



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:03 PM GMT

PDB ID : 2ISL
Title : BluB bound to reduced flavin (FMNH₂) 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 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>

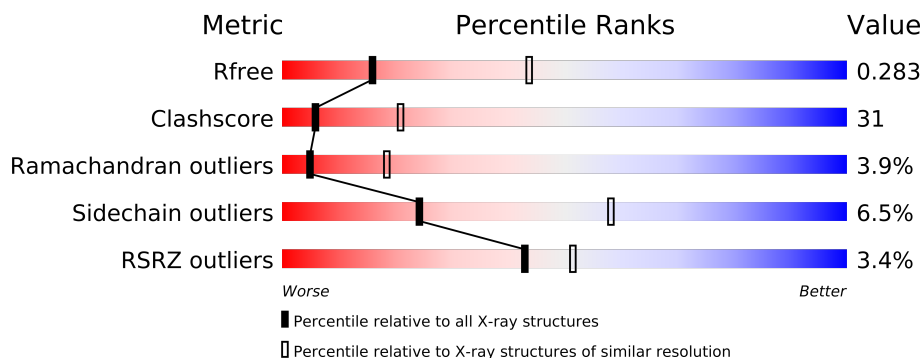
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 ≥ 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
3	OXY	C	605	-	X

2 Entry composition

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

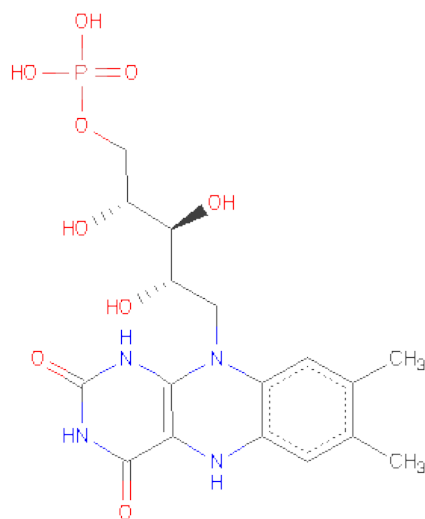
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
A	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
A	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
B	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
B	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
B	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
C	-2	GLY	-	CLONING ARTIFACT	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: $C_{17}H_{23}N_4O_9P$).



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: O₂).



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.

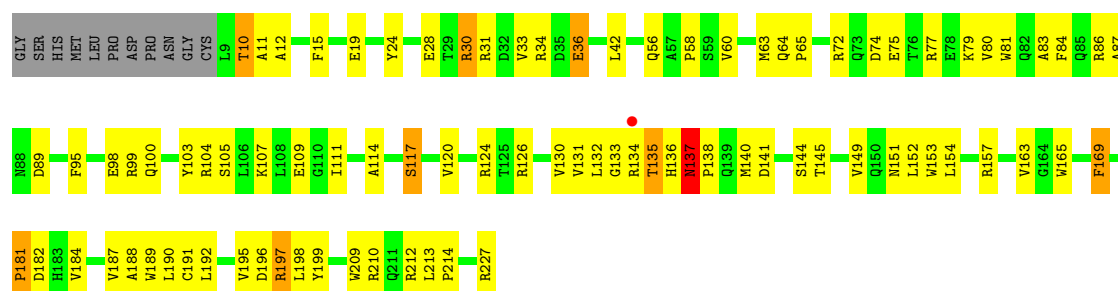
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	13	Total 13	O 13	0	0
4	C	12	Total 12	O 12	0	0
4	D	10	Total 10	O 10	0	0
4	E	4	Total 4	O 4	0	0
4	F	2	Total 2	O 2	0	0
4	G	7	Total 7	O 7	0	0
4	H	3	Total 3	O 3	0	0

3 Residue-property plots

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.

