Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 04:45 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

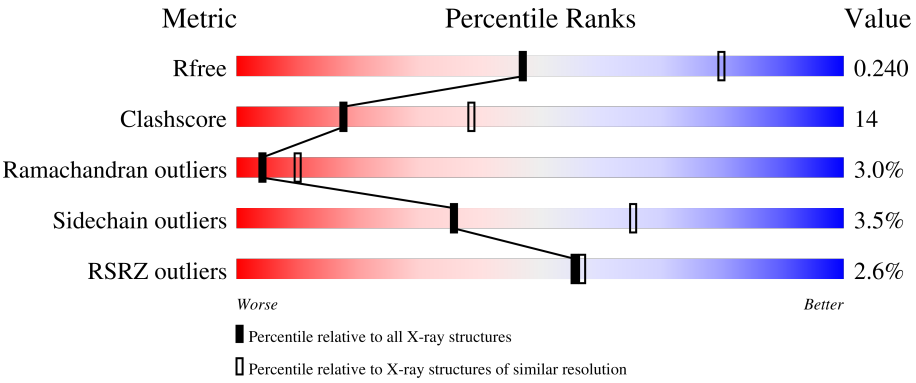
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	67% 26% 5%
1	B	401	2% 71% 23%
1	C	401	4% 67% 26%
1	D	401	72% 20%
1	E	401	3% 72% 20% 5%

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Mol	Chain	Length	Quality of chain
1	F	401	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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.

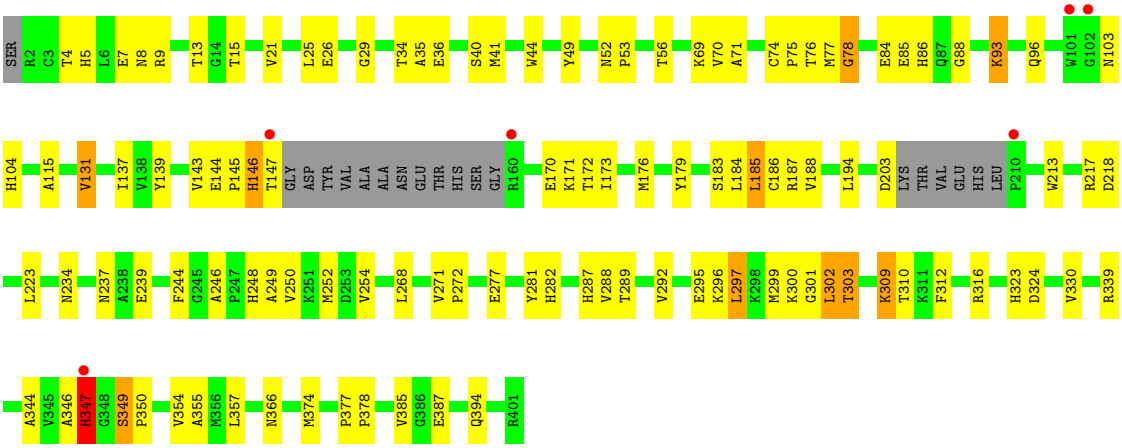
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	77	Total	O	0	0
			77	77		
2	C	64	Total	O	0	0
			64	64		
2	D	50	Total	O	0	0
			50	50		
2	E	49	Total	O	0	0
			49	49		
2	F	57	Total	O	0	0
			57	57		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

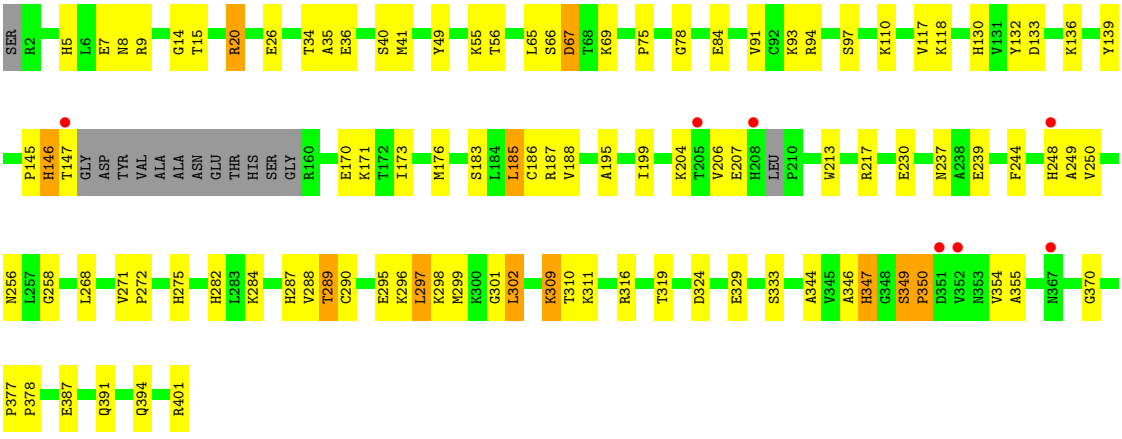
• Molecule 1: ENVELOPE PROTEIN

Chain A:



