



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:54 PM GMT

PDB ID : 3EGC
Title : Crystal structure of a putative ribose operon repressor from *Burkholderia thailandensis*
Authors : Bonanno, J.B.; Patskovsky, Y.; Gilmore, M.; Bain, K.T.; Hu, S.; Romero, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-09-10
Resolution : 2.35 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>

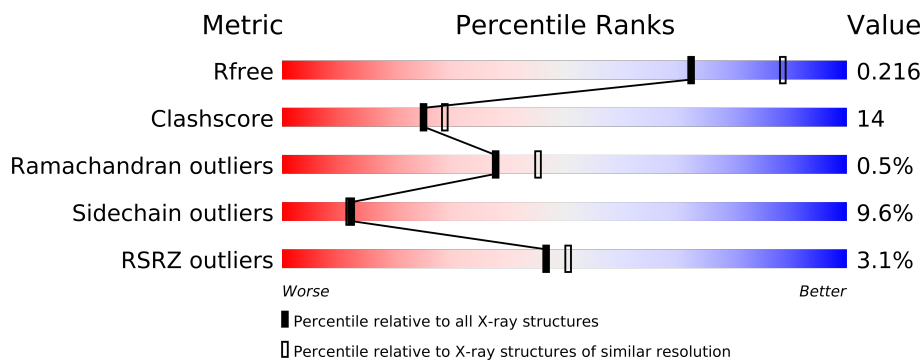
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	291	
1	B	291	
1	C	291	
1	D	291	
1	E	291	
1	F	291	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12302 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 putative ribose operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2006	1257	372	368	9			
1	B	261	Total	C	N	O	S	0	1	0
			2013	1262	374	368	9			
1	C	261	Total	C	N	O	S	0	0	0
			2006	1257	372	368	9			
1	D	262	Total	C	N	O	S	0	0	0
			2011	1260	373	369	9			
1	E	261	Total	C	N	O	S	0	0	0
			2006	1257	372	368	9			
1	F	262	Total	C	N	O	S	0	0	0
			2011	1260	373	369	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	expression tag	UNP Q2T0D1
A	344	GLY	-	expression tag	UNP Q2T0D1
A	345	HIS	-	expression tag	UNP Q2T0D1
A	346	HIS	-	expression tag	UNP Q2T0D1
A	347	HIS	-	expression tag	UNP Q2T0D1
A	348	HIS	-	expression tag	UNP Q2T0D1
A	349	HIS	-	expression tag	UNP Q2T0D1
A	350	HIS	-	expression tag	UNP Q2T0D1
B	60	MET	-	expression tag	UNP Q2T0D1
B	344	GLY	-	expression tag	UNP Q2T0D1
B	345	HIS	-	expression tag	UNP Q2T0D1
B	346	HIS	-	expression tag	UNP Q2T0D1
B	347	HIS	-	expression tag	UNP Q2T0D1
B	348	HIS	-	expression tag	UNP Q2T0D1
B	349	HIS	-	expression tag	UNP Q2T0D1
B	350	HIS	-	expression tag	UNP Q2T0D1
C	60	MET	-	expression tag	UNP Q2T0D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	344	GLY	-	expression tag	UNP Q2T0D1
C	345	HIS	-	expression tag	UNP Q2T0D1
C	346	HIS	-	expression tag	UNP Q2T0D1
C	347	HIS	-	expression tag	UNP Q2T0D1
C	348	HIS	-	expression tag	UNP Q2T0D1
C	349	HIS	-	expression tag	UNP Q2T0D1
C	350	HIS	-	expression tag	UNP Q2T0D1
D	60	MET	-	expression tag	UNP Q2T0D1
D	344	GLY	-	expression tag	UNP Q2T0D1
D	345	HIS	-	expression tag	UNP Q2T0D1
D	346	HIS	-	expression tag	UNP Q2T0D1
D	347	HIS	-	expression tag	UNP Q2T0D1
D	348	HIS	-	expression tag	UNP Q2T0D1
D	349	HIS	-	expression tag	UNP Q2T0D1
D	350	HIS	-	expression tag	UNP Q2T0D1
E	60	MET	-	expression tag	UNP Q2T0D1
E	344	GLY	-	expression tag	UNP Q2T0D1
E	345	HIS	-	expression tag	UNP Q2T0D1
E	346	HIS	-	expression tag	UNP Q2T0D1
E	347	HIS	-	expression tag	UNP Q2T0D1
E	348	HIS	-	expression tag	UNP Q2T0D1
E	349	HIS	-	expression tag	UNP Q2T0D1
E	350	HIS	-	expression tag	UNP Q2T0D1
F	60	MET	-	expression tag	UNP Q2T0D1
F	344	GLY	-	expression tag	UNP Q2T0D1
F	345	HIS	-	expression tag	UNP Q2T0D1
F	346	HIS	-	expression tag	UNP Q2T0D1
F	347	HIS	-	expression tag	UNP Q2T0D1
F	348	HIS	-	expression tag	UNP Q2T0D1
F	349	HIS	-	expression tag	UNP Q2T0D1
F	350	HIS	-	expression tag	UNP Q2T0D1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	52	Total O 52 52	0	0
2	C	56	Total O 56 56	0	0
2	D	46	Total O 46 46	0	0

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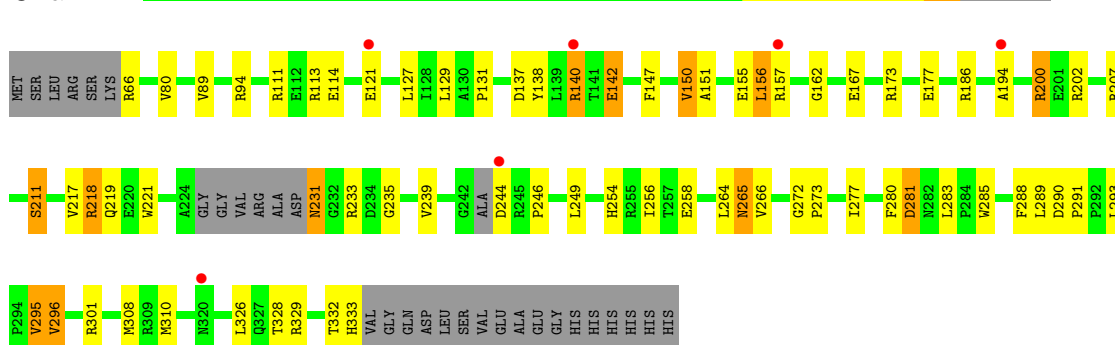
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	29	Total	O	0	0
			29	29		
2	F	19	Total	O	0	0
			19	19		

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.

