



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:16 PM GMT

PDB ID : 2ISK
Title : BluB bound to flavin anion (charge transfer complex)
Authors : Larsen, N.A.; Taga, M.E.; Howard-Jones, A.R.; Walsh, C.T.; Walker, G.C.
Deposited on : 2006-10-17
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

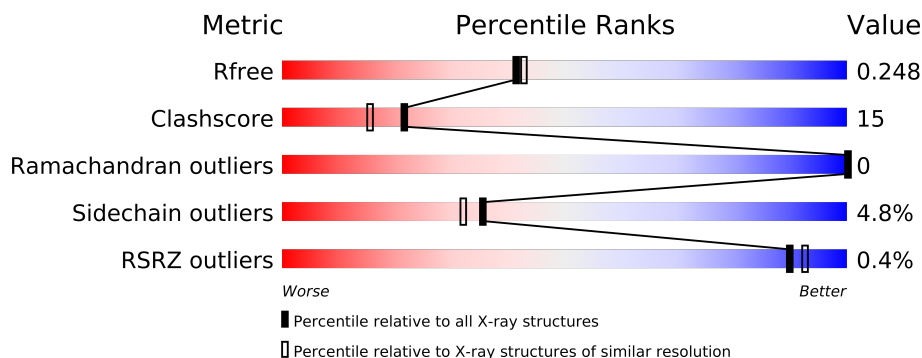
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	FNR	B	501	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15127 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

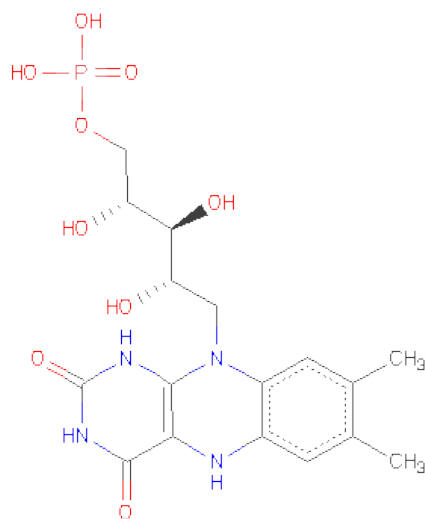
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
A	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
A	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
B	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
B	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
B	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
C	-2	GLY	-	CLONING ARTIFACT	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: C₁₇H₂₃N₄O₉P).



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 water.

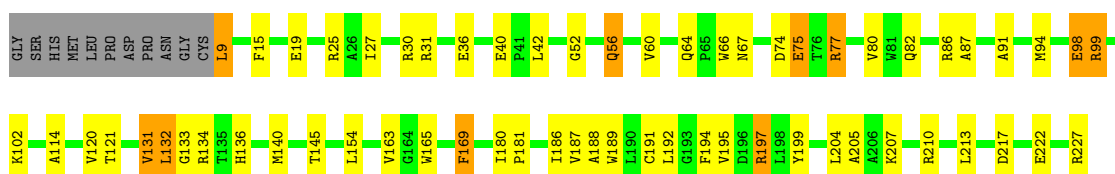
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	105	Total	O	0	0
			105	105		
3	C	126	Total	O	0	0
			126	126		
3	D	99	Total	O	0	0
			99	99		
3	E	131	Total	O	0	0
			131	131		
3	F	125	Total	O	0	0
			125	125		
3	G	107	Total	O	0	0
			107	107		
3	H	127	Total	O	0	0
			127	127		

3 Residue-property plots

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

Chain A:



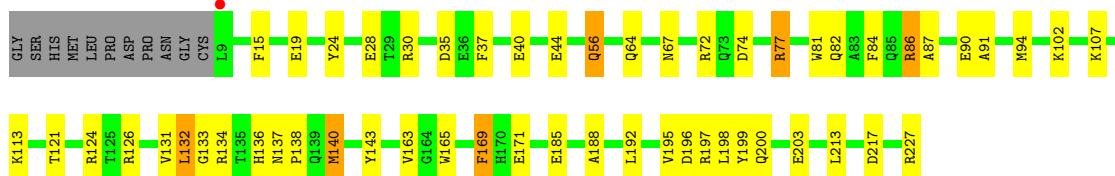
• Molecule 1: BluB

Chain B:



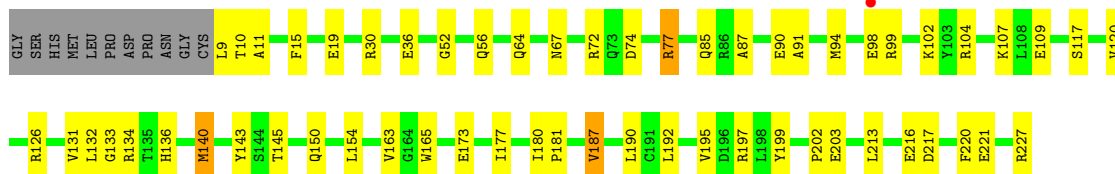
• Molecule 1: BluB

Chain C:



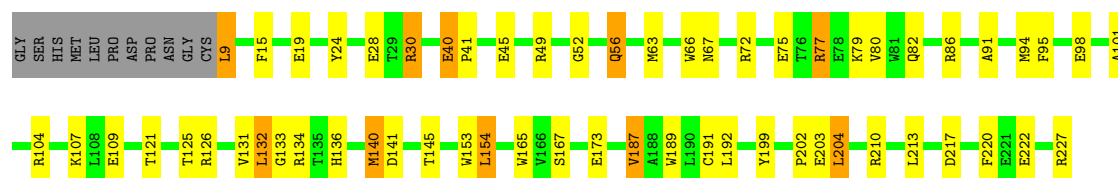
• Molecule 1: BluB

Chain D:



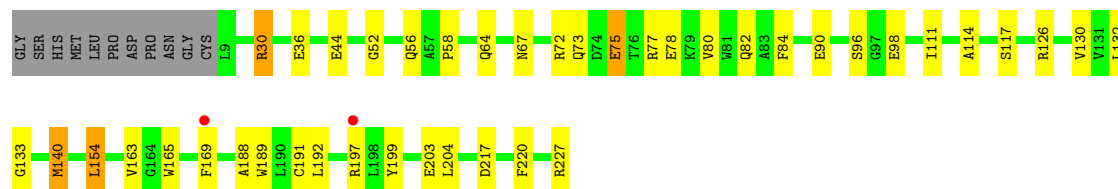
• Molecule 1: BluB

Chain E: 



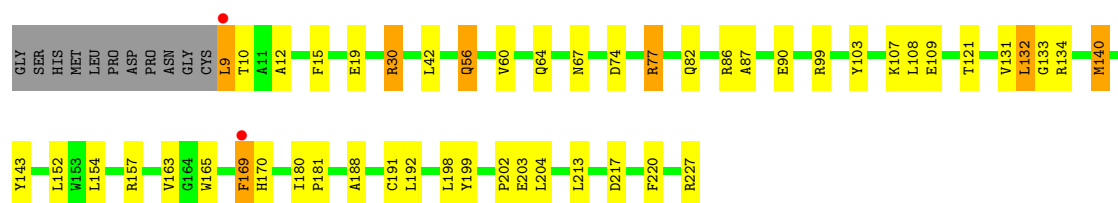
• Molecule 1: BluB

Chain F: 



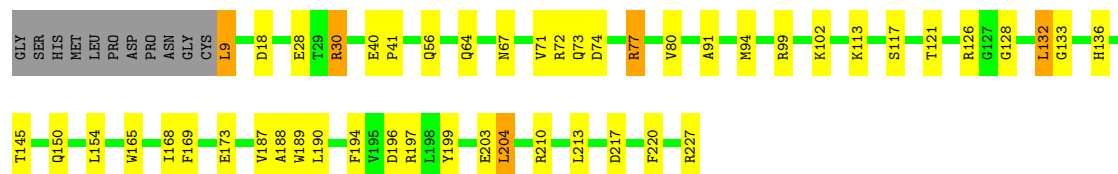
• Molecule 1: BluB

Chain G: 



