



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:05 PM GMT

PDB ID : 1URZ  
Title : LOW PH INDUCED, MEMBRANE FUSION CONFORMATION OF THE  
ENVELOPE PROTEIN OF TICK-BORNE ENCEPHALITIS VIRUS  
Authors : Bressanelli, S.; Rey, F.A.  
Deposited on : 2003-11-16  
Resolution : 2.70 Å(reported)

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

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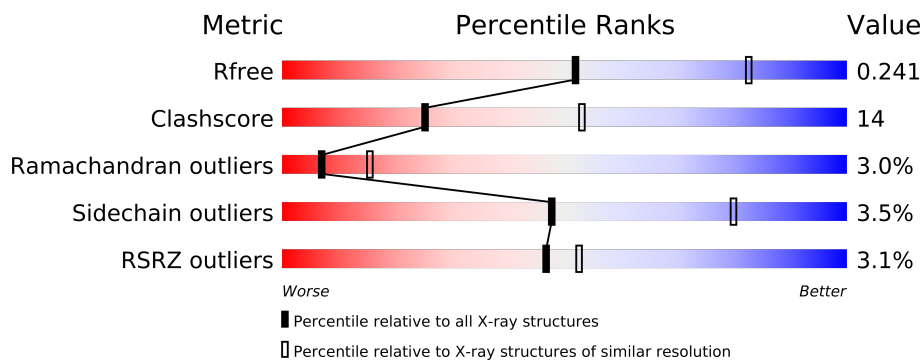
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	401	
1	B	401	
1	C	401	
1	D	401	
1	E	401	
1	F	401	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17986 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 ENVELOPE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2921	1836	514	550	21			
1	B	387	Total	C	N	O	S	0	0	0
			2946	1851	519	555	21			
1	C	385	Total	C	N	O	S	0	0	0
			2936	1845	517	553	21			
1	D	386	Total	C	N	O	S	0	0	0
			2941	1848	518	554	21			
1	E	382	Total	C	N	O	S	0	0	0
			2921	1836	514	550	21			
1	F	388	Total	C	N	O	S	0	0	0
			2951	1854	520	556	21			

- Molecule 2 is water.

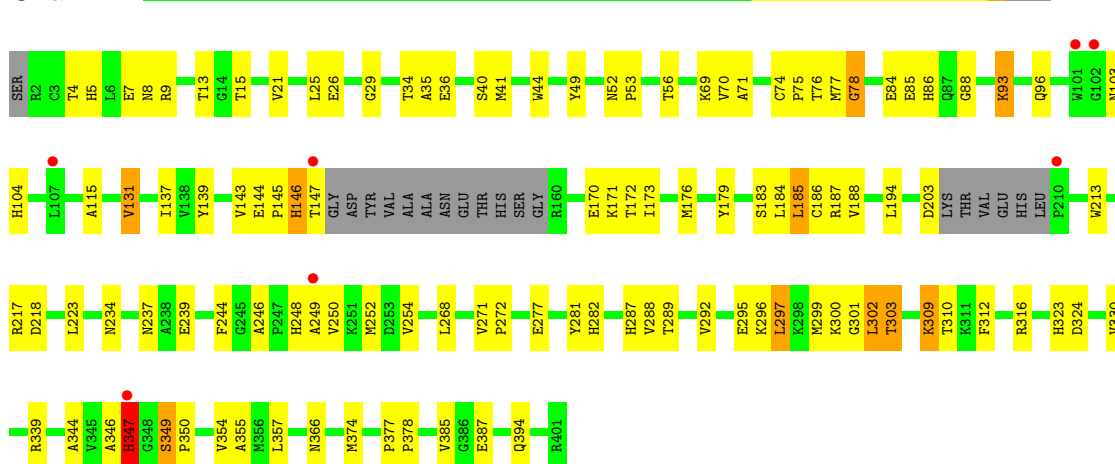
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	77	Total	O	0	0
			77	77		
2	C	64	Total	O	0	0
			64	64		
2	D	50	Total	O	0	0
			50	50		
2	E	49	Total	O	0	0
			49	49		
2	F	57	Total	O	0	0
			57	57		

### 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.

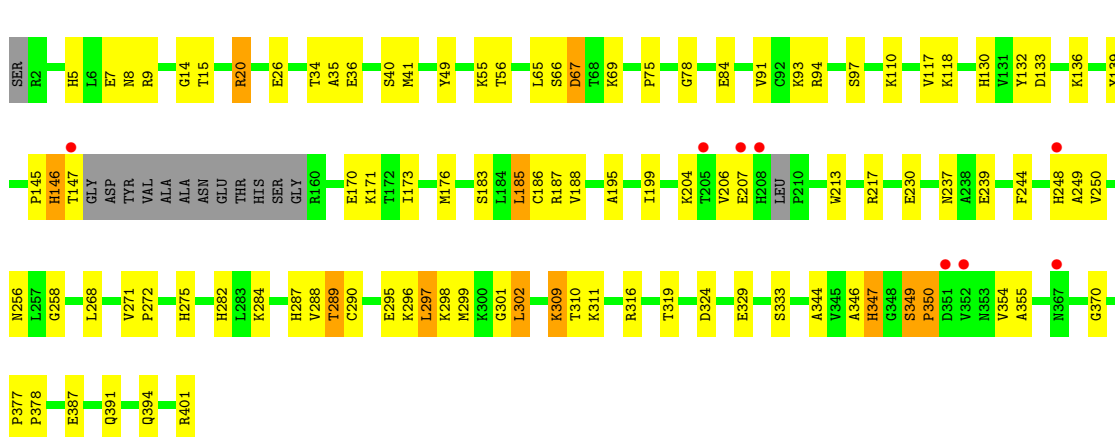
#### • Molecule 1: ENVELOPE PROTEIN

Chain A:



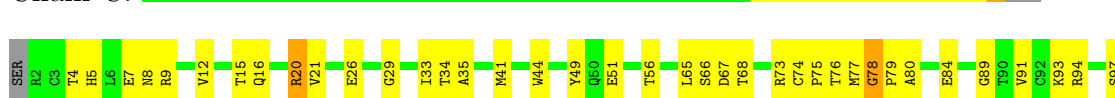
#### • Molecule 1: ENVELOPE PROTEIN

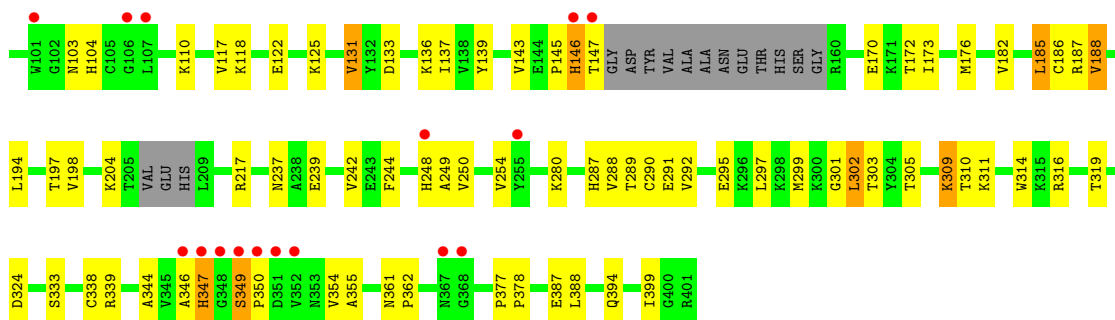
Chain B:



#### • Molecule 1: ENVELOPE PROTEIN

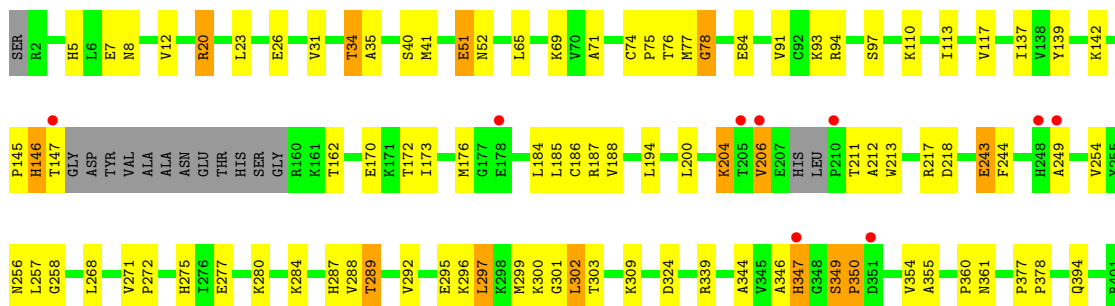
Chain C:





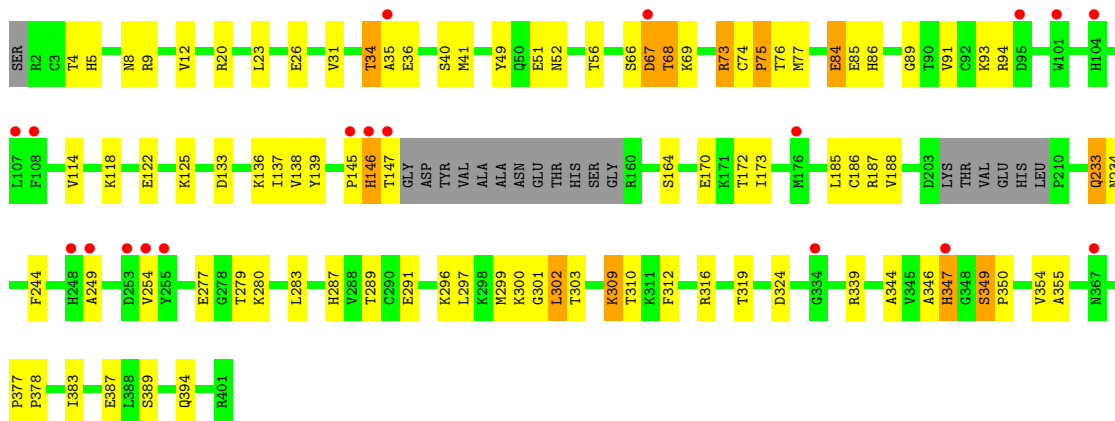
• Molecule 1: ENVELOPE PROTEIN

Chain D:



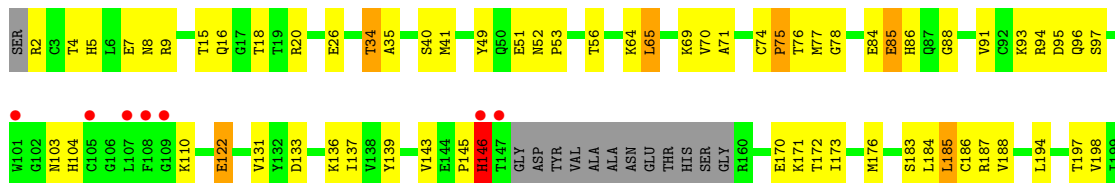
• Molecule 1: ENVELOPE PROTEIN

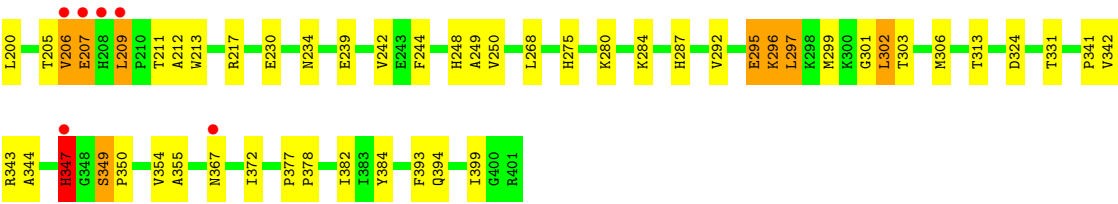
Chain E:



• Molecule 1: ENVELOPE PROTEIN

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.50Å 142.90Å 173.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.00-2.70) 96.8 (39.49-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.242 0.209 , 0.241	Depositor DCC
$R_{free}$ test set	4089 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 21.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 80895 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.39	0/2984	0.69	0/4046
1	B	0.40	0/3009	0.68	0/4081
1	C	0.37	0/2999	0.67	0/4068
1	D	0.38	0/3004	0.67	0/4074
1	E	0.37	0/2984	0.68	0/4046
1	F	0.37	0/3015	0.68	1/4092 (0.0%)
All	All	0.38	0/17995	0.68	1/24407 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	85	GLU	N-CA-C	-5.05	97.37	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	2921	0	2881	93	0
1	B	2946	0	2891	83	0
1	C	2936	0	2886	88	0
1	D	2941	0	2889	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2921	0	2881	78	0
1	F	2951	0	2893	85	0
2	A	73	0	0	6	0
2	B	77	0	0	5	0
2	C	64	0	0	0	0
2	D	50	0	0	0	0
2	E	49	0	0	2	0
2	F	57	0	0	2	0
All	All	17986	0	17321	477	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 14.