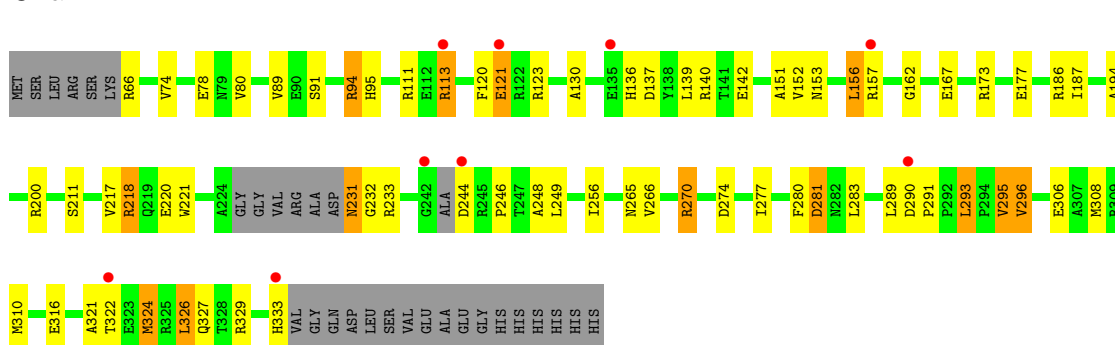
- Molecule 1: putative ribose operon repressor

Chain A:



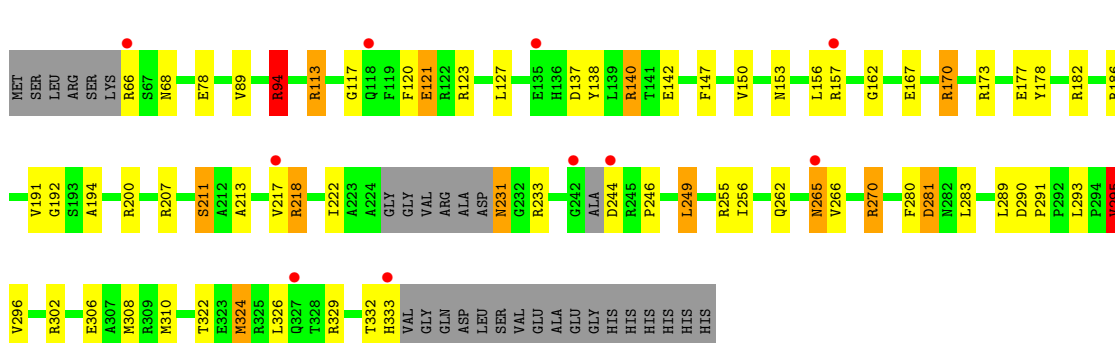
- Molecule 1: putative ribose operon repressor

Chain B:



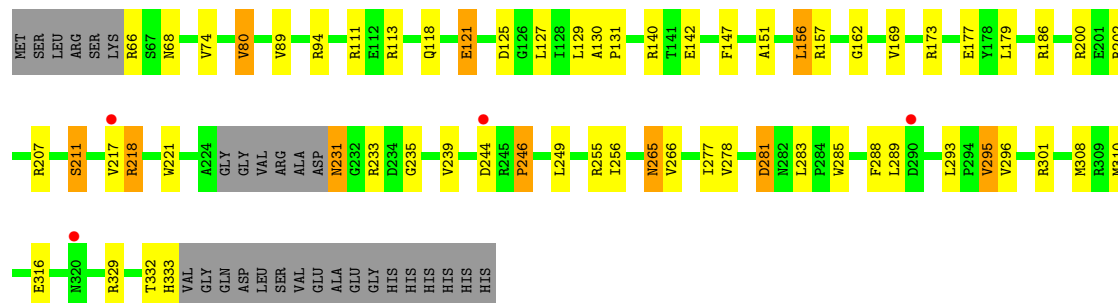
- Molecule 1: putative ribose operon repressor

Chain C:



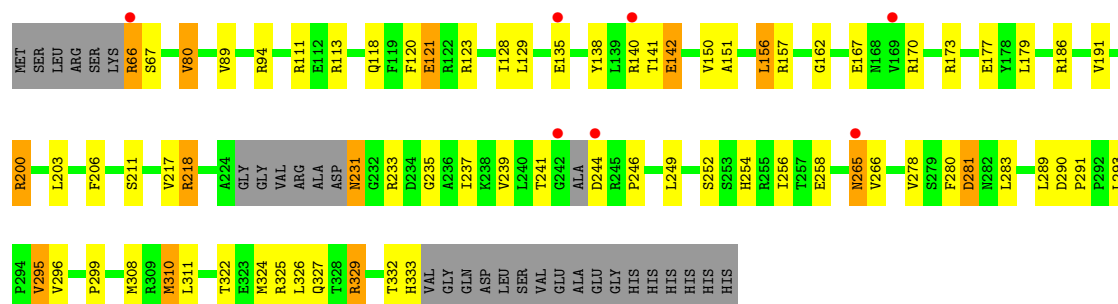
- Molecule 1: putative ribose operon repressor

Chain D:



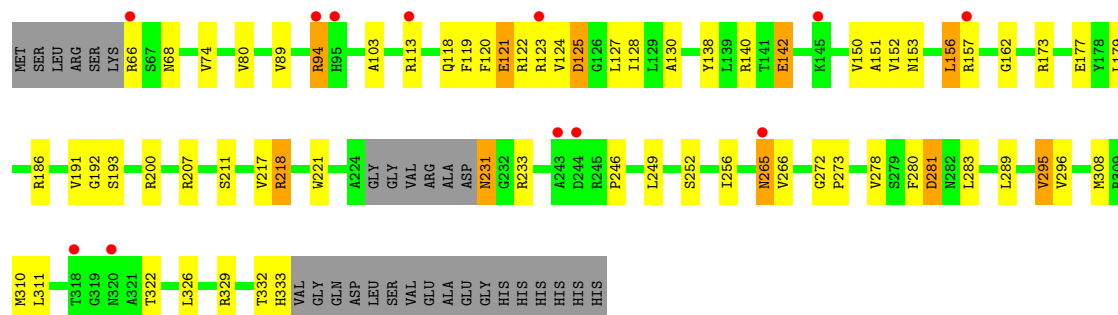
- Molecule 1: putative ribose operon repressor

Chain E:



- Molecule 1: putative ribose operon repressor

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.71Å 288.65Å 63.35Å 90.00° 113.59° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 46.47 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.35) 98.0 (46.47-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.95 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.257 , 0.299 0.204 , 0.216	Depositor DCC
R_{free} test set	3379 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.1	EDS
Estimated twinning fraction	0.397 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 67642 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.05	3/2038 (0.1%)	0.92	3/2756 (0.1%)
1	B	0.95	0/2049	0.99	6/2771 (0.2%)
1	C	0.91	1/2038 (0.0%)	0.96	10/2756 (0.4%)
1	D	0.94	1/2044 (0.0%)	0.89	3/2766 (0.1%)
1	E	0.92	0/2038	0.91	4/2756 (0.1%)
1	F	0.95	0/2044	0.89	2/2766 (0.1%)
All	All	0.95	5/12251 (0.0%)	0.93	28/16571 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLU	CD-OE1	-12.01	1.12	1.25
1	A	155	GLU	CD-OE2	-11.95	1.12	1.25
1	D	80	VAL	CB-CG2	-7.82	1.36	1.52
1	A	150	VAL	CB-CG2	-5.52	1.41	1.52
1	C	140	ARG	CG-CD	-5.09	1.39	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	ARG	NE-CZ-NH1	-16.66	111.97	120.30
1	A	155	GLU	OE1-CD-OE2	-16.62	103.35	123.30
1	B	113	ARG	NE-CZ-NH2	16.02	128.31	120.30
1	C	94	ARG	NE-CZ-NH1	-13.33	113.63	120.30
1	C	94	ARG	NE-CZ-NH2	12.34	126.47	120.30
1	D	94	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	B	94	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	E	94	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	F	94	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	113	ARG	CD-NE-CZ	7.04	133.46	123.60
1	E	325	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	94	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	202	ARG	NE-CZ-NH2	-6.62	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	310	MET	CG-SD-CE	6.53	110.64	100.20
1	C	270	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	270	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	E	94	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	94	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	F	125	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	155	GLU	CG-CD-OE2	5.87	130.03	118.30
1	C	113	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	170	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	113	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	295	VAL	CB-CA-C	-5.51	100.94	111.40
1	C	249	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	202	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	94	ARG	CG-CD-NE	5.28	122.88	111.80
1	C	94	ARG	CD-NE-CZ	5.16	130.82	123.60

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	2006	0	2028	81	0
1	B	2013	0	2035	76	1
1	C	2006	0	2028	61	2
1	D	2011	0	2034	40	0
1	E	2006	0	2028	85	1
1	F	2011	0	2034	49	1
2	A	47	0	0	3	0
2	B	52	0	0	8	0
2	C	56	0	0	9	0
2	D	46	0	0	3	1
2	E	29	0	0	4	0
2	F	19	0	0	4	0
All	All	12302	0	12187	335	4

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 14.