• Molecule 1: BluB

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.45Å 169.87Å 90.95Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 49.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.2 (20.00-2.10) 79.9 (49.75-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.250 0.202 , 0.248	Depositor DCC
R_{free} test set	4507 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.4	EDS
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 89692 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15127	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1780	0.62	0/2412
1	B	0.34	0/1780	0.60	0/2412
1	C	0.33	0/1780	0.59	0/2412
1	D	0.33	0/1780	0.60	0/2412
1	E	0.34	0/1780	0.62	0/2412
1	F	0.34	0/1780	0.60	0/2412
1	G	0.31	0/1780	0.57	0/2412
1	H	0.31	0/1780	0.60	0/2412
All	All	0.33	0/14240	0.60	0/19296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1716	77	0
1	B	1741	0	1716	62	0
1	C	1741	0	1716	58	0
1	D	1741	0	1716	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1741	0	1716	63	0
1	F	1741	0	1716	47	0
1	G	1741	0	1716	66	0
1	H	1741	0	1716	51	0
2	A	31	0	22	5	0
2	B	31	0	22	5	0
2	C	31	0	22	3	0
2	D	31	0	22	3	0
2	E	31	0	22	5	0
2	F	31	0	22	4	0
2	G	31	0	22	2	0
2	H	31	0	22	4	0
3	A	131	0	0	8	0
3	B	105	0	0	10	0
3	C	126	0	0	5	0
3	D	99	0	0	3	0
3	E	131	0	0	5	0
3	F	125	0	0	4	0
3	G	107	0	0	8	0
3	H	127	0	0	7	0
All	All	15127	0	13904	426	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (426) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:ALA:HA	1:A:94:MET:HE3	1.41	0.98
1:D:145:THR:HG21	1:D:187:VAL:HG11	1.43	0.97
1:E:145:THR:HG21	1:E:187:VAL:HG11	1.48	0.96
1:H:67:ASN:HD21	1:H:126:ARG:HH22	1.10	0.95
1:E:67:ASN:HD21	1:E:126:ARG:HH22	1.14	0.94
1:D:67:ASN:HD21	1:D:126:ARG:HH22	0.96	0.94
1:A:145:THR:HG21	1:A:187:VAL:HG11	1.51	0.90
1:B:131:VAL:HG13	1:B:134:ARG:HB3	1.52	0.88
1:D:67:ASN:HD21	1:D:126:ARG:NH2	1.73	0.87
1:A:64:GLN:HE22	1:B:213:LEU:H	1.22	0.86
1:E:131:VAL:HG13	1:E:134:ARG:HB3	1.59	0.85
1:G:82:GLN:NE2	1:G:86:ARG:HH21	1.75	0.85
1:E:91:ALA:HA	1:E:94:MET:HE3	1.57	0.84
1:A:145:THR:CG2	1:A:187:VAL:HG11	2.08	0.83
1:G:131:VAL:HG13	1:G:134:ARG:HB3	1.61	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:67:ASN:ND2	1:D:126:ARG:HH22	1.75	0.82
1:C:67:ASN:HD21	1:C:126:ARG:HH22	1.25	0.82
1:A:213:LEU:H	1:B:64:GLN:HE22	1.28	0.81
1:B:196:ASP:O	1:B:197:ARG:HD2	1.80	0.81
1:H:74:ASP:HA	1:H:77:ARG:NH1	1.97	0.80
1:H:91:ALA:HA	1:H:94:MET:HE3	1.64	0.80
1:C:217:ASP:HA	1:C:227:ARG:HH21	1.46	0.80
1:C:64:GLN:HE22	1:D:213:LEU:H	1.28	0.79
1:F:67:ASN:HD21	1:F:126:ARG:HH22	1.24	0.79
1:D:91:ALA:HA	1:D:94:MET:HE3	1.63	0.79
1:C:74:ASP:HA	1:C:77:ARG:NH1	1.99	0.78
1:C:131:VAL:HG13	1:C:134:ARG:HB3	1.65	0.77
1:C:140:MET:HE3	1:C:140:MET:HA	1.67	0.76
1:H:150:GLN:O	1:H:154:LEU:HD13	1.86	0.76
1:A:140:MET:HE2	1:B:167:SER:HB3	1.68	0.74
1:E:67:ASN:HD21	1:E:126:ARG:NH2	1.86	0.74
1:H:74:ASP:HA	1:H:77:ARG:HH12	1.53	0.74
1:G:213:LEU:H	1:H:64:GLN:HE22	1.36	0.73
1:A:75:GLU:HB2	3:A:770:HOH:O	1.88	0.73
1:F:36:GLU:HG3	1:F:197:ARG:CZ	2.19	0.72
1:D:150:GLN:O	1:D:154:LEU:HD13	1.88	0.72
1:G:64:GLN:HE22	1:H:213:LEU:H	1.35	0.72
1:D:74:ASP:HA	1:D:77:ARG:NH1	2.05	0.72
1:E:24:TYR:O	1:E:28:GLU:HG3	1.89	0.72
1:C:140:MET:HG3	2:D:503:FNR:H7M3	1.72	0.72
1:E:222:GLU:HG3	1:F:73:GLN:NE2	2.05	0.72
1:H:150:GLN:NE2	1:H:154:LEU:HD11	2.04	0.71
1:C:140:MET:HE1	1:C:143:TYR:HD2	1.56	0.71
1:A:140:MET:HE2	2:B:501:FNR:H7	1.71	0.71
1:A:222:GLU:HG3	1:B:73:GLN:NE2	2.05	0.71
1:C:74:ASP:HA	1:C:77:ARG:HH12	1.55	0.71
1:B:30:ARG:NH1	2:B:501:FNR:O2P	2.24	0.71
1:G:77:ARG:HD3	3:G:644:HOH:O	1.90	0.71
1:D:150:GLN:NE2	1:D:154:LEU:HD11	2.06	0.70
2:C:504:FNR:H7M3	1:D:140:MET:HG3	1.72	0.70
1:G:140:MET:HG3	2:H:507:FNR:H7M3	1.72	0.70
1:E:145:THR:HG21	1:E:187:VAL:CG1	2.21	0.70
1:H:9:LEU:N	1:H:9:LEU:HD23	2.07	0.70
1:E:213:LEU:H	1:F:64:GLN:HE22	1.39	0.70
1:G:163:VAL:HG22	1:G:192:LEU:HG	1.74	0.70
1:A:140:MET:CE	1:B:167:SER:HB3	2.22	0.69
1:C:217:ASP:HA	1:C:227:ARG:NH2	2.06	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:130:VAL:O	3:F:758:HOH:O	2.10	0.69
1:D:145:THR:CG2	1:D:187:VAL:HG11	2.19	0.69
1:H:217:ASP:HA	3:H:773:HOH:O	1.92	0.69
1:D:91:ALA:HA	1:D:94:MET:CE	2.23	0.68
2:E:506:FNR:H7	1:F:140:MET:HE2	1.76	0.68
2:A:502:FNR:H7M3	1:B:140:MET:HG3	1.76	0.68
1:A:98:GLU:HG3	1:A:99:ARG:N	2.08	0.67
1:H:67:ASN:ND2	1:H:126:ARG:HH22	1.88	0.67
1:H:67:ASN:HD21	1:H:126:ARG:NH2	1.89	0.67
1:G:87:ALA:CB	1:G:169:PHE:HA	2.24	0.67
1:E:217:ASP:HA	1:E:227:ARG:HH21	1.58	0.67
1:E:154:LEU:HD23	1:F:154:LEU:HD23	1.76	0.67
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.58	0.67
1:E:67:ASN:ND2	1:E:126:ARG:HH22	1.88	0.66
1:A:25:ARG:NH2	3:B:790:HOH:O	2.28	0.66
1:D:163:VAL:HG22	1:D:192:LEU:HG	1.77	0.66
1:B:204:LEU:HD13	3:B:543:HOH:O	1.95	0.66
1:G:227:ARG:HH11	1:G:227:ARG:HG2	1.61	0.66
1:C:140:MET:HE1	1:C:143:TYR:CD2	2.31	0.65
1:G:82:GLN:HE22	1:G:86:ARG:HH21	1.44	0.65
1:C:67:ASN:HD21	1:C:126:ARG:NH2	1.95	0.65
1:E:125:THR:HB	1:G:227:ARG:HG2	1.78	0.65
1:E:91:ALA:HA	1:E:94:MET:CE	2.26	0.64
1:C:140:MET:CE	1:C:143:TYR:HD2	2.11	0.64
1:G:74:ASP:HA	1:G:77:ARG:NH1	2.12	0.64
1:C:197:ARG:HB2	1:D:9:LEU:CD2	2.28	0.64
1:C:87:ALA:CB	1:C:169:PHE:HA	2.28	0.64
1:B:80:VAL:HG21	1:B:189:TRP:CH2	2.33	0.64
