



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:53 AM GMT

PDB ID : 2X0B  
Title : CRYSTAL STRUCTURE OF HUMAN ANGIOTENSINOGEN COM-  
PLEXED WITH RENIN  
Authors : Zhou, A.; Wei, Z.; Yan, Y.; Carrell, R.W.; Read, R.J.  
Deposited on : 2009-12-08  
Resolution : 4.33 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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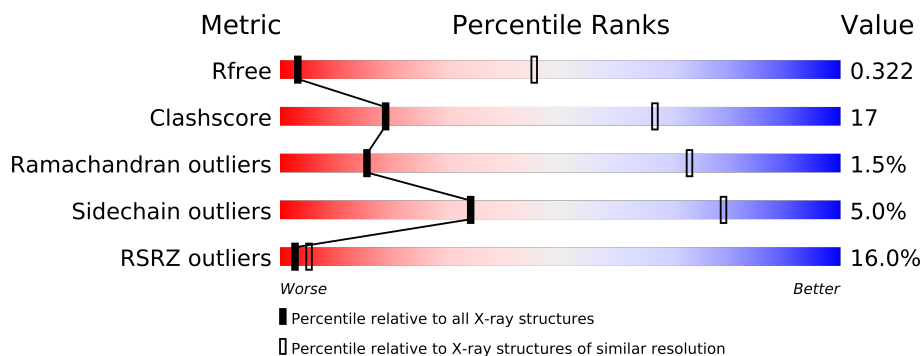
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.33 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	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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	383	
1	C	383	
1	E	383	
1	G	383	
2	B	452	
2	D	452	
2	F	452	
2	H	452	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23244 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	C	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	E	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	G	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			

- Molecule 2 is a protein called ANGIOTENSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	D	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	F	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	H	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			

There are 4 discrepancies between the modelled and reference sequences:

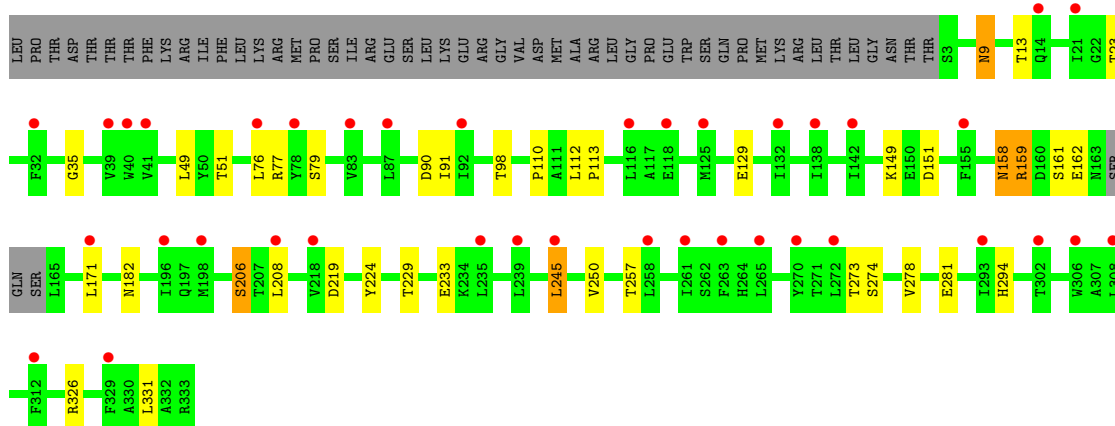
Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ASN	ASP	CONFLICT	UNP P01019
D	47	ASN	ASP	CONFLICT	UNP P01019
F	47	ASN	ASP	CONFLICT	UNP P01019
H	47	ASN	ASP	CONFLICT	UNP P01019

