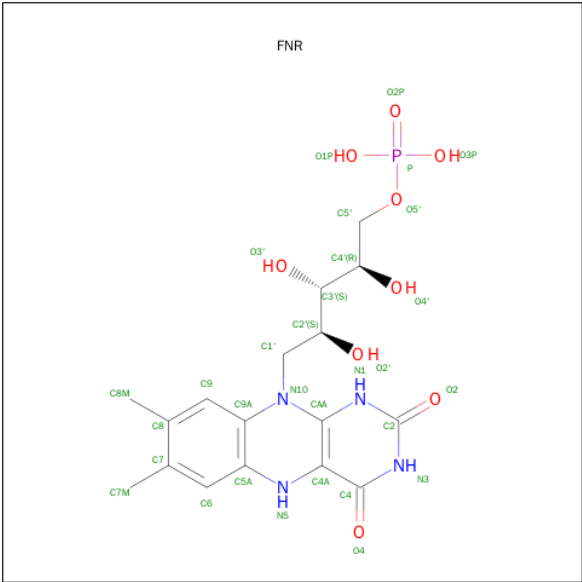
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
A	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
A	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
B	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
B	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
B	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
C	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
C	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
C	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
D	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
D	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
D	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
E	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
E	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
F	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
F	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
F	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
G	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
G	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
G	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
H	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
H	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
H	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8

- Molecule 2 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]P  
TERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR)  
(formula: C<sub>17</sub>H<sub>23</sub>N<sub>4</sub>O<sub>9</sub>P).



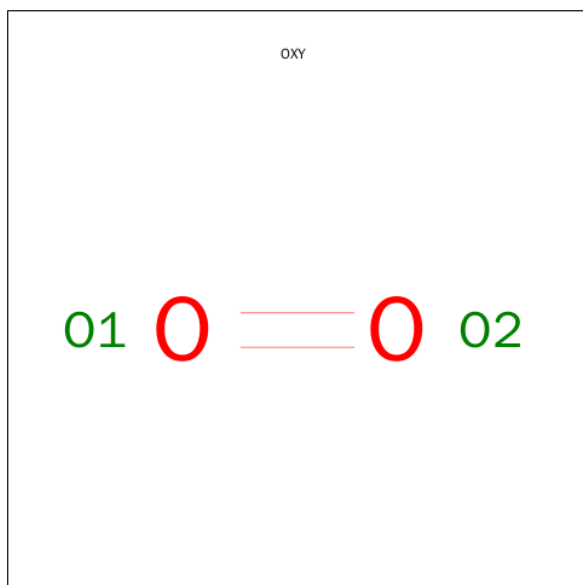
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			2	2		
3	G	1	Total	O	0	0
			2	2		
3	H	1	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			2	2		
3	A	1	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			2	2		

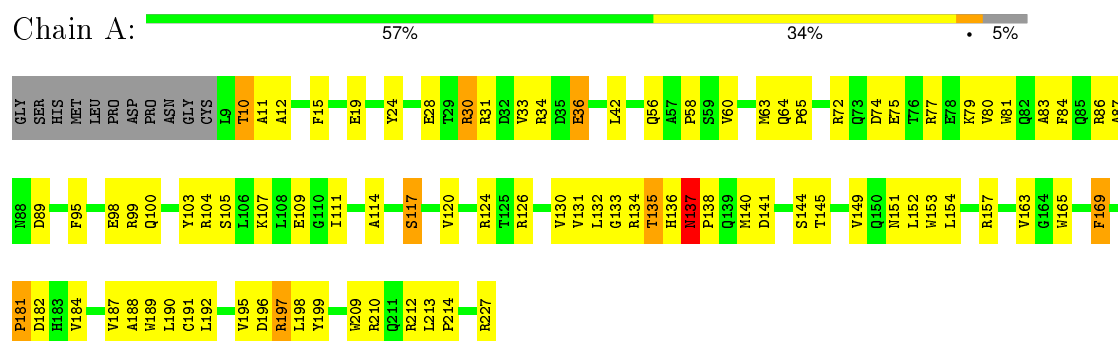
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	13	Total 13	O 13	0	0
4	C	12	Total 12	O 12	0	0
4	D	10	Total 10	O 10	0	0
4	E	4	Total 4	O 4	0	0
4	F	2	Total 2	O 2	0	0
4	G	7	Total 7	O 7	0	0
4	H	3	Total 3	O 3	0	0

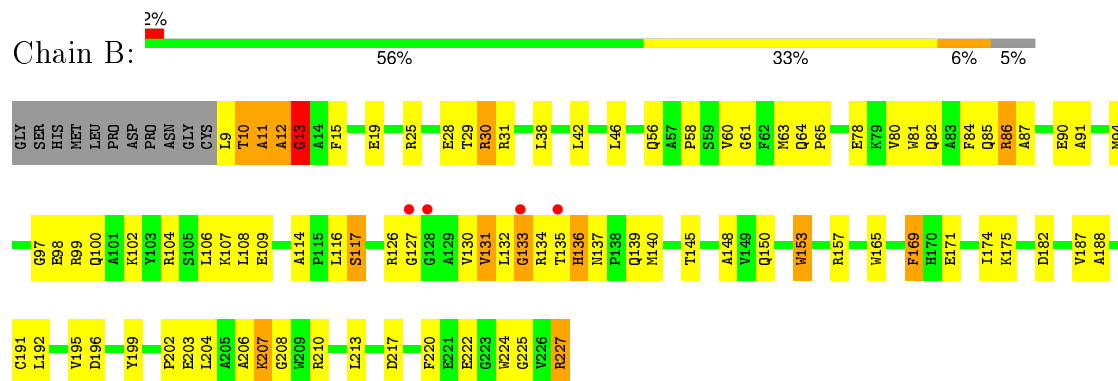
### 3 Residue-property plots [i](#)