1:F:217:ASP:HA	1:F:227:ARG:HH21	1.62	0.64
1:B:217:ASP:HA	1:B:227:ARG:NH2	2.14	0.63
1:E:165:TRP:CZ2	1:F:140:MET:HE3	2.33	0.63
1:B:131:VAL:HG11	1:B:134:ARG:NE	2.14	0.62
1:D:140:MET:HA	1:D:140:MET:HE3	1.81	0.62
1:C:67:ASN:ND2	1:C:126:ARG:HH22	1.95	0.62
1:F:67:ASN:HD21	1:F:126:ARG:NH2	1.97	0.62
1:C:77:ARG:HD3	3:C:563:HOH:O	2.00	0.62
1:A:140:MET:HE2	1:B:167:SER:CB	2.30	0.62
1:H:41:PRO:HG3	3:H:763:HOH:O	2.00	0.62
1:A:74:ASP:HA	1:A:77:ARG:NH1	2.15	0.61
1:C:67:ASN:HB2	1:C:121:THR:OG1	2.01	0.61
1:C:140:MET:HE2	2:D:503:FNR:H7M2	1.81	0.61
1:E:9:LEU:N	1:E:9:LEU:HD23	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:150:GLN:HE21	1:H:154:LEU:HD11	1.66	0.61
1:D:98:GLU:OE2	1:D:102:LYS:HE3	2.01	0.60
1:F:80:VAL:HG21	1:F:189:TRP:CH2	2.36	0.60
1:E:140:MET:HE2	2:F:505:FNR:H7	1.82	0.60
1:H:77:ARG:HD3	3:H:594:HOH:O	2.02	0.60
1:E:125:THR:HB	1:G:227:ARG:NH1	2.16	0.59
1:G:170:HIS:HA	3:G:1561:HOH:O	2.02	0.59
1:E:80:VAL:HG21	1:E:189:TRP:CH2	2.38	0.59
1:A:213:LEU:H	1:B:64:GLN:NE2	1.98	0.59
1:E:145:THR:CG2	1:E:187:VAL:HG11	2.29	0.59
1:C:64:GLN:NE2	1:D:213:LEU:H	1.99	0.59
1:D:140:MET:CE	1:D:143:TYR:HD2	2.15	0.59
1:A:199:TYR:CE2	1:B:9:LEU:HD12	2.38	0.59
1:B:14:ALA:O	3:B:790:HOH:O	2.16	0.58
1:E:77:ARG:HD3	3:E:562:HOH:O	2.01	0.58
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.67	0.58
1:H:91:ALA:HA	1:H:94:MET:CE	2.32	0.58
1:D:87:ALA:O	1:D:90:GLU:HB3	2.04	0.58
1:C:15:PHE:HB3	1:C:19:GLU:HB2	1.86	0.58
1:H:227:ARG:HH11	1:H:227:ARG:HG2	1.69	0.58
1:G:82:GLN:NE2	1:G:86:ARG:NH2	2.50	0.58
1:B:14:ALA:N	3:B:790:HOH:O	2.36	0.58
1:F:227:ARG:HG2	1:F:227:ARG:HH11	1.68	0.58
1:C:35:ASP:HB2	1:C:107:LYS:HD3	1.84	0.58
1:B:131:VAL:CG1	1:B:134:ARG:NE	2.67	0.58
1:A:64:GLN:NE2	1:B:213:LEU:H	1.95	0.58
1:F:114:ALA:HB1	1:F:192:LEU:O	2.04	0.58
1:D:120:VAL:O	1:D:187:VAL:HG13	2.03	0.57
1:B:90:GLU:OE1	1:B:170:HIS:NE2	2.37	0.57
1:D:145:THR:HG21	1:D:187:VAL:CG1	2.28	0.57
1:H:30:ARG:NH1	2:H:507:FNR:O2P	2.38	0.57
1:H:80:VAL:HG21	1:H:189:TRP:CH2	2.38	0.57
1:C:197:ARG:HB2	1:D:9:LEU:HD23	1.87	0.57
1:H:199:TYR:CZ	1:H:203:GLU:HG3	2.39	0.57
1:G:131:VAL:CG1	1:G:134:ARG:NE	2.67	0.57
1:B:24:TYR:O	1:B:28:GLU:HG3	2.05	0.57
1:D:150:GLN:HE21	1:D:154:LEU:HD11	1.68	0.57
1:A:52:GLY:O	1:A:56:GLN:HG2	2.05	0.57
2:C:504:FNR:H7M2	1:D:140:MET:HE2	1.87	0.57
1:A:9:LEU:N	1:A:9:LEU:HD23	2.20	0.57
1:H:165:TRP:CZ2	1:H:188:ALA:HB2	2.40	0.57
2:E:506:FNR:H7M3	1:F:140:MET:HG3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:132:LEU:HD23	1:E:133:GLY:N	2.19	0.57
3:G:1083:HOH:O	1:H:71:VAL:HG13	2.05	0.57
1:D:107:LYS:HE2	1:D:109:GLU:O	2.04	0.57
1:G:131:VAL:HG11	1:G:134:ARG:NE	2.20	0.56
1:D:132:LEU:HD23	1:D:133:GLY:N	2.20	0.56
1:G:140:MET:HE2	1:H:165:TRP:CZ2	2.40	0.56
1:H:113:LYS:HE3	3:H:1225:HOH:O	2.05	0.56
1:G:99:ARG:HD3	3:G:932:HOH:O	2.05	0.56
1:G:140:MET:CE	1:G:143:TYR:HD2	2.19	0.56
1:F:67:ASN:ND2	1:F:126:ARG:HH22	2.00	0.56
1:D:74:ASP:HA	1:D:77:ARG:HH12	1.69	0.56
1:G:56:GLN:OE1	1:H:28:GLU:HG2	2.06	0.56
1:C:77:ARG:HB2	1:C:77:ARG:HH11	1.69	0.55
1:C:163:VAL:HG22	1:C:192:LEU:HG	1.87	0.55
1:A:197:ARG:HB2	1:B:9:LEU:CD2	2.35	0.55
1:C:131:VAL:CG1	1:C:134:ARG:NE	2.70	0.55
1:F:163:VAL:HG22	1:F:192:LEU:HG	1.86	0.55
1:E:107:LYS:HE2	1:E:109:GLU:O	2.07	0.55
1:F:197:ARG:HG2	1:F:197:ARG:HH11	1.71	0.55
1:B:67:ASN:HB2	1:B:121:THR:OG1	2.07	0.55
1:G:132:LEU:HD23	1:G:133:GLY:N	2.21	0.55
1:B:204:LEU:HD22	2:B:501:FNR:O4'	2.07	0.55
2:A:502:FNR:H7M2	1:B:140:MET:HE3	1.87	0.55
1:G:87:ALA:HB2	1:G:169:PHE:HA	1.89	0.55
1:A:136:HIS:HE2	1:B:90:GLU:CG	2.20	0.55
1:C:140:MET:HE2	1:D:165:TRP:CZ2	2.42	0.55
1:E:15:PHE:HB3	1:E:19:GLU:HB2	1.89	0.55
1:G:227:ARG:HG2	1:G:227:ARG:NH1	2.21	0.55
1:G:140:MET:HE1	1:G:143:TYR:HD2	1.71	0.54
1:D:140:MET:HE1	1:D:143:TYR:CD2	2.42	0.54
1:H:220:PHE:HE1	1:H:227:ARG:NH1	2.05	0.54
1:C:165:TRP:CZ2	1:D:140:MET:HE2	2.42	0.54
1:A:25:ARG:CZ	3:B:790:HOH:O	2.55	0.54
1:C:200:GLN:HG2	1:D:10:THR:HG22	1.90	0.54
1:E:220:PHE:HE1	1:E:227:ARG:NH1	2.06	0.54
1:B:217:ASP:HA	1:B:227:ARG:HH21	1.72	0.54
1:D:140:MET:CE	1:D:143:TYR:CD2	2.91	0.53
1:E:204:LEU:HD21	1:F:132:LEU:HD13	1.90	0.53
1:E:191:CYS:C	1:E:192:LEU:HD12	2.28	0.53
1:C:165:TRP:CZ2	1:C:188:ALA:HB2	2.42	0.53
1:D:140:MET:HE1	1:D:143:TYR:HD2	1.74	0.53
1:A:197:ARG:HB2	1:B:9:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:VAL:HG11	1:B:134:ARG:CZ	2.38	0.53
1:G:64:GLN:NE2	1:H:213:LEU:H	2.05	0.53
1:C:171:GLU:OE2	1:C:185:GLU:HG3	2.08	0.53
1:G:15:PHE:HB3	1:G:19:GLU:HB2	1.91	0.53
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.25	0.52
1:B:132:LEU:HD23	1:B:133:GLY:N	2.25	0.52
1:H:77:ARG:HB2	1:H:77:ARG:HH11	1.74	0.52
1:A:77:ARG:HB2	1:A:77:ARG:HH11	1.75	0.52
1:A:132:LEU:HD23	1:A:133:GLY:N	2.24	0.52
1:F:30:ARG:NH1	2:F:505:FNR:O2P	2.31	0.52
1:C:140:MET:CE	1:C:143:TYR:CD2	2.91	0.52
1:C:24:TYR:O	1:C:28:GLU:HG3	2.10	0.52
1:B:87:ALA:O	1:B:90:GLU:HG2	2.09	0.52
1:A:217:ASP:HA	1:A:227:ARG:HH21	1.74	0.52
1:F:72:ARG:O	1:F:77:ARG:NH2	2.43	0.52
1:D:173:GLU:O	1:D:177:ILE:HG13	2.10	0.52
1:G:227:ARG:NE	3:G:685:HOH:O	2.39	0.51
1:G:132:LEU:HD22	3:H:509:HOH:O	2.10	0.51
1:C:102:LYS:HE2	3:C:1164:HOH:O	2.10	0.51
1:C:72:ARG:HG3	3:C:1135:HOH:O	2.10	0.51
1:E:132:LEU:HD22	3:F:1645:HOH:O	2.09	0.51
1:E:75:GLU:O	1:E:79:LYS:HG3	2.11	0.51