All (477) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:15:THR:HG22	1:F:16:GLN:HE21	1.31	0.92
1:E:233:GLN:HE21	1:E:234:ASN:H	1.14	0.91
1:C:15:THR:HG22	1:C:16:GLN:OE1	1.75	0.87
1:C:41:MET:HE2	1:C:145:PRO:HA	1.57	0.85
1:F:8:ASN:OD1	1:F:301:GLY:HA3	1.78	0.84
1:A:170:GLU:HG2	1:A:185:LEU:HD23	1.60	0.84
1:B:170:GLU:HG2	1:B:185:LEU:HD23	1.58	0.83
1:B:69:LYS:HE3	1:E:316:ARG:NH2	1.94	0.83
1:C:170:GLU:HG2	1:C:185:LEU:HD23	1.61	0.82
1:A:277:GLU:O	1:A:277:GLU:HG3	1.77	0.82
1:A:295:GLU:HG2	1:B:9:ARG:HG2	1.61	0.82
1:A:309:LYS:HG2	1:A:387:GLU:HG3	1.62	0.80
1:B:295:GLU:HG2	1:C:9:ARG:HG2	1.64	0.79
1:F:170:GLU:HG2	1:F:185:LEU:HD23	1.64	0.78
1:D:5:HIS:HB2	1:D:302:LEU:HD23	1.64	0.78
1:D:170:GLU:HG2	1:D:185:LEU:HD23	1.65	0.78
1:E:309:LYS:HG2	1:E:387:GLU:HG3	1.64	0.77
1:F:15:THR:HG22	1:F:16:GLN:NE2	2.01	0.74
1:E:316:ARG:HH12	1:E:319:THR:HG21	1.52	0.74
1:D:93:LYS:HB2	1:D:244:PHE:CD2	2.23	0.73
1:B:41:MET:HG3	1:B:176:MET:CE	2.20	0.72
1:E:93:LYS:HD3	1:E:94:ARG:N	2.03	0.72
1:D:206:VAL:CB	1:D:211:THR:HG21	2.20	0.72
1:A:186:CYS:HB3	1:A:288:VAL:CG1	2.20	0.72
1:D:41:MET:HE2	1:D:145:PRO:HA	1.70	0.71
1:B:309:LYS:HG2	1:B:387:GLU:HG3	1.72	0.71
1:A:25:LEU:HB3	2:A:2007:HOH:O	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:295:GLU:HG2	1:E:9:ARG:HG2	1.72	0.70
1:A:277:GLU:HG2	1:A:282:HIS:NE2	2.07	0.70
1:A:139:TYR:CZ	1:A:188:VAL:HG13	2.26	0.70
1:E:66:SER:OG	1:E:118:LYS:HB2	1.92	0.69
1:D:302:LEU:HD12	1:D:303:THR:H	1.57	0.68
1:D:302:LEU:HD12	1:D:303:THR:N	2.08	0.68
1:B:5:HIS:HB2	1:B:302:LEU:HD23	1.75	0.68
1:A:301:GLY:O	1:A:302:LEU:HB2	1.92	0.67
1:E:74:CYS:HB2	1:E:77:MET:HG2	1.76	0.67
1:F:139:TYR:CZ	1:F:188:VAL:HG13	2.29	0.67
1:A:88:GLY:HA3	1:A:234:ASN:ND2	2.10	0.67
1:A:8:ASN:OD1	1:A:301:GLY:HA3	1.93	0.67
1:B:20:ARG:HD3	1:C:12:VAL:HG23	1.77	0.67
1:E:170:GLU:HG2	1:E:185:LEU:HD23	1.75	0.67
1:D:12:VAL:HG23	1:F:20:ARG:HD3	1.76	0.66
1:E:56:THR:HA	1:F:399:ILE:HD13	1.78	0.66
1:D:8:ASN:OD1	1:D:301:GLY:HA3	1.95	0.66
1:E:233:GLN:NE2	1:E:234:ASN:H	1.90	0.66
1:D:41:MET:HG3	1:D:176:MET:CE	2.27	0.65
1:B:41:MET:HE2	1:B:145:PRO:HA	1.79	0.65
1:A:93:LYS:HB2	1:A:244:PHE:CD2	2.32	0.64
1:F:64:LYS:HB2	1:F:122:GLU:OE1	1.98	0.64
1:B:9:ARG:HD3	2:B:2001:HOH:O	1.96	0.64
1:B:8:ASN:OD1	1:B:301:GLY:HA3	1.97	0.64
1:A:170:GLU:HG2	1:A:185:LEU:CD2	2.27	0.64
1:C:8:ASN:OD1	1:C:301:GLY:HA3	1.98	0.64
1:B:173:ILE:HD12	1:C:9:ARG:HH21	1.61	0.64
1:E:378:PRO:HA	1:E:394:GLN:HB3	1.79	0.63
1:D:339:ARG:NH1	1:D:361:ASN:OD1	2.31	0.63
1:B:20:ARG:HG2	2:B:2063:HOH:O	1.97	0.63
1:A:36:GLU:OE2	1:A:300:LYS:HE2	1.98	0.63
1:F:344:ALA:HB3	1:F:355:ALA:HB2	1.81	0.62
1:D:20:ARG:HH11	1:D:20:ARG:HG3	1.64	0.62
1:D:20:ARG:NH1	1:D:20:ARG:HG3	2.13	0.62
1:B:170:GLU:HG2	1:B:185:LEU:CD2	2.28	0.62
1:E:8:ASN:OD1	1:E:301:GLY:HA3	1.99	0.62
1:C:41:MET:CE	1:C:145:PRO:HA	2.30	0.62
1:F:91:VAL:HG12	1:F:244:PHE:HE2	1.63	0.62
1:A:302:LEU:HD13	1:A:303:THR:N	2.15	0.61
1:E:170:GLU:OE1	1:F:187:ARG:NH2	2.32	0.61
1:A:277:GLU:HG2	1:A:282:HIS:CD2	2.34	0.61
1:F:170:GLU:HG2	1:F:185:LEU:CD2	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:5:HIS:CB	1:D:302:LEU:HD23	2.28	0.61
1:D:139:TYR:CZ	1:D:188:VAL:HG13	2.35	0.61
1:A:349:SER:H	1:A:350:PRO:CD	2.12	0.61
1:D:5:HIS:HB2	1:D:302:LEU:CD2	2.30	0.61
1:D:186:CYS:HB3	1:D:288:VAL:CG1	2.31	0.61
1:F:41:MET:HE2	1:F:145:PRO:HA	1.81	0.61
1:C:74:CYS:HB2	1:C:77:MET:HG2	1.82	0.61
1:F:2:ARG:N	1:F:367:ASN:HD21	1.99	0.61
1:C:5:HIS:HB2	1:C:302:LEU:HD23	1.82	0.61
1:B:186:CYS:HB3	1:B:288:VAL:HG13	1.82	0.60
1:E:233:GLN:CD	1:E:233:GLN:H	2.05	0.60
1:D:344:ALA:HB3	1:D:355:ALA:HB2	1.83	0.60
1:D:217:ARG:HH11	1:D:217:ARG:HG3	1.66	0.59
1:D:51:GLU:HG2	1:E:378:PRO:HG2	1.83	0.59
1:B:271:VAL:HG13	1:B:272:PRO:HD2	1.83	0.59
1:E:41:MET:HE2	1:E:145:PRO:HA	1.82	0.59
1:A:56:THR:HG23	1:A:131:VAL:HG22	1.84	0.59
1:B:69:LYS:HG3	1:B:84:GLU:OE2	2.02	0.59
1:D:187:ARG:NH2	1:F:170:GLU:OE1	2.35	0.59
1:B:36:GLU:HG3	1:B:298:LYS:HD3	1.83	0.59
1:E:316:ARG:HH11	1:E:316:ARG:HG2	1.68	0.58
1:E:91:VAL:HG12	1:E:244:PHE:HE2	1.68	0.58
1:B:5:HIS:HB2	1:B:302:LEU:CD2	2.34	0.58
1:B:344:ALA:HB3	1:B:355:ALA:HB2	1.84	0.58
1:B:217:ARG:NH1	1:B:217:ARG:HB2	2.18	0.58
1:A:70:VAL:HG12	1:A:71:ALA:N	2.19	0.58
1:F:378:PRO:HA	1:F:394:GLN:HB3	1.84	0.58
1:C:349:SER:H	1:C:350:PRO:CD	2.17	0.58
1:C:84:GLU:N	1:C:84:GLU:OE1	2.36	0.58
1:C:170:GLU:HG3	1:C:186:CYS:O	2.04	0.58
1:C:244:PHE:CE1	1:C:254:VAL:HG22	2.39	0.58
1:D:69:LYS:HG3	1:D:84:GLU:OE2	2.04	0.58
1:F:209:LEU:H	1:F:211:THR:HG23	1.68	0.58
1:A:84:GLU:OE1	1:A:84:GLU:N	2.36	0.58
1:F:93:LYS:HB2	1:F:244:PHE:CD2	2.40	0.57
1:A:143:VAL:HG11	1:A:176:MET:SD	2.44	0.57
1:C:309:LYS:HG3	1:C:310:THR:HG23	1.86	0.57
1:B:69:LYS:HE3	1:E:316:ARG:HH21	1.70	0.57
1:C:139:TYR:CZ	1:C:188:VAL:HG13	2.39	0.57
1:B:309:LYS:CG	1:B:387:GLU:HG3	2.34	0.57
1:F:84:GLU:N	1:F:84:GLU:OE1	2.38	0.57
1:C:93:LYS:HB2	1:C:244:PHE:CD2	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:52:ASN:OD1	1:E:279:THR:HB	2.04	0.56
1:F:145:PRO:O	1:F:146:HIS:HB3	2.04	0.56
1:E:36:GLU:OE2	1:E:300:LYS:HE2	2.05	0.56
1:A:170:GLU:OE1	1:B:187:ARG:NH2	2.38	0.56
1:B:170:GLU:OE1	1:C:187:ARG:NH2	2.39	0.56
1:F:349:SER:H	1:F:350:PRO:CD	2.19	0.56
1:C:68:THR:HA	1:C:117:VAL:HG12	1.88	0.56
1:D:145:PRO:O	1:D:146:HIS:HB3	2.05	0.56
1:E:349:SER:H	1:E:350:PRO:CD	2.19	0.55
1:F:143:VAL:HG11	1:F:176:MET:SD	2.46	0.55
1:D:378:PRO:HA	1:D:394:GLN:HB3	1.89	0.55
1:C:170:GLU:HG2	1:C:185:LEU:CD2	2.33	0.55
1:F:2:ARG:N	1:F:367:ASN:ND2	2.55	0.55
1:B:93:LYS:HB2	1:B:244:PHE:CD2	2.41	0.55
1:D:77:MET:O	1:D:78:GLY:O	2.23	0.55
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.71	0.55
1:D:349:SER:H	1:D:350:PRO:CD	2.18	0.55
1:D:35:ALA:HB2	1:D:299:MET:HE2	1.89	0.55
1:B:41:MET:CE	1:B:145:PRO:HA	2.36	0.55
1:A:349:SER:H	1:A:350:PRO:HD3	1.71	0.55
1:D:170:GLU:HG2	1:D:185:LEU:CD2	2.36	0.55
1:B:20:ARG:HD3	1:C:12:VAL:CG2	2.37	0.55
1:C:349:SER:H	1:C:350:PRO:HD3	1.72	0.55
1:A:69:LYS:HG3	1:A:84:GLU:OE2	2.08	0.55
1:B:378:PRO:HA	1:B:394:GLN:HB3	1.90	0.54
1:D:65:LEU:HB3	1:D:117:VAL:HG21	1.89	0.54
1:E:339:ARG:HG2	1:E:339:ARG:HH11	1.72	0.54
1:A:96:GLN:HE22	1:B:110:LYS:HG3	1.70	0.54
1:A:344:ALA:HB3	1:A:355:ALA:HB2	1.90	0.54
1:A:13:THR:HG22	2:A:2004:HOH:O	2.08	0.54
1:E:85:GLU:O	1:E:86:HIS:HB2	2.07	0.54
1:A:246:ALA:HB1	1:C:79:PRO:HG3	1.89	0.54
1:A:297:LEU:HD23	1:A:297:LEU:O	2.08	0.54
1:E:139:TYR:CZ	1:E:188:VAL:HG13	2.42	0.54
1:E:93:LYS:HD3	1:E:94:ARG:H	1.73	0.54
1:B:84:GLU:OE1	1:B:84:GLU:N	2.40	0.54
1:C:186:CYS:HB3	1:C:288:VAL:HG13	1.89	0.54
1:E:170:GLU:HG3	1:E:186:CYS:O	2.07	0.54
1:F:217:ARG:HH11	1:F:217:ARG:HG3	1.73	0.53
1:D:339:ARG:HG3	1:D:339:ARG:HH11	1.72	0.53
1:C:176:MET:HE2	1:C:182:VAL:HG11	1.91	0.53
1:A:330:VAL:HG11	1:A:385:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:74:CYS:HB2	1:D:77:MET:HG2	1.90	0.53
1:A:223:LEU:HA	2:A:2040:HOH:O	2.08	0.53
1:B:55:LYS:HG2	1:B:130:HIS:CE1	2.44	0.53
1:E:233:GLN:H	1:E:233:GLN:NE2	2.05	0.53
1:F:93:LYS:HD3	1:F:94:ARG:N	2.24	0.53
1:E:344:ALA:HB3	1:E:355:ALA:HB2	1.91	0.53
1:B:139:TYR:CZ	1:B:188:VAL:HG13	2.44	0.53