### 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.

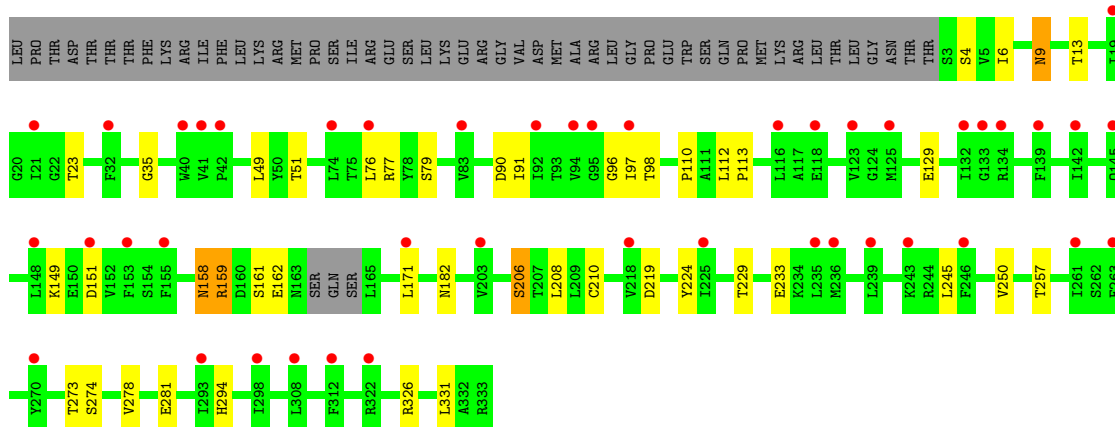
#### • Molecule 1: RENIN

Chain A: 



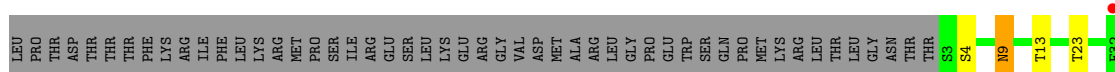
#### • Molecule 1: RENIN

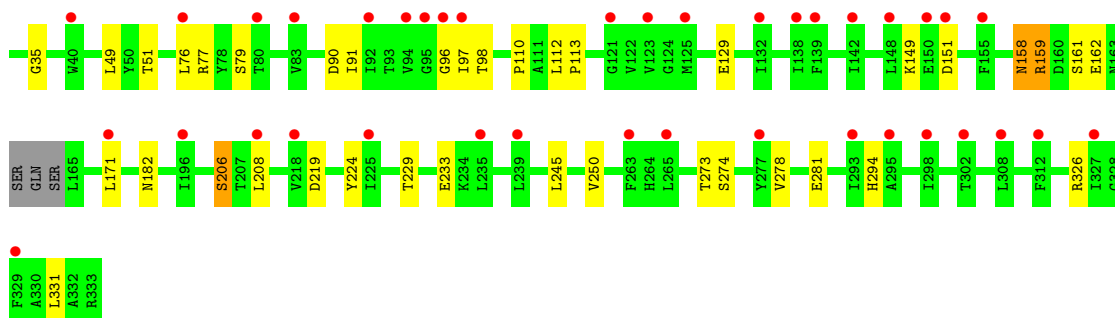
Chain C: 



#### • Molecule 1: RENIN

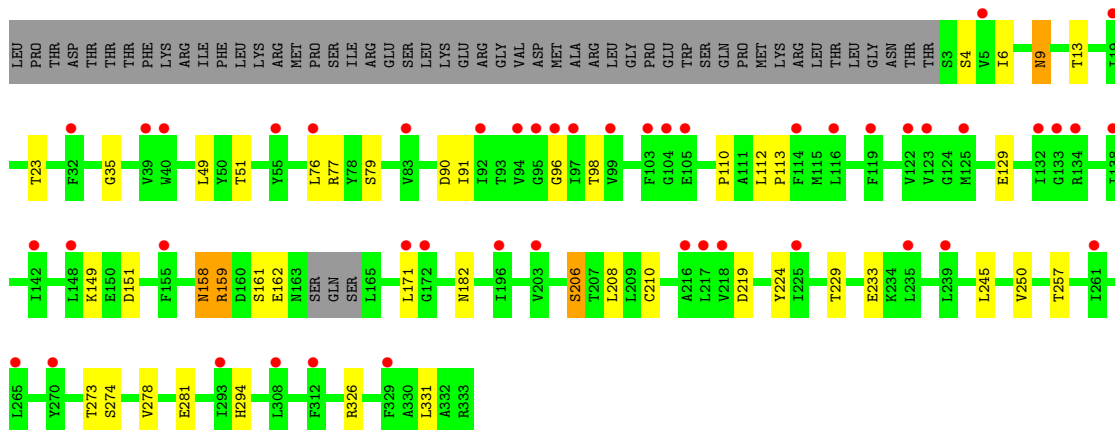
Chain E: 