1:A:98:GLU:HG3	1:A:99:ARG:H	1.75	0.51
1:C:213:LEU:H	1:D:64:GLN:HE22	1.59	0.51
1:C:132:LEU:HD23	1:C:133:GLY:N	2.26	0.51
1:B:131:VAL:CG1	1:B:134:ARG:HB3	2.33	0.51
1:A:74:ASP:HA	1:A:77:ARG:HH12	1.76	0.51
1:C:35:ASP:OD1	1:C:107:LYS:HE3	2.11	0.51
1:F:204:LEU:HD22	2:F:505:FNR:O4'	2.11	0.50
1:C:37:PHE:O	1:C:113:LYS:HE2	2.11	0.50
1:B:77:ARG:CB	1:B:77:ARG:HH11	2.24	0.50
1:C:199:TYR:CZ	1:C:203:GLU:HG3	2.46	0.50
1:D:220:PHE:HE1	1:D:227:ARG:HH12	1.59	0.50
1:D:131:VAL:CG2	1:D:134:ARG:HB3	2.40	0.50
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.76	0.50
1:B:107:LYS:HE2	1:B:109:GLU:O	2.11	0.50
1:G:191:CYS:C	1:G:192:LEU:HD12	2.31	0.50
1:B:166:VAL:O	1:B:169:PHE:HE1	1.95	0.50
1:G:30:ARG:NH1	2:G:508:FNR:O3P	2.41	0.50
1:C:90:GLU:OE2	1:D:136:HIS:HE1	1.94	0.50
1:B:14:ALA:C	3:B:790:HOH:O	2.49	0.50
1:A:77:ARG:HD3	3:A:593:HOH:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:ALA:HA	1:B:210:ARG:O	2.11	0.50
1:B:166:VAL:HG12	1:B:169:PHE:CE1	2.47	0.50
1:D:197:ARG:HH11	1:D:197:ARG:HG2	1.76	0.50
1:A:140:MET:CE	1:B:167:SER:CB	2.89	0.50
1:F:36:GLU:HA	1:F:197:ARG:NH2	2.27	0.50
1:C:81:TRP:O	1:C:84:PHE:HB3	2.12	0.50
1:E:52:GLY:O	1:E:56:GLN:HG3	2.12	0.50
1:A:140:MET:CE	2:B:501:FNR:H7	2.41	0.49
1:F:220:PHE:HE1	1:F:227:ARG:HH12	1.59	0.49
1:A:80:VAL:HG21	1:A:189:TRP:CH2	2.47	0.49
1:G:90:GLU:OE2	1:H:136:HIS:HE1	1.94	0.49
1:G:82:GLN:O	1:G:86:ARG:HG2	2.12	0.49
2:A:502:FNR:H7M2	1:B:140:MET:CE	2.43	0.49
1:G:67:ASN:HB2	1:G:121:THR:OG1	2.12	0.49
1:E:227:ARG:HH11	1:E:227:ARG:HG2	1.78	0.49
1:G:140:MET:HE1	1:G:143:TYR:CD2	2.48	0.49
1:E:125:THR:O	1:G:227:ARG:CZ	2.60	0.49
1:E:9:LEU:HB3	1:F:199:TYR:HA	1.95	0.48
1:E:131:VAL:CG1	1:E:134:ARG:NE	2.76	0.48
1:A:82:GLN:O	1:A:86:ARG:HG3	2.13	0.48
1:E:167:SER:HB3	1:F:140:MET:CE	2.44	0.48
1:E:213:LEU:H	1:F:64:GLN:NE2	2.07	0.48
1:E:95:PHE:HZ	3:F:758:HOH:O	1.97	0.48
1:A:102:LYS:HE2	1:A:207:LYS:O	2.14	0.48
1:A:15:PHE:HB3	1:A:19:GLU:HB2	1.95	0.48
1:G:165:TRP:CZ2	1:G:188:ALA:HB2	2.49	0.48
2:C:504:FNR:H5'1	3:C:579:HOH:O	2.13	0.48
1:A:77:ARG:CZ	3:A:898:HOH:O	2.62	0.47
1:B:52:GLY:O	1:B:56:GLN:HG2	2.13	0.47
1:E:167:SER:HB3	1:F:140:MET:HE2	1.96	0.47
1:D:217:ASP:HA	1:D:227:ARG:HH21	1.78	0.47
1:A:136:HIS:HE2	1:B:90:GLU:HG3	1.78	0.47
1:B:35:ASP:HB2	1:B:107:LYS:HD3	1.95	0.47
1:H:67:ASN:HB2	1:H:121:THR:OG1	2.14	0.47
1:A:120:VAL:O	1:A:187:VAL:HG12	2.14	0.47
1:G:199:TYR:HA	1:H:9:LEU:HB3	1.97	0.47
1:F:227:ARG:HG2	1:F:227:ARG:NH1	2.30	0.47
3:E:510:HOH:O	1:F:132:LEU:HD22	2.13	0.47
1:H:173:GLU:HB3	3:H:1432:HOH:O	2.14	0.47
1:G:10:THR:O	1:H:197:ARG:HA	2.14	0.47
1:F:220:PHE:HE1	1:F:227:ARG:NH1	2.13	0.47
1:A:195:VAL:HG23	3:A:1133:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:131:VAL:HG13	1:E:134:ARG:CB	2.36	0.47
1:A:140:MET:HE3	1:B:165:TRP:CE2	2.49	0.47
1:E:153:TRP:CZ3	1:F:58:PRO:HG3	2.51	0.46
1:G:60:VAL:HG22	1:G:132:LEU:O	2.16	0.46
1:G:30:ARG:HG2	1:G:154:LEU:HD23	1.97	0.46
1:A:25:ARG:NH1	3:B:790:HOH:O	2.48	0.46
1:B:131:VAL:HG13	1:B:134:ARG:CB	2.36	0.46
1:C:131:VAL:HG11	1:C:134:ARG:NE	2.29	0.46
1:D:77:ARG:HD3	3:D:665:HOH:O	2.14	0.46
1:G:140:MET:HE2	2:H:507:FNR:H7M2	1.96	0.46
1:F:191:CYS:C	1:F:192:LEU:HD12	2.35	0.46
1:G:202:PRO:HG3	2:G:508:FNR:O1P	2.16	0.46
1:A:132:LEU:HD22	3:B:1644:HOH:O	2.16	0.46
1:C:195:VAL:HG21	1:C:198:LEU:HD21	1.97	0.46
1:H:40:GLU:HG2	1:H:194:PHE:CD2	2.51	0.46
1:E:131:VAL:HG11	1:E:134:ARG:NE	2.31	0.46
1:D:134:ARG:O	1:D:134:ARG:HG2	2.15	0.46
1:G:227:ARG:NH2	3:G:685:HOH:O	2.49	0.46
1:A:191:CYS:C	1:A:192:LEU:HD12	2.36	0.46
1:E:210:ARG:HA	3:E:1138:HOH:O	2.16	0.45
1:A:87:ALA:CB	1:A:169:PHE:HA	2.45	0.45
1:D:154:LEU:N	1:D:154:LEU:CD1	2.79	0.45
1:D:221:GLU:HG3	1:D:227:ARG:O	2.16	0.45
1:A:42:LEU:N	1:A:42:LEU:HD12	2.31	0.45
1:G:131:VAL:HG11	1:G:134:ARG:CZ	2.45	0.45
1:F:132:LEU:HD23	1:F:133:GLY:N	2.31	0.45
1:A:131:VAL:HG13	1:A:134:ARG:HB3	1.98	0.45
1:D:52:GLY:O	1:D:56:GLN:HG2	2.16	0.45
1:B:198:LEU:HD23	3:B:1367:HOH:O	2.15	0.45
1:E:45:GLU:HG2	1:E:49:ARG:HH12	1.80	0.45
1:A:140:MET:HE3	2:B:501:FNR:H7M2	1.98	0.45
1:A:9:LEU:HB2	1:B:198:LEU:O	2.17	0.45
1:E:67:ASN:HB2	1:E:121:THR:OG1	2.17	0.45
1:F:36:GLU:HG2	1:F:197:ARG:HG3	1.99	0.45
1:A:67:ASN:HB2	1:A:121:THR:OG1	2.15	0.45
1:B:182:ASP:HB2	3:B:816:HOH:O	2.17	0.45
1:C:131:VAL:HG11	1:C:134:ARG:CZ	2.46	0.45
1:F:220:PHE:CE1	1:F:227:ARG:NH1	2.84	0.45
1:F:77:ARG:HD3	1:F:111:ILE:O	2.16	0.45
1:B:116:LEU:HD12	1:B:117:SER:H	1.82	0.45
1:E:98:GLU:O	1:E:101:ALA:HB3	2.17	0.45
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.28	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:30:ARG:HA	1:G:157:ARG:HD3	1.99	0.45
1:E:199:TYR:CZ	1:E:203:GLU:HG3	2.52	0.45
1:A:134:ARG:HG2	1:A:134:ARG:O	2.17	0.44
3:A:807:HOH:O	1:B:20:ARG:HD2	2.18	0.44
1:C:124:ARG:HG3	3:C:1418:HOH:O	2.17	0.44
1:E:131:VAL:CG1	1:E:134:ARG:HB3	2.40	0.44
1:F:36:GLU:HG3	1:F:197:ARG:NE	2.31	0.44
1:A:66:TRP:HA	1:A:121:THR:O	2.18	0.44
1:C:87:ALA:HB2	1:C:169:PHE:HA	2.00	0.44
1:B:191:CYS:C	1:B:192:LEU:HD12	2.38	0.44
1:E:40:GLU:H	1:E:40:GLU:HG2	1.50	0.44
1:G:82:GLN:HE21	1:G:82:GLN:HB3	1.61	0.44
1:G:140:MET:CE	1:G:143:TYR:CD2	3.00	0.44
1:C:136:HIS:NE2	1:D:90:GLU:OE2	2.50	0.44
1:A:136:HIS:NE2	1:B:90:GLU:OE1	2.50	0.44
1:G:15:PHE:HB3	1:G:19:GLU:CB	2.48	0.44
1:A:165:TRP:CZ2	1:A:188:ALA:HB2	2.52	0.44