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

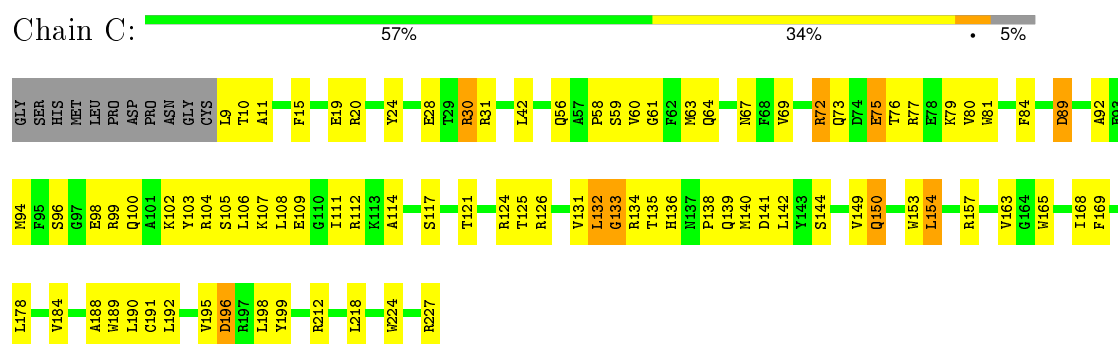
#### • Molecule 1: BluB



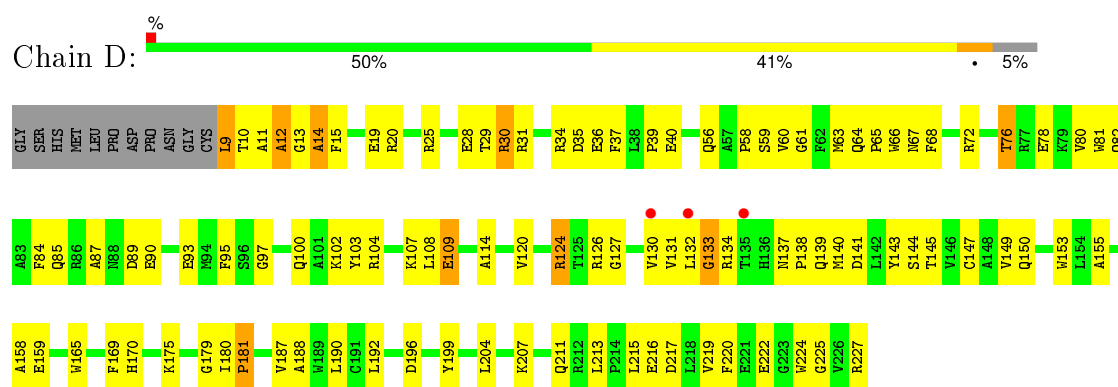
#### • Molecule 1: BluB



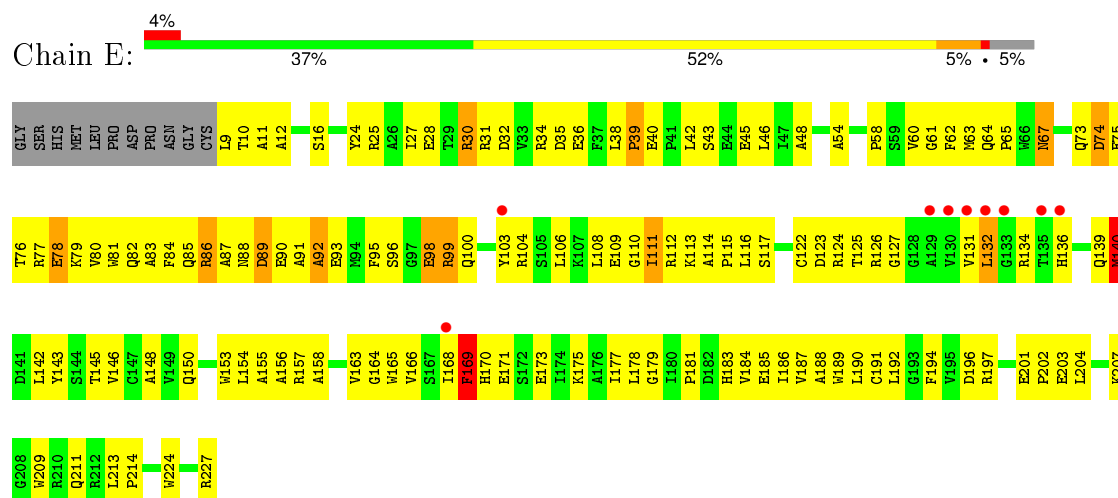
#### • Molecule 1: BluB



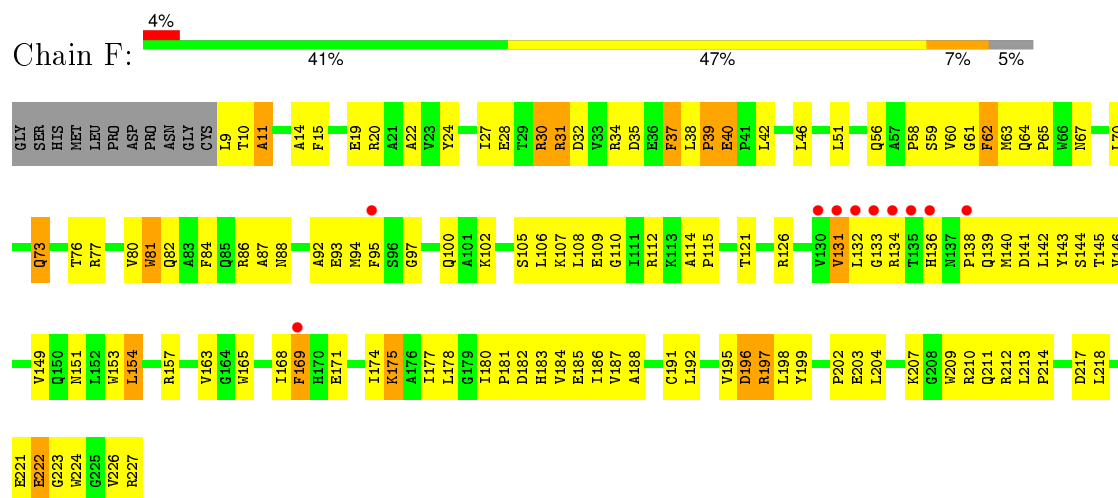
#### • Molecule 1: BluB



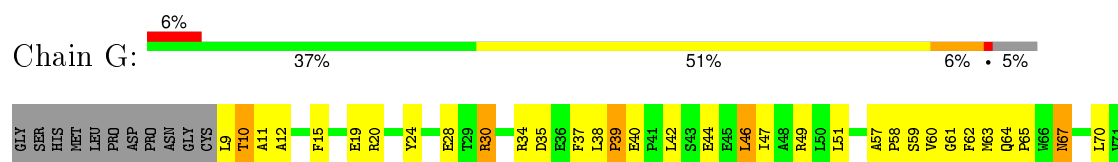
• Molecule 1: BluB

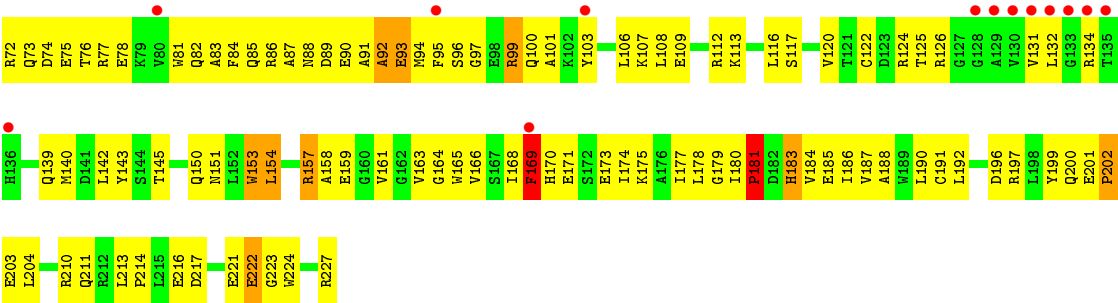


• Molecule 1: BluB

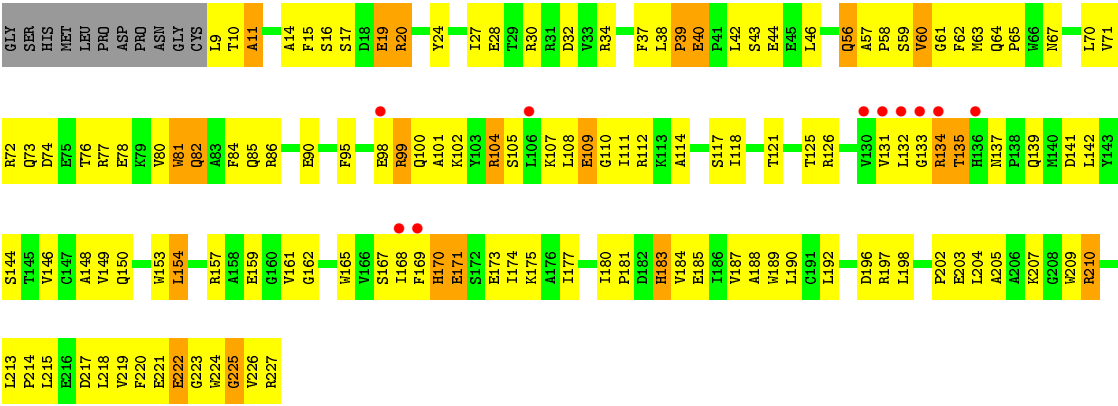


• Molecule 1: BluB





• Molecule 1: BluB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.07Å 173.84Å 91.98Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.90) 96.1 (49.03-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.285 0.212 , 0.283	Depositor DCC
$R_{free}$ test set	2162 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 0.8	EDS
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43289 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.42	0/1780	0.67	0/2412
1	B	0.44	0/1780	0.73	1/2412 (0.0%)
1	C	0.43	0/1780	0.68	0/2412
1	D	0.45	0/1780	0.72	1/2412 (0.0%)
1	E	0.36	0/1780	0.61	0/2412
1	F	0.36	0/1780	0.61	0/2412
1	G	0.35	0/1780	0.61	0/2412
1	H	0.34	0/1780	0.63	0/2412
All	All	0.39	0/14240	0.66	2/19296 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	GLY	N-CA-C	6.39	129.07	113.10
1	D	170	HIS	N-CA-C	-5.32	96.64	111.00

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	1741	0	1716	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1741	0	1716	119	0
1	C	1741	0	1716	93	0
1	D	1741	0	1716	107	0
1	E	1741	0	1716	157	0
1	F	1741	0	1716	149	0
1	G	1741	0	1716	161	0
1	H	1741	0	1716	156	0
2	A	31	0	21	4	0
2	B	31	0	21	3	0
2	C	31	0	21	3	0
2	D	31	0	21	3	0
2	E	31	0	21	6	0
2	F	31	0	21	5	0
2	G	31	0	21	5	0
2	H	31	0	21	5	0
3	A	2	0	0	2	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	1	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	2	0
3	H	2	0	0	0	0
4	A	12	0	0	1	0
4	B	13	0	0	1	0
4	C	12	0	0	3	0
4	D	10	0	0	3	0
4	E	4	0	0	4	0
4	F	2	0	0	0	0
4	G	7	0	0	4	0
4	H	3	0	0	1	0
All	All	14255	0	13896	877	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 31.