All (335) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:162:GLY:HA3	1:E:310:MET:CE	1.24	1.63
1:F:162:GLY:HA3	1:F:310:MET:CE	1.49	1.43
1:D:162:GLY:HA3	1:D:310:MET:CE	1.55	1.35
1:C:162:GLY:HA3	1:C:310:MET:CE	1.52	1.35
1:A:162:GLY:HA3	1:A:310:MET:CE	1.54	1.35
1:B:194:ALA:HB3	1:C:113:ARG:NH1	1.45	1.28
1:E:162:GLY:CA	1:E:310:MET:CE	2.13	1.25
1:B:113:ARG:NH1	1:C:194:ALA:HB3	1.55	1.19
1:E:162:GLY:CA	1:E:310:MET:HE3	1.71	1.18
1:B:157:ARG:HH22	1:C:137:ASP:CB	1.56	1.18
1:E:162:GLY:HA3	1:E:310:MET:HE1	1.26	1.17
1:A:89:VAL:HG13	1:A:308:MET:HE2	1.25	1.14
1:B:157:ARG:NH2	1:C:137:ASP:CB	2.12	1.12
1:E:162:GLY:HA3	1:E:310:MET:HE3	1.19	1.12
1:C:89:VAL:HG13	1:C:308:MET:HE2	1.30	1.11
1:B:162:GLY:HA3	1:B:310:MET:CE	1.80	1.11
1:A:157:ARG:CZ	1:E:123:ARG:NE	2.12	1.11
1:B:137:ASP:CB	1:C:157:ARG:HH22	1.63	1.09
1:B:310:MET:HE3	1:B:322:THR:H	1.05	1.08
1:B:137:ASP:CB	1:C:157:ARG:NH2	2.16	1.08
1:A:162:GLY:HA3	1:A:310:MET:HE3	1.15	1.07
1:D:162:GLY:HA3	1:D:310:MET:HE1	1.11	1.06
1:F:94:ARG:HD3	2:F:362:HOH:O	1.54	1.05
1:F:162:GLY:CA	1:F:310:MET:CE	2.35	1.05
1:F:173:ARG:O	1:F:177:GLU:HG3	1.56	1.04
1:B:310:MET:HE3	1:B:322:THR:N	1.72	1.04
1:B:173:ARG:O	1:B:177:GLU:HG3	1.58	1.04
1:E:89:VAL:HG13	1:E:308:MET:HE2	1.41	1.03
1:B:113:ARG:HH11	1:C:194:ALA:HB3	0.86	1.03
1:B:194:ALA:HB3	1:C:113:ARG:HH11	1.03	1.02
1:F:162:GLY:HA3	1:F:310:MET:HE1	1.03	1.02
1:C:162:GLY:HA3	1:C:310:MET:HE1	1.04	1.02
1:F:162:GLY:CA	1:F:310:MET:HE1	1.90	1.01
1:B:310:MET:CE	1:B:322:THR:H	1.73	1.01
1:D:162:GLY:HA3	1:D:310:MET:HE3	1.43	1.00
1:B:162:GLY:HA3	1:B:310:MET:HE1	1.43	1.00
1:A:219:GLN:HB2	1:E:135:GLU:OE1	1.64	0.98
1:F:151:ALA:HB2	1:F:156:LEU:HD22	1.43	0.98
1:C:162:GLY:CA	1:C:310:MET:CE	2.42	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ARG:HH11	1:E:123:ARG:HG3	1.27	0.98
1:B:162:GLY:CA	1:B:310:MET:HE1	1.93	0.97
1:A:281:ASP:O	1:A:295:VAL:HG11	1.64	0.97
1:E:162:GLY:HA3	1:E:310:MET:HE2	1.44	0.96
1:A:157:ARG:NH1	1:E:123:ARG:NE	2.13	0.96
1:A:157:ARG:NH1	1:E:123:ARG:CD	2.27	0.96
1:C:173:ARG:O	1:C:177:GLU:HG3	1.64	0.96
1:D:151:ALA:HB2	1:D:156:LEU:HD22	1.44	0.95
1:A:162:GLY:HA3	1:A:310:MET:HE1	1.46	0.94
1:B:113:ARG:HH11	1:C:194:ALA:CB	1.80	0.93
1:E:281:ASP:O	1:E:295:VAL:HG11	1.69	0.93
1:C:162:GLY:CA	1:C:310:MET:HE1	1.97	0.93
1:A:157:ARG:NH1	1:E:123:ARG:HG3	1.84	0.93
1:A:162:GLY:CA	1:A:310:MET:HE3	1.97	0.92
1:E:173:ARG:O	1:E:177:GLU:HG3	1.70	0.92
1:B:162:GLY:HA3	1:B:310:MET:HE2	1.52	0.92
1:C:162:GLY:HA3	1:C:310:MET:HE3	1.49	0.91
1:D:162:GLY:CA	1:D:310:MET:HE1	1.99	0.90
1:A:162:GLY:CA	1:A:310:MET:CE	2.47	0.90
1:A:80:VAL:HG23	1:B:80:VAL:HG23	1.51	0.90
1:E:80:VAL:HG23	1:F:80:VAL:HG23	1.52	0.89
1:A:219:GLN:CB	1:E:135:GLU:OE1	2.21	0.89
1:A:89:VAL:HG13	1:A:308:MET:CE	2.05	0.87
1:A:157:ARG:CZ	1:E:123:ARG:HE	1.85	0.86
1:C:89:VAL:HG13	1:C:308:MET:CE	2.05	0.86
1:F:89:VAL:HG13	1:F:308:MET:CE	2.07	0.85
1:E:151:ALA:HB2	1:E:156:LEU:HD22	1.60	0.84
1:E:162:GLY:HA2	1:E:310:MET:HE3	1.59	0.83
1:E:67:SER:HB2	2:E:373:HOH:O	1.78	0.82
1:A:157:ARG:NH1	1:E:123:ARG:CG	2.41	0.82
1:F:89:VAL:HG13	1:F:308:MET:HE2	1.61	0.82
1:E:89:VAL:HG13	1:E:308:MET:CE	2.10	0.81
1:B:89:VAL:HG13	1:B:308:MET:CE	2.12	0.80
1:A:157:ARG:NH2	1:E:123:ARG:HE	1.79	0.79
1:D:173:ARG:O	1:D:177:GLU:HG3	1.80	0.79
1:B:310:MET:HE3	1:B:321:ALA:HA	1.63	0.79
1:F:162:GLY:HA3	1:F:310:MET:HE3	1.60	0.79
1:B:151:ALA:HB2	1:B:156:LEU:HD22	1.62	0.79
1:D:169:VAL:HG23	2:D:356:HOH:O	1.83	0.79
1:A:157:ARG:HH11	1:E:123:ARG:CG	1.95	0.79
1:E:120:PHE:O	1:E:123:ARG:HD3	1.82	0.78
1:A:151:ALA:HB2	1:A:156:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:162:GLY:CA	1:F:310:MET:HE3	2.13	0.78
1:B:162:GLY:CA	1:B:310:MET:CE	2.56	0.77
1:A:173:ARG:O	1:A:177:GLU:HG3	1.85	0.77
1:A:157:ARG:NH2	1:E:123:ARG:NE	2.33	0.76
1:D:156:LEU:O	1:D:157:ARG:HB2	1.86	0.76
1:E:329:ARG:NH2	2:E:363:HOH:O	2.18	0.76
1:C:281:ASP:O	1:C:295:VAL:HG11	1.86	0.75
1:E:218:ARG:HH11	1:E:244:ASP:HB2	1.52	0.74
1:B:89:VAL:HG13	1:B:308:MET:HE1	1.69	0.74
1:B:194:ALA:CB	1:C:113:ARG:NH1	2.40	0.74
1:B:121:GLU:HG2	2:B:359:HOH:O	1.88	0.74
1:B:91:SER:O	1:B:95[B]:HIS:CD2	2.39	0.73
1:C:162:GLY:CA	1:C:310:MET:HE3	2.10	0.73
1:A:194:ALA:HB1	1:E:141:THR:O	1.88	0.72
1:F:152:VAL:HG23	2:F:368:HOH:O	1.88	0.72
1:B:316:GLU:OE1	2:B:370:HOH:O	2.06	0.72
1:E:156:LEU:O	1:E:157:ARG:HB2	1.90	0.71
1:A:94:ARG:NH2	1:B:111:ARG:O	2.24	0.71
1:A:281:ASP:O	1:A:295:VAL:CG1	2.37	0.71
1:B:310:MET:HE3	1:B:321:ALA:CA	2.21	0.71
1:A:89:VAL:CG1	1:A:308:MET:HE2	2.14	0.70
1:A:194:ALA:CB	1:E:141:THR:O	2.40	0.70
1:A:137:ASP:CB	1:E:66:ARG:NH2	2.55	0.70
1:E:281:ASP:O	1:E:295:VAL:CG1	2.39	0.69
1:D:89:VAL:HG13	1:D:308:MET:CE	2.23	0.69
1:A:157:ARG:NH2	1:E:123:ARG:HH21	1.90	0.69
1:B:113:ARG:NH1	1:C:194:ALA:CB	2.47	0.69
1:A:157:ARG:NH2	1:E:123:ARG:NH2	2.41	0.68
1:A:157:ARG:CZ	1:E:123:ARG:CZ	2.71	0.68
1:B:162:GLY:HA2	1:B:310:MET:HE1	1.74	0.68
1:A:162:GLY:CA	1:A:310:MET:HE1	2.21	0.68