1:E:82:GLN:O	1:E:86:ARG:HG3	2.17	0.44
1:D:197:ARG:HG2	1:D:197:ARG:NH1	2.33	0.44
1:D:199:TYR:CZ	1:D:203:GLU:HG3	2.53	0.44
1:A:145:THR:HG22	1:A:187:VAL:HG11	1.95	0.44
1:B:165:TRP:CZ2	1:B:188:ALA:HB2	2.53	0.44
1:H:9:LEU:CD2	1:H:9:LEU:N	2.79	0.44
1:A:163:VAL:HG22	1:A:192:LEU:HG	1.99	0.44
1:G:217:ASP:HA	3:G:685:HOH:O	2.18	0.43
1:H:220:PHE:CE1	1:H:227:ARG:NH1	2.85	0.43
1:E:136:HIS:HE1	1:F:90:GLU:OE2	2.01	0.43
1:D:117:SER:HA	1:D:190:LEU:O	2.17	0.43
1:E:40:GLU:HA	1:E:41:PRO:HD3	1.92	0.43
1:A:40:GLU:OE1	1:E:173:GLU:OE2	2.36	0.43
1:G:42:LEU:HD12	1:G:42:LEU:N	2.33	0.43
1:E:140:MET:HE3	2:F:505:FNR:H7M2	2.00	0.43
1:A:60:VAL:HG22	1:A:132:LEU:O	2.18	0.43
1:E:104:ARG:NH2	3:E:728:HOH:O	2.41	0.43
2:E:506:FNR:H7M2	1:F:140:MET:HE3	2.01	0.43
1:B:180:ILE:HA	1:B:181:PRO:HD3	1.79	0.43
1:B:57:ALA:HB2	1:B:148:ALA:HA	2.01	0.43
1:G:103:TYR:CE1	1:H:132:LEU:HG	2.54	0.43
1:E:66:TRP:HA	1:E:121:THR:O	2.18	0.43
1:F:199:TYR:CZ	1:F:203:GLU:HG3	2.54	0.43
1:A:31:ARG:HD2	1:A:199:TYR:O	2.18	0.43
1:G:107:LYS:HE2	1:G:109:GLU:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:502:FNR:H7	1:B:140:MET:HE2	1.99	0.43
1:F:78:GLU:O	1:F:82:GLN:HG3	2.18	0.43
1:H:145:THR:HG21	1:H:187:VAL:HG21	2.01	0.43
1:A:120:VAL:O	1:A:187:VAL:CG1	2.67	0.43
1:D:202:PRO:HG3	2:D:503:FNR:O1P	2.17	0.43
1:G:74:ASP:HA	1:G:77:ARG:HH12	1.84	0.43
1:A:36:GLU:HG2	1:B:9:LEU:HD11	2.00	0.43
1:C:86:ARG:HA	1:C:86:ARG:HD3	1.90	0.43
1:A:180:ILE:HA	1:A:181:PRO:HD3	1.83	0.43
1:F:227:ARG:HE	1:H:128:GLY:HA2	1.84	0.42
1:F:52:GLY:O	1:F:56:GLN:HG2	2.19	0.42
1:D:10:THR:OG1	1:D:11:ALA:N	2.51	0.42
1:D:203:GLU:HB2	3:D:791:HOH:O	2.18	0.42
1:A:180:ILE:HD12	1:A:186:ILE:HD11	2.01	0.42
1:B:78:GLU:HG3	1:B:82:GLN:HE21	1.84	0.42
1:G:140:MET:HE3	1:G:140:MET:HA	2.01	0.42
1:E:45:GLU:CG	1:E:49:ARG:HH12	2.32	0.42
1:H:197:ARG:NH1	3:H:762:HOH:O	2.52	0.42
1:G:108:LEU:HD13	1:H:132:LEU:HD21	2.01	0.42
1:G:220:PHE:CE1	1:G:227:ARG:NH2	2.87	0.42
1:G:12:ALA:O	1:H:196:ASP:HA	2.19	0.42
1:D:154:LEU:N	1:D:154:LEU:HD12	2.35	0.42
1:A:205:ALA:HA	1:A:210:ARG:O	2.20	0.42
1:H:102:LYS:HB2	1:H:102:LYS:HE3	1.88	0.42
1:H:204:LEU:HD22	2:H:507:FNR:O4'	2.19	0.42
1:A:204:LEU:HD12	2:A:502:FNR:O4'	2.20	0.42
1:G:99:ARG:HD2	1:G:99:ARG:HA	1.86	0.42
1:E:202:PRO:HB3	2:E:506:FNR:H5'2	2.01	0.42
1:D:216:GLU:HG2	1:D:217:ASP:N	2.35	0.42
1:C:82:GLN:OE1	1:C:86:ARG:NH2	2.52	0.42
1:A:56:GLN:HB3	1:A:56:GLN:HE21	1.62	0.42
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.78	0.42
1:C:197:ARG:HB2	1:D:9:LEU:HD21	2.02	0.42
1:E:140:MET:HE3	1:F:165:TRP:CZ2	2.55	0.42
1:G:198:LEU:O	1:H:9:LEU:HB2	2.20	0.41
1:F:165:TRP:CZ2	1:F:188:ALA:HB2	2.55	0.41
1:F:75:GLU:HG3	3:F:1450:HOH:O	2.19	0.41
1:D:15:PHE:HB3	1:D:19:GLU:HB2	2.01	0.41
1:G:9:LEU:N	1:G:9:LEU:HD23	2.35	0.41
1:G:213:LEU:H	1:H:64:GLN:NE2	2.12	0.41
1:A:210:ARG:HG3	3:A:1528:HOH:O	2.20	0.41
1:C:196:ASP:OD1	1:C:197:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:PHE:CB	1:E:86:ARG:HD3	2.50	0.41
1:D:36:GLU:O	1:D:195:VAL:HG12	2.19	0.41
1:D:104:ARG:HD3	3:D:1142:HOH:O	2.20	0.41
1:G:180:ILE:HA	1:G:181:PRO:HD3	1.80	0.41
1:H:117:SER:HA	1:H:190:LEU:O	2.20	0.41
1:D:180:ILE:HA	1:D:181:PRO:HD3	1.80	0.41
1:D:220:PHE:CE1	1:D:227:ARG:NH1	2.88	0.41
1:A:99:ARG:NH2	3:A:1528:HOH:O	2.53	0.41
3:G:1083:HOH:O	1:H:73:GLN:HB2	2.20	0.41
1:G:152:LEU:C	1:G:152:LEU:HD23	2.41	0.41
1:G:199:TYR:CZ	1:G:203:GLU:HG3	2.56	0.41
1:A:9:LEU:CD2	1:A:9:LEU:N	2.84	0.41
1:E:63:MET:SD	1:E:141:ASP:HB3	2.60	0.41
1:C:77:ARG:HH11	1:C:77:ARG:CB	2.33	0.41
1:E:30:ARG:NH1	2:E:506:FNR:O2P	2.46	0.41
1:A:227:ARG:HB3	3:A:1053:HOH:O	2.21	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.35	0.41
1:C:91:ALA:O	1:C:94:MET:HB2	2.21	0.41
1:C:137:ASN:HA	1:C:138:PRO:HD2	1.94	0.41
1:H:227:ARG:HG2	1:H:227:ARG:NH1	2.34	0.41
1:E:72:ARG:NH2	3:E:1203:HOH:O	2.53	0.41
1:A:36:GLU:CG	1:B:9:LEU:HD11	2.51	0.40
1:H:132:LEU:HD23	1:H:133:GLY:N	2.35	0.40
1:C:56:GLN:HB3	1:C:56:GLN:HE21	1.64	0.40
1:G:192:LEU:HD12	1:G:192:LEU:N	2.36	0.40
1:D:131:VAL:HG23	1:D:134:ARG:HB3	2.03	0.40
1:A:114:ALA:HB1	1:A:192:LEU:O	2.21	0.40
1:C:40:GLU:HG3	1:C:40:GLU:O	2.20	0.40
1:D:85:GLN:OE1	1:D:85:GLN:HA	2.21	0.40
1:A:213:LEU:N	1:B:64:GLN:HE22	2.07	0.40
1:F:84:PHE:HB2	1:F:169:PHE:CE2	2.56	0.40
1:H:168:ILE:O	1:H:168:ILE:HG22	2.20	0.40
1:A:27:ILE:HG23	1:B:151:ASN:ND2	2.36	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%)	211 (97%)	6 (3%)	0	100	100
1	B	217/230 (94%)	216 (100%)	1 (0%)	0	100	100
1	C	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
1	D	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
1	E	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	F	217/230 (94%)	215 (99%)	2 (1%)	0	100	100
1	G	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
1	H	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
All	All	1736/1840 (94%)	1703 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	166 (93%)	12 (7%)	23	18
1	B	178/187 (95%)	173 (97%)	5 (3%)	56	59
1	C	178/187 (95%)	170 (96%)	8 (4%)	38	35
1	D	178/187 (95%)	172 (97%)	6 (3%)	49	49
1	E	178/187 (95%)	168 (94%)	10 (6%)	30	25
1	F	178/187 (95%)	170 (96%)	8 (4%)	38	35
1	G	178/187 (95%)	170 (96%)	8 (4%)	38	35
1	H	178/187 (95%)	167 (94%)	11 (6%)	26	21
All	All	1424/1496 (95%)	1356 (95%)	68 (5%)	35	32