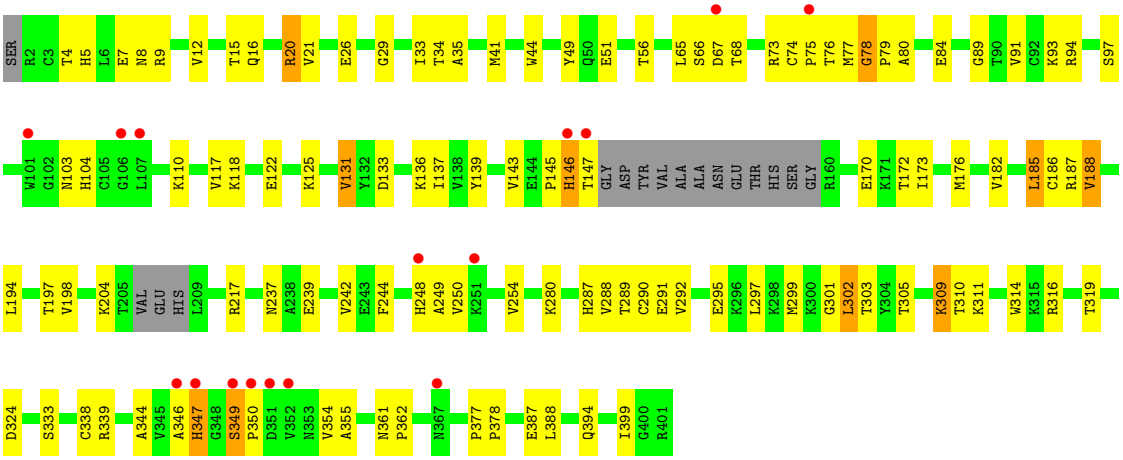
• Molecule 1: ENVELOPE PROTEIN

Chain B:



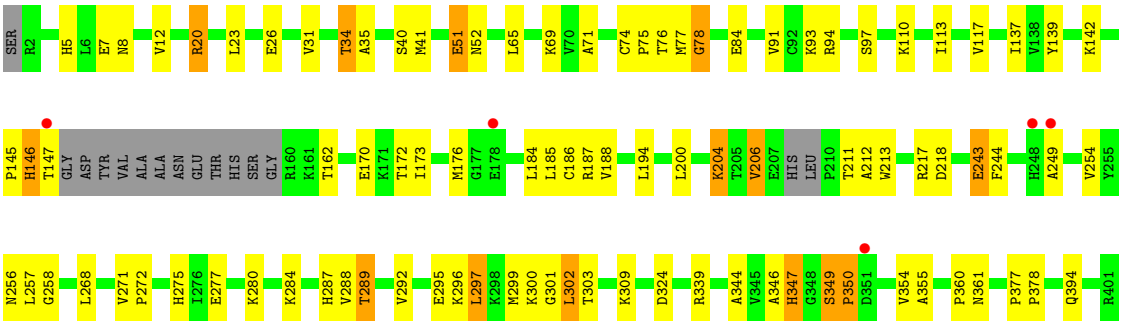
• Molecule 1: ENVELOPE PROTEIN

Chain C:



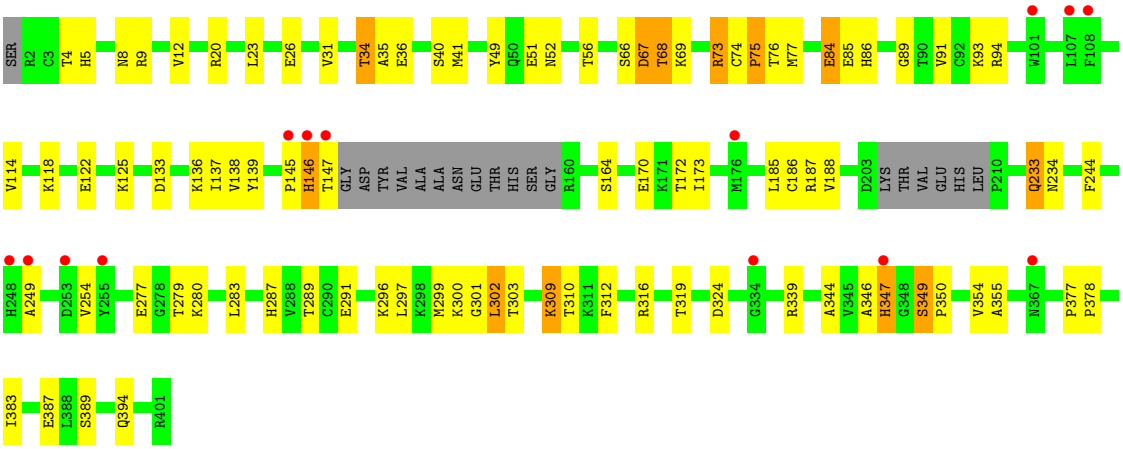
• Molecule 1: ENVELOPE PROTEIN

Chain D:



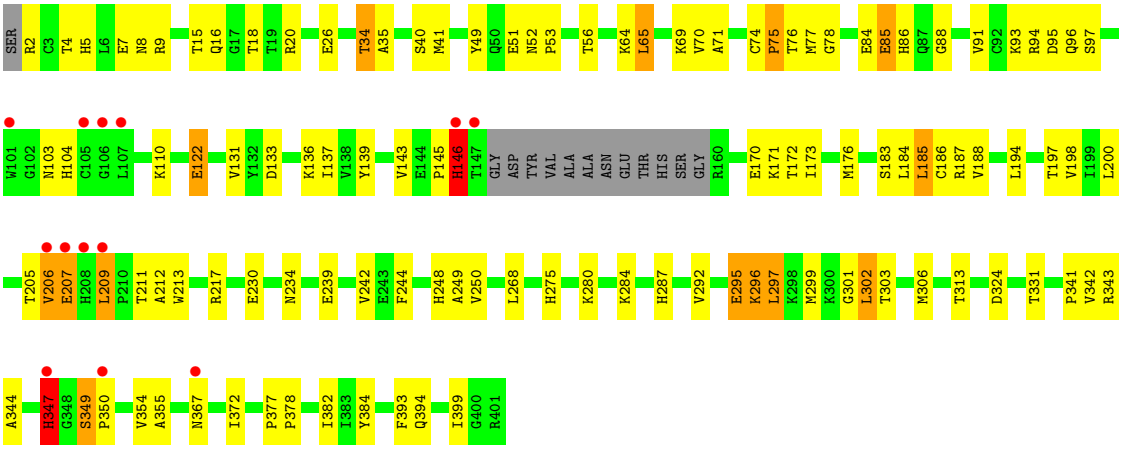
• Molecule 1: ENVELOPE PROTEIN

Chain E:



• Molecule 1: ENVELOPE PROTEIN

Chain F:


SER R2 C3 T4 H5 L6 E7 N8 R9 T15 Q16 G17 T18 T19 R20 E26 T34 A35 S40 M41 Y49 Q50 E51 N52 P53 T56 K64 L65 K69 V70 A71 C74 P75 T76 M77 G78 E84 E85 H86 Q87 G88 V91 C92 K93 R94 D95 Q96 S97
W101 G102 N103 H104 C105 G106 L107 K110 E122 V131 Y132 D133 K136 I137 V138 Y139 V143 E144 P145 H146 T147 GLY ASP TYR VAL ALA ALA ASN GLU THR HIS SER GLY R160 E170 K171 T172 I173 M176 S183 L184 L185 C186 R187 V188 L194 T197 V198 I199 L200
T205 V206 E207 H208 L209 P210 T211 A212 W213 R217 E230 N234 E239 V242 E243 F244 H248 A249 V250 L268 H275 K280 K284 H287 V292 E295 K296 L297 K298 M299 K300 G301 L302 T303 M306 T313 D324 T331 P341 V342 R343
A344 H347 G348 S349 P350 V354 A355 N367 I372 P377 P378 I382 I383 Y384 F393 Q394 I399 G400 R401