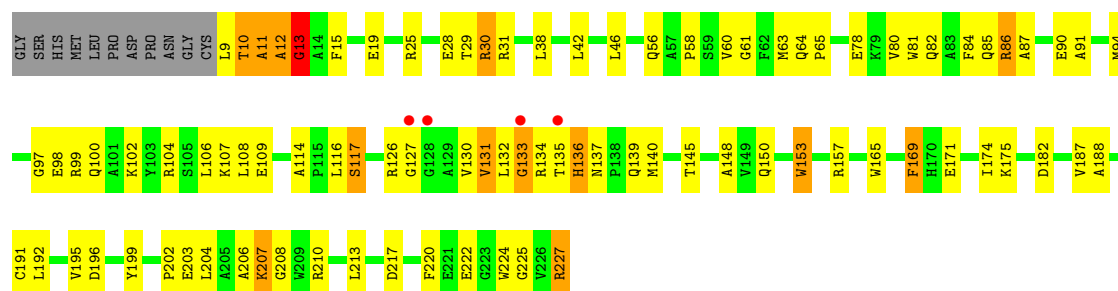
• Molecule 1: BluB

Chain A:



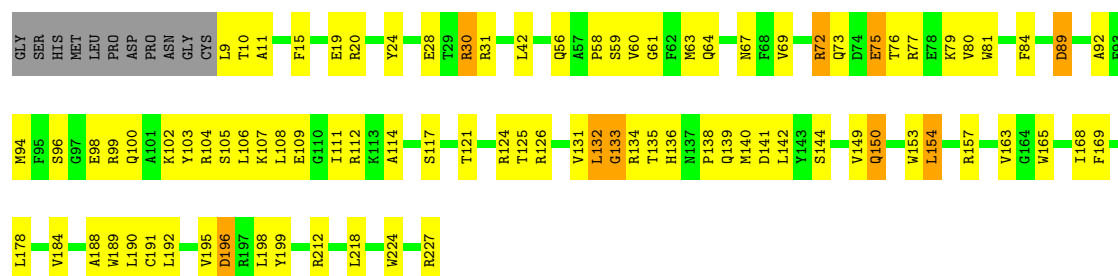
• Molecule 1: BluB

Chain B:



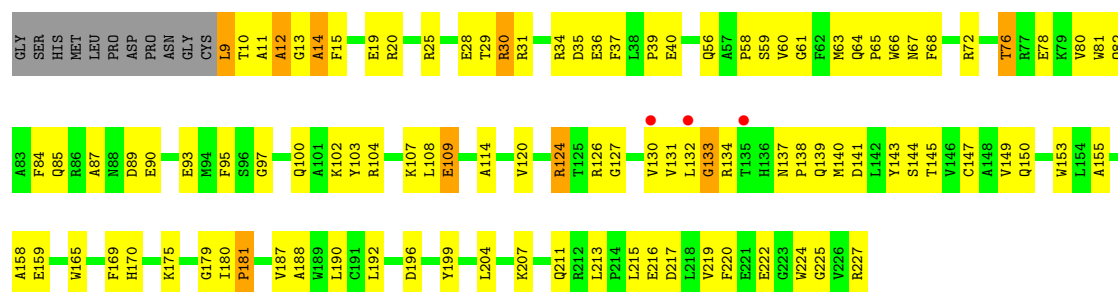
• Molecule 1: BluB

Chain C:



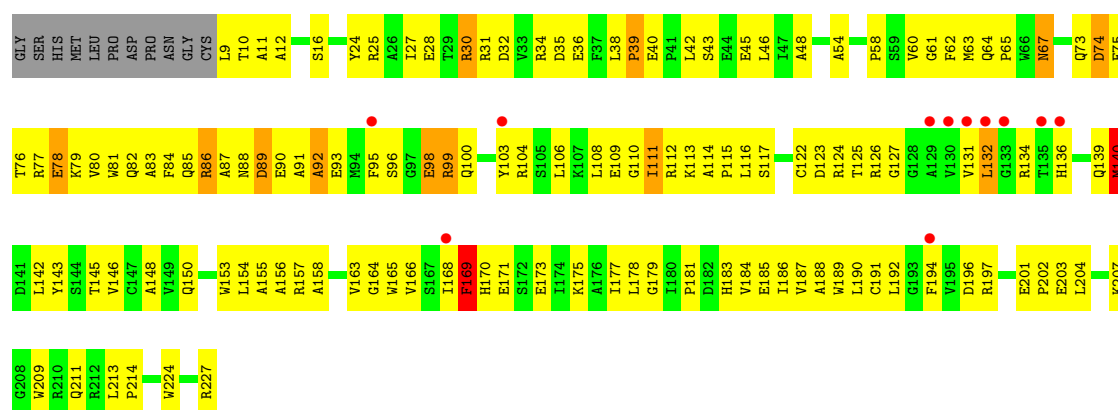
• Molecule 1: BluB

Chain D:



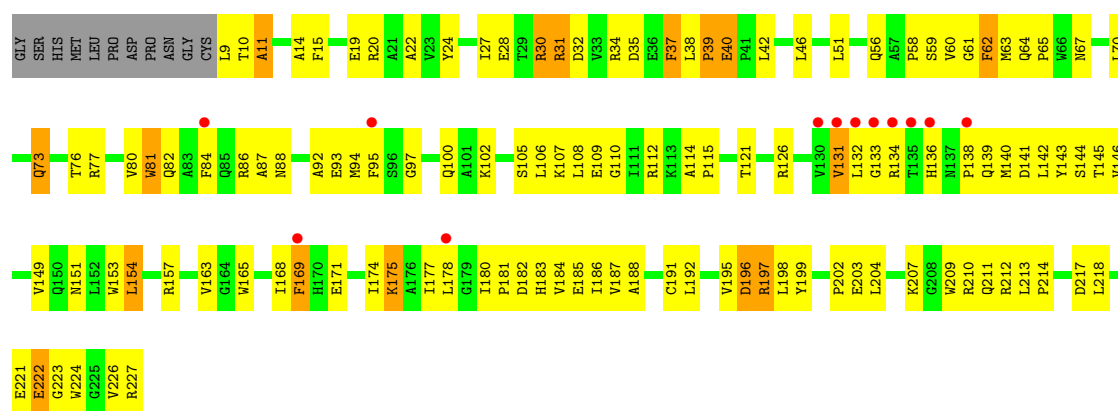
• Molecule 1: BluB

Chain E:



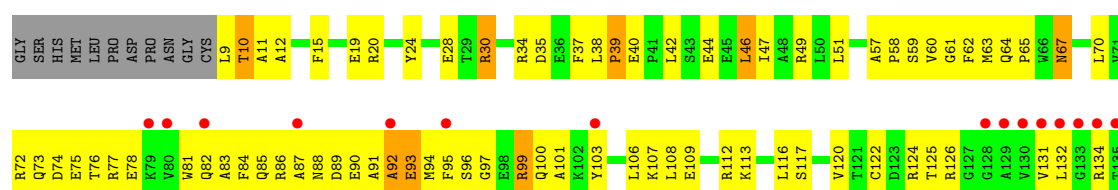
• Molecule 1: BluB

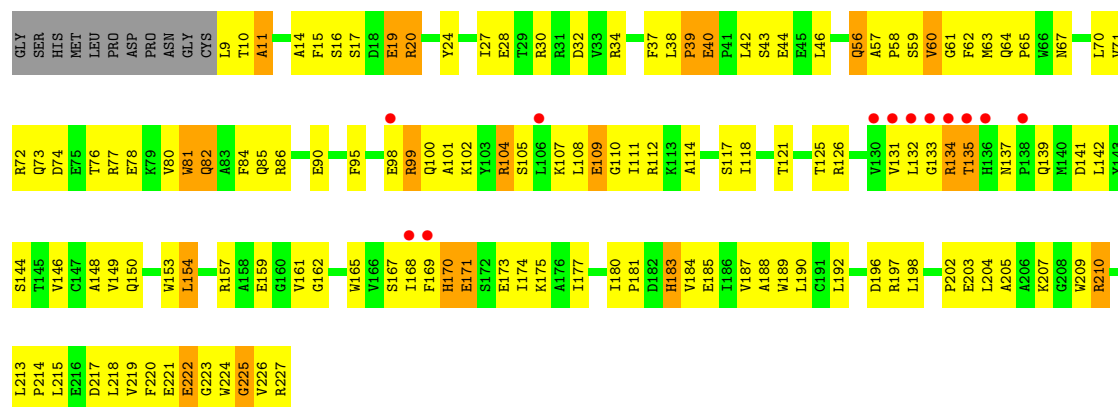
Chain F:



• Molecule 1: BluB

Chain G:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 96.2 (49.03-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	41.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -1.1	EDS
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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, 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 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	102	0
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

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 31.