1:E:89:VAL:CG1	1:E:308:MET:HE2	2.22	0.67
1:D:162:GLY:CA	1:D:310:MET:CE	2.52	0.67
1:D:89:VAL:HG13	1:D:308:MET:HE2	1.77	0.67
1:F:156:LEU:O	1:F:157:ARG:HB2	1.94	0.67
1:E:231:ASN:O	1:E:256:ILE:HA	1.95	0.66
1:B:194:ALA:CB	1:C:113:ARG:HH11	1.95	0.66
1:A:114:GLU:HG3	2:A:391:HOH:O	1.93	0.66
1:D:162:GLY:CA	1:D:310:MET:HE3	2.24	0.65
1:D:281:ASP:O	1:D:295:VAL:HG11	1.97	0.65
1:F:89:VAL:CG1	1:F:308:MET:CE	2.75	0.65
1:A:157:ARG:NH1	1:E:123:ARG:HE	1.85	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:ALA:HB1	1:E:141:THR:C	2.17	0.64
1:F:130:ALA:HB2	2:F:368:HOH:O	1.98	0.63
1:C:94:ARG:HH12	1:D:111:ARG:HB3	1.63	0.63
1:F:89:VAL:HG13	1:F:308:MET:HE1	1.79	0.63
1:F:332:THR:O	1:F:333:HIS:HB2	1.99	0.63
1:A:186:ARG:HB3	1:A:246:PRO:HA	1.82	0.62
1:E:118:GLN:O	1:E:121:GLU:HG3	2.01	0.61
1:C:213:ALA:HA	2:C:360:HOH:O	2.01	0.61
1:A:89:VAL:CG1	1:A:308:MET:CE	2.77	0.61
1:B:89:VAL:HG13	1:B:308:MET:HE2	1.82	0.60
1:C:127:LEU:HG	1:C:147:PHE:CE1	2.37	0.60
1:A:156:LEU:O	1:A:157:ARG:HB2	2.02	0.60
1:A:157:ARG:NH2	1:E:123:ARG:CZ	2.64	0.60
1:E:186:ARG:HB3	1:E:246:PRO:HA	1.84	0.59
1:B:220:GLU:O	2:B:383:HOH:O	2.17	0.59
1:E:322:THR:HG22	2:E:361:HOH:O	2.02	0.59
1:F:265:ASN:C	1:F:265:ASN:HD22	2.06	0.59
1:C:333:HIS:HA	2:C:399:HOH:O	2.03	0.59
1:F:191:VAL:HG12	1:F:252:SER:HB3	1.85	0.59
1:C:191:VAL:HG22	2:C:387:HOH:O	2.01	0.59
1:F:89:VAL:CG1	1:F:308:MET:HE2	2.31	0.58
1:E:280:PHE:O	1:E:281:ASP:HB2	2.03	0.58
1:B:156:LEU:O	1:B:157:ARG:HB2	2.03	0.58
1:F:310:MET:HE3	1:F:322:THR:H	1.68	0.58
1:F:281:ASP:O	1:F:295:VAL:HG11	2.03	0.58
1:E:150:VAL:HB	1:E:310:MET:HE1	1.85	0.57
1:C:68:ASN:ND2	2:C:397:HOH:O	2.37	0.57
1:E:162:GLY:CA	1:E:310:MET:HE1	2.01	0.57
1:F:130:ALA:CB	2:F:368:HOH:O	2.51	0.57
1:B:120:PHE:O	1:B:123:ARG:HD3	2.05	0.57
1:E:332:THR:O	1:E:333:HIS:HB2	2.05	0.57
1:A:157:ARG:CZ	1:E:123:ARG:HG3	2.35	0.56
1:A:200:ARG:CZ	1:E:120:PHE:HE2	2.18	0.56
1:D:89:VAL:CG1	1:D:308:MET:HE2	2.36	0.56
1:B:310:MET:CE	1:B:321:ALA:HA	2.33	0.56
1:D:233:ARG:HH11	1:D:266:VAL:HG21	1.69	0.56
1:E:111:ARG:O	1:F:94:ARG:NH2	2.38	0.56
1:E:237:ILE:O	1:E:241:THR:HG23	2.06	0.56
1:A:280:PHE:O	1:A:281:ASP:HB2	2.06	0.56
1:A:231:ASN:O	1:A:256:ILE:HA	2.05	0.56
1:B:186:ARG:HB3	1:B:246:PRO:HA	1.88	0.56
1:D:89:VAL:CG1	1:D:308:MET:CE	2.84	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:231:ASN:O	1:B:256:ILE:HA	2.07	0.55
1:C:156:LEU:O	1:C:157:ARG:HB2	2.06	0.55
1:B:306:GLU:HG3	1:B:324:MET:HE1	1.89	0.55
1:E:179:LEU:HD11	1:E:278:VAL:HG22	1.89	0.54
1:F:162:GLY:HA2	1:F:310:MET:HE3	1.88	0.54
1:F:280:PHE:O	1:F:281:ASP:HB2	2.08	0.54
1:C:280:PHE:O	1:C:281:ASP:HB2	2.07	0.54
1:A:137:ASP:CB	1:E:66:ARG:CZ	2.86	0.54
1:E:254:HIS:O	1:E:258:GLU:HG3	2.08	0.54
1:A:280:PHE:HA	1:A:296:VAL:HG13	1.89	0.54
1:B:281:ASP:O	1:B:295:VAL:HG11	2.08	0.54
1:B:327:GLN:HB3	2:B:371:HOH:O	2.07	0.54
1:C:332:THR:O	1:C:333:HIS:HB2	2.08	0.53
1:A:233:ARG:HH11	1:A:266:VAL:HG21	1.74	0.53
1:C:231:ASN:O	1:C:256:ILE:HA	2.08	0.53
1:A:140:ARG:NH1	1:E:66:ARG:HD2	2.24	0.53
1:E:191:VAL:HG12	1:E:252:SER:HB3	1.90	0.53
1:B:310:MET:HE3	1:B:321:ALA:C	2.29	0.53
1:B:218:ARG:HH11	1:B:244:ASP:HB2	1.73	0.53
1:C:94:ARG:NH1	1:D:111:ARG:HB3	2.24	0.52
1:C:121:GLU:HA	1:C:123:ARG:NH1	2.23	0.52
1:A:301:ARG:NH1	1:B:78:GLU:OE1	2.42	0.52
1:F:231:ASN:O	1:F:256:ILE:HA	2.09	0.52
1:D:68:ASN:N	1:D:125:ASP:OD1	2.40	0.52
1:A:137:ASP:CB	1:E:66:ARG:HH22	2.23	0.51
1:C:255:ARG:NH1	2:C:389:HOH:O	2.43	0.51
1:B:74:VAL:HA	1:B:130:ALA:HB3	1.92	0.51
1:C:218:ARG:HH11	1:C:244:ASP:HB2	1.74	0.51
1:E:167:GLU:OE1	1:E:170:ARG:NH2	2.43	0.51
1:F:152:VAL:O	1:F:153:ASN:HB3	2.10	0.51
1:F:68:ASN:N	1:F:125:ASP:OD1	2.41	0.51
1:F:233:ARG:HH11	1:F:266:VAL:HG21	1.76	0.51
1:E:162:GLY:C	1:E:310:MET:HE1	2.31	0.51
1:C:265:ASN:C	1:C:265:ASN:HD22	2.14	0.50
1:B:277:ILE:HG22	1:B:293:LEU:HD21	1.92	0.50
1:D:316:GLU:OE2	2:D:383:HOH:O	2.20	0.50
1:E:322:THR:CG2	2:E:361:HOH:O	2.59	0.49
1:D:74:VAL:HA	1:D:130:ALA:HB3	1.94	0.49
1:C:233:ARG:HD3	1:C:262:GLN:HB3	1.94	0.49
1:F:89:VAL:CG1	1:F:308:MET:HE1	2.39	0.49
1:A:218:ARG:HH11	1:A:244:ASP:HB2	1.77	0.49
1:E:235:GLY:O	1:E:239:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:ARG:O	1:B:221:TRP:HB2	2.13	0.49
1:B:310:MET:HE1	1:B:322:THR:O	2.13	0.49
1:F:74:VAL:HA	1:F:130:ALA:HB3	1.95	0.49
1:C:127:LEU:HG	1:C:147:PHE:HE1	1.75	0.49
1:C:117:GLY:O	1:C:121:GLU:HG3	2.12	0.49
1:A:157:ARG:NH1	1:E:123:ARG:HD2	2.22	0.49
1:D:218:ARG:HH11	1:D:244:ASP:HB2	1.77	0.49
1:B:280:PHE:O	1:B:281:ASP:HB2	2.14	0.48
1:E:121:GLU:HA	1:E:123:ARG:NH1	2.28	0.48
1:E:265:ASN:HD22	1:E:265:ASN:C	2.16	0.48
1:E:89:VAL:CG1	1:E:308:MET:CE	2.86	0.48
1:B:280:PHE:HA	1:B:296:VAL:HG13	1.95	0.48
1:C:231:ASN:HD22	1:C:231:ASN:HA	1.36	0.48
1:A:219:GLN:HB3	1:E:135:GLU:OE1	2.09	0.48
1:F:186:ARG:HB3	1:F:246:PRO:HA	1.95	0.48
1:D:277:ILE:HG22	1:D:293:LEU:HD21	1.94	0.48
1:D:127:LEU:HG	1:D:147:PHE:CE1	2.49	0.48
1:A:140:ARG:NH1	1:E:66:ARG:CD	2.76	0.48
1:D:89:VAL:HG13	1:D:308:MET:HE1	1.92	0.48