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.242 0.206 , 0.240	Depositor DCC
R_{free} test set	4090 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17986	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
1	E	2921	0	2881	78	0
1	F	2951	0	2893	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (477) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:A:277:GLU:HG3	1:A:277:GLU:O	1.77	0.82
1:C:170:GLU:HG2	1:C:185:LEU:HD23	1.61	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:D:5:HIS:HB2	1:D:302:LEU:HD23	1.64	0.78
1:F:170:GLU:HG2	1:F:185: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	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLU:HG2	1:E:9:ARG:HG2	1.72	0.70
1:A:139:TYR:CZ	1:A:188:VAL:HG13	2.26	0.70
1:A:277:GLU:HG2	1:A:282:HIS:NE2	2.07	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:HG3	1:D:20:ARG:HH11	1.64	0.62
1:D:20:ARG:HG3	1:D:20:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:F:170:GLU:HG2	1:F:185:LEU:CD2	2.30	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:D:344:ALA:HB3	1:D:355:ALA:HB2	1.83	0.60
1:E:233:GLN:CD	1:E:233:GLN:H	2.05	0.60
1:D:217:ARG:HG3	1:D:217:ARG:HH11	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:B:36:GLU:HG3	1:B:298:LYS:HD3	1.83	0.59
1:D:187:ARG:NH2	1:F:170:GLU:OE1	2.35	0.59
1:E:316:ARG:HH11	1:E:316:ARG:HG2	1.68	0.58
1:B:5:HIS:HB2	1:B:302:LEU:CD2	2.34	0.58
1:E:91:VAL:HG12	1:E:244:PHE:HE2	1.68	0.58
1:A:70:VAL:HG12	1:A:71:ALA:N	2.19	0.58
1:B:217:ARG:HB2	1:B:217:ARG:NH1	2.18	0.58
1:B:344:ALA:HB3	1:B:355:ALA:HB2	1.84	0.58
1:C:84:GLU:N	1:C:84:GLU:OE1	2.36	0.58
1:C:349:SER:H	1:C:350:PRO:CD	2.17	0.58
1:F:378:PRO:HA	1:F:394:GLN:HB3	1.84	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:A:84:GLU:N	1:A:84:GLU:OE1	2.36	0.58
1:F:209:LEU:H	1:F:211:THR:HG23	1.68	0.58
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:F:93:LYS:HB2	1:F:244:PHE:CD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:52:ASN:OD1	1:E:279:THR:HB	2.04	0.56
1:E:36:GLU:OE2	1:E:300:LYS:HE2	2.05	0.56
1:F:145:PRO:O	1:F:146:HIS:HB3	2.04	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:B:93:LYS:HB2	1:B:244:PHE:CD2	2.41	0.55
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.71	0.55
1:D:77:MET:O	1:D:78:GLY:O	2.23	0.55
1:F:2:ARG:N	1:F:367:ASN:ND2	2.55	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:A:349:SER:H	1:A:350:PRO:HD3	1.71	0.55
1:B:41:MET:CE	1:B:145:PRO:HA	2.36	0.55
1:A:69:LYS:HG3	1:A:84:GLU:OE2	2.08	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:D:170:GLU:HG2	1:D:185:LEU:CD2	2.36	0.55
1:B:378:PRO:HA	1:B:394:GLN:HB3	1.90	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:D:65:LEU:HB3	1:D:117:VAL:HG21	1.89	0.54
1:E:339:ARG:HH11	1:E:339:ARG:HG2	1.72	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:HG3	1:F:217:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG11	1:A:385:VAL:HG11	1.90	0.53
1:C:176:MET:HE2	1:C:182:VAL:HG11	1.91	0.53
1:D:339:ARG:HG3	1:D:339:ARG:HH11	1.72	0.53
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:B:139:TYR:CZ	1:B:188:VAL:HG13	2.44	0.53
1:E:233:GLN:NE2	1:E:233:GLN:H	2.05	0.53
1:E:344:ALA:HB3	1:E:355:ALA:HB2	1.91	0.53
1:F:93:LYS:HD3	1:F:94:ARG:N	2.24	0.53
1:A:244:PHE:CE1	1:A:254:VAL:HG22	2.44	0.53
1:F:15:THR:CG2	1:F:16:GLN:HE21	2.14	0.53
1:A:145:PRO:O	1:A:146:HIS:HB3	2.08	0.53
1:E:20:ARG:HD3	1:E:291:GLU:OE2	2.08	0.53
1:F:301:GLY:O	1:F:302:LEU:HB2	2.09	0.53
1:B:41:MET:HG3	1:B:176:MET:HE2	1.91	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:D:35:ALA:HB2	1:D:299:MET:CE	2.38	0.53