All (877) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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%)	10	36
1	B	217/230 (94%)	196 (90%)	12 (6%)	9 (4%)	4	17
1	C	217/230 (94%)	200 (92%)	15 (7%)	2 (1%)	25	66
1	D	217/230 (94%)	190 (88%)	18 (8%)	9 (4%)	4	17
1	E	217/230 (94%)	182 (84%)	25 (12%)	10 (5%)	4	14
1	F	217/230 (94%)	178 (82%)	28 (13%)	11 (5%)	3	10
1	G	217/230 (94%)	180 (83%)	26 (12%)	11 (5%)	3	10
1	H	217/230 (94%)	184 (85%)	22 (10%)	11 (5%)	3	10
All	All	1736/1840 (94%)	1511 (87%)	157 (9%)	68 (4%)	5	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	30	66
1	B	178/187 (95%)	172 (97%)	6 (3%)	49	86
1	C	178/187 (95%)	165 (93%)	13 (7%)	20	51
1	D	178/187 (95%)	169 (95%)	9 (5%)	33	72
1	E	178/187 (95%)	164 (92%)	14 (8%)	18	46
1	F	178/187 (95%)	165 (93%)	13 (7%)	20	51
1	G	178/187 (95%)	166 (93%)	12 (7%)	23	56
1	H	178/187 (95%)	163 (92%)	15 (8%)	16	42
All	All	1424/1496 (95%)	1332 (94%)	92 (6%)	24	58

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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 ⓘ