All (877) 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:131:VAL:HG11	1:B:134:ARG:HE	1.05	1.09
1:E:86:ARG:HD2	1:E:87:ALA:N	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:HE22	1:B:213:LEU:H	1.09	0.98
1:G:63:MET:HG3	1:G:65:PRO:HD3	1.47	0.95
1:H:38:LEU:HB3	1:H:39:PRO:HD2	1.49	0.94
1:H:204:LEU:H	1:H:204:LEU:HD12	1.34	0.91
1:C:196:ASP:O	1:D:12:ALA:HA	1.70	0.90
1:H:81:TRP:HD1	1:H:111:ILE:HB	1.35	0.90
1:B:131:VAL:HG11	1:B:134:ARG:NE	1.85	0.90
1:E:86:ARG:HD2	1:E:87:ALA:H	1.30	0.90
1:E:86:ARG:HH21	1:E:169:PHE:HB2	1.37	0.88
1:H:17:SER:HA	1:H:20:ARG:HD3	1.53	0.88
1:G:64:GLN:HE22	1:H:213:LEU:H	1.21	0.86
1:G:96:SER:N	1:G:100:GLN:HB2	1.90	0.86
1:G:12:ALA:HB3	1:H:197:ARG:HA	1.56	0.85
1:G:174:ILE:HA	1:G:177:ILE:HD12	1.58	0.85
1:G:78:GLU:HG3	1:G:82:GLN:HE21	1.42	0.85
1:C:212:ARG:HD3	1:D:64:GLN:HE22	1.42	0.82
1:B:217:ASP:HB2	1:B:227:ARG:HH21	1.45	0.82
1:F:38:LEU:HB3	1:F:39:PRO:HD2	1.61	0.82
1:B:130:VAL:HG12	1:B:131:VAL:H	1.45	0.81
1:B:85:GLN:O	1:B:86:ARG:HB2	1.81	0.80
1:F:185:GLU:HG2	1:F:186:ILE:N	1.96	0.80
1:G:116:LEU:HD12	1:G:117:SER:H	1.44	0.80
1:G:106:LEU:HD13	1:G:204:LEU:HD22	1.64	0.79
1:F:82:GLN:HB3	1:F:86:ARG:NH1	1.96	0.79
1:F:39:PRO:HG2	1:F:40:GLU:H	1.45	0.79
1:F:32:ASP:O	1:F:34:ARG:HD2	1.83	0.78
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.47	0.78
2:C:504:FNR:H7	1:D:140:MET:HE2	1.64	0.78
1:F:163:VAL:HG22	1:F:192:LEU:HG	1.64	0.78
1:H:34:ARG:HH22	1:H:204:LEU:HD11	1.49	0.77
1:E:116:LEU:HD12	1:E:117:SER:H	1.49	0.77
1:H:71:VAL:HB	1:H:117:SER:HB3	1.66	0.77
1:C:134:ARG:HG3	1:C:138:PRO:HA	1.65	0.76
1:H:224:TRP:O	1:H:226:VAL:HG23	1.86	0.76
1:H:37:PHE:CD2	1:H:114:ALA:HB2	2.21	0.76
1:G:116:LEU:HD12	1:G:117:SER:N	2.00	0.76
1:E:197:ARG:HA	1:F:11:ALA:HA	1.68	0.76
1:B:203:GLU:OE2	1:B:207:LYS:HE3	1.86	0.76
1:H:34:ARG:NH2	1:H:204:LEU:HD11	2.02	0.75
1:G:63:MET:HE2	1:G:65:PRO:HB3	1.68	0.75
1:G:95:PHE:HB2	1:G:100:GLN:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:502:FNR:H7	1:B:140:MET:HE2	1.67	0.74
1:G:64:GLN:NE2	1:H:213:LEU:H	1.85	0.74
1:E:123:ASP:HA	1:E:184:VAL:HG22	1.69	0.74
1:E:39:PRO:HA	1:E:115:PRO:HD3	1.69	0.74
1:F:42:LEU:HB3	1:F:46:LEU:HD23	1.69	0.74
1:E:173:GLU:O	1:E:177:ILE:HG13	1.87	0.74
1:A:196:ASP:O	1:B:12:ALA:HA	1.88	0.74
1:A:136:HIS:O	1:A:137:ASN:HB2	1.87	0.74
1:G:74:ASP:HA	1:G:77:ARG:NE	2.03	0.73
1:C:64:GLN:HE22	1:D:213:LEU:H	1.34	0.73
1:C:73:GLN:HG2	1:D:222:GLU:OE1	1.89	0.73
1:A:63:MET:HG3	1:A:65:PRO:HD3	1.71	0.73
1:G:46:LEU:HD23	1:G:49:ARG:NH2	2.03	0.73
1:C:195:VAL:HG21	1:C:198:LEU:HD21	1.71	0.72
1:A:210:ARG:HE	1:B:63:MET:HA	1.54	0.72
1:E:38:LEU:HB3	1:E:40:GLU:OE1	1.89	0.72
1:H:39:PRO:HG2	1:H:40:GLU:H	1.53	0.72
1:H:84:PHE:HE2	1:H:109:GLU:HG2	1.54	0.71
1:G:163:VAL:HG22	1:G:192:LEU:HG	1.72	0.71
1:G:28:GLU:HG2	1:H:56:GLN:HE22	1.55	0.71
1:G:85:GLN:HA	1:G:88:ASN:HB3	1.72	0.71
1:B:217:ASP:HB2	1:B:227:ARG:NH2	2.05	0.71
1:F:62:PHE:O	1:F:64:GLN:HG3	1.89	0.71
1:E:106:LEU:O	1:E:106:LEU:HD12	1.90	0.71
1:E:196:ASP:O	1:F:11:ALA:HB1	1.90	0.70
1:E:213:LEU:H	1:F:64:GLN:HE22	1.36	0.70
1:D:15:PHE:HB3	1:D:19:GLU:HB2	1.73	0.70
1:D:134:ARG:HG3	1:D:138:PRO:HA	1.72	0.70
1:E:32:ASP:OD1	1:E:164:GLY:HA2	1.91	0.70
1:F:42:LEU:HD12	1:F:42:LEU:H	1.55	0.70
1:B:131:VAL:CG1	1:B:134:ARG:HE	1.96	0.70
1:F:221:GLU:O	1:F:223:GLY:N	2.24	0.70
1:H:81:TRP:O	1:H:85:GLN:HG2	1.91	0.69
1:E:158:ALA:HB1	1:F:20:ARG:HB3	1.74	0.69
1:G:83:ALA:HA	1:G:86:ARG:CZ	2.22	0.69
1:H:17:SER:CA	1:H:20:ARG:HD3	2.22	0.69
1:G:125:THR:HA	1:G:134:ARG:HH22	1.58	0.69
1:H:149:VAL:HG13	1:H:190:LEU:HD11	1.74	0.69
1:E:116:LEU:HD12	1:E:117:SER:N	2.08	0.69
1:A:163:VAL:HG22	1:A:192:LEU:HG	1.75	0.68
1:G:46:LEU:HD23	1:G:49:ARG:HH21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HE3	1:D:207:LYS:O	1.94	0.68
1:C:103:TYR:HE1	1:D:132:LEU:HG	1.58	0.68
1:C:132:LEU:HD23	1:D:204:LEU:HD21	1.74	0.68
1:G:34:ARG:HH12	1:G:203:GLU:HB3	1.58	0.68
1:H:76:THR:O	1:H:80:VAL:HG23	1.93	0.68
1:F:185:GLU:HG2	1:F:186:ILE:H	1.57	0.68
1:A:28:GLU:CG	1:B:56:GLN:HE22	2.07	0.68
1:A:165:TRP:CZ2	1:A:188:ALA:HB2	2.30	0.67
1:F:60:VAL:HG21	1:F:133:GLY:HA3	1.75	0.67
1:E:27:ILE:HG23	1:F:151:ASN:ND2	2.09	0.67
1:G:81:TRP:CH2	1:G:85:GLN:HG3	2.29	0.67
1:G:94:MET:SD	1:H:135:THR:HG21	2.34	0.67
1:F:84:PHE:CE2	1:F:109:GLU:HG2	2.29	0.67
1:E:95:PHE:HB2	1:E:100:GLN:HB3	1.77	0.67
1:E:178:LEU:HD22	1:F:222:GLU:O	1.94	0.67
1:C:94:MET:HG2	1:D:130:VAL:HG11	1.78	0.66
1:E:122:CYS:HB2	1:E:145:THR:HG21	1.77	0.66
1:F:73:GLN:HE21	1:F:73:GLN:HA	1.59	0.66
1:B:135:THR:HG22	4:B:524:HOH:O	1.95	0.66
1:G:38:LEU:HB3	1:G:40:GLU:OE2	1.95	0.66
1:H:60:VAL:HG21	1:H:133:GLY:HA3	1.78	0.66
1:H:204:LEU:N	1:H:204:LEU:HD12	2.11	0.65
1:F:226:VAL:HG12	1:F:227:ARG:N	2.11	0.65
1:H:134:ARG:NE	1:H:141:ASP:HB3	2.11	0.65
1:H:204:LEU:H	1:H:204:LEU:CD1	2.08	0.65
1:H:62:PHE:O	1:H:64:GLN:HG3	1.97	0.65
1:A:198:LEU:O	1:B:9:LEU:HA	1.97	0.65
1:C:60:VAL:HG22	1:C:132:LEU:O	1.96	0.65
1:A:28:GLU:HG2	1:B:56:GLN:HE22	1.61	0.65
1:H:60:VAL:CG2	1:H:133:GLY:HA3	2.27	0.65
1:A:140:MET:HE2	2:B:501:FNR:H7	1.78	0.65
1:F:95:PHE:C	1:F:100:GLN:HB2	2.16	0.65
1:G:216:GLU:HG2	1:G:217:ASP:OD2	1.96	0.65
1:F:199:TYR:CE1	1:F:203:GLU:HG3	2.31	0.65
1:E:91:ALA:C	1:E:93:GLU:H	1.99	0.65
1:A:132:LEU:HD23	1:A:133:GLY:N	2.11	0.65
1:B:202:PRO:HB3	2:B:501:FNR:H5'2	1.79	0.65
1:H:203:GLU:HG2	1:H:207:LYS:HD3	1.79	0.65
1:G:74:ASP:HA	1:G:77:ARG:HE	1.62	0.64
1:E:74:ASP:O	1:E:77:ARG:HG2	1.97	0.64
1:E:83:ALA:O	1:E:86:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:O	1:D:12:ALA:CA	2.46	0.64
1:E:64:GLN:HE22	1:F:213:LEU:H	1.44	0.64
1:B:63:MET:HE2	1:B:126:ARG:HB3	1.79	0.64
1:H:95:PHE:C	1:H:100:GLN:HB2	2.17	0.64
1:E:209:TRP:CE2	1:F:132:LEU:HD11	2.33	0.64
1:H:32:ASP:O	1:H:34:ARG:HD2	1.98	0.64
1:B:132:LEU:O	1:B:134:ARG:N	2.32	0.64
1:E:175:LYS:O	1:E:179:GLY:N	2.30	0.64
1:F:63:MET:HE2	1:F:126:ARG:HB3	1.79	0.63
1:E:60:VAL:HG11	1:E:140:MET:HB3	1.79	0.63
1:G:9:LEU:O	1:G:10:THR:HB	1.98	0.63
1:E:67:ASN:HD22	1:F:218:LEU:HB3	1.63	0.63
1:G:44:GLU:HA	1:G:47:ILE:HD12	1.81	0.63
2:E:506:FNR:H6	1:F:59:SER:O	1.99	0.63
1:G:120:VAL:O	1:G:187:VAL:HG22	1.97	0.63
1:F:76:THR:O	1:F:80:VAL:HG23	1.98	0.63
1:H:42:LEU:HB3	1:H:46:LEU:HD23	1.81	0.63
1:A:227:ARG:NH1	1:H:126:ARG:HA	2.13	0.63
1:E:42:LEU:HD23	1:E:46:LEU:HD23	1.81	0.63
1:H:81:TRP:CD1	1:H:111:ILE:HB	2.27	0.62
1:C:165:TRP:CZ2	1:C:188:ALA:HB2	2.34	0.62
1:H:165:TRP:CZ2	1:H:188:ALA:HB2	2.33	0.62
1:G:87:ALA:HB3	1:G:169:PHE:HA	1.81	0.62
1:F:174:ILE:O	1:F:177:ILE:HG22	1.98	0.62
1:G:63:MET:CE	1:G:65:PRO:HB3	2.29	0.62
1:H:38:LEU:HB3	1:H:39:PRO:CD	2.27	0.62
1:G:74:ASP:O	1:G:77:ARG:HG2	2.00	0.62
1:B:171:GLU:O	1:B:175:LYS:HG3	1.98	0.62
1:G:60:VAL:O	1:G:63:MET:HG2	2.00	0.62
1:G:173:GLU:O	1:G:177:ILE:HG13	1.99	0.62
1:E:63:MET:HE2	1:E:65:PRO:HB3	1.81	0.62
1:H:131:VAL:HG22	1:H:132:LEU:H	1.65	0.62
1:C:61:GLY:HA2	1:C:132:LEU:HB2	1.82	0.62
1:E:192:LEU:N	1:E:192:LEU:HD12	2.15	0.61
1:G:143:TYR:CE2	1:H:187:VAL:HG13	2.35	0.61
1:F:61:GLY:CA	1:F:132:LEU:HD13	2.31	0.61
1:F:60:VAL:CG2	1:F:133:GLY:HA3	2.30	0.61
1:E:171:GLU:HG2	1:E:175:LYS:HG3	1.81	0.61
1:A:227:ARG:HH11	1:A:227:ARG:HG3	1.64	0.61
1:B:175:LYS:HZ3	1:B:182:ASP:HA	1.66	0.61
1:A:60:VAL:HG22	1:A:132:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HD2	1:D:159:GLU:OE2	2.01	0.61
1:G:87:ALA:CB	1:G:169:PHE:HA	2.30	0.61
1:F:175:LYS:HD2	1:F:180:ILE:HG21	1.82	0.61
1:C:61:GLY:CA	1:C:132:LEU:HB2	2.31	0.61
1:E:108:LEU:HD21	1:F:132:LEU:HD23	1.82	0.61
1:C:58:PRO:HG3	1:D:153:TRP:CZ3	2.36	0.61
1:B:227:ARG:HH11	1:B:227:ARG:HG2	1.66	0.61
1:B:86:ARG:O	1:B:90:GLU:HG3	2.01	0.61
2:A:502:FNR:H7	1:B:140:MET:CE	2.30	0.61
1:B:11:ALA:O	1:B:12:ALA:O	2.19	0.61
1:H:9:LEU:HD22	1:H:9:LEU:O	2.01	0.61
1:G:30:ARG:HA	1:G:157:ARG:HG3	1.83	0.60
1:D:78:GLU:HG3	1:D:82:GLN:HE21	1.65	0.60
1:G:132:LEU:HB3	3:G:603:OXY:O1	2.02	0.60
1:H:131:VAL:HG22	1:H:132:LEU:N	2.16	0.60
1:E:90:GLU:HB2	1:F:136:HIS:NE2	2.16	0.60
1:A:132:LEU:HD22	3:A:606:OXY:O1	2.02	0.60
1:A:64:GLN:NE2	1:B:213:LEU:H	1.91	0.60
1:C:73:GLN:HG2	1:D:222:GLU:CD	2.21	0.60
1:G:40:GLU:N	1:G:40:GLU:OE2	2.32	0.60
1:B:165:TRP:CZ2	1:B:188:ALA:HB2	2.36	0.60
1:C:112:ARG:HG2	4:C:553:HOH:O	2.01	0.60
1:G:151:ASN:ND2	1:H:27:ILE:HG23	2.17	0.60
1:C:96:SER:N	1:C:100:GLN:HB2	2.17	0.60
1:A:31:ARG:HD2	1:A:199:TYR:O	2.02	0.59
1:C:15:PHE:HB3	1:C:19:GLU:HB2	1.84	0.59
1:D:132:LEU:O	1:D:134:ARG:N	2.30	0.59
1:E:67:ASN:ND2	1:F:218:LEU:HB3	2.17	0.59
1:A:87:ALA:CB	1:A:169:PHE:HA	2.32	0.59
1:F:65:PRO:HA	1:F:126:ARG:HD2	1.85	0.59
1:F:227:ARG:HG2	1:F:227:ARG:HH11	1.68	0.59
1:G:154:LEU:HD23	1:H:154:LEU:HD23	1.84	0.59
1:C:199:TYR:HA	1:D:9:LEU:HA	1.83	0.59
1:B:100:GLN:NE2	1:B:104:ARG:HH21	2.00	0.59
1:G:15:PHE:HB2	1:G:20:ARG:HG3	1.84	0.59
1:E:202:PRO:HG2	1:F:62:PHE:CZ	2.37	0.59
1:E:84:PHE:CE1	1:E:168:ILE:HB	2.38	0.59
4:A:548:HOH:O	1:B:132:LEU:HA	2.01	0.59
1:B:9:LEU:N	1:B:9:LEU:HD12	2.17	0.59
1:B:139:GLN:HA	1:B:139:GLN:HE21	1.68	0.59
1:D:63:MET:HE3	1:D:65:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:HH11	1:C:227:ARG:CG	2.16	0.58
1:F:175:LYS:HD2	1:F:180:ILE:CG2	2.33	0.58
1:F:226:VAL:HG12	1:F:227:ARG:H	1.66	0.58
1:F:131:VAL:HG12	1:F:134:ARG:H	1.67	0.58
1:F:61:GLY:HA2	1:F:132:LEU:HD13	1.85	0.58
1:H:205:ALA:HA	1:H:210:ARG:O	2.04	0.58
1:G:9:LEU:HD22	1:H:197:ARG:HG3	1.85	0.58
1:D:165:TRP:HA	1:D:190:LEU:HD23	1.85	0.58
1:G:224:TRP:CZ3	1:H:184:VAL:HG11	2.39	0.58
1:F:24:TYR:O	1:F:28:GLU:HG3	2.03	0.58
1:G:108:LEU:N	1:G:108:LEU:HD12	2.18	0.58
1:A:132:LEU:HD22	3:A:606:OXY:O2	2.03	0.58
1:E:10:THR:O	1:F:197:ARG:HG3	2.03	0.58
1:C:153:TRP:CZ3	1:D:58:PRO:HG3	2.38	0.58
1:C:60:VAL:CG2	1:C:133:GLY:HA3	2.33	0.58
1:E:42:LEU:HG	1:E:194:PHE:CE2	2.38	0.58
1:D:155:ALA:O	1:D:158:ALA:HB3	2.04	0.58
1:A:63:MET:HE2	1:A:65:PRO:HB3	1.84	0.58
1:G:58:PRO:HG3	1:H:153:TRP:CZ3	2.39	0.58
1:D:13:GLY:O	1:D:14:ALA:CB	2.52	0.58
1:F:38:LEU:HB3	1:F:39:PRO:CD	2.34	0.58
1:E:163:VAL:HG22	1:E:192:LEU:HG	1.86	0.58
1:B:25:ARG:O	1:B:29:THR:HG23	2.04	0.58
1:B:220:PHE:CE1	1:B:225:GLY:HA2	2.38	0.58
1:A:64:GLN:HB2	1:B:213:LEU:HD12	1.86	0.57
1:B:63:MET:HG3	1:B:65:PRO:HD3	1.86	0.57
1:B:130:VAL:O	1:B:131:VAL:HB	2.05	0.57
1:C:20:ARG:O	1:C:24:TYR:HD1	1.87	0.57
1:F:131:VAL:HG22	1:F:132:LEU:H	1.68	0.57
1:G:73:GLN:HE21	1:H:222:GLU:HG3	1.67	0.57
1:B:63:MET:CG	1:B:65:PRO:HD3	2.35	0.57
1:G:95:PHE:HB2	1:G:100:GLN:CA	2.33	0.57
1:F:165:TRP:CZ2	1:F:188:ALA:HB2	2.40	0.57
1:C:131:VAL:HG22	1:C:132:LEU:N	2.20	0.57
1:E:65:PRO:HA	1:E:126:ARG:HD2	1.87	0.57
1:C:28:GLU:CG	1:D:56:GLN:HE22	2.17	0.57
1:E:75:GLU:HA	1:E:78:GLU:HB2	1.87	0.57
1:G:165:TRP:CZ2	1:G:188:ALA:HB2	2.40	0.57
1:G:108:LEU:HB3	2:G:508:FNR:H3	1.70	0.57
1:G:224:TRP:CZ2	1:H:184:VAL:HG21	2.40	0.57
1:G:197:ARG:HA	1:H:11:ALA:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:HG21	1:B:187:VAL:HG21	1.87	0.57
1:F:84:PHE:HZ	1:F:108:LEU:HB2	1.70	0.57
1:C:94:MET:HG3	1:D:130:VAL:HG21	1.87	0.57
1:A:15:PHE:HB3	1:A:19:GLU:HB2	1.87	0.57
1:E:154:LEU:O	1:E:157:ARG:HB3	2.05	0.57
1:H:99:ARG:HH11	1:H:99:ARG:HG2	1.70	0.56
1:G:145:THR:CG2	1:G:187:VAL:HG21	2.35	0.56
1:B:78:GLU:HG3	1:B:82:GLN:NE2	2.20	0.56
1:E:86:ARG:CZ	1:E:170:HIS:H	2.18	0.56
1:H:80:VAL:HG12	1:H:111:ILE:HD13	1.86	0.56
1:E:86:ARG:NH2	1:E:170:HIS:H	2.03	0.56
1:D:131:VAL:HG22	1:D:132:LEU:H	1.71	0.56
1:H:214:PRO:O	1:H:217:ASP:HB2	2.05	0.56
1:F:134:ARG:NH1	1:F:141:ASP:HB3	2.20	0.56
1:H:43:SER:O	1:H:46:LEU:HB3	2.05	0.56
1:F:214:PRO:O	1:F:217:ASP:HB2	2.04	0.56
1:A:103:TYR:HE1	1:B:132:LEU:HD22	1.70	0.56
1:A:153:TRP:CZ3	1:B:58:PRO:HG3	2.40	0.56
1:H:221:GLU:O	1:H:223:GLY:N	2.34	0.56
1:E:224:TRP:CH2	1:F:184:VAL:HG21	2.40	0.56
1:C:9:LEU:N	4:C:535:HOH:O	2.38	0.56
1:E:38:LEU:O	1:E:40:GLU:N	2.39	0.56
1:D:15:PHE:O	1:D:20:ARG:NH1	2.38	0.56
1:E:63:MET:CE	1:E:65:PRO:HB3	2.35	0.56
1:C:114:ALA:HB1	1:C:192:LEU:O	2.05	0.56
1:E:165:TRP:HD1	1:E:166:VAL:N	2.03	0.56
1:F:73:GLN:NE2	1:F:73:GLN:HA	2.20	0.56
1:G:35:ASP:HB2	1:G:107:LYS:HD3	1.87	0.56
1:C:139:GLN:HE22	1:D:139:GLN:NE2	2.03	0.56
1:F:67:ASN:HB2	1:F:121:THR:OG1	2.06	0.56
1:H:77:ARG:HB2	1:H:111:ILE:HG22	1.87	0.55
1:G:12:ALA:N	4:G:541:HOH:O	2.39	0.55
1:E:197:ARG:HB3	1:F:11:ALA:HB2	1.88	0.55
1:E:150:GLN:HE21	1:E:154:LEU:CD1	2.18	0.55
1:F:95:PHE:HB2	1:F:100:GLN:HA	1.89	0.55
1:D:78:GLU:O	1:D:82:GLN:HG3	2.06	0.55
1:C:144:SER:OG	2:D:503:FNR:H8M3	2.06	0.55
1:G:125:THR:CA	1:G:134:ARG:HH22	2.20	0.55
1:F:73:GLN:HE21	1:F:73:GLN:CA	2.19	0.55
1:G:159:GLU:O	1:G:161:VAL:HG23	2.06	0.55
1:E:58:PRO:HG3	1:F:153:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:NH2	1:E:170:HIS:N	2.55	0.55
1:A:131:VAL:HG12	1:A:134:ARG:HE	1.71	0.55
1:E:87:ALA:CB	1:E:169:PHE:HA	2.37	0.55
1:H:84:PHE:CE2	1:H:109:GLU:HG2	2.40	0.55
1:E:209:TRP:NE1	1:F:132:LEU:HD11	2.22	0.55