1:D:332:THR:O	1:D:333:HIS:HB2	2.14	0.47
1:D:186:ARG:HB3	1:D:246:PRO:HA	1.96	0.47
1:C:162:GLY:HA2	1:C:310:MET:HE3	1.94	0.47
1:E:128:ILE:HG13	1:E:311:LEU:HD22	1.96	0.47
1:C:333:HIS:HD2	2:C:399:HOH:O	1.95	0.47
1:D:285:TRP:HA	1:D:288:PHE:CD2	2.49	0.47
1:A:129:LEU:O	1:A:131:PRO:HD3	2.15	0.47
1:E:218:ARG:HH11	1:E:244:ASP:CB	2.24	0.47
1:C:120:PHE:O	1:C:123:ARG:HD3	2.14	0.47
1:C:167:GLU:OE1	1:C:170:ARG:NH2	2.48	0.47
1:B:231:ASN:HD22	1:B:231:ASN:HA	1.43	0.47
1:A:94:ARG:HH12	1:B:111:ARG:HB3	1.80	0.47
1:D:218:ARG:HD3	1:D:221:TRP:CZ2	2.49	0.47
1:C:233:ARG:HH11	1:C:266:VAL:HG21	1.79	0.47
1:D:231:ASN:O	1:D:256:ILE:HA	2.15	0.46
1:E:280:PHE:O	1:E:281:ASP:CB	2.63	0.46
1:F:179:LEU:HD11	1:F:278:VAL:HG22	1.98	0.46
1:A:235:GLY:O	1:A:239:VAL:HG13	2.14	0.46
1:A:288:PHE:O	2:A:362:HOH:O	2.20	0.46
1:E:200:ARG:HH21	1:E:200:ARG:HG2	1.81	0.46
1:A:254:HIS:O	1:A:258:GLU:HG3	2.15	0.46
1:B:89:VAL:CG1	1:B:308:MET:CE	2.88	0.45
1:A:231:ASN:HA	1:A:231:ASN:HD22	1.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:333:HIS:CD2	2:C:399:HOH:O	2.67	0.45
1:C:222:ILE:CG2	2:C:387:HOH:O	2.63	0.45
1:B:233:ARG:HH11	1:B:266:VAL:HG21	1.81	0.45
1:E:128:ILE:HD12	1:E:308:MET:HE1	1.98	0.45
1:F:119:PHE:O	1:F:124:VAL:HG22	2.16	0.45
1:D:265:ASN:HD22	1:D:265:ASN:C	2.19	0.45
1:A:150:VAL:HB	1:A:310:MET:HE1	1.98	0.45
1:F:191:VAL:HA	1:F:252:SER:OG	2.17	0.45
1:F:218:ARG:HD3	1:F:221:TRP:CZ2	2.51	0.45
1:C:207:ARG:O	1:C:211:SER:HB2	2.17	0.45
1:B:157:ARG:N	2:B:390:HOH:O	2.50	0.44
1:E:231:ASN:HD22	1:E:231:ASN:HA	1.48	0.44
1:D:235:GLY:O	1:D:239:VAL:HG13	2.17	0.44
1:A:265:ASN:C	1:A:265:ASN:HD22	2.21	0.44
1:C:186:ARG:HB3	1:C:246:PRO:HA	1.98	0.44
1:B:136:HIS:HB3	1:B:139:LEU:HD12	2.00	0.44
1:C:222:ILE:HG23	2:C:387:HOH:O	2.16	0.44
1:D:179:LEU:HD11	1:D:278:VAL:HG22	2.00	0.44
1:D:129:LEU:O	1:D:131:PRO:HD3	2.17	0.44
1:A:167:GLU:HG2	1:A:328:THR:HG23	1.99	0.44
1:B:232:GLY:HA2	2:B:388:HOH:O	2.16	0.44
1:C:280:PHE:O	1:C:281:ASP:CB	2.65	0.44
1:B:121:GLU:HA	1:B:123:ARG:NH1	2.33	0.44
1:F:121:GLU:HA	1:F:123:ARG:NH1	2.33	0.44
1:B:218:ARG:HD3	1:B:221:TRP:CZ2	2.53	0.43
1:F:120:PHE:O	1:F:123:ARG:HD3	2.18	0.43
1:B:167:GLU:O	1:B:167:GLU:HG3	2.18	0.43
1:D:118:GLN:O	1:D:121:GLU:HG3	2.18	0.43
1:B:310:MET:CE	1:B:322:THR:N	2.52	0.43
1:E:129:LEU:O	1:E:151:ALA:HA	2.18	0.43
1:E:138:TYR:O	1:E:142:GLU:HB2	2.18	0.43
1:A:94:ARG:NH1	1:B:111:ARG:HB3	2.33	0.43
1:B:194:ALA:HB3	1:C:113:ARG:HH12	1.64	0.43
1:F:332:THR:O	1:F:333:HIS:CB	2.67	0.43
1:F:231:ASN:HD22	1:F:231:ASN:HA	1.55	0.43
1:E:299:PRO:HG3	1:E:327:GLN:O	2.19	0.43
1:C:150:VAL:HB	1:C:310:MET:HE1	2.01	0.43
1:B:152:VAL:O	1:B:153:ASN:HB3	2.19	0.43
1:A:157:ARG:NE	1:E:123:ARG:HG3	2.34	0.43
1:A:280:PHE:O	1:A:281:ASP:CB	2.67	0.43
1:D:281:ASP:O	1:D:295:VAL:CG1	2.66	0.43
1:C:290:ASP:HA	1:C:291:PRO:HA	1.90	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:128:ILE:HG13	1:F:311:LEU:HD22	2.01	0.42
1:A:127:LEU:HG	1:A:147:PHE:CE1	2.54	0.42
1:B:333:HIS:HB3	2:B:400:HOH:O	2.19	0.42
1:A:272:GLY:HA3	1:A:273:PRO:HD3	1.90	0.42
1:B:270:ARG:N	1:B:274:ASP:OD2	2.53	0.42
1:A:207:ARG:O	1:A:211:SER:HB2	2.20	0.42
1:A:137:ASP:CB	1:E:66:ARG:NH1	2.83	0.42
1:C:192:GLY:N	1:C:256:ILE:HD11	2.34	0.42
1:A:301:ARG:HD3	1:B:78:GLU:OE2	2.20	0.42
1:F:138:TYR:O	1:F:142:GLU:HB2	2.19	0.42
1:F:113:ARG:HG3	1:F:138:TYR:CE1	2.54	0.42
1:C:178:TYR:CE2	1:C:182:ARG:HD2	2.55	0.42
1:A:218:ARG:HD3	1:A:221:TRP:CZ2	2.54	0.42
1:A:332:THR:O	1:A:333:HIS:HB2	2.19	0.42
1:A:138:TYR:O	1:A:142:GLU:HB2	2.19	0.42
1:C:113:ARG:HG3	1:C:138:TYR:CE1	2.56	0.41
1:D:231:ASN:HA	1:D:231:ASN:HD22	1.58	0.41
1:F:118:GLN:O	1:F:122:ARG:HG3	2.21	0.41
1:B:187:ILE:HG12	1:B:248:ALA:HB3	2.01	0.41
1:E:141:THR:OG1	1:E:142:GLU:OE2	2.38	0.41
1:E:167:GLU:O	1:E:167:GLU:HG3	2.20	0.41
1:B:290:ASP:HA	1:B:291:PRO:HA	1.93	0.41
1:C:306:GLU:HG3	1:C:324:MET:HE1	2.02	0.41
1:B:324:MET:HE1	1:B:326:LEU:HD11	2.03	0.41
1:F:272:GLY:HA3	1:F:273:PRO:HD3	1.89	0.41
1:B:91:SER:O	1:B:95[B]:HIS:HD2	1.98	0.41
1:A:285:TRP:HD1	2:B:373:HOH:O	2.02	0.41
1:F:192:GLY:O	1:F:193:SER:C	2.59	0.41
1:A:301:ARG:HH11	1:B:78:GLU:CD	2.24	0.41
1:C:324:MET:CE	1:C:326:LEU:HD21	2.50	0.41
1:A:290:ASP:HA	1:A:291:PRO:HA	1.94	0.41
1:E:203:LEU:O	1:E:206:PHE:HB3	2.19	0.41
1:A:277:ILE:HG22	1:A:293:LEU:HD21	2.02	0.41
1:D:207:ARG:O	1:D:211:SER:HB2	2.21	0.40
1:E:290:ASP:HA	1:E:291:PRO:HA	1.95	0.40
1:A:167:GLU:HB2	2:A:351:HOH:O	2.21	0.40
1:E:233:ARG:HH11	1:E:266:VAL:HG21	1.87	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.97	0.40
1:C:78:GLU:OE2	1:D:301:ARG:HD3	2.21	0.40
1:F:103:ALA:HB2	1:F:119:PHE:CZ	2.56	0.40
1:D:255:ARG:NH1	2:D:363:HOH:O	2.55	0.40
1:A:111:ARG:HB3	1:B:94:ARG:HH12	1.87	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:218:ARG:NH2	1:F:207:ARG:NH2[1_556]	1.77	0.43
1:B:123:ARG:CG	1:B:270:ARG:NH1[1_454]	2.00	0.20
1:C:302:ARG:NH1	2:D:352:HOH:O[1_455]	2.09	0.11
1:C:123:ARG:CG	1:C:270:ARG:NH1[1_556]	2.11	0.09