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	30	ARG
1	A	56	GLN
1	A	75	GLU
1	A	77	ARG
1	A	98	GLU
1	A	99	ARG
1	A	131	VAL
1	A	132	LEU
1	A	154	LEU
1	A	169	PHE
1	A	197	ARG
1	B	30	ARG
1	B	96	SER
1	B	117	SER
1	B	140	MET
1	B	154	LEU
1	C	30	ARG
1	C	44	GLU
1	C	56	GLN
1	C	77	ARG
1	C	86	ARG
1	C	132	LEU
1	C	140	MET
1	C	169	PHE
1	D	30	ARG
1	D	72	ARG
1	D	77	ARG
1	D	99	ARG
1	D	140	MET
1	D	187	VAL
1	E	9	LEU
1	E	30	ARG
1	E	40	GLU
1	E	56	GLN
1	E	77	ARG
1	E	132	LEU
1	E	140	MET
1	E	154	LEU
1	E	187	VAL
1	E	204	LEU
1	F	30	ARG
1	F	44	GLU

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Mol	Chain	Res	Type
1	F	75	GLU
1	F	96	SER
1	F	98	GLU
1	F	117	SER
1	F	140	MET
1	F	154	LEU
1	G	9	LEU
1	G	30	ARG
1	G	56	GLN
1	G	77	ARG
1	G	132	LEU
1	G	140	MET
1	G	169	PHE
1	G	204	LEU
1	H	9	LEU
1	H	18	ASP
1	H	30	ARG
1	H	56	GLN
1	H	72	ARG
1	H	77	ARG
1	H	99	ARG
1	H	132	LEU
1	H	169	PHE
1	H	204	LEU
1	H	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	GLN
1	A	211	GLN
1	B	56	GLN
1	B	64	GLN
1	B	73	GLN
1	B	82	GLN
1	C	56	GLN
1	C	64	GLN
1	C	67	ASN
1	C	211	GLN
1	D	64	GLN
1	D	67	ASN