1:H:171:GLU:OE2	1:H:185:GLU:HG3	2.06	0.55
1:G:84:PHE:CE1	1:G:168:ILE:HB	2.42	0.55
1:E:142:LEU:O	1:E:146:VAL:HG23	2.07	0.55
1:A:120:VAL:O	1:A:187:VAL:HG12	2.07	0.55
1:H:221:GLU:HG3	1:H:227:ARG:O	2.07	0.55
1:A:195:VAL:HG21	1:A:198:LEU:HD21	1.89	0.55
1:G:143:TYR:OH	1:H:142:LEU:HD13	2.07	0.55
1:E:9:LEU:N	1:E:9:LEU:HD23	2.21	0.55
1:H:86:ARG:NH2	1:H:173:GLU:OE1	2.39	0.55
1:C:20:ARG:HB2	1:C:20:ARG:HH11	1.72	0.55
1:G:179:GLY:O	1:G:181:PRO:HD3	2.06	0.55
1:A:80:VAL:HG21	1:A:189:TRP:CH2	2.41	0.55
1:H:9:LEU:HD13	1:H:9:LEU:O	2.07	0.54
1:F:134:ARG:HE	1:F:138:PRO:HA	1.72	0.54
1:A:149:VAL:HG13	1:A:190:LEU:HD11	1.87	0.54
1:D:145:THR:HG21	1:D:187:VAL:HG21	1.90	0.54
1:E:165:TRP:CZ2	1:E:188:ALA:HB2	2.43	0.54
1:D:220:PHE:CE1	1:D:225:GLY:HA2	2.42	0.54
1:G:64:GLN:HE22	1:H:213:LEU:N	1.98	0.54
1:A:196:ASP:C	1:B:12:ALA:HA	2.28	0.54
1:A:184:VAL:HG21	1:B:224:TRP:CH2	2.43	0.54
1:H:165:TRP:CZ2	2:H:507:FNR:H7M2	2.43	0.54
1:G:108:LEU:HD22	1:G:168:ILE:HD11	1.90	0.54
1:C:125:THR:O	1:F:227:ARG:HG3	2.07	0.54
1:D:25:ARG:O	1:D:29:THR:HG23	2.07	0.54
1:A:103:TYR:CE1	1:B:132:LEU:HD22	2.42	0.54
1:A:63:MET:HA	1:B:210:ARG:HE	1.73	0.54
1:D:31:ARG:HD2	1:D:199:TYR:O	2.08	0.54
1:A:75:GLU:HG2	1:A:79:LYS:HE2	1.90	0.54
1:C:131:VAL:O	1:C:135:THR:HG23	2.07	0.54
1:H:183:HIS:CD2	1:H:184:VAL:HG23	2.42	0.54
1:E:30:ARG:HH22	1:F:58:PRO:HB3	1.72	0.54
1:G:70:LEU:HD23	1:G:70:LEU:N	2.23	0.54
1:C:28:GLU:HA	1:D:56:GLN:NE2	2.23	0.54
1:E:179:GLY:O	1:F:224:TRP:HB3	2.07	0.53
1:B:131:VAL:CG1	1:B:134:ARG:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HB2	1:H:125:THR:HB	1.90	0.53
1:H:117:SER:OG	1:H:189:TRP:CZ2	2.56	0.53
1:F:174:ILE:HA	1:F:177:ILE:HG22	1.91	0.53
1:C:140:MET:HE2	2:D:503:FNR:H7	1.88	0.53
1:G:213:LEU:H	1:H:64:GLN:HE22	1.56	0.53
1:H:100:GLN:CD	1:H:104:ARG:HH21	2.12	0.53
1:E:60:VAL:HB	1:E:132:LEU:O	2.08	0.53
1:C:150:GLN:HG2	1:D:147:CYS:SG	2.49	0.53
1:D:149:VAL:HG13	1:D:190:LEU:HD11	1.91	0.53
1:G:171:GLU:OE1	1:G:175:LYS:HD2	2.09	0.53
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.73	0.53
1:G:60:VAL:HG22	1:G:132:LEU:O	2.09	0.53
1:E:165:TRP:CZ2	1:F:140:MET:HE3	2.44	0.53
1:G:124:ARG:NH1	1:G:142:LEU:HG	2.23	0.53
1:A:63:MET:CE	1:A:65:PRO:HB3	2.38	0.53
1:D:134:ARG:CG	1:D:138:PRO:HA	2.39	0.53
1:F:171:GLU:OE2	1:F:185:GLU:HG3	2.09	0.53
1:C:102:LYS:HE3	1:C:102:LYS:HA	1.91	0.53
1:F:84:PHE:HD1	1:F:168:ILE:O	1.91	0.53
1:A:132:LEU:HD13	1:B:204:LEU:HD21	1.91	0.52
1:C:72:ARG:C	1:C:77:ARG:HH12	2.12	0.52
1:B:130:VAL:HG12	1:B:131:VAL:N	2.20	0.52
1:B:85:GLN:O	1:B:86:ARG:CB	2.53	0.52
1:G:153:TRP:CZ3	1:H:58:PRO:HG3	2.44	0.52
1:C:191:CYS:C	1:C:192:LEU:HD12	2.30	0.52
1:A:56:GLN:HE22	1:B:28:GLU:HG2	1.74	0.52
1:B:136:HIS:C	1:B:137:ASN:HD22	2.13	0.52
1:D:132:LEU:C	1:D:134:ARG:H	2.11	0.52
1:G:178:LEU:HD22	1:H:222:GLU:O	2.10	0.52
1:A:58:PRO:HG3	1:B:153:TRP:CZ3	2.44	0.52
1:A:144:SER:OG	2:B:501:FNR:H8M3	2.09	0.52
1:E:124:ARG:O	1:E:134:ARG:NH2	2.43	0.52
1:E:139:GLN:OE1	1:F:142:LEU:HD13	2.09	0.52
1:G:122:CYS:SG	1:G:142:LEU:HD23	2.49	0.52
1:G:184:VAL:HG11	1:H:224:TRP:CH2	2.44	0.52
1:F:95:PHE:O	1:F:100:GLN:HB2	2.10	0.52
1:E:63:MET:HE2	1:E:126:ARG:HB3	1.90	0.52
1:C:67:ASN:HB2	1:C:121:THR:OG1	2.10	0.52
1:D:108:LEU:O	1:D:109:GLU:HB3	2.10	0.52
1:C:196:ASP:O	1:D:12:ALA:N	2.43	0.52
1:E:38:LEU:CB	1:E:40:GLU:OE1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:O	1:A:28:GLU:HB2	2.09	0.52
1:G:222:GLU:HG2	1:H:73:GLN:HE22	1.75	0.52
1:B:131:VAL:HG22	1:B:132:LEU:N	2.25	0.52
1:C:64:GLN:NE2	1:D:213:LEU:H	2.04	0.52
1:G:20:ARG:O	1:G:24:TYR:HD1	1.93	0.52
1:D:67:ASN:HB2	4:D:526:HOH:O	2.08	0.52
1:E:54:ALA:HB1	1:E:148:ALA:HB1	1.91	0.52
1:G:165:TRP:CZ2	2:G:508:FNR:H7M2	2.45	0.52
1:G:88:ASN:HA	1:G:168:ILE:HG21	1.91	0.52
1:F:39:PRO:CG	1:F:40:GLU:H	2.20	0.52
1:F:165:TRP:CZ2	2:F:505:FNR:H7M2	2.45	0.52
1:E:77:ARG:O	1:E:80:VAL:HB	2.10	0.52
1:F:9:LEU:N	1:F:9:LEU:HD23	2.25	0.52
1:G:92:ALA:HB2	1:G:103:TYR:CD2	2.45	0.51
1:G:108:LEU:HD22	1:G:168:ILE:CD1	2.39	0.51
1:E:96:SER:O	1:E:99:ARG:HB2	2.10	0.51
1:G:64:GLN:O	1:G:126:ARG:NH1	2.38	0.51
1:A:196:ASP:O	1:B:12:ALA:CA	2.57	0.51
1:F:204:LEU:HG	1:F:209:TRP:HB3	1.91	0.51
1:F:81:TRP:CZ2	1:F:112:ARG:NH2	2.79	0.51
1:H:38:LEU:CB	1:H:39:PRO:HD2	2.32	0.51
1:C:59:SER:HA	1:C:144:SER:OG	2.10	0.51
1:A:63:MET:HE1	1:A:126:ARG:O	2.11	0.51
1:G:139:GLN:NE2	1:G:143:TYR:OH	2.44	0.51
1:H:24:TYR:O	1:H:28:GLU:HG3	2.09	0.51
1:E:86:ARG:NH2	1:E:169:PHE:HB2	2.17	0.51
1:G:202:PRO:HB3	2:G:508:FNR:H5'1	1.93	0.51
1:G:196:ASP:O	1:H:11:ALA:HB1	2.11	0.51
1:E:9:LEU:HB2	1:F:198:LEU:O	2.11	0.51
1:H:98:GLU:O	1:H:101:ALA:HB3	2.10	0.51
1:G:34:ARG:NH1	1:G:203:GLU:HB3	2.25	0.51
1:G:63:MET:SD	1:G:131:VAL:HG21	2.50	0.51
1:H:203:GLU:HG2	1:H:207:LYS:CD	2.41	0.51
1:E:203:GLU:O	1:E:207:LYS:HD3	2.11	0.51
1:G:91:ALA:O	1:G:93:GLU:N	2.42	0.51
1:E:103:TYR:CE1	1:E:108:LEU:HD11	2.46	0.51
1:D:34:ARG:HH21	2:D:503:FNR:HN1	1.58	0.51
1:A:56:GLN:NE2	1:B:28:GLU:HG2	2.25	0.51
1:F:145:THR:O	1:F:149:VAL:HG23	2.10	0.51
1:E:189:TRP:O	1:E:190:LEU:HD23	2.11	0.50
1:E:30:ARG:NH2	1:F:58:PRO:HD3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:PRO:HG2	1:H:62:PHE:CZ	2.46	0.50
1:G:47:ILE:O	1:G:51:LEU:HG	2.11	0.50
1:A:227:ARG:HG3	1:H:125:THR:O	2.12	0.50
1:C:56:GLN:OE1	1:D:28:GLU:HG2	2.12	0.50
1:E:85:GLN:O	1:E:88:ASN:HB3	2.12	0.50
1:E:39:PRO:HB3	1:E:113:LYS:O	2.11	0.50
1:C:28:GLU:HG2	1:D:56:GLN:HE22	1.77	0.50
1:F:87:ALA:CB	1:F:169:PHE:HA	2.42	0.50
1:A:95:PHE:O	1:A:100:GLN:NE2	2.44	0.50
1:F:42:LEU:HD12	1:F:42:LEU:N	2.24	0.50
1:D:95:PHE:O	1:D:100:GLN:NE2	2.42	0.50
1:C:163:VAL:HG22	1:C:192:LEU:HG	1.93	0.50
1:A:42:LEU:N	1:A:42:LEU:HD12	2.27	0.50
1:A:131:VAL:CG1	1:A:134:ARG:HE	2.24	0.50
1:E:27:ILE:HG23	1:F:151:ASN:HD22	1.77	0.50
1:E:90:GLU:HB2	1:F:136:HIS:CE1	2.47	0.50
1:B:139:GLN:HA	1:B:139:GLN:NE2	2.27	0.49
1:F:106:LEU:HD23	1:F:207:LYS:HE3	1.93	0.49
1:E:143:TYR:CE2	1:F:187:VAL:HG13	2.47	0.49
1:G:221:GLU:O	1:G:223:GLY:N	2.43	0.49
1:F:84:PHE:O	1:F:88:ASN:N	2.44	0.49
1:C:20:ARG:HB2	1:C:20:ARG:NH1	2.27	0.49
1:H:220:PHE:CE1	1:H:225:GLY:HA2	2.47	0.49
1:F:177:ILE:HG23	1:F:178:LEU:HG	1.94	0.49
1:D:9:LEU:HD23	1:D:10:THR:H	1.76	0.49
1:B:42:LEU:HB3	1:B:46:LEU:HD23	1.95	0.49
1:A:75:GLU:O	1:A:79:LYS:HG3	2.12	0.49
1:G:39:PRO:HD3	4:G:527:HOH:O	2.11	0.49
1:G:124:ARG:O	1:G:134:ARG:NH2	2.45	0.49
1:G:132:LEU:HD23	3:G:603:OXY:O2	2.12	0.49
1:C:124:ARG:NE	1:C:141:ASP:OD2	2.33	0.49
1:H:84:PHE:CE2	1:H:109:GLU:HB3	2.48	0.49
1:H:202:PRO:O	1:H:205:ALA:HB3	2.13	0.49
1:H:74:ASP:O	1:H:78:GLU:HB2	2.13	0.49
1:G:9:LEU:HA	1:H:198:LEU:O	2.13	0.49
1:G:174:ILE:HD13	1:G:177:ILE:HD12	1.94	0.49
1:C:131:VAL:HG13	1:C:134:ARG:HB3	1.93	0.49
1:F:131:VAL:HG12	1:F:134:ARG:HB2	1.94	0.49
1:G:30:ARG:NH2	1:H:58:PRO:HD3	2.27	0.49
1:E:73:GLN:O	1:E:76:THR:HB	2.12	0.49
1:F:92:ALA:O	1:F:94:MET:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:HG23	1:D:133:GLY:HA3	1.95	0.49
1:F:84:PHE:CZ	1:F:108:LEU:HB2	2.48	0.49
1:G:221:GLU:HB2	1:G:227:ARG:OXT	2.13	0.49
1:E:73:GLN:HB2	1:E:76:THR:OG1	2.13	0.49
1:G:171:GLU:OE2	1:G:186:ILE:HB	2.12	0.49
1:D:68:PHE:CD1	1:D:120:VAL:HG22	2.48	0.49
1:B:60:VAL:CG2	1:B:133:GLY:HA3	2.43	0.49
1:E:64:GLN:OE1	1:F:213:LEU:HG	2.13	0.48
1:E:84:PHE:HE1	1:E:168:ILE:HB	1.77	0.48
1:B:191:CYS:C	1:B:192:LEU:HD12	2.32	0.48
1:A:83:ALA:HA	1:A:86:ARG:NH2	2.28	0.48
1:G:61:GLY:HA2	1:G:132:LEU:HB2	1.94	0.48
1:A:114:ALA:HB1	1:A:192:LEU:O	2.13	0.48
1:E:9:LEU:O	1:E:9:LEU:HG	2.12	0.48
1:E:165:TRP:CD1	1:E:166:VAL:N	2.81	0.48
1:G:113:LYS:HG2	4:G:527:HOH:O	2.13	0.48
1:C:89:ASP:O	1:C:92:ALA:HB3	2.13	0.48
1:G:83:ALA:O	1:G:86:ARG:HG2	2.13	0.48
1:E:197:ARG:HA	1:F:11:ALA:CA	2.40	0.48
1:A:80:VAL:HG12	1:A:111:ILE:HD13	1.96	0.48
1:C:106:LEU:HB3	1:C:108:LEU:HD21	1.95	0.48
1:H:137:ASN:OD1	1:H:139:GLN:HB2	2.13	0.48
1:C:138:PRO:O	1:C:141:ASP:OD1	2.31	0.48
1:E:9:LEU:N	4:E:572:HOH:O	2.46	0.48
1:D:89:ASP:O	1:D:93:GLU:HG3	2.14	0.48
1:B:107:LYS:HE2	1:B:109:GLU:O	2.13	0.48
1:H:197:ARG:HH11	1:H:197:ARG:HG2	1.79	0.48
1:G:83:ALA:HA	1:G:86:ARG:NE	2.28	0.48
1:A:134:ARG:O	1:A:135:THR:CB	2.61	0.48
1:F:37:PHE:CD2	1:F:114:ALA:HB2	2.48	0.48
1:G:158:ALA:HA	1:H:15:PHE:CD1	2.48	0.48
1:B:38:LEU:HD23	1:B:195:VAL:HA	1.96	0.48
1:F:31:ARG:HE	1:F:31:ARG:HA	1.78	0.48
1:A:72:ARG:N	1:B:222:GLU:OE2	2.46	0.48
1:A:63:MET:CG	1:A:65:PRO:HD3	2.42	0.48
1:E:110:GLY:O	1:E:114:ALA:N	2.37	0.48
1:C:140:MET:HE3	1:D:165:TRP:CZ2	2.48	0.48
1:H:86:ARG:O	1:H:90:GLU:HG3	2.13	0.48
1:D:59:SER:HA	1:D:144:SER:HB3	1.96	0.48
1:E:30:ARG:HA	1:E:157:ARG:HD3	1.96	0.48
1:C:94:MET:CG	1:D:130:VAL:HG11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LYS:HE2	1:D:109:GLU:O	2.14	0.48
1:B:11:ALA:C	1:B:12:ALA:O	2.50	0.48
1:C:94:MET:HG2	1:D:130:VAL:CG1	2.43	0.48
1:E:108:LEU:CD2	1:F:132:LEU:HD23	2.43	0.48
1:A:64:GLN:HE22	1:B:213:LEU:N	1.93	0.47
1:H:168:ILE:HG13	2:H:507:FNR:O4	2.14	0.47
1:F:163:VAL:HA	1:F:191:CYS:O	2.14	0.47
1:A:130:VAL:HG11	1:B:94:MET:SD	2.54	0.47
1:C:73:GLN:CG	1:D:222:GLU:OE1	2.61	0.47
1:G:89:ASP:O	1:G:91:ALA:N	2.47	0.47
1:G:61:GLY:CA	1:G:132:LEU:HB2	2.44	0.47
1:H:16:SER:O	1:H:17:SER:C	2.51	0.47
1:F:132:LEU:H	1:F:132:LEU:HD12	1.78	0.47
1:G:224:TRP:CH2	1:H:184:VAL:HG21	2.49	0.47
1:E:136:HIS:CD2	1:F:87:ALA:HB1	2.50	0.47
1:B:61:GLY:HA2	1:B:132:LEU:HD12	1.95	0.47
1:F:202:PRO:HB3	2:F:505:FNR:H5'2	1.96	0.47
1:H:162:GLY:O	1:H:192:LEU:HA	2.15	0.47
1:A:84:PHE:CE2	1:A:109:GLU:HG2	2.50	0.47
1:G:86:ARG:NE	1:G:173:GLU:OE1	2.47	0.47
1:B:9:LEU:O	1:B:10:THR:HB	2.15	0.47
1:E:79:LYS:HA	1:E:82:GLN:NE2	2.29	0.47
1:C:30:ARG:HG2	1:C:154:LEU:HD12	1.95	0.47
1:H:223:GLY:O	1:H:226:VAL:HB	2.15	0.47
1:E:165:TRP:HD1	1:E:166:VAL:H	1.62	0.47
1:B:87:ALA:CB	1:B:169:PHE:HA	2.45	0.47
1:B:169:PHE:O	1:B:169:PHE:HD1	1.97	0.47
1:G:67:ASN:ND2	1:H:218:LEU:O	2.48	0.47
1:A:209:TRP:CZ2	1:B:132:LEU:HD21	2.50	0.47
2:E:506:FNR:H8M3	1:F:144:SER:OG	2.15	0.47
1:G:200:GLN:HG3	1:H:9:LEU:N	2.30	0.47
1:E:78:GLU:O	1:E:82:GLN:HG3	2.14	0.47
1:H:57:ALA:HB2	1:H:148:ALA:HA	1.97	0.47
1:H:39:PRO:O	1:H:40:GLU:C	2.54	0.47
1:A:192:LEU:N	1:A:192:LEU:HD12	2.29	0.47
1:E:64:GLN:NE2	1:F:213:LEU:H	2.10	0.47
1:F:80:VAL:O	1:F:81:TRP:C	2.53	0.47
1:E:28:GLU:HG2	1:F:56:GLN:HE22	1.80	0.47
1:H:204:LEU:HB3	1:H:209:TRP:HB3	1.97	0.47
1:G:12:ALA:O	1:H:196:ASP:O	2.33	0.47
1:F:82:GLN:HB3	1:F:86:ARG:HH12	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:PHE:O	1:H:221:GLU:HG2	2.16	0.47
1:G:192:LEU:HD12	1:G:192:LEU:N	2.30	0.47
1:C:69:VAL:HG11	1:C:178:LEU:HD13	1.97	0.47
1:F:131:VAL:CG1	1:F:134:ARG:H	2.28	0.46
1:E:61:GLY:O	1:E:62:PHE:C	2.53	0.46
1:E:127:GLY:HA2	1:F:210:ARG:NH1	2.30	0.46
1:G:99:ARG:C	1:G:101:ALA:H	2.18	0.46
1:C:75:GLU:O	1:C:79:LYS:HG2	2.14	0.46
1:C:134:ARG:CG	1:C:138:PRO:HA	2.41	0.46
1:E:171:GLU:HG2	1:E:175:LYS:CG	2.43	0.46
1:G:145:THR:HG21	1:G:187:VAL:HG21	1.97	0.46
1:F:183:HIS:ND1	1:F:184:VAL:HG23	2.30	0.46
1:G:72:ARG:HB3	1:G:72:ARG:HH11	1.81	0.46
1:H:16:SER:O	1:H:20:ARG:HD2	2.16	0.46
1:E:64:GLN:NE2	1:F:212:ARG:HD3	2.30	0.46
1:A:10:THR:HG22	1:A:11:ALA:O	2.15	0.46
1:H:82:GLN:HA	1:H:85:GLN:HG2	1.98	0.46
1:E:31:ARG:NE	2:E:506:FNR:O3P	2.38	0.46
1:H:100:GLN:HG2	1:H:104:ARG:HH21	1.81	0.46
1:E:146:VAL:HB	1:F:146:VAL:HG11	1.96	0.46
1:G:30:ARG:HH21	1:H:58:PRO:HD3	1.80	0.46
1:A:212:ARG:HA	1:B:64:GLN:HE22	1.81	0.46
1:D:131:VAL:HG13	1:D:132:LEU:O	2.16	0.46
1:D:30:ARG:C	1:D:31:ARG:HG2	2.36	0.46
1:D:132:LEU:HB3	3:D:601:OXY:O1	2.16	0.46
1:E:40:GLU:O	1:E:115:PRO:CB	2.63	0.46
1:E:122:CYS:CB	1:E:145:THR:HG21	2.45	0.46
1:B:127:GLY:HA2	1:G:217:ASP:OD2	2.15	0.46
1:E:114:ALA:CB	1:E:191:CYS:HB3	2.45	0.46
1:D:30:ARG:NH1	1:D:31:ARG:HA	2.30	0.46
1:H:15:PHE:HD2	1:H:19:GLU:HB3	1.80	0.46
1:B:116:LEU:HD12	1:B:117:SER:H	1.81	0.46
1:H:107:LYS:O	1:H:108:LEU:HD23	2.16	0.46
1:B:42:LEU:HD12	1:B:42:LEU:N	2.31	0.46
1:B:131:VAL:HG13	1:B:134:ARG:HB3	1.97	0.46
1:B:175:LYS:NZ	1:B:182:ASP:HA	2.30	0.46
1:E:125:THR:HG23	1:E:183:HIS:HB2	1.98	0.46
1:E:136:HIS:NE2	1:F:87:ALA:HB1	2.31	0.46
1:A:81:TRP:O	1:A:84:PHE:HB3	2.16	0.46
1:B:227:ARG:HH11	1:B:227:ARG:CG	2.29	0.46
1:G:74:ASP:OD1	1:G:75:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:VAL:HG13	1:F:132:LEU:N	2.31	0.46
1:C:77:ARG:HD2	1:C:111:ILE:O	2.15	0.46
1:C:99:ARG:HB3	4:C:533:HOH:O	2.15	0.46
1:C:149:VAL:HG13	1:C:190:LEU:HD11	1.98	0.46
1:D:60:VAL:HG22	1:D:132:LEU:O	2.15	0.45
1:C:227:ARG:NH1	1:C:227:ARG:CG	2.76	0.45
1:E:81:TRP:HA	1:E:111:ILE:HD12	1.98	0.45
1:A:131:VAL:HG22	1:A:132:LEU:N	2.31	0.45
1:H:9:LEU:HB3	4:H:558:HOH:O	2.14	0.45
1:C:80:VAL:HG21	1:C:189:TRP:CH2	2.51	0.45
1:A:152:LEU:O	1:A:152:LEU:HD23	2.16	0.45
1:D:150:GLN:HA	1:D:150:GLN:OE1	2.15	0.45
1:E:45:GLU:O	1:E:48:ALA:HB3	2.16	0.45
1:E:155:ALA:O	1:E:156:ALA:C	2.55	0.45