1:F:15:THR:CG2	1:F:16:GLN:HE21	2.14	0.53
1:A:244:PHE:CE1	1:A:254:VAL:HG22	2.44	0.53
1:E:20:ARG:HD3	1:E:291:GLU:OE2	2.08	0.53
1:A:145:PRO:O	1:A:146:HIS:HB3	2.08	0.53
1:F:301:GLY:O	1:F:302:LEU:HB2	2.09	0.53
1:E:310:THR:HG22	1:E:387:GLU:OE1	2.09	0.53
1:B:41:MET:HG3	1:B:176:MET:HE2	1.91	0.53
1:D:35:ALA:HB2	1:D:299:MET:CE	2.38	0.53
1:B:130:HIS:HB2	1:B:199:ILE:HB	1.90	0.53
1:C:344:ALA:HB3	1:C:355:ALA:HB2	1.91	0.53
1:C:137:ILE:HD12	1:C:194:LEU:HD11	1.90	0.52
1:A:85:GLU:O	1:A:86:HIS:HB2	2.08	0.52
1:F:41:MET:CE	1:F:145:PRO:HA	2.39	0.52
1:F:5:HIS:HB2	1:F:302:LEU:HD23	1.90	0.52
1:E:74:CYS:O	1:E:76:THR:N	2.35	0.52
1:D:349:SER:H	1:D:350:PRO:HD3	1.74	0.52
1:B:97:SER:O	1:B:110:LYS:HA	2.09	0.52
1:A:378:PRO:HA	1:A:394:GLN:HB3	1.90	0.52
1:B:349:SER:H	1:B:350:PRO:CD	2.21	0.52
1:D:97:SER:O	1:D:110:LYS:HA	2.10	0.52
1:C:93:LYS:HD3	1:C:94:ARG:N	2.24	0.52
1:C:145:PRO:O	1:C:146:HIS:HB3	2.10	0.52
1:D:297:LEU:HD23	1:D:297:LEU:O	2.10	0.52
1:D:344:ALA:CB	1:D:355:ALA:HB2	2.39	0.51
1:C:137:ILE:HD12	1:C:194:LEU:CD1	2.41	0.51
1:C:56:THR:HG23	1:C:131:VAL:HG22	1.92	0.51
1:F:74:CYS:O	1:F:76:THR:N	2.41	0.51
1:D:170:GLU:OE1	1:E:187:ARG:NH2	2.44	0.51
1:C:301:GLY:O	1:C:302:LEU:HB2	2.09	0.51
1:E:244:PHE:CE1	1:E:254:VAL:HG22	2.45	0.51
1:E:301:GLY:O	1:E:302:LEU:HB2	2.09	0.51
1:C:35:ALA:HB2	1:C:299:MET:CE	2.41	0.51
1:E:349:SER:H	1:E:350:PRO:HD3	1.76	0.51
1:B:55:LYS:HD2	1:B:230:GLU:OE1	2.09	0.51
1:C:378:PRO:HA	1:C:394:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:5:HIS:HB2	1:E:302:LEU:HD23	1.93	0.50
1:C:316:ARG:HH21	1:D:69:LYS:HE3	1.75	0.50
2:B:2038:HOH:O	1:C:9:ARG:HD3	2.10	0.50
1:B:93:LYS:HD3	1:B:94:ARG:N	2.27	0.50
1:B:349:SER:H	1:B:350:PRO:HD3	1.76	0.50
1:C:172:THR:HG22	1:C:173:ILE:N	2.27	0.50
1:E:93:LYS:O	1:E:114:VAL:HG23	2.11	0.50
1:E:145:PRO:O	1:E:146:HIS:HB3	2.12	0.50
1:A:271:VAL:HG13	1:A:272:PRO:HD2	1.94	0.50
1:C:139:TYR:CG	1:C:188:VAL:HG22	2.47	0.49
1:A:244:PHE:CD1	1:A:254:VAL:HG22	2.47	0.49
1:A:349:SER:N	1:A:350:PRO:CD	2.73	0.49
1:C:91:VAL:HG12	1:C:244:PHE:HE2	1.77	0.49
1:A:187:ARG:NH2	1:C:170:GLU:OE1	2.45	0.49
1:E:74:CYS:C	1:E:76:THR:H	2.15	0.49
1:D:354:VAL:HB	1:D:377:PRO:HG2	1.94	0.49
1:A:248:HIS:O	1:A:250:VAL:N	2.45	0.49
1:D:41:MET:CE	1:D:145:PRO:HA	2.38	0.49
1:B:344:ALA:CB	1:B:355:ALA:HB2	2.42	0.49
1:A:35:ALA:HB2	1:A:299:MET:CE	2.42	0.49
1:F:70:VAL:HG12	1:F:71:ALA:N	2.26	0.49
1:C:74:CYS:C	1:C:76:THR:H	2.15	0.49
1:D:271:VAL:HG13	1:D:272:PRO:HD2	1.93	0.49
1:F:7:GLU:HA	1:F:302:LEU:O	2.12	0.49
1:E:73:ARG:HG3	1:E:77:MET:HB2	1.95	0.49
1:A:74:CYS:O	1:A:76:THR:N	2.45	0.49
1:F:26:GLU:HA	1:F:287:HIS:HB3	1.94	0.49
1:D:7:GLU:HA	1:D:302:LEU:O	2.12	0.49
1:B:401:ARG:NE	2:B:2077:HOH:O	2.46	0.49
1:A:346:ALA:O	1:A:347:HIS:C	2.51	0.49
1:C:77:MET:O	1:C:78:GLY:O	2.31	0.49
1:F:349:SER:H	1:F:350:PRO:HD3	1.77	0.49
1:C:74:CYS:O	1:C:76:THR:N	2.45	0.48
1:E:316:ARG:NH1	1:E:319:THR:HG21	2.25	0.48
1:D:12:VAL:HG21	1:F:20:ARG:HB2	1.95	0.48
1:E:41:MET:CE	1:E:145:PRO:HA	2.43	0.48
1:B:275:HIS:CD2	1:B:284:LYS:HG3	2.48	0.48
1:E:49:TYR:CZ	1:E:280:LYS:HE3	2.48	0.48
1:C:73:ARG:HG2	1:C:80:ALA:HB2	1.95	0.48
1:F:349:SER:N	1:F:350:PRO:CD	2.76	0.48
1:F:213:TRP:CD2	1:F:268:LEU:HD13	2.47	0.48
1:D:93:LYS:HD3	1:D:94:ARG:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:349:SER:N	1:C:350:PRO:CD	2.76	0.48
1:B:49:TYR:HB3	1:B:282:HIS:ND1	2.28	0.48
1:B:310:THR:HG22	1:B:387:GLU:OE1	2.13	0.48
1:C:26:GLU:HA	1:C:287:HIS:CB	2.43	0.48
1:C:288:VAL:HG12	1:C:290:CYS:SG	2.53	0.48
1:B:256:ASN:OD1	1:B:258:GLY:N	2.40	0.48
1:A:184:LEU:HD23	1:A:292:VAL:HG22	1.95	0.48
1:D:26:GLU:HA	1:D:287:HIS:CB	2.43	0.48
1:D:217:ARG:HG3	1:D:217:ARG:NH1	2.28	0.48
1:A:147:THR:HG23	1:A:147:THR:O	2.14	0.48
1:B:349:SER:N	1:B:350:PRO:CD	2.77	0.48
1:C:314:TRP:CD1	1:C:388:LEU:HD11	2.49	0.48
1:A:366:ASN:N	1:A:366:ASN:HD22	2.11	0.48
1:F:344:ALA:CB	1:F:355:ALA:HB2	2.44	0.48
1:F:306:MET:CE	1:F:341:PRO:HB3	2.44	0.48
1:E:172:THR:HG22	1:E:173:ILE:N	2.28	0.47
1:D:349:SER:N	1:D:350:PRO:CD	2.76	0.47
1:F:393:PHE:HB3	2:F:2054:HOH:O	2.13	0.47
1:F:342:VAL:HG21	1:F:372:ILE:HD13	1.96	0.47
1:E:312:PHE:HB2	2:E:2037:HOH:O	2.15	0.47
1:B:145:PRO:O	1:B:146:HIS:HB3	2.13	0.47
1:E:137:ILE:HG22	1:E:139:TYR:CE1	2.50	0.47
1:B:311:LYS:HB3	1:B:333:SER:OG	2.15	0.47
1:A:357:LEU:HD23	1:A:374:MET:HB3	1.96	0.47
1:A:316:ARG:NE	2:A:2053:HOH:O	2.48	0.47
1:E:26:GLU:HA	1:E:287:HIS:CB	2.44	0.47
1:A:323:HIS:ND1	2:A:2054:HOH:O	2.35	0.47
1:F:26:GLU:HA	1:F:287:HIS:CB	2.44	0.47
1:F:18:THR:HA	1:F:295:GLU:OE1	2.15	0.47
1:F:172:THR:HG22	1:F:173:ILE:N	2.29	0.47
1:A:115:ALA:HB3	1:A:252:MET:HE3	1.95	0.47
1:D:91:VAL:HG12	1:D:244:PHE:HE2	1.79	0.47
1:A:176:MET:HB2	1:A:179:TYR:HB2	1.97	0.47
1:C:7:GLU:HA	1:C:302:LEU:O	2.14	0.47
1:E:349:SER:N	1:E:350:PRO:CD	2.77	0.47
1:F:354:VAL:HB	1:F:377:PRO:HG2	1.97	0.47
1:E:84:GLU:OE1	1:E:84:GLU:N	2.48	0.47
1:D:142:LYS:NZ	1:D:162:THR:OG1	2.46	0.47
1:A:41:MET:CE	1:A:145:PRO:HA	2.44	0.46
1:C:354:VAL:HB	1:C:377:PRO:HG2	1.97	0.46
1:D:147:THR:HG23	1:D:147:THR:O	2.15	0.46
1:A:295:GLU:HG2	1:B:9:ARG:CG	2.37	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:VAL:HG12	1:B:244:PHE:HE2	1.80	0.46
1:F:85:GLU:O	1:F:86:HIS:HB2	2.15	0.46
1:B:35:ALA:HB2	1:B:299:MET:CE	2.46	0.46
1:C:103:ASN:O	1:C:104:HIS:HB2	2.16	0.46
1:B:40:SER:O	1:B:41:MET:HE2	2.16	0.46
1:F:75:PRO:O	1:F:76:THR:HG23	2.16	0.46
1:A:172:THR:HG22	1:A:173:ILE:N	2.31	0.46
1:D:200:LEU:HD23	1:D:268:LEU:HD11	1.97	0.46
1:F:97:SER:O	1:F:110:LYS:HA	2.14	0.46
1:E:91:VAL:HG12	1:E:244:PHE:CE2	2.50	0.46
1:B:297:LEU:HD23	1:B:297:LEU:O	2.15	0.46
1:F:347:HIS:CE1	1:F:382:ILE:HD11	2.50	0.46
1:D:12:VAL:CG2	1:F:20:ARG:HD3	2.43	0.46
1:D:23:LEU:HD22	1:D:31:VAL:HG21	1.97	0.46
1:A:354:VAL:HB	1:A:377:PRO:HG2	1.98	0.46
1:B:213:TRP:CD2	1:B:268:LEU:HD13	2.51	0.46
1:F:239:GLU:HA	1:F:242:VAL:O	2.16	0.46
1:A:186:CYS:HB3	1:A:288:VAL:HG11	1.98	0.46
1:E:244:PHE:CD1	1:E:254:VAL:HG22	2.51	0.46
1:E:133:ASP:HB3	1:E:136:LYS:HB2	1.97	0.46
1:E:67:ASP:O	1:E:68:THR:CB	2.64	0.45
1:C:311:LYS:HB3	1:C:333:SER:OG	2.16	0.45
1:C:29:GLY:O	1:C:44:TRP:HB2	2.15	0.45
1:F:170:GLU:HG3	1:F:186:CYS:O	2.16	0.45
1:E:173:ILE:HD12	1:F:9:ARG:HH21	1.81	0.45
1:F:65:LEU:HD11	1:F:242:VAL:HG21	1.99	0.45
1:E:23:LEU:HD22	1:E:31:VAL:HG11	1.99	0.45
1:A:139:TYR:CE1	1:A:188:VAL:CG1	3.00	0.45
1:A:309:LYS:O	1:A:309:LYS:HG2	2.15	0.45
1:F:217:ARG:HG3	1:F:217:ARG:NH1	2.31	0.45
1:D:275:HIS:CD2	1:D:284:LYS:HG3	2.50	0.45
1:B:66:SER:OG	1:B:118:LYS:HB2	2.16	0.45
1:F:95:ASP:OD1	1:F:96:GLN:N	2.39	0.45
1:C:186:CYS:HB3	1:C:288:VAL:CG1	2.46	0.45
1:C:310:THR:HG22	1:C:387:GLU:OE1	2.16	0.45
1:E:26:GLU:HA	1:E:287:HIS:HB3	1.99	0.45
1:A:29:GLY:O	1:A:44:TRP:HB2	2.16	0.45
1:B:7:GLU:HA	1:B:302:LEU:O	2.17	0.45
1:F:34:THR:HB	1:F:40:SER:OG	2.16	0.45
1:F:53:PRO:HB2	1:F:131:VAL:O	2.16	0.45
1:E:89:GLY:HA2	2:E:2030:HOH:O	2.16	0.45
1:E:49:TYR:CE2	1:E:280:LYS:HE3	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:31:VAL:O	1:D:31:VAL:HG23	2.16	0.45
1:D:256:ASN:C	1:D:258:GLY:H	2.20	0.45