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	-	33,33,33	1.95	9 (27%)	44,50,50	1.33	5 (11%)
3	OXY	A	606	-	1,1,1	1.34	0	0,0,0	0.00	-
2	FNR	B	501	-	33,33,33	2.03	9 (27%)	44,50,50	1.31	5 (11%)
3	OXY	B	602	-	1,1,1	1.20	0	0,0,0	0.00	-
2	FNR	C	504	-	33,33,33	1.99	9 (27%)	44,50,50	1.28	5 (11%)
3	OXY	C	605	-	1,1,1	1.34	0	0,0,0	0.00	-
2	FNR	D	503	-	33,33,33	2.03	8 (24%)	44,50,50	1.27	4 (9%)
3	OXY	D	601	-	1,1,1	1.10	0	0,0,0	0.00	-
2	FNR	E	506	-	33,33,33	1.95	8 (24%)	44,50,50	1.21	4 (9%)
3	OXY	E	607	-	1,1,1	1.32	0	0,0,0	0.00	-
2	FNR	F	505	-	33,33,33	1.99	8 (24%)	44,50,50	1.22	5 (11%)
3	OXY	F	608	-	1,1,1	1.35	0	0,0,0	0.00	-
2	FNR	G	508	-	33,33,33	1.95	9 (27%)	44,50,50	1.29	5 (11%)
3	OXY	G	603	-	1,1,1	1.22	0	0,0,0	0.00	-
2	FNR	H	507	-	33,33,33	2.00	9 (27%)	44,50,50	1.22	4 (9%)
3	OXY	H	604	-	1,1,1	1.24	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	0/0/3/3
3	OXY	A	606	-	-	0/0/0/0	0/0/0/0
2	FNR	B	501	-	-	0/18/18/18	0/0/3/3
3	OXY	B	602	-	-	0/0/0/0	0/0/0/0
2	FNR	C	504	-	-	0/18/18/18	0/0/3/3
3	OXY	C	605	-	-	0/0/0/0	0/0/0/0
2	FNR	D	503	-	-	0/18/18/18	0/0/3/3
3	OXY	D	601	-	-	0/0/0/0	0/0/0/0
2	FNR	E	506	-	-	0/18/18/18	0/0/3/3
3	OXY	E	607	-	-	0/0/0/0	0/0/0/0
2	FNR	F	505	-	-	0/18/18/18	0/0/3/3
3	OXY	F	608	-	-	0/0/0/0	0/0/0/0
2	FNR	G	508	-	-	0/18/18/18	0/0/3/3
3	OXY	G	603	-	-	0/0/0/0	0/0/0/0
2	FNR	H	507	-	-	0/18/18/18	0/0/3/3
3	OXY	H	604	-	-	0/0/0/0	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	508	FNR	C4-C4A	7.05	1.52	1.41
2	B	501	FNR	C4-C4A	6.93	1.52	1.41
2	F	505	FNR	C4-C4A	6.82	1.52	1.41
2	H	507	FNR	C4-C4A	6.73	1.52	1.41
2	C	504	FNR	C4-C4A	6.50	1.51	1.41
2	E	506	FNR	C4-C4A	6.35	1.51	1.41
2	D	503	FNR	C4-C4A	6.28	1.51	1.41
2	A	502	FNR	C4-C4A	5.97	1.51	1.41
2	A	502	FNR	C2-N3	3.98	1.45	1.37
2	D	503	FNR	C4A-CAA	3.96	1.49	1.39
2	D	503	FNR	C1'-C2'	3.86	1.55	1.51
2	F	505	FNR	C2-N3	3.82	1.44	1.37
2	F	505	FNR	C4A-CAA	3.68	1.48	1.39
2	D	503	FNR	C2-N3	3.65	1.44	1.37
2	C	504	FNR	C4A-CAA	3.62	1.48	1.39
2	H	507	FNR	C4A-CAA	3.61	1.48	1.39
2	B	501	FNR	C2-N3	3.58	1.44	1.37
2	E	506	FNR	C4A-CAA	3.56	1.48	1.39
2	A	502	FNR	C4A-CAA	3.55	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FNR	C1'-C2'	3.53	1.54	1.51
2	B	501	FNR	C4A-CAA	3.52	1.48	1.39
2	E	506	FNR	C2-N3	3.51	1.44	1.37
2	G	508	FNR	C4A-CAA	3.49	1.48	1.39
2	G	508	FNR	C2-N3	3.49	1.44	1.37
2	C	504	FNR	C2-N3	3.47	1.44	1.37
2	H	507	FNR	C2-N3	3.45	1.44	1.37
2	E	506	FNR	C1'-C2'	3.38	1.54	1.51
2	A	502	FNR	C1'-C2'	3.16	1.54	1.51
2	F	505	FNR	C4-N3	3.09	1.42	1.37
2	C	504	FNR	C5'-C4'	3.01	1.56	1.51
2	C	504	FNR	P-O1P	-2.97	1.43	1.54
2	H	507	FNR	C1'-C2'	2.96	1.54	1.51
2	A	502	FNR	P-O1P	-2.95	1.43	1.54
2	C	504	FNR	C1'-C2'	2.90	1.54	1.51
2	G	508	FNR	C1'-C2'	2.83	1.54	1.51
2	H	507	FNR	P-O1P	-2.72	1.44	1.54
2	E	506	FNR	CAA-N1	-2.72	1.33	1.37
2	D	503	FNR	C9A-N10	2.67	1.42	1.38
2	E	506	FNR	C9A-N10	2.65	1.42	1.38
2	H	507	FNR	C9A-N10	2.64	1.42	1.38
2	D	503	FNR	P-O1P	-2.64	1.45	1.54
2	A	502	FNR	C4-N3	2.59	1.41	1.37
2	A	502	FNR	C5'-C4'	2.57	1.55	1.51
2	E	506	FNR	C4-N3	2.56	1.41	1.37
2	H	507	FNR	C4-N3	2.55	1.41	1.37
2	E	506	FNR	P-O1P	-2.51	1.45	1.54
2	G	508	FNR	P-O1P	-2.51	1.45	1.54
2	G	508	FNR	C4-N3	2.42	1.41	1.37
2	C	504	FNR	C9A-N10	2.40	1.42	1.38
2	F	505	FNR	P-O1P	-2.35	1.46	1.54
2	B	501	FNR	C4-N3	2.32	1.41	1.37
2	C	504	FNR	CAA-N1	-2.29	1.34	1.37
2	B	501	FNR	P-O1P	-2.28	1.46	1.54
2	G	508	FNR	CAA-N1	-2.27	1.34	1.37
2	F	505	FNR	C1'-C2'	2.27	1.53	1.51
2	C	504	FNR	C4-N3	2.26	1.41	1.37
2	G	508	FNR	C9A-N10	2.24	1.42	1.38
2	A	502	FNR	CAA-N1	-2.23	1.34	1.37
2	F	505	FNR	CAA-N1	-2.23	1.34	1.37
2	A	502	FNR	C9A-N10	2.20	1.42	1.38
2	H	507	FNR	C5'-C4'	2.19	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FNR	C1'-N10	-2.18	1.45	1.48
2	F	505	FNR	C6-C5A	2.16	1.45	1.39
2	B	501	FNR	C2'-C3'	-2.15	1.49	1.53
2	B	501	FNR	C6-C5A	2.13	1.45	1.39
2	H	507	FNR	CAA-N1	-2.12	1.34	1.37
2	D	503	FNR	C6-C5A	2.10	1.45	1.39
2	G	508	FNR	C6-C5A	2.09	1.45	1.39
2	D	503	FNR	C4-N3	2.09	1.40	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	506	FNR	C4A-CAA-N1	3.73	123.61	118.87
2	B	501	FNR	C4A-CAA-N1	3.59	123.42	118.87
2	A	502	FNR	C4A-CAA-N1	3.54	123.36	118.87
2	F	505	FNR	C4A-CAA-N1	3.52	123.33	118.87
2	G	508	FNR	C4A-CAA-N1	3.48	123.29	118.87
2	D	503	FNR	C4-C4A-CAA	3.48	116.93	114.55
2	A	502	FNR	C9A-C5A-N5	3.39	122.30	117.75
2	H	507	FNR	C4A-CAA-N1	3.34	123.10	118.87
2	C	504	FNR	C9A-C5A-N5	3.33	122.23	117.75
2	C	504	FNR	C4A-CAA-N1	3.28	123.03	118.87
2	D	503	FNR	C9A-C5A-N5	3.24	122.10	117.75
2	H	507	FNR	C9A-C5A-N5	3.22	122.08	117.75
2	B	501	FNR	C9A-C5A-N5	3.13	121.96	117.75
2	G	508	FNR	C9A-C5A-N5	3.11	121.93	117.75
2	E	506	FNR	C9A-C5A-N5	3.11	121.92	117.75
2	F	505	FNR	C9A-C5A-N5	3.08	121.89	117.75
2	D	503	FNR	C4A-CAA-N1	2.97	122.63	118.87
2	A	502	FNR	C4-C4A-CAA	2.89	116.53	114.55
2	C	504	FNR	O3P-P-O5'	2.88	114.59	106.65
2	A	502	FNR	O3P-P-O5'	2.70	114.10	106.65
2	E	506	FNR	C4-C4A-CAA	2.60	116.33	114.55
2	C	504	FNR	C4-C4A-CAA	2.59	116.32	114.55
2	F	505	FNR	C4-C4A-CAA	2.59	116.32	114.55
2	G	508	FNR	C4-C4A-CAA	2.58	116.32	114.55
2	B	501	FNR	C4-C4A-CAA	2.53	116.28	114.55
2	H	507	FNR	C4-C4A-CAA	2.47	116.24	114.55
2	D	503	FNR	CAA-C4A-N5	2.44	122.77	117.77
2	E	506	FNR	CAA-C4A-N5	2.44	122.77	117.77
2	C	504	FNR	CAA-C4A-N5	2.42	122.72	117.77
2	A	502	FNR	CAA-C4A-N5	2.40	122.70	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	505	FNR	O3P-P-O5'	2.34	113.10	106.65
2	H	507	FNR	CAA-C4A-N5	2.32	122.52	117.77
2	G	508	FNR	O3P-P-O5'	2.31	113.03	106.65
2	G	508	FNR	CAA-C4A-N5	2.25	122.39	117.77
2	F	505	FNR	CAA-C4A-N5	2.24	122.36	117.77
2	B	501	FNR	O3P-P-O5'	2.22	112.78	106.65
2	B	501	FNR	CAA-C4A-N5	2.16	122.19	117.77