1:B:63:MET:CE	1:B:126:ARG:HB3	2.46	0.45
1:H:100:GLN:CG	1:H:104:ARG:HH21	2.29	0.45
1:G:197:ARG:HB3	1:H:11:ALA:HB2	1.98	0.45
1:G:81:TRP:NE1	1:G:112:ARG:CZ	2.80	0.45
2:C:504:FNR:H8M1	1:D:58:PRO:C	2.37	0.45
1:G:217:ASP:N	1:G:217:ASP:OD2	2.49	0.45
1:H:61:GLY:HA3	1:H:132:LEU:HB2	1.99	0.45
1:D:124:ARG:NE	1:D:141:ASP:OD2	2.50	0.45
1:E:131:VAL:HG13	1:E:131:VAL:O	2.17	0.45
1:F:77:ARG:O	1:F:80:VAL:HB	2.16	0.45
1:G:157:ARG:O	1:G:157:ARG:HD3	2.15	0.45
1:G:81:TRP:CE2	1:G:112:ARG:CZ	3.00	0.45
1:E:204:LEU:HD21	1:F:132:LEU:HD22	1.97	0.45
1:E:191:CYS:C	1:E:192:LEU:HD12	2.37	0.45
1:E:125:THR:HA	1:E:134:ARG:HH12	1.81	0.45
1:H:67:ASN:HB2	1:H:121:THR:OG1	2.16	0.45
1:H:167:SER:N	2:H:507:FNR:O4	2.50	0.45
1:G:170:HIS:HB2	1:G:173:GLU:OE2	2.16	0.45
1:E:204:LEU:HD12	1:E:204:LEU:N	2.32	0.45
1:F:139:GLN:O	1:F:142:LEU:N	2.50	0.45
1:C:218:LEU:HD13	1:D:66:TRP:O	2.17	0.45
1:H:39:PRO:CG	1:H:40:GLU:H	2.28	0.45
1:A:34:ARG:HH21	2:A:502:FNR:HN1	1.65	0.45
1:D:81:TRP:O	1:D:84:PHE:HB3	2.17	0.45
1:F:143:TYR:CD1	1:F:143:TYR:N	2.83	0.45
1:H:215:LEU:O	1:H:219:VAL:HG23	2.17	0.45
1:E:25:ARG:HG2	1:F:15:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:LYS:HA	1:F:180:ILE:HB	1.98	0.45
1:D:9:LEU:N	4:D:513:HOH:O	2.49	0.45
1:H:173:GLU:O	1:H:177:ILE:HG13	2.16	0.45
1:D:76:THR:O	1:D:80:VAL:HG23	2.17	0.45
1:H:77:ARG:NH1	1:H:114:ALA:O	2.50	0.45
1:E:80:VAL:HG21	1:E:189:TRP:CH2	2.52	0.45
1:G:28:GLU:HG2	1:H:56:GLN:NE2	2.28	0.45
1:H:146:VAL:O	1:H:149:VAL:N	2.50	0.45
1:B:145:THR:O	1:B:148:ALA:HB3	2.16	0.45
1:E:24:TYR:O	1:E:28:GLU:HB2	2.17	0.45
1:A:213:LEU:H	1:B:64:GLN:HE22	1.63	0.45
1:F:15:PHE:HD2	1:F:19:GLU:HB3	1.82	0.45
1:E:34:ARG:HG3	1:E:34:ARG:HH11	1.82	0.45
1:H:84:PHE:CD2	1:H:109:GLU:HB3	2.52	0.44
1:H:71:VAL:HG21	1:H:189:TRP:CH2	2.52	0.44
1:E:123:ASP:N	4:E:530:HOH:O	2.41	0.44
1:E:32:ASP:OD2	2:E:506:FNR:H1'1	2.17	0.44
1:A:30:ARG:HH21	1:B:58:PRO:N	2.15	0.44
1:F:102:LYS:HD2	1:F:105:SER:OG	2.16	0.44
1:A:214:PRO:HB2	1:G:210:ARG:HH12	1.82	0.44
1:B:65:PRO:HA	1:B:126:ARG:HD2	1.99	0.44
1:F:226:VAL:CG1	1:F:227:ARG:N	2.79	0.44
1:D:30:ARG:HH12	1:D:31:ARG:HA	1.82	0.44
1:C:96:SER:CA	1:C:100:GLN:HB2	2.47	0.44
1:E:92:ALA:HB1	1:E:104:ARG:HE	1.83	0.44
1:A:33:VAL:HG13	1:A:36:GLU:HG2	1.99	0.44
1:H:109:GLU:H	1:H:109:GLU:HG3	1.62	0.44
1:D:60:VAL:CG1	1:D:63:MET:HE1	2.48	0.44
1:G:154:LEU:CD2	1:H:154:LEU:HD23	2.45	0.44
1:C:140:MET:HE3	1:D:165:TRP:CE2	2.52	0.44
1:B:199:TYR:CZ	1:B:203:GLU:HG3	2.52	0.44
1:E:204:LEU:HD21	1:F:132:LEU:CD2	2.48	0.44
1:B:99:ARG:O	1:B:102:LYS:N	2.50	0.44
1:E:150:GLN:HE21	1:E:154:LEU:HD11	1.82	0.44
1:G:63:MET:O	1:G:64:GLN:C	2.56	0.44
1:G:201:GLU:O	1:G:202:PRO:C	2.56	0.44
1:F:61:GLY:HA3	1:F:132:LEU:HD13	1.98	0.44
1:D:39:PRO:HG2	1:D:40:GLU:OE2	2.17	0.44
1:D:196:ASP:N	4:D:540:HOH:O	2.39	0.44
1:H:170:HIS:O	1:H:171:GLU:C	2.56	0.44
1:H:15:PHE:HB3	1:H:19:GLU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ALA:HB1	1:D:192:LEU:O	2.18	0.44
1:D:37:PHE:CD2	1:D:114:ALA:HB2	2.53	0.44
1:G:131:VAL:HG22	1:G:134:ARG:HD3	2.00	0.44
1:H:111:ILE:HD11	1:H:169:PHE:CZ	2.52	0.44
1:A:135:THR:HG21	1:B:94:MET:HE2	2.00	0.44
1:H:134:ARG:NH2	1:H:141:ASP:CG	2.71	0.44
1:F:131:VAL:HG12	1:F:134:ARG:CB	2.47	0.44
1:A:213:LEU:H	1:B:64:GLN:NE2	2.16	0.44
1:H:111:ILE:HD11	1:H:169:PHE:HZ	1.83	0.44
2:G:508:FNR:H8M3	1:H:144:SER:OG	2.18	0.44
1:C:103:TYR:O	1:C:105:SER:N	2.51	0.44
1:E:81:TRP:CE2	1:E:112:ARG:CZ	3.00	0.44
1:A:227:ARG:CG	1:A:227:ARG:HH11	2.30	0.44
1:C:192:LEU:N	1:C:192:LEU:HD12	2.32	0.44
1:E:146:VAL:HG11	1:F:146:VAL:HB	2.00	0.44
1:B:108:LEU:O	1:B:109:GLU:HB3	2.17	0.44
1:C:168:ILE:HG13	2:C:504:FNR:O4	2.18	0.44
1:E:80:VAL:HG12	1:E:111:ILE:HD13	1.99	0.44
1:A:140:MET:HE1	1:B:165:TRP:NE1	2.33	0.44
1:E:42:LEU:HD23	1:E:46:LEU:CD2	2.45	0.44
1:F:175:LYS:NZ	1:F:175:LYS:HB3	2.32	0.44
1:B:99:ARG:O	1:B:100:GLN:C	2.55	0.44
1:C:136:HIS:CD2	1:D:87:ALA:HB1	2.52	0.44
1:A:134:ARG:O	1:A:135:THR:HB	2.17	0.43
1:F:63:MET:C	1:F:64:GLN:HG3	2.38	0.43
1:C:58:PRO:HD3	1:D:30:ARG:HH21	1.83	0.43
1:D:165:TRP:CZ2	1:D:188:ALA:HB2	2.53	0.43
1:B:145:THR:CG2	1:B:187:VAL:HG21	2.47	0.43
1:D:68:PHE:HD1	1:D:120:VAL:HG22	1.81	0.43
1:E:86:ARG:O	1:E:90:GLU:HG3	2.19	0.43
1:B:84:PHE:O	1:B:87:ALA:HB3	2.18	0.43
1:H:175:LYS:HE3	1:H:180:ILE:CG2	2.48	0.43
1:A:12:ALA:O	1:B:196:ASP:HA	2.18	0.43
1:G:81:TRP:CZ2	1:G:85:GLN:HG3	2.52	0.43
1:E:91:ALA:O	1:E:93:GLU:N	2.50	0.43
1:A:117:SER:HG	1:A:189:TRP:HE1	1.64	0.43
1:B:206:ALA:C	1:B:208:GLY:H	2.21	0.43
1:G:191:CYS:C	1:G:192:LEU:HD12	2.39	0.43
1:A:140:MET:HE1	1:B:165:TRP:HE1	1.83	0.43
1:E:12:ALA:O	1:F:196:ASP:HA	2.19	0.43
1:A:157:ARG:NH1	1:B:13:GLY:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:ARG:NH2	2:H:507:FNR:O2P	2.51	0.43
1:G:145:THR:HG22	1:G:187:VAL:HG21	1.99	0.43
1:H:171:GLU:O	1:H:174:ILE:N	2.46	0.43
1:A:214:PRO:HB2	1:G:210:ARG:NH1	2.33	0.43
1:G:150:GLN:HG2	1:H:150:GLN:HB3	2.00	0.43
1:C:42:LEU:HD12	1:C:42:LEU:N	2.32	0.43
1:G:134:ARG:O	1:G:134:ARG:HG2	2.18	0.43
1:B:91:ALA:HA	1:B:94:MET:HE3	2.00	0.43
1:A:140:MET:HE3	1:B:165:TRP:CZ2	2.53	0.43
1:E:86:ARG:NH1	1:E:170:HIS:HB2	2.34	0.43
1:G:9:LEU:O	1:G:10:THR:CB	2.67	0.43
1:F:224:TRP:O	1:F:224:TRP:CD1	2.71	0.43
1:E:10:THR:OG1	1:E:11:ALA:N	2.50	0.43
1:D:84:PHE:HB2	1:D:169:PHE:HE2	1.84	0.43
1:C:84:PHE:CE2	1:C:109:GLU:HG2	2.53	0.43
1:A:98:GLU:HG3	1:A:99:ARG:N	2.33	0.43
1:G:95:PHE:HE2	1:G:103:TYR:CD2	2.37	0.43
1:H:217:ASP:HA	1:H:227:ARG:NH2	2.34	0.43
1:G:199:TYR:HA	1:H:9:LEU:HA	2.01	0.43
1:F:51:LEU:HD11	1:F:70:LEU:HD21	2.01	0.43
1:A:95:PHE:CE1	1:B:130:VAL:HB	2.54	0.43
1:H:30:ARG:HA	1:H:157:ARG:HD3	2.01	0.43
1:A:145:THR:CG2	1:A:187:VAL:HG11	2.49	0.43
1:D:145:THR:CG2	1:D:187:VAL:HG21	2.48	0.43
1:C:76:THR:O	1:C:80:VAL:HG23	2.19	0.43
1:G:78:GLU:CG	1:G:82:GLN:HE21	2.20	0.42
1:E:165:TRP:CZ2	2:E:506:FNR:H7M2	2.53	0.42
1:E:171:GLU:OE1	1:E:186:ILE:HG13	2.19	0.42
1:E:30:ARG:HH22	1:F:58:PRO:CB	2.31	0.42
1:C:224:TRP:CD1	1:D:181:PRO:HD3	2.53	0.42
1:C:10:THR:OG1	1:C:11:ALA:N	2.52	0.42
1:H:102:LYS:O	1:H:105:SER:OG	2.32	0.42
1:G:84:PHE:O	1:G:88:ASN:N	2.52	0.42
1:E:63:MET:O	1:E:64:GLN:C	2.57	0.42
1:G:57:ALA:HB1	1:G:58:PRO:HD2	2.00	0.42
1:F:30:ARG:HA	1:F:157:ARG:HD3	2.01	0.42
1:D:126:ARG:CG	1:D:127:GLY:N	2.82	0.42
1:E:86:ARG:HH12	1:E:170:HIS:HB2	1.85	0.42
1:A:191:CYS:C	1:A:192:LEU:HD12	2.39	0.42
1:E:9:LEU:CD2	1:E:9:LEU:N	2.82	0.42
1:G:59:SER:OG	1:G:62:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:THR:HG22	1:G:76:THR:O	2.19	0.42
1:H:84:PHE:CE1	1:H:168:ILE:HB	2.54	0.42
1:G:81:TRP:CD1	1:G:112:ARG:NE	2.88	0.42
1:F:108:LEU:HA	2:F:505:FNR:O2	2.19	0.42
1:F:42:LEU:HD23	1:F:46:LEU:CD2	2.49	0.42
1:A:132:LEU:HD23	1:A:133:GLY:H	1.83	0.42
1:A:63:MET:HA	1:B:210:ARG:NE	2.33	0.42
1:F:19:GLU:O	1:F:22:ALA:N	2.52	0.42
1:D:215:LEU:O	1:D:219:VAL:HG23	2.20	0.42
1:H:204:LEU:HD13	2:H:507:FNR:O4'	2.19	0.42
1:H:81:TRP:CD2	1:H:85:GLN:NE2	2.87	0.42
1:C:132:LEU:O	1:C:134:ARG:N	2.43	0.42
1:E:67:ASN:HA	1:E:67:ASN:HD22	1.51	0.42
1:E:171:GLU:CD	1:E:175:LYS:HD2	2.40	0.42
1:D:9:LEU:HD23	1:D:10:THR:N	2.35	0.42
1:C:30:ARG:HG2	1:C:154:LEU:CD1	2.49	0.42
1:B:81:TRP:O	1:B:84:PHE:HB3	2.19	0.42
1:F:32:ASP:CG	2:F:505:FNR:H1'1	2.40	0.42
1:E:67:ASN:HB2	4:E:530:HOH:O	2.18	0.42
1:G:197:ARG:HA	1:H:11:ALA:CA	2.49	0.42
1:A:152:LEU:HD23	1:A:152:LEU:C	2.40	0.42
1:B:157:ARG:NH1	1:B:157:ARG:O	2.51	0.42
1:G:10:THR:OG1	1:G:11:ALA:N	2.53	0.42
1:F:39:PRO:O	1:F:40:GLU:C	2.58	0.42
1:A:197:ARG:HA	1:B:11:ALA:O	2.20	0.42
1:E:91:ALA:C	1:E:93:GLU:N	2.68	0.42
1:D:13:GLY:O	1:D:14:ALA:HB3	2.19	0.42
1:B:15:PHE:HB3	1:B:19:GLU:HB2	2.01	0.42
1:B:98:GLU:HA	1:B:98:GLU:OE2	2.19	0.42
1:E:87:ALA:HB3	1:E:169:PHE:HA	2.01	0.42
1:C:227:ARG:HG3	1:C:227:ARG:NH1	2.24	0.42
1:A:135:THR:C	1:A:137:ASN:H	2.22	0.42
1:G:42:LEU:HD11	1:G:46:LEU:HD12	2.00	0.42
1:H:61:GLY:C	1:H:63:MET:N	2.70	0.42
1:A:181:PRO:HD3	1:B:224:TRP:CD1	2.55	0.42
1:B:114:ALA:HB1	1:B:192:LEU:O	2.20	0.42
1:A:12:ALA:N	1:B:196:ASP:O	2.52	0.42
1:D:131:VAL:HG22	1:D:132:LEU:N	2.33	0.42
1:D:60:VAL:CG2	1:D:133:GLY:HA3	2.49	0.42
1:B:30:ARG:C	1:B:31:ARG:HG2	2.40	0.42
1:A:213:LEU:HD12	1:B:64:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:NE	1:A:141:ASP:OD2	2.47	0.42
1:E:201:GLU:O	1:E:202:PRO:C	2.58	0.42
1:H:44:GLU:OE1	1:H:72:ARG:NH2	2.53	0.42
1:A:74:ASP:OD1	1:A:77:ARG:NH2	2.52	0.42
1:A:103:TYR:C	1:A:105:SER:H	2.23	0.41
1:D:144:SER:O	1:D:147:CYS:HB2	2.19	0.41
1:H:70:LEU:HD23	1:H:118:ILE:HG23	2.02	0.41
1:G:84:PHE:CE2	1:G:109:GLU:HB3	2.55	0.41
1:G:165:TRP:HD1	1:G:166:VAL:N	2.17	0.41
1:H:117:SER:OG	1:H:189:TRP:CE2	2.73	0.41
1:D:39:PRO:O	1:D:40:GLU:C	2.59	0.41
1:F:107:LYS:HD2	1:F:107:LYS:HA	1.90	0.41
1:E:227:ARG:HH11	1:E:227:ARG:HG2	1.85	0.41
1:A:151:ASN:OD1	1:B:150:GLN:NE2	2.51	0.41
1:G:15:PHE:HB3	1:G:19:GLU:HB2	2.02	0.41
1:F:114:ALA:HA	1:F:115:PRO:HD3	1.92	0.41
1:C:99:ARG:HD2	1:C:99:ARG:HA	1.90	0.41
1:D:180:ILE:HA	1:D:181:PRO:HD3	1.83	0.41
1:H:77:ARG:HD2	1:H:111:ILE:O	2.19	0.41
1:G:117:SER:HA	1:G:190:LEU:O	2.20	0.41
1:B:31:ARG:HH21	1:B:202:PRO:HG3	1.85	0.41
1:F:132:LEU:HD12	1:F:132:LEU:N	2.35	0.41
1:B:80:VAL:HG13	1:B:174:ILE:CD1	2.51	0.41
2:A:502:FNR:C7M	1:B:140:MET:HE3	2.51	0.41
1:E:40:GLU:HB3	4:E:543:HOH:O	2.19	0.41
1:A:134:ARG:HD2	1:A:138:PRO:HA	2.02	0.41
1:E:213:LEU:HA	1:E:214:PRO:HD3	1.87	0.41
1:G:38:LEU:O	1:G:40:GLU:N	2.53	0.41
1:C:157:ARG:HH12	1:D:14:ALA:H	1.67	0.41
1:G:185:GLU:HG2	1:G:186:ILE:N	2.35	0.41
1:D:108:LEU:O	1:D:109:GLU:CB	2.68	0.41
1:G:183:HIS:CD2	1:G:183:HIS:H	2.38	0.41
1:G:103:TYR:HE1	1:G:108:LEU:HD21	1.85	0.41
1:F:165:TRP:CE2	2:F:505:FNR:H7M2	2.56	0.41
1:H:63:MET:HE2	1:H:126:ARG:HB3	2.03	0.41
1:H:159:GLU:O	1:H:161:VAL:HG23	2.20	0.41
1:C:184:VAL:HG21	1:D:224:TRP:CH2	2.55	0.41
1:G:164:GLY:HA3	4:G:532:HOH:O	2.20	0.41
1:B:131:VAL:HG11	1:B:134:ARG:HB3	2.03	0.41
1:H:99:ARG:HD2	1:H:209:TRP:CZ3	2.55	0.41
1:H:42:LEU:HD23	1:H:46:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:O	1:B:106:LEU:HG	2.21	0.41
1:E:30:ARG:NH2	1:F:58:PRO:CD	2.83	0.41
1:D:175:LYS:O	1:D:179:GLY:N	2.53	0.41
1:A:103:TYR:O	1:A:105:SER:N	2.53	0.41
1:G:131:VAL:CG2	1:G:134:ARG:HD3	2.51	0.41
1:G:92:ALA:HB2	1:G:103:TYR:CE2	2.56	0.41
1:G:213:LEU:HA	1:G:214:PRO:HD3	1.83	0.41
1:D:137:ASN:HA	1:D:138:PRO:HD2	1.86	0.41
1:D:63:MET:HE2	1:D:65:PRO:HD3	2.03	0.41
2:E:506:FNR:N5	1:F:60:VAL:HG23	2.36	0.41
1:E:60:VAL:HG11	1:E:140:MET:CB	2.50	0.41
1:G:73:GLN:HG3	1:H:222:GLU:CD	2.41	0.41
1:C:72:ARG:C	1:C:77:ARG:NH1	2.75	0.41
1:B:87:ALA:HB2	1:B:169:PHE:HA	2.02	0.41
1:D:84:PHE:HB2	1:D:169:PHE:CE2	2.56	0.41
1:C:81:TRP:O	1:C:84:PHE:HB3	2.21	0.41
1:C:142:LEU:HD13	1:D:143:TYR:OH	2.21	0.41
1:D:103:TYR:CD2	1:D:103:TYR:C	2.95	0.41
1:F:195:VAL:O	1:F:195:VAL:HG23	2.20	0.41
1:F:27:ILE:HA	1:F:154:LEU:HD11	2.02	0.41
1:G:96:SER:CA	1:G:100:GLN:HB2	2.51	0.41
1:E:189:TRP:C	1:E:190:LEU:HD23	2.41	0.41
1:F:63:MET:CE	1:F:65:PRO:HB3	2.51	0.41
1:F:102:LYS:O	1:F:106:LEU:HG	2.20	0.41
1:D:87:ALA:HA	1:D:90:GLU:HG3	2.03	0.41
1:D:60:VAL:HG13	1:D:60:VAL:O	2.21	0.40
1:E:89:ASP:C	1:E:91:ALA:N	2.75	0.40
1:G:30:ARG:NH2	1:H:58:PRO:CD	2.84	0.40
1:B:99:ARG:HD2	1:B:99:ARG:HA	1.92	0.40
1:H:15:PHE:HB3	1:H:19:GLU:HB3	2.04	0.40
2:G:508:FNR:H6	1:H:59:SER:O	2.21	0.40
1:D:61:GLY:HA2	1:D:132:LEU:HB2	2.03	0.40
1:F:39:PRO:CG	1:F:40:GLU:N	2.84	0.40
1:H:71:VAL:HG21	1:H:189:TRP:HH2	1.87	0.40
1:H:60:VAL:HG22	1:H:133:GLY:HA3	2.01	0.40
1:H:63:MET:HG2	1:H:65:PRO:HB3	2.04	0.40
1:E:36:GLU:CD	1:E:36:GLU:N	2.74	0.40
1:A:131:VAL:HG22	1:A:132:LEU:H	1.86	0.40
1:C:24:TYR:O	1:C:28:GLU:HB2	2.21	0.40
1:D:217:ASP:OD2	1:F:210:ARG:NH2	2.55	0.40
1:C:63:MET:HE3	1:C:126:ARG:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:SER:HA	1:E:190:LEU:O	2.21	0.40
1:B:10:THR:O	1:B:11:ALA:HB3	2.21	0.40
1:A:28:GLU:HG3	1:B:56:GLN:NE2	2.37	0.40
1:E:150:GLN:HE21	1:E:154:LEU:HD13	1.83	0.40
1:F:92:ALA:C	1:F:94:MET:H	2.20	0.40
1:D:63:MET:O	1:D:64:GLN:C	2.60	0.40
1:C:131:VAL:CG2	1:C:132:LEU:N	2.84	0.40
1:G:180:ILE:HG22	1:G:184:VAL:O	2.22	0.40
1:G:28:GLU:CG	1:H:56:GLN:HE22	2.30	0.40
1:E:145:THR:OG1	1:E:187:VAL:HG21	2.21	0.40
1:F:95:PHE:O	1:F:100:GLN:HG3	2.21	0.40
1:D:78:GLU:HG3	1:D:82:GLN:NE2	2.34	0.40
1:E:43:SER:HB2	1:E:45:GLU:OE2	2.22	0.40
1:F:35:ASP:CG	1:F:35:ASP:O	2.60	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	217/230 (94%)	201 (93%)	11 (5%)	5 (2%)	8	30
1	B	217/230 (94%)	196 (90%)	12 (6%)	9 (4%)	3	14
1	C	217/230 (94%)	200 (92%)	15 (7%)	2 (1%)	21	57
1	D	217/230 (94%)	190 (88%)	18 (8%)	9 (4%)	3	14
1	E	217/230 (94%)	182 (84%)	25 (12%)	10 (5%)	3	11
1	F	217/230 (94%)	178 (82%)	28 (13%)	11 (5%)	2	9
1	G	217/230 (94%)	180 (83%)	26 (12%)	11 (5%)	2	9
1	H	217/230 (94%)	184 (85%)	22 (10%)	11 (5%)	2	9
All	All	1736/1840 (94%)	1511 (87%)	157 (9%)	68 (4%)	4	15