1:E:310:THR:HG22	1:E:387:GLU:OE1	2.09	0.53
1:A:85:GLU:O	1:A:86:HIS:HB2	2.08	0.52
1:C:137:ILE:HD12	1:C:194:LEU:HD11	1.90	0.52
1:F:41:MET:CE	1:F:145:PRO:HA	2.39	0.52
1:A:378:PRO:HA	1:A:394:GLN:HB3	1.90	0.52
1:B:97:SER:O	1:B:110:LYS:HA	2.09	0.52
1:D:349:SER:H	1:D:350:PRO:HD3	1.74	0.52
1:E:74:CYS:O	1:E:76:THR:N	2.35	0.52
1:F:5:HIS:HB2	1:F:302:LEU:HD23	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:C:137:ILE:HD12	1:C:194:LEU:CD1	2.41	0.51
1:D:344:ALA:CB	1:D:355:ALA:HB2	2.39	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:C:301:GLY:O	1:C:302:LEU:HB2	2.09	0.51
1:D:170:GLU:OE1	1:E:187:ARG:NH2	2.44	0.51
1:C:35:ALA:HB2	1:C:299:MET:CE	2.41	0.51
1:E:244:PHE:CE1	1:E:254:VAL:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:GLY:O	1:E:302:LEU:HB2	2.09	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
1:E:349:SER:H	1:E:350:PRO:HD3	1.76	0.51
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:A:271:VAL:HG13	1:A:272:PRO:HD2	1.94	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: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:A:248:HIS:O	1:A:250:VAL:N	2.45	0.49
1:D:354:VAL:HB	1:D:377:PRO:HG2	1.94	0.49
1:E:74:CYS:C	1:E:76:THR:H	2.15	0.49
1:A:35:ALA:HB2	1:A:299:MET:CE	2.42	0.49
1:B:344:ALA:CB	1:B:355:ALA:HB2	2.42	0.49
1:D:41:MET:CE	1:D:145:PRO:HA	2.38	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:A:74:CYS:O	1:A:76:THR:N	2.45	0.49
1:E:73:ARG:HG3	1:E:77:MET:HB2	1.95	0.49
1:F:26:GLU:HA	1:F:287:HIS:HB3	1.94	0.49
1:A:346:ALA:O	1:A:347:HIS:C	2.51	0.49
1:B:401:ARG:NE	2:B:2077:HOH:O	2.46	0.49
1:D:7:GLU:HA	1:D:302:LEU:O	2.12	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:B:275:HIS:CD2	1:B:284:LYS:HG3	2.48	0.48
1:C:73:ARG:HG2	1:C:80:ALA:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:TYR:CZ	1:E:280:LYS:HE3	2.48	0.48
1:E:316:ARG:NH1	1:E:319:THR:HG21	2.25	0.48
1:F:213:TRP:CD2	1:F:268:LEU:HD13	2.47	0.48
1:F:349:SER:N	1:F:350:PRO:CD	2.76	0.48
1:B:49:TYR:HB3	1:B:282:HIS:ND1	2.28	0.48
1:C:349:SER:N	1:C:350:PRO:CD	2.76	0.48
1:D:93:LYS:HD3	1:D:94:ARG:N	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:A:184:LEU:HD23	1:A:292:VAL:HG22	1.95	0.48
1:B:256:ASN:OD1	1:B:258:GLY:N	2.40	0.48
1:C:288:VAL:HG12	1:C:290:CYS:SG	2.53	0.48
1:D:26:GLU:HA	1:D:287:HIS:CB	2.43	0.48
1:A:147:THR:HG23	1:A:147:THR:O	2.14	0.48
1:D:217:ARG:HG3	1:D:217:ARG:NH1	2.28	0.48
1:A:366:ASN:N	1:A:366:ASN:HD22	2.11	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:F:306:MET:CE	1:F:341:PRO:HB3	2.44	0.48
1:F:344:ALA:CB	1:F:355:ALA:HB2	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:E:312:PHE:HB2	2:E:2037:HOH:O	2.15	0.47
1:F:342:VAL:HG21	1:F:372:ILE:HD13	1.96	0.47
1:A:357:LEU:HD23	1:A:374:MET:HB3	1.96	0.47
1:B:145:PRO:O	1:B:146:HIS:HB3	2.13	0.47
1:B:311:LYS:HB3	1:B:333:SER:OG	2.15	0.47
1:E:137:ILE:HG22	1:E:139:TYR:CE1	2.50	0.47
1:A:316:ARG:NE	2:A:2053:HOH:O	2.48	0.47
1:A:323:HIS:ND1	2:A:2054:HOH:O	2.35	0.47
1:E:26:GLU:HA	1:E:287:HIS:CB	2.44	0.47
1:A:115:ALA:HB3	1:A:252:MET:HE3	1.95	0.47
1:F:18:THR:HA	1:F:295:GLU:OE1	2.15	0.47
1:F:26:GLU:HA	1:F:287:HIS:CB	2.44	0.47
1:F:172:THR:HG22	1:F:173:ILE:N	2.29	0.47
1:A:176:MET:HB2	1:A:179:TYR:HB2	1.97	0.47
1:D:91:VAL:HG12	1:D:244:PHE:HE2	1.79	0.47
1:C:7:GLU:HA	1:C:302:LEU:O	2.14	0.47
1:D:142:LYS:NZ	1:D:162:THR:OG1	2.46	0.47
1:E:84:GLU:OE1	1:E:84:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:D:147:THR:HG23	2.15	0.46
1:A:295:GLU:HG2	1:B:9:ARG:CG	2.37	0.46