1:C:33:ILE:HG13	1:C:33:ILE:O	2.17	0.45
1:E:75:PRO:O	1:E:76:THR:HG23	2.15	0.45
1:E:35:ALA:HB2	1:E:299:MET:HE2	1.98	0.45
1:C:122:GLU:O	1:C:125:LYS:HB2	2.17	0.45
1:C:133:ASP:HB3	1:C:136:LYS:HB2	1.99	0.45
1:B:147:THR:HG23	1:B:147:THR:O	2.17	0.45
1:A:170:GLU:HG3	1:A:186:CYS:O	2.17	0.44
1:E:316:ARG:NH1	1:E:316:ARG:HG2	2.31	0.44
1:C:339:ARG:HG2	1:C:339:ARG:NH1	2.32	0.44
1:A:366:ASN:N	1:A:366:ASN:ND2	2.64	0.44
1:A:213:TRP:CD2	1:A:268:LEU:HD13	2.53	0.44
1:F:133:ASP:HB3	1:F:136:LYS:HB2	2.00	0.44
1:F:275:HIS:CD2	1:F:284:LYS:HG3	2.53	0.44
1:B:139:TYR:CE1	1:B:188:VAL:HG13	2.53	0.44
1:C:197:THR:HG22	1:C:198:VAL:N	2.33	0.44
1:C:346:ALA:O	1:C:347:HIS:C	2.55	0.44
1:C:66:SER:OG	1:C:67:ASP:N	2.50	0.44
1:E:34:THR:HB	1:E:40:SER:OG	2.18	0.44
1:A:137:ILE:HD12	1:A:194:LEU:HD11	2.00	0.44
1:D:51:GLU:HG2	1:E:378:PRO:CG	2.45	0.44
1:C:143:VAL:HG11	1:C:176:MET:SD	2.58	0.44
1:F:49:TYR:CZ	1:F:280:LYS:HE3	2.52	0.44
1:B:186:CYS:HB3	1:B:288:VAL:CG1	2.48	0.44
1:A:339:ARG:HH11	1:A:339:ARG:HG3	1.82	0.44
1:D:40:SER:O	1:D:41:MET:HE2	2.17	0.44
1:C:237:ASN:HA	1:C:239:GLU:OE2	2.18	0.44
1:B:26:GLU:HA	1:B:287:HIS:CB	2.48	0.44
1:B:237:ASN:HA	1:B:239:GLU:OE2	2.18	0.44
1:D:20:ARG:HD2	1:E:12:VAL:HG23	1.99	0.43
1:A:344:ALA:CB	1:A:355:ALA:HB2	2.48	0.43
1:D:256:ASN:C	1:D:258:GLY:N	2.72	0.43
1:C:248:HIS:O	1:C:250:VAL:N	2.51	0.43
1:D:170:GLU:HG3	1:D:186:CYS:O	2.18	0.43
1:E:301:GLY:O	1:E:302:LEU:CB	2.66	0.43
1:A:9:ARG:HD3	1:C:295:GLU:OE2	2.18	0.43
1:D:139:TYR:CG	1:D:188:VAL:HG22	2.53	0.43
1:F:35:ALA:HB2	1:F:299:MET:HE2	1.99	0.43
1:A:310:THR:HG22	1:A:387:GLU:OE1	2.18	0.43
1:A:35:ALA:HB2	1:A:299:MET:HE1	2.00	0.43
1:C:49:TYR:CZ	1:C:280:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:89:GLY:O	1:C:118:LYS:HA	2.19	0.43
1:A:7:GLU:HA	1:A:302:LEU:O	2.18	0.43
1:E:122:GLU:O	1:E:125:LYS:HB2	2.18	0.43
1:D:346:ALA:O	1:D:347:HIS:C	2.56	0.43
1:B:56:THR:HA	1:C:399:ILE:HD13	2.01	0.43
1:F:171:LYS:HE2	1:F:183:SER:HB2	1.99	0.43
1:D:26:GLU:OE2	1:D:360:PRO:HD2	2.18	0.43
1:B:26:GLU:HA	1:B:287:HIS:HB3	2.00	0.43
1:C:288:VAL:CG1	1:C:290:CYS:SG	3.07	0.43
1:A:297:LEU:C	1:A:297:LEU:HD23	2.39	0.43
1:C:305:THR:O	1:C:338:CYS:HB2	2.19	0.43
1:D:173:ILE:HD12	1:E:9:ARG:HH21	1.83	0.43
1:F:137:ILE:HD12	1:F:194:LEU:HD11	1.99	0.43
1:F:301:GLY:O	1:F:302:LEU:CB	2.67	0.43
1:D:204:LYS:C	1:D:206:VAL:N	2.71	0.43
1:C:93:LYS:C	1:C:93:LYS:HD3	2.39	0.43
1:F:172:THR:HG22	1:F:173:ILE:H	1.84	0.43
1:F:197:THR:HG22	1:F:198:VAL:N	2.33	0.43
1:B:65:LEU:HB3	1:B:117:VAL:HG21	2.00	0.43
1:D:93:LYS:HD3	1:D:93:LYS:C	2.39	0.43
1:F:139:TYR:CE1	1:F:188:VAL:CG1	3.01	0.43
1:D:184:LEU:HD23	1:D:292:VAL:HG22	2.00	0.43
1:C:5:HIS:CB	1:C:302:LEU:HD23	2.47	0.42
1:B:295:GLU:HG3	2:B:2038:HOH:O	2.18	0.42
1:F:297:LEU:HD23	2:F:2003:HOH:O	2.19	0.42
1:E:346:ALA:O	1:E:347:HIS:C	2.57	0.42
1:D:243:GLU:OE1	1:D:257:LEU:HD11	2.19	0.42
1:A:49:TYR:HB3	1:A:282:HIS:ND1	2.35	0.42
1:B:20:ARG:HB2	1:C:12:VAL:HG21	2.01	0.42
1:B:346:ALA:O	1:B:347:HIS:C	2.58	0.42
1:B:217:ARG:CB	1:B:217:ARG:HH11	2.32	0.42
1:A:40:SER:O	1:A:41:MET:HE2	2.20	0.42
1:B:354:VAL:HB	1:B:377:PRO:HG2	2.01	0.42
1:D:74:CYS:O	1:D:76:THR:N	2.53	0.42
1:A:74:CYS:C	1:A:76:THR:H	2.22	0.42
1:A:217:ARG:HH21	1:C:217:ARG:HH21	1.66	0.42
1:B:288:VAL:HG12	1:B:290:CYS:SG	2.59	0.42
1:C:344:ALA:CB	1:C:355:ALA:HB2	2.49	0.42
1:C:172:THR:HG22	1:C:173:ILE:H	1.84	0.42
1:A:137:ILE:HG22	1:A:139:TYR:CE1	2.54	0.42
1:B:217:ARG:CZ	1:B:217:ARG:HB2	2.50	0.42
1:B:354:VAL:HB	1:B:377:PRO:CG	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:PRO:HD2	1:A:281:TYR:CD1	2.54	0.42
1:E:354:VAL:HB	1:E:377:PRO:HG2	2.01	0.42
1:D:289:THR:HG21	1:F:170:GLU:OE2	2.19	0.42
1:E:93:LYS:HB2	1:E:244:PHE:CD2	2.55	0.42
1:C:301:GLY:O	1:C:302:LEU:CB	2.68	0.42
1:A:41:MET:HE2	1:A:145:PRO:HA	2.02	0.42
1:C:26:GLU:HA	1:C:287:HIS:HB3	2.01	0.42
1:D:137:ILE:HD12	1:D:194:LEU:HD11	2.02	0.42
1:F:313:THR:OG1	1:F:331:THR:HB	2.19	0.42
1:C:65:LEU:HD21	1:C:242:VAL:CG2	2.50	0.42
1:E:69:LYS:HG3	1:E:84:GLU:OE2	2.20	0.42
1:B:171:LYS:HE2	1:B:183:SER:HB2	2.01	0.42
1:A:26:GLU:HA	1:A:287:HIS:CB	2.50	0.41
1:C:147:THR:HG23	1:C:147:THR:O	2.20	0.41
1:D:26:GLU:HA	1:D:287:HIS:HB3	2.02	0.41
1:B:217:ARG:CB	1:B:217:ARG:NH1	2.81	0.41
1:E:147:THR:HG23	1:E:147:THR:O	2.20	0.41
1:A:77:MET:O	1:A:78:GLY:O	2.37	0.41
1:D:244:PHE:CD1	1:D:254:VAL:HG22	2.55	0.41
1:D:91:VAL:HG12	1:D:244:PHE:CE2	2.56	0.41
1:F:69:LYS:HG3	1:F:84:GLU:OE2	2.20	0.41
1:F:5:HIS:CB	1:F:302:LEU:HD23	2.50	0.41
1:A:36:GLU:CD	1:A:300:LYS:HE2	2.41	0.41
1:B:288:VAL:CG1	1:B:290:CYS:SG	3.09	0.41
1:F:213:TRP:CE3	1:F:268:LEU:HD13	2.56	0.41
1:C:97:SER:O	1:C:110:LYS:HA	2.20	0.41
1:E:4:THR:CG2	1:E:5:HIS:N	2.84	0.41
1:A:312:PHE:HB2	2:A:2051:HOH:O	2.21	0.41
1:F:295:GLU:HA	1:F:295:GLU:OE1	2.21	0.41
1:A:171:LYS:HE2	1:A:183:SER:HB2	2.03	0.41
1:D:200:LEU:O	1:D:212:ALA:HA	2.20	0.41
1:A:103:ASN:O	1:A:104:HIS:HB2	2.20	0.41
1:A:26:GLU:HA	1:A:287:HIS:HB3	2.03	0.41
1:D:244:PHE:CE1	1:D:254:VAL:HG22	2.55	0.41
1:A:139:TYR:CZ	1:A:188:VAL:CG1	3.02	0.41
1:A:139:TYR:CE1	1:A:188:VAL:HG13	2.56	0.41
1:D:213:TRP:CD2	1:D:268:LEU:HD13	2.56	0.41
1:F:343:ARG:HG2	1:F:384:TYR:HB2	2.01	0.41
1:F:88:GLY:HA3	1:F:234:ASN:ND2	2.35	0.41
1:A:4:THR:CG2	1:A:5:HIS:N	2.84	0.41
1:B:195:ALA:O	1:B:217:ARG:HD2	2.21	0.41
1:A:21:VAL:HB	1:A:292:VAL:HB	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:34:THR:O	1:D:300:LYS:HB2	2.20	0.41
1:D:287:HIS:CD2	1:D:289:THR:HG22	2.56	0.40
1:F:206:VAL:O	1:F:207:GLU:C	2.59	0.40
1:F:248:HIS:O	1:F:250:VAL:N	2.54	0.40
1:B:133:ASP:HB3	1:B:136:LYS:HB2	2.03	0.40
1:D:172:THR:HG22	1:D:173:ILE:N	2.36	0.40
1:C:20:ARG:NE	1:C:291:GLU:CD	2.75	0.40
1:B:329:GLU:HA	1:B:370:GLY:O	2.21	0.40
1:F:184:LEU:HD23	1:F:292:VAL:HG22	2.02	0.40
1:D:93:LYS:HB2	1:D:244:PHE:CE2	2.56	0.40
1:E:137:ILE:HD13	1:E:283:LEU:HD11	2.03	0.40
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.82	0.40
1:A:218:ASP:OD1	1:C:217:ARG:NH2	2.54	0.40
1:D:71:ALA:O	1:D:113:ILE:HA	2.21	0.40
1:F:103:ASN:O	1:F:104:HIS:HB2	2.21	0.40
1:F:200:LEU:O	1:F:212:ALA:HA	2.21	0.40
1:C:21:VAL:HB	1:C:292:VAL:HB	2.03	0.40
1:F:296:LYS:O	1:F:296:LYS:HG3	2.21	0.40
1:D:277:GLU:OE2	1:D:280:LYS:HD2	2.22	0.40
1:A:170:GLU:OE2	1:B:289:THR:HG21	2.21	0.40
1:A:139:TYR:CE1	1:A:188:VAL:HG11	2.57	0.40
1:F:139:TYR:CE1	1:F:188:VAL:HG13	2.55	0.40
1:B:14:GLY:HA3	1:C:12:VAL:HG13	2.04	0.40
1:E:383:ILE:O	1:E:389:SER:HA	2.21	0.40
1:D:218:ASP:OD2	1:F:56:THR:HG21	2.22	0.40
1:E:138:VAL:HG13	1:E:164:SER:HB3	2.02	0.40
1:C:361:ASN:HA	1:C:362:PRO:HD2	1.95	0.40
1:B:132:TYR:CE2	1:B:199:ILE:HD11	2.57	0.40
1:B:248:HIS:O	1:B:250:VAL:N	2.55	0.40
1:A:237:ASN:HA	1:A:239:GLU:OE2	2.21	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	376/401 (94%)	349 (93%)	18 (5%)	9 (2%)	9	22
1	B	381/401 (95%)	344 (90%)	23 (6%)	14 (4%)	5	11
1	C	379/401 (94%)	348 (92%)	22 (6%)	9 (2%)	9	22
1	D	380/401 (95%)	350 (92%)	17 (4%)	13 (3%)	6	12
1	E	376/401 (94%)	344 (92%)	22 (6%)	10 (3%)	8	19
1	F	384/401 (96%)	352 (92%)	19 (5%)	13 (3%)	6	12
All	All	2276/2406 (95%)	2087 (92%)	121 (5%)	68 (3%)	7	15