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	255/291 (88%)	248 (97%)	6 (2%)	1 (0%)	43	52
1	B	256/291 (88%)	251 (98%)	4 (2%)	1 (0%)	43	52
1	C	255/291 (88%)	248 (97%)	5 (2%)	2 (1%)	27	31
1	D	258/291 (89%)	248 (96%)	9 (4%)	1 (0%)	43	52
1	E	255/291 (88%)	247 (97%)	7 (3%)	1 (0%)	43	52
1	F	258/291 (89%)	250 (97%)	7 (3%)	1 (0%)	43	52
All	All	1537/1746 (88%)	1492 (97%)	38 (2%)	7 (0%)	38	45

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	ASP
1	A	281	ASP
1	C	281	ASP
1	D	281	ASP
1	E	281	ASP
1	C	153	ASN
1	F	281	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/233 (90%)	190 (91%)	19 (9%)	14	13
1	B	210/233 (90%)	190 (90%)	20 (10%)	12	12
1	C	209/233 (90%)	189 (90%)	20 (10%)	12	12
1	D	209/233 (90%)	189 (90%)	20 (10%)	12	12
1	E	209/233 (90%)	187 (90%)	22 (10%)	10	10
1	F	209/233 (90%)	189 (90%)	20 (10%)	12	12
All	All	1255/1398 (90%)	1134 (90%)	121 (10%)	12	12