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	137	ASN
1	B	12	ALA
1	B	86	ARG
1	B	133	GLY
1	D	11	ALA
1	D	12	ALA
1	D	14	ALA
1	D	181	PRO
1	E	16	SER
1	E	111	ILE
1	F	11	ALA
1	F	181	PRO
1	F	222	GLU
1	G	10	THR
1	G	181	PRO
1	G	222	GLU
1	H	11	ALA
1	H	135	THR
1	A	104	ARG
1	A	135	THR
1	B	10	THR
1	B	131	VAL
1	D	97	GLY
1	D	133	GLY
1	E	39	PRO
1	E	74	ASP
1	E	132	LEU
1	E	169	PHE
1	F	14	ALA
1	F	39	PRO
1	F	93	GLU
1	F	97	GLY
1	F	131	VAL
1	G	90	GLU
1	G	93	GLU
1	G	169	PHE
1	H	14	ALA
1	H	171	GLU
1	H	181	PRO
1	B	13	GLY
1	C	104	ARG

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Mol	Chain	Res	Type
1	E	92	ALA
1	G	39	PRO
1	G	92	ALA
1	G	97	GLY
1	H	110	GLY
1	B	11	ALA
1	B	97	GLY
1	D	104	ARG
1	D	109	GLU
1	H	40	GLU
1	A	181	PRO
1	C	133	GLY
1	D	124	ARG
1	E	140	MET
1	E	181	PRO
1	F	37	PHE
1	F	40	GLU
1	H	39	PRO
1	H	222	GLU
1	B	207	LYS
1	E	98	GLU
1	G	37	PHE
1	H	19	GLU
1	F	110	GLY
1	H	225	GLY
1	G	202	PRO