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	GLY
1	A	302	LEU
1	A	349	SER
1	B	206	VAL
1	B	302	LEU
1	B	349	SER
1	C	204	LYS
1	C	302	LEU
1	C	349	SER
1	D	78	GLY
1	D	204	LYS
1	D	302	LEU
1	D	349	SER
1	E	68	THR
1	E	302	LEU
1	E	349	SER
1	F	78	GLY
1	F	302	LEU
1	F	349	SER
1	A	75	PRO
1	A	249	ALA
1	A	296	LYS
1	B	78	GLY
1	B	296	LYS
1	C	78	GLY
1	D	206	VAL
1	F	209	LEU
1	A	309	LYS
1	A	347	HIS
1	B	67	ASP

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Mol	Chain	Res	Type
1	B	204	LYS
1	B	207	GLU
1	B	249	ALA
1	B	309	LYS
1	B	347	HIS
1	C	75	PRO
1	C	249	ALA
1	C	309	LYS
1	C	347	HIS
1	D	75	PRO
1	D	296	LYS
1	D	309	LYS
1	D	347	HIS
1	E	75	PRO
1	E	296	LYS
1	E	309	LYS
1	E	347	HIS
1	F	75	PRO
1	F	205	THR
1	F	207	GLU
1	F	249	ALA
1	F	296	LYS
1	A	146	HIS
1	B	146	HIS
1	C	146	HIS
1	D	249	ALA
1	E	67	ASP
1	E	146	HIS
1	E	249	ALA
1	F	347	HIS
1	B	75	PRO
1	D	146	HIS
1	F	146	HIS
1	D	52	ASN
1	F	206	VAL
1	F	52	ASN
1	B	350	PRO
1	D	350	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	315/331 (95%)	303 (96%)	12 (4%)	44	76
1	B	315/331 (95%)	304 (96%)	11 (4%)	48	80
1	C	315/331 (95%)	303 (96%)	12 (4%)	44	76
1	D	315/331 (95%)	308 (98%)	7 (2%)	64	90
1	E	315/331 (95%)	305 (97%)	10 (3%)	51	82
1	F	315/331 (95%)	301 (96%)	14 (4%)	39	71
All	All	1890/1986 (95%)	1824 (96%)	66 (4%)	48	80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	34	THR
1	A	52	ASN
1	A	93	LYS
1	A	131	VAL
1	A	185	LEU
1	A	203	ASP
1	A	289	THR
1	A	297	LEU
1	A	303	THR
1	A	324	ASP
1	A	347	HIS
1	B	15	THR
1	B	20	ARG
1	B	34	THR
1	B	67	ASP
1	B	185	LEU
1	B	289	THR
1	B	297	LEU
1	B	316	ARG
1	B	319	THR
1	B	324	ASP
1	B	391	GLN