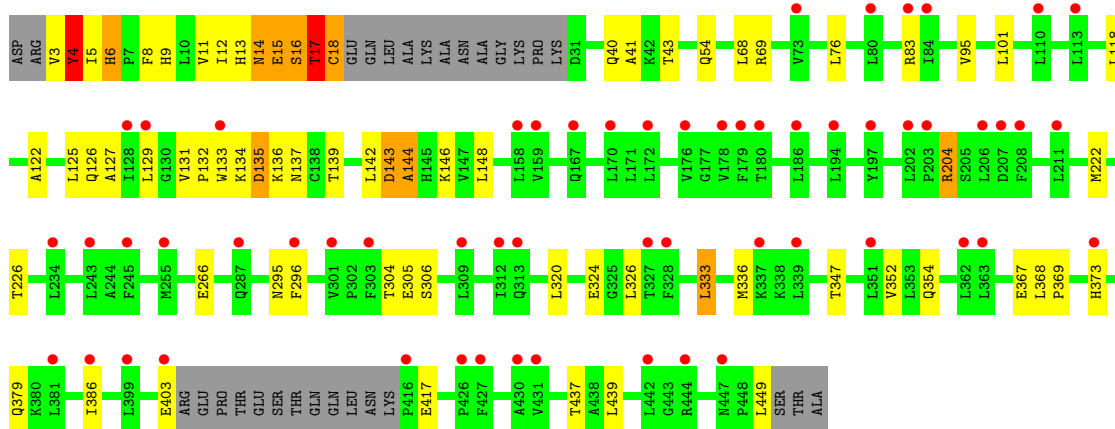
• Molecule 1: RENIN

Chain G: 



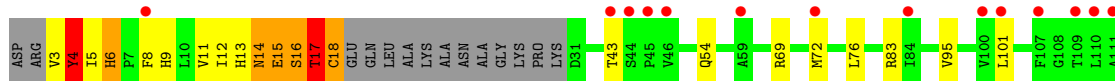
• Molecule 2: ANGIOTENSINOGEN

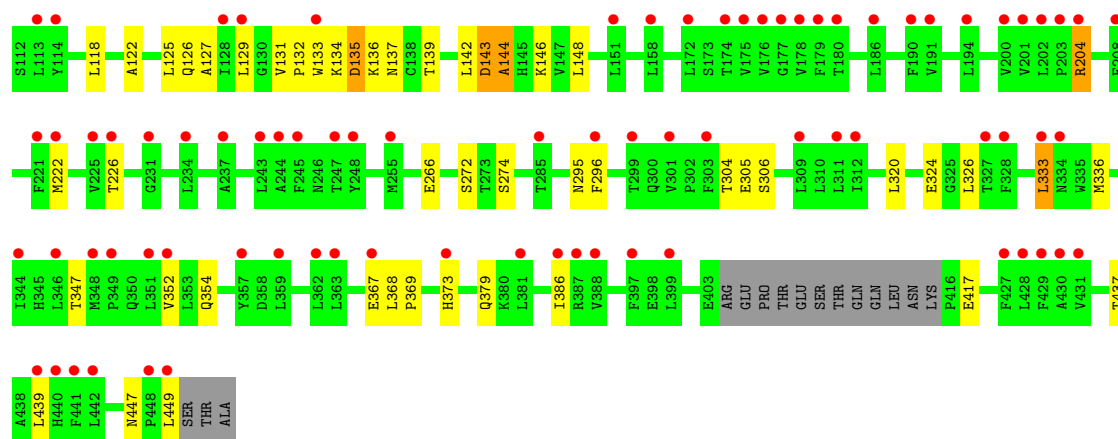
Chain B: 