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%)	-0.52	1 (0%) 88 93	5, 19, 49, 71	0
1	B	219/230 (95%)	-0.38	4 (1%) 65 74	7, 23, 50, 75	0
1	C	219/230 (95%)	-0.51	0 100 100	6, 18, 48, 67	0
1	D	219/230 (95%)	-0.40	3 (1%) 72 80	6, 22, 50, 78	0
1	E	219/230 (95%)	0.26	11 (5%) 28 33	23, 50, 83, 88	0
1	F	219/230 (95%)	0.15	12 (5%) 24 29	23, 47, 76, 88	0
1	G	219/230 (95%)	0.32	17 (7%) 13 16	19, 48, 83, 89	0
1	H	219/230 (95%)	0.14	12 (5%) 24 29	21, 48, 79, 89	0
All	All	1752/1840 (95%)	-0.12	60 (3%) 43 51	5, 32, 77, 89	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	131	VAL	7.8
1	E	133	GLY	7.4
1	F	130	VAL	6.1
1	E	168	ILE	5.9
1	G	133	GLY	5.9
1	H	130	VAL	5.7
1	G	136	HIS	5.7
1	E	132	LEU	5.6
1	F	133	GLY	5.5
1	E	131	VAL	5.3
1	E	135	THR	5.3
1	G	132	LEU	5.2
1	F	134	ARG	5.1
1	G	130	VAL	4.9
1	G	129	ALA	4.8
1	F	132	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	136	HIS	4.8
1	F	136	HIS	4.7
1	B	133	GLY	4.5
1	F	131	VAL	4.5
1	H	131	VAL	4.3
1	G	128	GLY	4.2
1	D	130	VAL	4.2
1	H	133	GLY	4.1
1	G	169	PHE	3.8
1	D	135	THR	3.7
1	H	136	HIS	3.6
1	G	135	THR	3.5
1	H	134	ARG	3.2
1	G	134	ARG	3.2
1	G	103	TYR	3.1
1	G	95	PHE	3.1
1	G	80	VAL	3.0
1	E	130	VAL	3.0
1	B	127	GLY	2.9
1	H	132	LEU	2.7
1	F	95	PHE	2.7
1	E	103	TYR	2.6
1	F	135	THR	2.5
1	F	169	PHE	2.5
1	D	132	LEU	2.5
1	F	138	PRO	2.4
1	E	129	ALA	2.4
1	B	128	GLY	2.4
1	H	98	GLU	2.4
1	H	135	THR	2.2
1	H	169	PHE	2.2
1	G	92	ALA	2.2
1	B	135	THR	2.2
1	G	82	GLN	2.2
1	G	87	ALA	2.1
1	E	95	PHE	2.1
1	E	194	PHE	2.1
1	G	79	LYS	2.1
1	F	178	LEU	2.1
1	H	168	ILE	2.1
1	F	84	PHE	2.1
1	A	134	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	106	LEU	2.0
1	H	138	PRO	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 ⓘ