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Mol	Chain	Res	Type
1	C	4	THR
1	C	20	ARG
1	C	34	THR
1	C	51	GLU
1	C	131	VAL
1	C	185	LEU
1	C	188	VAL
1	C	289	THR
1	C	297	LEU
1	C	303	THR
1	C	319	THR
1	C	324	ASP
1	D	20	ARG
1	D	34	THR
1	D	51	GLU
1	D	243	GLU
1	D	289	THR
1	D	297	LEU
1	D	324	ASP
1	E	34	THR
1	E	51	GLU
1	E	73	ARG
1	E	84	GLU
1	E	233	GLN
1	E	277	GLU
1	E	289	THR
1	E	297	LEU
1	E	303	THR
1	E	324	ASP
1	F	4	THR
1	F	34	THR
1	F	51	GLU
1	F	65	LEU
1	F	77	MET
1	F	122	GLU
1	F	146	HIS
1	F	185	LEU
1	F	230	GLU
1	F	295	GLU
1	F	297	LEU
1	F	303	THR
1	F	324	ASP

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Mol	Chain	Res	Type
1	F	347	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	52	ASN
1	A	96	GLN
1	A	221	ASN
1	A	234	ASN
1	A	275	HIS
1	A	366	ASN
1	B	16	GLN
1	B	96	GLN
1	B	130	HIS
1	B	221	ASN
1	B	275	HIS
1	B	366	ASN
1	B	391	GLN
1	C	96	GLN
1	C	221	ASN
1	C	233	GLN
1	C	234	ASN
1	C	275	HIS
1	C	366	ASN
1	D	16	GLN
1	D	52	ASN
1	D	96	GLN
1	D	130	HIS
1	D	234	ASN
1	D	275	HIS
1	D	366	ASN
1	E	16	GLN
1	E	96	GLN
1	E	221	ASN
1	E	233	GLN
1	E	275	HIS
1	E	282	HIS
1	E	366	ASN
1	F	16	GLN
1	F	52	ASN
1	F	96	GLN