### 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	178/187 (95%)	168 (94%)	10 (6%)	26	60
1	B	178/187 (95%)	172 (97%)	6 (3%)	44	79
1	C	178/187 (95%)	165 (93%)	13 (7%)	17	45
1	D	178/187 (95%)	169 (95%)	9 (5%)	29	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	178/187 (95%)	164 (92%)	14 (8%)	15	41
1	F	178/187 (95%)	165 (93%)	13 (7%)	17	45
1	G	178/187 (95%)	166 (93%)	12 (7%)	20	50
1	H	178/187 (95%)	163 (92%)	15 (8%)	14	37
All	All	1424/1496 (95%)	1332 (94%)	92 (6%)	21	52

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	36	GLU
1	A	89	ASP
1	A	107	LYS
1	A	117	SER
1	A	137	ASN
1	A	154	LEU
1	A	169	PHE
1	A	182	ASP
1	A	197	ARG
1	B	30	ARG
1	B	117	SER
1	B	136	HIS
1	B	153	TRP
1	B	169	PHE
1	B	227	ARG
1	C	30	ARG
1	C	31	ARG
1	C	72	ARG
1	C	75	GLU
1	C	89	ASP
1	C	98	GLU
1	C	107	LYS
1	C	117	SER
1	C	132	LEU
1	C	150	GLN
1	C	154	LEU
1	C	169	PHE
1	C	196	ASP
1	D	9	LEU
1	D	30	ARG
1	D	35	ASP

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Mol	Chain	Res	Type
1	D	36	GLU
1	D	72	ARG
1	D	76	THR
1	D	85	GLN
1	D	211	GLN
1	D	216	GLU
1	E	30	ARG
1	E	35	ASP
1	E	67	ASN
1	E	78	GLU
1	E	86	ARG
1	E	89	ASP
1	E	98	GLU
1	E	99	ARG
1	E	109	GLU
1	E	140	MET
1	E	153	TRP
1	E	169	PHE
1	E	185	GLU
1	E	211	GLN
1	F	10	THR
1	F	30	ARG
1	F	31	ARG
1	F	62	PHE
1	F	73	GLN
1	F	81	TRP
1	F	154	LEU
1	F	169	PHE
1	F	175	LYS
1	F	182	ASP
1	F	196	ASP
1	F	197	ARG
1	F	211	GLN
1	G	30	ARG
1	G	46	LEU
1	G	67	ASN
1	G	99	ARG
1	G	140	MET
1	G	153	TRP
1	G	154	LEU
1	G	157	ARG
1	G	169	PHE

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Mol	Chain	Res	Type
1	G	181	PRO
1	G	183	HIS
1	G	211	GLN
1	H	10	THR
1	H	20	ARG
1	H	56	GLN
1	H	60	VAL
1	H	81	TRP
1	H	82	GLN
1	H	99	ARG
1	H	104	ARG
1	H	109	GLU
1	H	112	ARG
1	H	134	ARG
1	H	154	LEU
1	H	170	HIS
1	H	183	HIS
1	H	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	GLN
1	A	82	GLN
1	A	100	GLN
1	A	139	GLN
1	B	56	GLN
1	B	64	GLN
1	B	100	GLN
1	B	137	ASN
1	B	139	GLN
1	B	200	GLN
1	C	64	GLN
1	C	100	GLN
1	D	56	GLN
1	D	82	GLN
1	D	136	HIS
1	D	139	GLN
1	E	64	GLN
1	E	67	ASN
1	E	82	GLN

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Mol	Chain	Res	Type
1	E	85	GLN
1	E	100	GLN
1	E	150	GLN
1	E	200	GLN
1	F	64	GLN
1	F	73	GLN
1	F	150	GLN
1	F	151	ASN
1	F	211	GLN
1	G	64	GLN
1	G	67	ASN
1	G	73	GLN
1	G	82	GLN
1	G	100	GLN
1	G	139	GLN
1	G	150	GLN
1	G	170	HIS
1	H	56	GLN
1	H	64	GLN
1	H	85	GLN
1	H	151	ASN
1	H	183	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FNR	A	502	-	30,33,33	1.90	7 (23%)	33,50,50	3.05	7 (21%)
3	OXY	A	606	-	1,1,1	1.37	0	0,0,0	0.00	-
2	FNR	B	501	-	30,33,33	1.99	9 (30%)	33,50,50	3.19	8 (24%)
3	OXY	B	602	-	1,1,1	1.28	0	0,0,0	0.00	-
2	FNR	C	504	-	30,33,33	1.98	8 (26%)	33,50,50	3.06	7 (21%)
3	OXY	C	605	-	1,1,1	1.37	0	0,0,0	0.00	-
2	FNR	D	503	-	30,33,33	2.01	7 (23%)	33,50,50	3.06	5 (15%)
3	OXY	D	601	-	1,1,1	1.23	0	0,0,0	0.00	-
2	FNR	E	506	-	30,33,33	1.87	6 (20%)	33,50,50	3.08	5 (15%)
3	OXY	E	607	-	1,1,1	1.36	0	0,0,0	0.00	-
2	FNR	F	505	-	30,33,33	2.01	7 (23%)	33,50,50	3.06	7 (21%)
3	OXY	F	608	-	1,1,1	1.37	0	0,0,0	0.00	-
2	FNR	G	508	-	30,33,33	1.91	7 (23%)	33,50,50	3.08	8 (24%)
3	OXY	G	603	-	1,1,1	1.30	0	0,0,0	0.00	-
2	FNR	H	507	-	30,33,33	2.00	8 (26%)	33,50,50	3.07	6 (18%)
3	OXY	H	604	-	1,1,1	1.31	0	0,0,0	0.00	-