1:B:35:ALA:HB2	1:B:299:MET:CE	2.46	0.46
1:B:91:VAL:HG12	1:B:244:PHE:HE2	1.80	0.46
1:C:103:ASN:O	1:C:104:HIS:HB2	2.16	0.46
1:F:85:GLU:O	1:F:86:HIS:HB2	2.15	0.46
1:A:172:THR:HG22	1:A:173:ILE:N	2.31	0.46
1:B:40:SER:O	1:B:41:MET:HE2	2.16	0.46
1:D:200:LEU:HD23	1:D:268:LEU:HD11	1.97	0.46
1:F:75:PRO:O	1:F:76:THR:HG23	2.16	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:133:ASP:HB3	1:E:136:LYS:HB2	1.97	0.46
1:E:244:PHE:CD1	1:E:254:VAL:HG22	2.51	0.46
1:C:29:GLY:O	1:C:44:TRP:HB2	2.15	0.45
1:C:311:LYS:HB3	1:C:333:SER:OG	2.16	0.45
1:E:67:ASP:O	1:E:68:THR:CB	2.64	0.45
1:E:23:LEU:HD22	1:E:31:VAL:HG11	1.99	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:F:170:GLU:HG3	1:F:186:CYS:O	2.16	0.45
1:A:139:TYR:CE1	1:A:188:VAL:CG1	3.00	0.45
1:A:309:LYS:HG2	1:A:309:LYS:O	2.15	0.45
1:D:275:HIS:CD2	1:D:284:LYS:HG3	2.50	0.45
1:F:217:ARG:HG3	1:F:217:ARG:NH1	2.31	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:A:29:GLY:O	1:A:44:TRP:HB2	2.16	0.45
1:C:186:CYS:HB3	1:C:288:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:7:GLU:HA	1:B:302:LEU:O	2.17	0.45
1:E:89:GLY:HA2	2:E:2030:HOH:O	2.16	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:C:33:ILE:O	1:C:33:ILE:HG13	2.17	0.45
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:E:49:TYR:CE2	1:E:280:LYS:HE3	2.50	0.45
1:C:122:GLU:O	1:C:125:LYS:HB2	2.17	0.45
1:E:35:ALA:HB2	1:E:299:MET:HE2	1.98	0.45
1:E:75:PRO:O	1:E:76:THR:HG23	2.15	0.45
1:B:147:THR:HG23	1:B:147:THR:O	2.17	0.45
1:C:133:ASP:HB3	1:C:136:LYS:HB2	1.99	0.45
1:A:170:GLU:HG3	1:A:186:CYS:O	2.17	0.44
1:E:316:ARG:HG2	1:E:316:ARG:NH1	2.31	0.44
1:A:213:TRP:CD2	1:A:268:LEU:HD13	2.53	0.44
1:A:366:ASN:N	1:A:366:ASN:ND2	2.64	0.44
1:C:339:ARG:HG2	1:C:339:ARG:NH1	2.32	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:66:SER:OG	1:C:67:ASP:N	2.50	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: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:C:143:VAL:HG11	1:C:176:MET:SD	2.58	0.44
1:D:51:GLU:HG2	1:E:378:PRO:CG	2.45	0.44
1:F:49:TYR:CZ	1:F:280:LYS:HE3	2.52	0.44
1:A:339:ARG:HG3	1:A:339:ARG:HH11	1.82	0.44
1:B:186:CYS:HB3	1:B:288:VAL:CG1	2.48	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:C:237:ASN:HA	1:C:239:GLU:OE2	2.18	0.44
1:D:40:SER:O	1:D:41:MET:HE2	2.17	0.44
1:A:344:ALA:CB	1:A:355:ALA:HB2	2.48	0.43
1:C:248:HIS:O	1:C:250:VAL:N	2.51	0.43
1:D:20:ARG:HD2	1:E:12:VAL:HG23	1.99	0.43
1:D:256:ASN:C	1:D:258:GLY:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HD3	1:C:295:GLU:OE2	2.18	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: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:35:ALA:HB2	1:A:299:MET:HE1	2.00	0.43
1:A:310:THR:HG22	1:A:387:GLU:OE1	2.18	0.43
1:C:49:TYR:CZ	1:C:280:LYS:HE3	2.53	0.43
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:B:56:THR:HA	1:C:399:ILE:HD13	2.01	0.43
1:D:346:ALA:O	1:D:347:HIS:C	2.56	0.43
1:E:122:GLU:O	1:E:125:LYS:HB2	2.18	0.43
1:F:171:LYS:HE2	1:F:183:SER:HB2	1.99	0.43
1:B:26:GLU:HA	1:B:287:HIS:HB3	2.00	0.43
1:D:26:GLU:OE2	1:D:360:PRO:HD2	2.18	0.43
1:A:297:LEU:HD23	1:A:297:LEU:C	2.39	0.43
1:C:288:VAL:CG1	1:C:290:CYS:SG	3.07	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:B:65:LEU:HB3	1:B:117:VAL:HG21	2.00	0.43
1:C:93:LYS:HD3	1:C:93:LYS:C	2.39	0.43
1:D:204:LYS:C	1:D:206:VAL:N	2.71	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:F:301:GLY:O	1:F:302:LEU:CB	2.67	0.43
1:D:93:LYS:HD3	1:D:93:LYS:C	2.39	0.43
1:D:184:LEU:HD23	1:D:292:VAL:HG22	2.00	0.43