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Mol	Chain	Res	Type
1	F	221	ASN
1	F	233	GLN
1	F	234	ASN
1	F	275	HIS
1	F	347	HIS
1	F	366	ASN

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	382/401 (95%)	-0.19	7 (1%) 65 71	13, 33, 67, 89	0
1	B	387/401 (96%)	-0.15	8 (2%) 60 67	12, 35, 70, 94	0
1	C	385/401 (96%)	-0.05	16 (4%) 35 39	12, 37, 71, 94	0
1	D	386/401 (96%)	-0.05	9 (2%) 57 64	16, 41, 74, 98	0
1	E	382/401 (95%)	0.10	19 (4%) 28 30	13, 41, 75, 95	0
1	F	388/401 (96%)	-0.03	13 (3%) 43 48	13, 37, 76, 99	0
All	All	2310/2406 (96%)	-0.06	72 (3%) 47 52	12, 37, 74, 99	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	147	THR	7.6
1	F	206	VAL	5.3
1	C	147	THR	5.2
1	E	146	HIS	4.7
1	A	347	HIS	4.3
1	B	205	THR	4.1
1	F	207	GLU	4.0
1	F	147	THR	4.0
1	D	147	THR	4.0
1	E	347	HIS	4.0
1	F	209	LEU	3.8
1	A	210	PRO	3.8
1	C	367	ASN	3.7
1	E	367	ASN	3.5
1	E	101	TRP	3.5
1	C	106	GLY	3.5
1	E	248	HIS	3.3
1	E	107	LEU	3.3
1	A	147	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	107	LEU	3.3
1	C	347	HIS	3.1
1	C	352	VAL	3.1
1	B	352	VAL	3.1
1	B	207	GLU	3.0
1	C	349	SER	3.0
1	F	208	HIS	3.0
1	E	108	PHE	2.9
1	E	176	MET	2.9
1	F	367	ASN	2.9
1	E	255	TYR	2.8
1	C	351	ASP	2.8
1	C	101	TRP	2.8
1	D	178	GLU	2.8
1	C	350	PRO	2.7
1	B	351	ASP	2.7
1	C	255	TYR	2.7
1	D	248	HIS	2.7
1	C	107	LEU	2.7
1	C	346	ALA	2.7
1	D	347	HIS	2.6
1	F	146	HIS	2.6
1	F	347	HIS	2.6
1	D	206	VAL	2.6
1	B	208	HIS	2.6
1	C	146	HIS	2.6
1	C	248	HIS	2.5
1	F	101	TRP	2.5
1	F	108	PHE	2.5
1	D	351	ASP	2.4
1	A	107	LEU	2.4
1	D	205	THR	2.3
1	A	101	TRP	2.3
1	D	249	ALA	2.3
1	B	147	THR	2.3
1	C	348	GLY	2.3
1	F	105	CYS	2.3
1	E	145	PRO	2.3
1	E	253	ASP	2.2
1	B	367	ASN	2.2
1	C	368	GLY	2.2
1	E	334	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	254	VAL	2.2
1	E	104	HIS	2.1
1	E	249	ALA	2.1
1	D	210	PRO	2.1
1	E	67	ASP	2.1
1	B	248	HIS	2.1
1	E	95	ASP	2.0
1	E	35	ALA	2.0
1	F	109	GLY	2.0
1	A	249	ALA	2.0
1	A	102	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.