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
3	OXY	C	605	2/2	0.28	2.59	18,18,18,19	0
3	OXY	A	606	2/2	0.25	1.10	21,21,21,22	0
2	FNR	D	503	31/31	0.16	0.41	20,24,26,28	0
2	FNR	G	508	31/31	0.19	0.19	38,45,49,50	0
2	FNR	C	504	31/31	0.16	0.14	23,28,30,30	0
2	FNR	A	502	31/31	0.17	0.08	18,25,29,30	0
2	FNR	B	501	31/31	0.15	-0.00	23,28,31,31	0
3	OXY	D	601	2/2	0.19	-0.03	10,10,10,11	0
2	FNR	E	506	31/31	0.19	-0.07	44,50,52,54	0
3	OXY	B	602	2/2	0.18	-0.28	8,8,8,9	0
3	OXY	H	604	2/2	0.20	-0.41	32,32,32,32	0
2	FNR	F	505	31/31	0.17	-0.52	37,44,47,50	0
2	FNR	H	507	31/31	0.14	-0.64	34,39,41,43	0
3	OXY	F	608	2/2	0.16	-0.68	33,33,33,35	0
3	OXY	G	603	2/2	0.18	-0.71	27,27,27,27	0
3	OXY	E	607	2/2	0.23	-0.80	25,25,25,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.