1:F:139:TYR:CE1	1:F:188:VAL:CG1	3.01	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:D:243:GLU:OE1	1:D:257:LEU:HD11	2.19	0.42
1:E:346:ALA:O	1:E:347:HIS:C	2.57	0.42
1:F:297:LEU:HD23	2:F:2003:HOH:O	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:A:40:SER:O	1:A:41:MET:HE2	2.20	0.42
1:B:217:ARG:HH11	1:B:217:ARG:CB	2.32	0.42
1:B:354:VAL:HB	1:B:377:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:74:CYS:O	1:D:76:THR:N	2.53	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:53:PRO:HD2	1:A:281:TYR:CD1	2.54	0.42
1:A:137:ILE:HG22	1:A:139:TYR:CE1	2.54	0.42
1:B:217:ARG:HB2	1:B:217:ARG:CZ	2.50	0.42
1:B:354:VAL:HB	1:B:377:PRO:CG	2.50	0.42
1:E:354:VAL:HB	1:E:377:PRO:HG2	2.01	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:C:65:LEU:HD21	1:C:242:VAL:CG2	2.50	0.42
1:C:301:GLY:O	1:C:302:LEU:CB	2.68	0.42
1:D:137:ILE:HD12	1:D:194:LEU:HD11	2.02	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:F:313:THR:OG1	1:F:331:THR:HB	2.19	0.42
1:B:171:LYS:HE2	1:B:183:SER:HB2	2.01	0.42
1:E:69:LYS:HG3	1:E:84:GLU:OE2	2.20	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:A:77:MET:O	1:A:78:GLY:O	2.37	0.41
1:B:217:ARG:NH1	1:B:217:ARG:CB	2.81	0.41
1:D:26:GLU:HA	1:D:287:HIS:HB3	2.02	0.41
1:E:147:THR:HG23	1:E:147:THR:O	2.20	0.41
1:D:91:VAL:HG12	1:D:244:PHE:CE2	2.56	0.41
1:D:244:PHE:CD1	1:D:254:VAL:HG22	2.55	0.41
1:F:69:LYS:HG3	1:F:84:GLU:OE2	2.20	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:C:97:SER:O	1:C:110:LYS:HA	2.20	0.41
1:F:5:HIS:CB	1:F:302:LEU:HD23	2.50	0.41
1:F:213:TRP:CE3	1:F:268:LEU:HD13	2.56	0.41
1:A:312:PHE:HB2	2:A:2051:HOH:O	2.21	0.41
1:E:4:THR:CG2	1:E:5:HIS:N	2.84	0.41
1:A:171:LYS:HE2	1:A:183:SER:HB2	2.03	0.41
1:F:295:GLU:OE1	1:F:295:GLU:HA	2.21	0.41
1:A:103:ASN:O	1:A:104:HIS:HB2	2.20	0.41
1:D:200:LEU:O	1:D:212:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:HA	1:A:287:HIS:HB3	2.03	0.41
1:A:4:THR:CG2	1:A:5:HIS:N	2.84	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:D:244:PHE:CE1	1:D:254:VAL:HG22	2.55	0.41
1:F:88:GLY:HA3	1:F:234:ASN:ND2	2.35	0.41
1:F:343:ARG:HG2	1:F:384:TYR:HB2	2.01	0.41
1:A:21:VAL:HB	1:A:292:VAL:HB	2.04	0.41
1:B:195:ALA:O	1:B:217:ARG:HD2	2.21	0.41
1:D:34:THR:O	1:D:300:LYS:HB2	2.20	0.41
1:B:133:ASP:HB3	1:B:136:LYS:HB2	2.03	0.40
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:329:GLU:HA	1:B:370:GLY:O	2.21	0.40
1:C:20:ARG:NE	1:C:291:GLU:CD	2.75	0.40
1:D:172:THR:HG22	1:D:173:ILE:N	2.36	0.40
1:F:184:LEU:HD23	1:F:292:VAL:HG22	2.02	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:C:21:VAL:HB	1:C:292:VAL:HB	2.03	0.40
1:D:71:ALA:O	1:D:113:ILE:HA	2.21	0.40
1:D:93:LYS:HB2	1:D:244:PHE:CE2	2.56	0.40
1:D:277:GLU:OE2	1:D:280:LYS:HD2	2.22	0.40
1:E:137:ILE:HD13	1:E:283:LEU:HD11	2.03	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:F:296:LYS:O	1:F:296:LYS:HG3	2.21	0.40
1:A:139:TYR:CE1	1:A:188:VAL:HG11	2.57	0.40
1:A:170:GLU:OE2	1:B:289:THR:HG21	2.21	0.40
1:B:14:GLY:HA3	1:C:12:VAL:HG13	2.04	0.40
1:C:361:ASN:HA	1:C:362:PRO:HD2	1.95	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:E:383:ILE:O	1:E:389:SER:HA	2.21	0.40
1:F:139:TYR:CE1	1:F:188:VAL:HG13	2.55	0.40
1:A:237:ASN:HA	1:A:239:GLU:OE2	2.21	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	6 15
1	B	381/401 (95%)	344 (90%)	23 (6%)	14 (4%)	3 7
1	C	379/401 (94%)	348 (92%)	22 (6%)	9 (2%)	6 15
1	D	380/401 (95%)	350 (92%)	17 (4%)	13 (3%)	3 8
1	E	376/401 (94%)	344 (92%)	22 (6%)	10 (3%)	5 12
1	F	384/401 (96%)	352 (92%)	19 (5%)	13 (3%)	3 8
All	All	2276/2406 (95%)	2087 (92%)	121 (5%)	68 (3%)	4 10