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Mol	Chain	Res	Type
1	D	82	GLN
1	D	136	HIS
1	D	139	GLN
1	D	150	GLN
1	D	211	GLN
1	E	67	ASN
1	E	136	HIS
1	E	211	GLN
1	F	56	GLN
1	F	64	GLN
1	F	67	ASN
1	F	73	GLN
1	F	100	GLN
1	F	211	GLN
1	G	64	GLN
1	G	82	GLN
1	G	136	HIS
1	H	56	GLN
1	H	64	GLN
1	H	67	ASN
1	H	82	GLN
1	H	136	HIS
1	H	150	GLN
1	H	211	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	-	33,33,33	2.21	10 (30%)	44,50,50	2.27	13 (29%)
2	FNR	B	501	-	33,33,33	2.26	12 (36%)	44,50,50	1.55	7 (15%)
2	FNR	C	504	-	33,33,33	2.26	10 (30%)	44,50,50	2.33	13 (29%)
2	FNR	D	503	-	33,33,33	2.11	11 (33%)	44,50,50	1.75	11 (25%)
2	FNR	E	506	-	33,33,33	2.21	11 (33%)	44,50,50	1.45	7 (15%)
2	FNR	F	505	-	33,33,33	2.28	10 (30%)	44,50,50	1.52	7 (15%)
2	FNR	G	508	-	33,33,33	2.17	12 (36%)	44,50,50	1.69	10 (22%)
2	FNR	H	507	-	33,33,33	2.12	8 (24%)	44,50,50	1.58	8 (18%)

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	0/0/3/3
2	FNR	B	501	-	-	0/18/18/18	0/0/3/3
2	FNR	C	504	-	-	0/18/18/18	0/0/3/3
2	FNR	D	503	-	-	0/18/18/18	0/0/3/3
2	FNR	E	506	-	-	0/18/18/18	0/0/3/3
2	FNR	F	505	-	-	0/18/18/18	0/0/3/3
2	FNR	G	508	-	-	0/18/18/18	0/0/3/3
2	FNR	H	507	-	-	0/18/18/18	0/0/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	508	FNR	C9A-N10	5.62	1.47	1.38
2	E	506	FNR	C4A-N5	5.52	1.45	1.36
2	C	504	FNR	C4A-N5	5.45	1.45	1.36
2	A	502	FNR	C4A-N5	5.39	1.45	1.36
2	F	505	FNR	C9A-N10	5.28	1.46	1.38
2	F	505	FNR	C4A-N5	5.12	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FNR	C9A-N10	4.99	1.46	1.38
2	E	506	FNR	C9A-N10	4.95	1.46	1.38
2	D	503	FNR	C4A-N5	4.93	1.44	1.36
2	C	504	FNR	C1'-C2'	4.92	1.56	1.51
2	B	501	FNR	C4A-N5	4.87	1.44	1.36
2	B	501	FNR	C1'-C2'	4.83	1.56	1.51
2	H	507	FNR	C4A-N5	4.78	1.44	1.36
2	F	505	FNR	C1'-C2'	4.75	1.56	1.51
2	A	502	FNR	C9A-N10	4.60	1.45	1.38
2	H	507	FNR	C9A-N10	4.59	1.45	1.38
2	C	504	FNR	C9A-N10	4.54	1.45	1.38
2	H	507	FNR	C1'-C2'	4.53	1.55	1.51
2	G	508	FNR	C4A-N5	4.51	1.43	1.36
2	D	503	FNR	C9A-N10	4.16	1.45	1.38
2	A	502	FNR	C4-N3	4.12	1.44	1.37
2	E	506	FNR	C4-N3	4.03	1.44	1.37
2	D	503	FNR	C4-N3	4.02	1.44	1.37
2	D	503	FNR	C5A-N5	4.02	1.44	1.36
2	F	505	FNR	C4-N3	4.00	1.43	1.37
2	A	502	FNR	C1'-C2'	3.95	1.55	1.51
2	G	508	FNR	C5A-N5	3.94	1.44	1.36
2	A	502	FNR	C5A-N5	3.86	1.44	1.36
2	B	501	FNR	C4-N3	3.84	1.43	1.37
2	C	504	FNR	C4-N3	3.83	1.43	1.37
2	F	505	FNR	C5A-N5	3.83	1.43	1.36
2	B	501	FNR	C5A-N5	3.82	1.43	1.36
2	E	506	FNR	C5A-N5	3.80	1.43	1.36
2	C	504	FNR	C5A-N5	3.78	1.43	1.36
2	D	503	FNR	C4'-C3'	3.77	1.61	1.53
2	H	507	FNR	C5A-N5	3.71	1.43	1.36
2	G	508	FNR	C4-N3	3.50	1.43	1.37
2	H	507	FNR	C4-N3	3.47	1.43	1.37
2	E	506	FNR	C1'-C2'	3.09	1.54	1.51
2	C	504	FNR	C2'-C3'	-3.04	1.47	1.53
2	G	508	FNR	C1'-C2'	2.92	1.54	1.51
2	G	508	FNR	C4'-C3'	2.87	1.59	1.53
2	G	508	FNR	C1'-N10	-2.77	1.45	1.48
2	A	502	FNR	C2'-C3'	-2.66	1.48	1.53
2	E	506	FNR	C6-C7	2.64	1.45	1.37
2	B	501	FNR	C5'-C4'	2.64	1.55	1.51
2	D	503	FNR	O3'-C3'	2.62	1.49	1.43
2	D	503	FNR	C6-C7	2.61	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	504	FNR	C6-C7	2.61	1.45	1.37
2	A	502	FNR	C6-C7	2.59	1.44	1.37
2	F	505	FNR	C6-C7	2.57	1.44	1.37
2	B	501	FNR	CAA-N10	2.57	1.44	1.38
2	G	508	FNR	CAA-N1	2.52	1.40	1.37
2	G	508	FNR	C9-C9A	2.47	1.45	1.40
2	B	501	FNR	C6-C7	2.46	1.44	1.37
2	H	507	FNR	CAA-N10	2.44	1.44	1.38
2	H	507	FNR	C6-C7	2.43	1.44	1.37
2	D	503	FNR	C1'-C2'	2.39	1.53	1.51
2	A	502	FNR	C5'-C4'	-2.37	1.47	1.51
2	E	506	FNR	C9-C9A	2.36	1.45	1.40
2	G	508	FNR	C6-C7	2.34	1.44	1.37
2	B	501	FNR	C9-C9A	2.33	1.45	1.40
2	F	505	FNR	C5'-C4'	2.30	1.55	1.51
2	F	505	FNR	C9-C9A	2.28	1.45	1.40
2	C	504	FNR	CAA-N10	2.26	1.43	1.38
2	E	506	FNR	CAA-N10	2.25	1.43	1.38
2	B	501	FNR	C4-C4A	2.24	1.44	1.41
2	B	501	FNR	C4'-C3'	2.23	1.58	1.53
2	C	504	FNR	C5'-C4'	-2.22	1.48	1.51
2	D	503	FNR	C1'-N10	-2.21	1.45	1.48
2	D	503	FNR	CAA-N10	2.20	1.43	1.38
2	F	505	FNR	CAA-N10	2.19	1.43	1.38
2	G	508	FNR	O3'-C3'	2.18	1.48	1.43
2	A	502	FNR	CAA-N10	2.17	1.43	1.38
2	D	503	FNR	C9-C9A	2.12	1.45	1.40
2	A	502	FNR	C9-C9A	2.11	1.44	1.40
2	F	505	FNR	C4'-C3'	2.10	1.57	1.53
2	E	506	FNR	O3'-C3'	2.10	1.48	1.43
2	G	508	FNR	CAA-N10	2.08	1.43	1.38
2	H	507	FNR	C5'-C4'	2.07	1.55	1.51
2	E	506	FNR	O4-C4	-2.07	1.20	1.24
2	C	504	FNR	C9-C9A	2.06	1.44	1.40
2	B	501	FNR	P-O2P	-2.05	1.44	1.51
2	E	506	FNR	C4-C4A	2.03	1.44	1.41