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	113	ARG
1	A	121	GLU
1	A	140	ARG
1	A	142	GLU
1	A	156	LEU
1	A	200	ARG
1	A	211	SER
1	A	217	VAL
1	A	218	ARG
1	A	231	ASN
1	A	249	LEU
1	A	265	ASN
1	A	283	LEU
1	A	289	LEU
1	A	295	VAL
1	A	296	VAL
1	A	326	LEU
1	A	329	ARG
1	B	66	ARG
1	B	121	GLU
1	B	140	ARG
1	B	142	GLU

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Mol	Chain	Res	Type
1	B	156	LEU
1	B	200	ARG
1	B	211	SER
1	B	217	VAL
1	B	218	ARG
1	B	231	ASN
1	B	249	LEU
1	B	265	ASN
1	B	283	LEU
1	B	289	LEU
1	B	293	LEU
1	B	295	VAL
1	B	296	VAL
1	B	324	MET
1	B	326	LEU
1	B	329	ARG
1	C	66	ARG
1	C	94	ARG
1	C	121	GLU
1	C	140	ARG
1	C	142	GLU
1	C	200	ARG
1	C	211	SER
1	C	217	VAL
1	C	218	ARG
1	C	231	ASN
1	C	249	LEU
1	C	265	ASN
1	C	283	LEU
1	C	289	LEU
1	C	293	LEU
1	C	295	VAL
1	C	296	VAL
1	C	322	THR
1	C	324	MET
1	C	329	ARG
1	D	66	ARG
1	D	80	VAL
1	D	113	ARG
1	D	121	GLU
1	D	140	ARG
1	D	142	GLU

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Mol	Chain	Res	Type
1	D	156	LEU
1	D	200	ARG
1	D	211	SER
1	D	217	VAL
1	D	218	ARG
1	D	231	ASN
1	D	246	PRO
1	D	249	LEU
1	D	265	ASN
1	D	283	LEU
1	D	289	LEU
1	D	295	VAL
1	D	296	VAL
1	D	329	ARG
1	E	66	ARG
1	E	80	VAL
1	E	113	ARG
1	E	121	GLU
1	E	140	ARG
1	E	142	GLU
1	E	156	LEU
1	E	200	ARG
1	E	211	SER
1	E	217	VAL
1	E	218	ARG
1	E	231	ASN
1	E	249	LEU
1	E	265	ASN
1	E	283	LEU
1	E	289	LEU
1	E	293	LEU
1	E	295	VAL
1	E	296	VAL
1	E	324	MET
1	E	326	LEU
1	E	329	ARG
1	F	66	ARG
1	F	121	GLU
1	F	127	LEU
1	F	140	ARG
1	F	142	GLU
1	F	150	VAL

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Mol	Chain	Res	Type
1	F	156	LEU
1	F	200	ARG
1	F	211	SER
1	F	217	VAL
1	F	218	ARG
1	F	231	ASN
1	F	249	LEU
1	F	265	ASN
1	F	283	LEU
1	F	289	LEU
1	F	295	VAL
1	F	296	VAL
1	F	326	LEU
1	F	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	262	GLN
1	A	265	ASN
1	A	333	HIS
1	B	136	HIS
1	B	231	ASN
1	B	262	GLN
1	B	265	ASN
1	B	333	HIS
1	C	68	ASN
1	C	136	HIS
1	C	231	ASN
1	C	262	GLN
1	C	265	ASN
1	C	333	HIS
1	D	231	ASN
1	D	262	GLN
1	D	265	ASN
1	E	153	ASN
1	E	231	ASN
1	E	262	GLN
1	E	265	ASN
1	F	136	HIS
1	F	231	ASN

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Mol	Chain	Res	Type
1	F	262	GLN
1	F	265	ASN
1	F	305	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 ⓘ

There are no ligands in this entry.

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	261/291 (89%)	0.47	6 (2%) 57 61	25, 35, 45, 52	0
1	B	261/291 (89%)	0.46	9 (3%) 43 47	25, 36, 46, 51	0
1	C	261/291 (89%)	0.49	10 (3%) 38 42	25, 36, 46, 52	0
1	D	262/291 (90%)	0.40	4 (1%) 70 74	25, 35, 46, 52	0
1	E	261/291 (89%)	0.42	7 (2%) 52 55	25, 36, 45, 52	0
1	F	262/291 (90%)	0.40	12 (4%) 31 35	25, 36, 46, 52	0
All	All	1568/1746 (89%)	0.44	48 (3%) 47 50	25, 36, 46, 52	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	244	ASP	5.0
1	B	244	ASP	4.5
1	F	66	ARG	4.4
1	B	242	GLY	4.3
1	D	244	ASP	3.8
1	C	244	ASP	3.7
1	E	242	GLY	3.5
1	C	333	HIS	3.5
1	B	333	HIS	3.5
1	A	121	GLU	3.4
1	E	66	ARG	3.4
1	A	244	ASP	3.3
1	A	140	ARG	3.3
1	F	318	THR	3.1
1	F	94	ARG	3.0
1	B	290	ASP	2.9
1	C	265	ASN	2.9
1	D	290	ASP	2.9
1	A	194	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	327	GLN	2.8
1	F	244	ASP	2.8
1	F	95	HIS	2.7
1	E	169	VAL	2.7
1	F	123	ARG	2.7
1	B	157	ARG	2.6
1	B	135	GLU	2.6
1	C	66	ARG	2.6
1	E	135	GLU	2.6
1	F	265	ASN	2.5
1	C	118	GLN	2.5
1	C	157	ARG	2.5
1	A	320	ASN	2.4
1	E	140	ARG	2.4
1	E	265	ASN	2.4
1	F	113	ARG	2.3
1	B	113	ARG	2.3
1	B	121	GLU	2.3
1	A	157	ARG	2.3
1	B	322	THR	2.3
1	F	320	ASN	2.2
1	F	243	ALA	2.2
1	C	242	GLY	2.2
1	C	135	GLU	2.1
1	C	217	VAL	2.1
1	F	157	ARG	2.1
1	D	320	ASN	2.1
1	D	217	VAL	2.0
1	F	145	LYS	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.