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	FNR	A	502	-	-	0/18/18/18	0/3/3/3
3	OXY	A	606	-	-	0/0/0/0	0/0/0/0
2	FNR	B	501	-	-	0/18/18/18	0/3/3/3
3	OXY	B	602	-	-	0/0/0/0	0/0/0/0
2	FNR	C	504	-	-	0/18/18/18	0/3/3/3
3	OXY	C	605	-	-	0/0/0/0	0/0/0/0
2	FNR	D	503	-	-	0/18/18/18	0/3/3/3
3	OXY	D	601	-	-	0/0/0/0	0/0/0/0
2	FNR	E	506	-	-	0/18/18/18	0/3/3/3
3	OXY	E	607	-	-	0/0/0/0	0/0/0/0
2	FNR	F	505	-	-	0/18/18/18	0/3/3/3
3	OXY	F	608	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FNR	G	508	-	-	0/18/18/18	0/3/3/3
3	OXY	G	603	-	-	0/0/0/0	0/0/0/0
2	FNR	H	507	-	-	0/18/18/18	0/3/3/3
3	OXY	H	604	-	-	0/0/0/0	0/0/0/0

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	504	FNR	P-O1P	-3.02	1.43	1.54
2	A	502	FNR	P-O1P	-3.01	1.43	1.54
2	H	507	FNR	P-O1P	-2.77	1.44	1.54
2	D	503	FNR	P-O1P	-2.69	1.45	1.54
2	B	501	FNR	C1'-N10	-2.59	1.45	1.48
2	E	506	FNR	P-O1P	-2.56	1.45	1.54
2	G	508	FNR	P-O1P	-2.56	1.45	1.54
2	F	505	FNR	P-O1P	-2.39	1.46	1.54
2	B	501	FNR	P-O1P	-2.32	1.46	1.54
2	B	501	FNR	C2'-C3'	-2.18	1.49	1.53
2	F	505	FNR	CAA-N10	2.01	1.41	1.39
2	B	501	FNR	C5A-N5	2.05	1.38	1.35
2	F	505	FNR	C5A-N5	2.05	1.38	1.35
2	C	504	FNR	C6-C5A	2.10	1.44	1.41
2	A	502	FNR	CAA-N10	2.12	1.41	1.39
2	G	508	FNR	C5A-N5	2.12	1.38	1.35
2	E	506	FNR	C6-C5A	2.13	1.45	1.41
2	B	501	FNR	C9A-N10	2.17	1.41	1.38
2	H	507	FNR	C6-C5A	2.24	1.45	1.41
2	H	507	FNR	C5'-C4'	2.28	1.55	1.51
2	A	502	FNR	C9A-N10	2.40	1.42	1.38
2	G	508	FNR	C6-C5A	2.42	1.45	1.41
2	D	503	FNR	C6-C5A	2.44	1.45	1.41
2	G	508	FNR	C9A-N10	2.44	1.42	1.38
2	H	507	FNR	CAA-N10	2.46	1.42	1.39
2	B	501	FNR	C6-C5A	2.49	1.45	1.41
2	C	504	FNR	CAA-N10	2.49	1.42	1.39
2	F	505	FNR	C6-C5A	2.54	1.45	1.41
2	C	504	FNR	C9A-N10	2.61	1.42	1.38
2	A	502	FNR	C5'-C4'	2.68	1.55	1.51
2	H	507	FNR	C9A-N10	2.87	1.42	1.38
2	E	506	FNR	C9A-N10	2.88	1.42	1.38
2	D	503	FNR	C9A-N10	2.90	1.42	1.38
2	C	504	FNR	C5'-C4'	3.14	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	FNR	CAA-N10	3.16	1.42	1.39
2	G	508	FNR	C4A-CAA	3.93	1.48	1.41
2	B	501	FNR	C4A-CAA	3.97	1.48	1.41
2	A	502	FNR	C4A-CAA	4.01	1.48	1.41
2	E	506	FNR	C4A-CAA	4.02	1.48	1.41
2	H	507	FNR	C4A-CAA	4.10	1.48	1.41
2	C	504	FNR	C4A-CAA	4.10	1.48	1.41
2	D	503	FNR	C4-N3	4.11	1.40	1.33
2	F	505	FNR	C4A-CAA	4.18	1.48	1.41
2	C	504	FNR	C4-N3	4.26	1.41	1.33
2	B	501	FNR	C4-N3	4.31	1.41	1.33
2	G	508	FNR	C4-N3	4.40	1.41	1.33
2	H	507	FNR	C4-N3	4.52	1.41	1.33
2	E	506	FNR	C4-N3	4.52	1.41	1.33
2	D	503	FNR	C4A-CAA	4.55	1.49	1.41
2	A	502	FNR	C4-N3	4.56	1.41	1.33
2	A	502	FNR	C4-C4A	4.86	1.51	1.41
2	F	505	FNR	C4-N3	5.00	1.42	1.33
2	D	503	FNR	C4-C4A	5.11	1.51	1.41
2	E	506	FNR	C4-C4A	5.17	1.51	1.41
2	C	504	FNR	C4-C4A	5.29	1.51	1.41
2	H	507	FNR	C4-C4A	5.48	1.52	1.41
2	F	505	FNR	C4-C4A	5.55	1.52	1.41
2	B	501	FNR	C4-C4A	5.64	1.52	1.41
2	G	508	FNR	C4-C4A	5.74	1.52	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	FNR	C4A-CAA-N10	-9.12	115.14	120.52
2	H	507	FNR	C4A-CAA-N10	-8.77	115.35	120.52
2	B	501	FNR	C4A-CAA-N10	-8.77	115.35	120.52
2	F	505	FNR	C4A-CAA-N10	-8.70	115.39	120.52
2	C	504	FNR	C4A-CAA-N10	-8.54	115.49	120.52
2	A	502	FNR	C4A-CAA-N10	-8.46	115.54	120.52
2	E	506	FNR	C4A-CAA-N10	-8.38	115.58	120.52
2	G	508	FNR	C4A-CAA-N10	-8.20	115.69	120.52
2	E	506	FNR	C4A-C4-N3	-6.64	114.50	123.59
2	B	501	FNR	C4A-C4-N3	-6.53	114.67	123.59
2	F	505	FNR	C4A-C4-N3	-6.47	114.74	123.59
2	G	508	FNR	C4A-C4-N3	-6.45	114.77	123.59
2	A	502	FNR	C4A-C4-N3	-6.35	114.90	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	507	FNR	C4A-C4-N3	-6.30	114.97	123.59
2	D	503	FNR	C4A-C4-N3	-6.23	115.08	123.59
2	C	504	FNR	C4A-C4-N3	-6.20	115.11	123.59
2	H	507	FNR	C4-C4A-CAA	-5.78	116.24	119.94
2	B	501	FNR	C4-C4A-CAA	-5.71	116.28	119.94
2	G	508	FNR	C4-C4A-CAA	-5.66	116.32	119.94
2	F	505	FNR	C4-C4A-CAA	-5.66	116.32	119.94
2	C	504	FNR	C4-C4A-CAA	-5.66	116.32	119.94
2	E	506	FNR	C4-C4A-CAA	-5.65	116.33	119.94
2	A	502	FNR	C4-C4A-CAA	-5.34	116.53	119.94
2	D	503	FNR	C4-C4A-CAA	-4.71	116.93	119.94
2	A	502	FNR	O5'-P-O2P	-2.21	101.52	107.14
2	C	504	FNR	O5'-P-O2P	-2.19	101.58	107.14
2	B	501	FNR	O5'-P-O2P	-2.09	101.83	107.14
2	G	508	FNR	O5'-P-O2P	-2.05	101.92	107.14
2	H	507	FNR	C4-C4A-N5	2.02	121.17	118.72
2	G	508	FNR	C4-C4A-N5	2.05	121.21	118.72
2	F	505	FNR	C4-C4A-N5	2.08	121.24	118.72
2	B	501	FNR	O3P-P-O5'	2.16	112.78	106.56
2	B	501	FNR	C4-C4A-N5	2.23	121.43	118.72
2	G	508	FNR	O3P-P-O5'	2.24	113.03	106.56
2	F	505	FNR	O3P-P-O5'	2.27	113.10	106.56
2	A	502	FNR	C4A-N5-C5A	2.34	119.46	116.76
2	C	504	FNR	C4A-N5-C5A	2.47	119.61	116.76
2	G	508	FNR	C4A-N5-C5A	2.52	119.66	116.76
2	E	506	FNR	C4A-N5-C5A	2.53	119.67	116.76
2	A	502	FNR	O3P-P-O5'	2.62	114.10	106.56
2	F	505	FNR	C4A-N5-C5A	2.70	119.87	116.76
2	B	501	FNR	C4A-N5-C5A	2.79	119.97	116.76
2	C	504	FNR	O3P-P-O5'	2.79	114.59	106.56
2	H	507	FNR	C4A-N5-C5A	2.87	120.06	116.76
2	D	503	FNR	C4A-N5-C5A	2.90	120.10	116.76
2	F	505	FNR	C4-N3-C2	11.46	125.15	115.25
2	A	502	FNR	C4-N3-C2	11.51	125.20	115.25
2	H	507	FNR	C4-N3-C2	11.54	125.22	115.25
2	C	504	FNR	C4-N3-C2	11.54	125.22	115.25
2	G	508	FNR	C4-N3-C2	11.73	125.38	115.25
2	D	503	FNR	C4-N3-C2	11.79	125.44	115.25
2	E	506	FNR	C4-N3-C2	11.92	125.55	115.25
2	B	501	FNR	C4-N3-C2	12.20	125.80	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	FNR	4	0
3	A	606	OXY	2	0
2	B	501	FNR	3	0
2	C	504	FNR	3	0
2	D	503	FNR	3	0
3	D	601	OXY	1	0
2	E	506	FNR	6	0
2	F	505	FNR	5	0
2	G	508	FNR	5	0
3	G	603	OXY	2	0
2	H	507	FNR	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/230 (95%)	-0.54	0 100 100	5, 19, 49, 71	0
1	B	219/230 (95%)	-0.42	4 (1%) 71 68	7, 23, 50, 75	0
1	C	219/230 (95%)	-0.54	0 100 100	6, 18, 48, 67	0
1	D	219/230 (95%)	-0.43	3 (1%) 78 76	6, 22, 50, 78	0
1	E	219/230 (95%)	0.19	9 (4%) 41 34	23, 50, 83, 88	0
1	F	219/230 (95%)	0.07	10 (4%) 36 30	23, 47, 76, 88	0
1	G	219/230 (95%)	0.24	13 (5%) 26 19	19, 48, 83, 89	0
1	H	219/230 (95%)	0.07	10 (4%) 36 30	21, 48, 79, 89	0
All	All	1752/1840 (95%)	-0.17	49 (2%) 56 50	5, 32, 77, 89	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	133	GLY	7.0
1	G	131	VAL	6.7
1	G	133	GLY	6.2
1	E	168	ILE	5.6
1	F	130	VAL	5.6
1	E	132	LEU	5.5
1	E	135	THR	5.4
1	G	132	LEU	5.3
1	G	136	HIS	5.3
1	H	130	VAL	5.2
1	E	131	VAL	5.0
1	F	133	GLY	4.8
1	F	132	LEU	4.8
1	E	136	HIS	4.7
1	F	136	HIS	4.6
1	G	130	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLY	4.3
1	G	129	ALA	4.2
1	F	134	ARG	4.1
1	H	131	VAL	3.9
1	G	128	GLY	3.9
1	F	131	VAL	3.8
1	D	135	THR	3.6
1	G	169	PHE	3.6
1	G	135	THR	3.4
1	D	130	VAL	3.4
1	H	133	GLY	3.3
1	H	136	HIS	3.2
1	G	103	TYR	3.1
1	G	95	PHE	2.9
1	G	80	VAL	2.9
1	E	130	VAL	2.6
1	F	95	PHE	2.6
1	H	134	ARG	2.5
1	D	132	LEU	2.5
1	B	127	GLY	2.5
1	G	134	ARG	2.5
1	H	132	LEU	2.4
1	E	103	TYR	2.4
1	F	135	THR	2.4
1	F	169	PHE	2.3
1	B	135	THR	2.2
1	H	169	PHE	2.1
1	H	98	GLU	2.1
1	E	129	ALA	2.0
1	H	168	ILE	2.0
1	F	138	PRO	2.0
1	H	106	LEU	2.0
1	B	128	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	OXY	C	605	2/2	0.98	0.28	2.53	18,18,18,19	0
3	OXY	A	606	2/2	0.98	0.26	0.94	21,21,21,22	0
2	FNR	D	503	31/31	0.97	0.16	0.42	20,24,26,28	0
2	FNR	C	504	31/31	0.97	0.16	0.14	23,28,30,30	0
2	FNR	G	508	31/31	0.94	0.19	0.13	38,45,49,50	0
2	FNR	A	502	31/31	0.96	0.17	0.06	18,25,29,30	0
2	FNR	B	501	31/31	0.97	0.15	-0.05	23,28,31,31	0
3	OXY	D	601	2/2	0.98	0.18	-0.09	10,10,10,11	0
2	FNR	E	506	31/31	0.94	0.19	-0.09	44,50,52,54	0
3	OXY	B	602	2/2	0.98	0.18	-0.31	8,8,8,9	0
3	OXY	H	604	2/2	0.97	0.20	-0.42	32,32,32,32	0
2	FNR	F	505	31/31	0.95	0.17	-0.52	37,44,47,50	0
2	FNR	H	507	31/31	0.96	0.15	-0.58	34,39,41,43	0
3	OXY	F	608	2/2	0.96	0.16	-0.69	33,33,33,35	0
3	OXY	G	603	2/2	0.99	0.17	-0.79	27,27,27,27	0
3	OXY	E	607	2/2	0.98	0.22	-0.84	25,25,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.