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	FNR	C5'-C4'-C3'	-8.71	95.62	112.06
2	A	502	FNR	C5'-C4'-C3'	-8.22	96.55	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	FNR	O1P-P-O5'	-5.52	91.42	106.65
2	B	501	FNR	C4-C4A-CAA	5.24	118.14	114.55
2	C	504	FNR	O1P-P-O5'	-5.23	92.21	106.65
2	C	504	FNR	C4-C4A-CAA	5.14	118.07	114.55
2	G	508	FNR	C5'-C4'-C3'	-5.12	102.40	112.06
2	D	503	FNR	C5'-C4'-C3'	-5.04	102.54	112.06
2	H	507	FNR	C4-C4A-CAA	5.02	117.99	114.55
2	F	505	FNR	C4-C4A-CAA	4.90	117.90	114.55
2	E	506	FNR	C4-C4A-CAA	4.80	117.84	114.55
2	G	508	FNR	C4-C4A-CAA	4.73	117.79	114.55
2	A	502	FNR	C4-C4A-CAA	4.71	117.77	114.55
2	D	503	FNR	C4-C4A-CAA	4.57	117.68	114.55
2	A	502	FNR	O3P-P-O2P	4.09	123.80	110.44
2	C	504	FNR	O3P-P-O2P	3.99	123.47	110.44
2	C	504	FNR	C4'-C3'-C2'	3.43	120.99	113.25
2	B	501	FNR	P-O5'-C5'	3.16	127.33	118.19
2	C	504	FNR	O4'-C4'-C5'	3.13	116.55	110.12
2	G	508	FNR	O4'-C4'-C5'	3.12	116.54	110.12
2	A	502	FNR	C4'-C3'-C2'	3.10	120.24	113.25
2	F	505	FNR	P-O5'-C5'	3.08	127.10	118.19
2	A	502	FNR	O4'-C4'-C5'	3.02	116.33	110.12
2	H	507	FNR	C1'-N10-CAA	3.00	121.94	118.93
2	F	505	FNR	O3P-P-O2P	2.94	120.07	110.44
2	H	507	FNR	O3P-P-O2P	2.94	120.03	110.44
2	B	501	FNR	O3P-P-O2P	2.86	119.79	110.44
2	E	506	FNR	O3P-P-O2P	2.84	119.72	110.44
2	A	502	FNR	C1'-C2'-C3'	-2.80	101.81	109.82
2	C	504	FNR	C1'-C2'-C3'	-2.77	101.88	109.82
2	D	503	FNR	C1'-N10-CAA	2.72	121.66	118.93
2	C	504	FNR	C1'-N10-CAA	2.72	121.66	118.93
2	D	503	FNR	O3P-P-O5'	-2.71	99.16	106.65
2	G	508	FNR	C4'-C3'-C2'	2.68	119.31	113.25
2	A	502	FNR	C1'-N10-CAA	2.65	121.59	118.93
2	E	506	FNR	O1P-P-O5'	-2.64	99.35	106.65
2	H	507	FNR	O1P-P-O5'	-2.64	99.36	106.65
2	D	503	FNR	C4'-C3'-C2'	2.62	119.18	113.25
2	B	501	FNR	C4-N3-C2	-2.61	120.07	125.36
2	C	504	FNR	C2'-C1'-N10	2.60	115.90	112.45
2	F	505	FNR	C4-N3-C2	-2.52	120.24	125.36
2	E	506	FNR	C4-N3-C2	-2.52	120.25	125.36
2	H	507	FNR	P-O5'-C5'	2.50	125.42	118.19
2	D	503	FNR	C4-N3-C2	-2.49	120.32	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	506	FNR	C1'-N10-CAA	2.48	121.42	118.93
2	C	504	FNR	C4-N3-C2	-2.48	120.34	125.36
2	A	502	FNR	C4-N3-C2	-2.47	120.35	125.36
2	H	507	FNR	C4-N3-C2	-2.44	120.42	125.36
2	F	505	FNR	O1P-P-O5'	-2.41	99.99	106.65
2	D	503	FNR	C1'-N10-C9A	-2.40	116.54	118.87
2	D	503	FNR	C8M-C8-C9	-2.40	114.59	120.38
2	H	507	FNR	C2'-C1'-N10	2.36	115.58	112.45
2	D	503	FNR	O4'-C4'-C5'	2.35	114.96	110.12
2	E	506	FNR	P-O5'-C5'	2.35	124.98	118.19
2	F	505	FNR	C2'-C1'-N10	2.33	115.54	112.45
2	B	501	FNR	C1'-N10-CAA	2.29	121.23	118.93
2	G	508	FNR	C4-N3-C2	-2.27	120.75	125.36
2	A	502	FNR	C2'-C1'-N10	2.25	115.43	112.45
2	H	507	FNR	C8M-C8-C9	-2.18	115.12	120.38
2	G	508	FNR	O3'-C3'-C2'	-2.17	103.25	108.74
2	A	502	FNR	O3P-P-O5'	2.15	112.59	106.65
2	A	502	FNR	C8M-C8-C9	-2.15	115.20	120.38
2	G	508	FNR	C2'-C1'-N10	2.14	115.30	112.45
2	C	504	FNR	O3P-P-O5'	2.14	112.54	106.65
2	D	503	FNR	C4A-CAA-N1	2.13	121.57	118.87
2	G	508	FNR	C4A-CAA-N1	2.12	121.56	118.87
2	G	508	FNR	C1'-C2'-C3'	-2.11	103.77	109.82
2	B	501	FNR	C8M-C8-C9	-2.11	115.29	120.38
2	E	506	FNR	C8M-C8-C9	-2.10	115.31	120.38
2	F	505	FNR	C8M-C8-C9	-2.08	115.37	120.38
2	G	508	FNR	C8M-C8-C9	-2.06	115.41	120.38
2	A	502	FNR	O4'-C4'-C3'	2.05	114.16	109.05
2	C	504	FNR	C1'-N10-C9A	-2.05	116.88	118.87
2	C	504	FNR	C8M-C8-C9	-2.04	115.46	120.38
2	D	503	FNR	C8M-C8-C7	2.04	125.45	120.74
2	B	501	FNR	C9A-C5A-N5	2.03	120.48	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/230 (95%)	-0.31	0 100 100	9, 16, 30, 42	0
1	B	219/230 (95%)	-0.31	1 (0%) 88 91	9, 18, 29, 43	0
1	C	219/230 (95%)	-0.23	1 (0%) 88 91	11, 20, 36, 48	0
1	D	219/230 (95%)	-0.24	1 (0%) 88 91	11, 19, 31, 39	0
1	E	219/230 (95%)	-0.35	0 100 100	9, 16, 28, 38	0
1	F	219/230 (95%)	-0.25	2 (0%) 81 85	10, 18, 30, 42	0
1	G	219/230 (95%)	-0.24	2 (0%) 81 85	12, 21, 37, 46	0
1	H	219/230 (95%)	-0.32	0 100 100	11, 19, 31, 42	0
All	All	1752/1840 (95%)	-0.28	7 (0%) 90 92	9, 18, 32, 48	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	LEU	3.4
1	F	197	ARG	2.3
1	D	98	GLU	2.2
1	G	169	PHE	2.2
1	B	169	PHE	2.2
1	C	9	LEU	2.1
1	F	169	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FNR	B	501	31/31	0.14	2.32	13,17,24,27	0
2	FNR	A	502	31/31	0.13	1.72	12,17,20,24	0
2	FNR	E	506	31/31	0.14	1.64	12,17,31,36	0
2	FNR	D	503	31/31	0.14	1.31	11,17,28,31	0
2	FNR	C	504	31/31	0.15	1.30	14,18,23,27	0
2	FNR	G	508	31/31	0.13	1.13	10,15,30,32	0
2	FNR	H	507	31/31	0.14	1.02	8,13,27,31	0
2	FNR	F	505	31/31	0.12	0.62	14,17,24,28	0

6.5 Other polymers

There are no such residues in this entry.