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	33	62
1	B	315/331 (95%)	304 (96%)	11 (4%)	36	65
1	C	315/331 (95%)	303 (96%)	12 (4%)	33	62
1	D	315/331 (95%)	308 (98%)	7 (2%)	52	79
1	E	315/331 (95%)	305 (97%)	10 (3%)	39	68
1	F	315/331 (95%)	301 (96%)	14 (4%)	28	56
All	All	1890/1986 (95%)	1824 (96%)	66 (4%)	36	65

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	F	347	HIS

Sometimes 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

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Mol	Chain	Res	Type
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
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 molecules 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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	382/401 (95%)	-0.22	6 (1%)	72 74	13, 33, 67, 89	0
1	B	387/401 (96%)	-0.15	7 (1%)	68 70	12, 35, 70, 94	0
1	C	385/401 (96%)	-0.01	16 (4%)	36 35	12, 37, 71, 94	0
1	D	386/401 (96%)	-0.02	5 (1%)	77 78	16, 41, 74, 98	0
1	E	382/401 (95%)	0.10	14 (3%)	41 41	13, 41, 75, 95	0
1	F	388/401 (96%)	-0.05	13 (3%)	45 45	13, 37, 76, 99	0
All	All	2310/2406 (96%)	-0.06	61 (2%)	56 57	12, 37, 74, 99	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	147	THR	7.3
1	C	147	THR	5.1
1	F	147	THR	5.0
1	D	147	THR	4.8
1	F	206	VAL	4.6
1	E	248	HIS	4.5
1	E	146	HIS	4.4
1	A	147	THR	4.0
1	A	347	HIS	3.6
1	C	367	ASN	3.4
1	C	106	GLY	3.4
1	F	146	HIS	3.3
1	F	207	GLU	3.3
1	E	347	HIS	3.3
1	F	367	ASN	3.2
1	D	249	ALA	3.2
1	B	205	THR	3.1
1	B	147	THR	3.1
1	C	248	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	367	ASN	3.0
1	D	248	HIS	3.0
1	E	249	ALA	3.0
1	C	107	LEU	3.0
1	F	209	LEU	2.9
1	C	352	VAL	2.9
1	B	352	VAL	2.9
1	C	346	ALA	2.9
1	F	107	LEU	2.8
1	C	347	HIS	2.8
1	E	253	ASP	2.7
1	E	367	ASN	2.7
1	E	107	LEU	2.6
1	C	146	HIS	2.6
1	E	334	GLY	2.6
1	F	101	TRP	2.6
1	F	208	HIS	2.5
1	D	178	GLU	2.5
1	C	101	TRP	2.5
1	E	101	TRP	2.5
1	C	75	PRO	2.5
1	C	349	SER	2.5
1	C	67	ASP	2.4
1	C	251	LYS	2.4
1	F	105	CYS	2.4
1	E	255	TYR	2.4
1	C	350	PRO	2.4
1	B	351	ASP	2.3
1	E	108	PHE	2.3
1	F	347	HIS	2.3
1	E	176	MET	2.3
1	C	351	ASP	2.3
1	A	102	GLY	2.2
1	D	351	ASP	2.2
1	A	210	PRO	2.2
1	A	160	ARG	2.2
1	B	208	HIS	2.1
1	E	145	PRO	2.1
1	F	350	PRO	2.1
1	F	106	GLY	2.1
1	B	248	HIS	2.0
1	A	101	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.