• Molecule 2: ANGIOTENSINOGEN

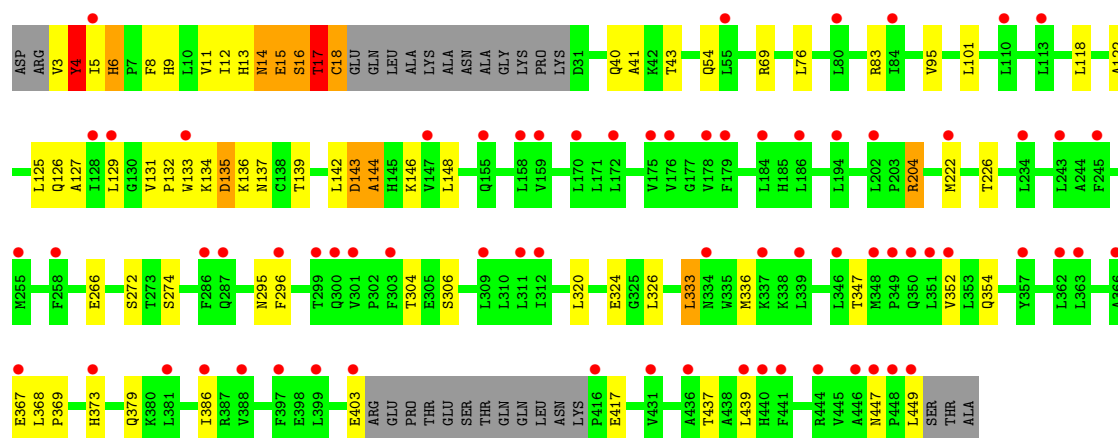
Chain D: 





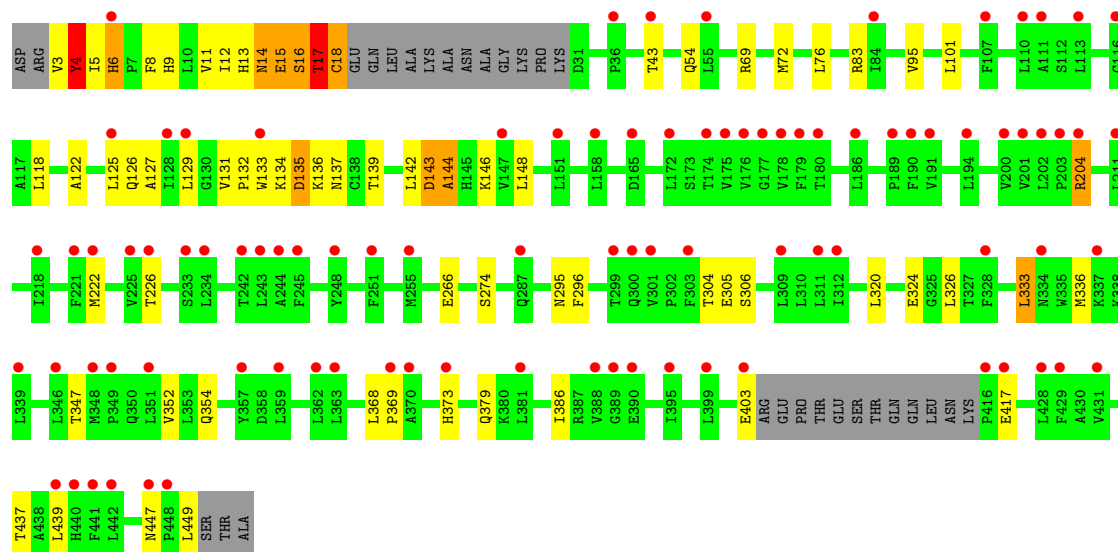
• Molecule 2: ANGIOTENSINOGEN

Chain F:



• Molecule 2: ANGIOTENSINOGEN

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.47 Å   212.47 Å   474.06 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	48.52 – 4.33 48.52 – 4.34	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.52-4.33) 84.2 (48.52-4.34)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 4.29 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_249)	Depositor
R, $R_{free}$	0.309 , 0.334 0.293 , 0.322	Depositor DCC
$R_{free}$ test set	2253 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	200.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 272.0	EDS
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 44561 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	325.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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	0.35	0/2599	0.67	0/3523
1	C	0.35	0/2599	0.67	0/3523
1	E	0.35	0/2599	0.67	0/3523
1	G	0.35	0/2599	0.67	0/3523
2	B	0.31	0/3345	0.51	5/4557 (0.1%)
2	D	0.31	0/3345	0.51	5/4557 (0.1%)
2	F	0.31	0/3345	0.51	5/4557 (0.1%)
2	H	0.31	0/3345	0.51	5/4557 (0.1%)
All	All	0.33	0/23776	0.59	20/32320 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	PHE	CZ-CE2-CD2	6.16	127.50	120.10
2	F	8	PHE	CZ-CE2-CD2	6.13	127.45	120.10
2	B	8	PHE	CZ-CE2-CD2	6.12	127.44	120.10
2	D	8	PHE	CZ-CE2-CD2	6.08	127.39	120.10
2	H	8	PHE	CG-CD1-CE1	5.27	126.60	120.80
2	B	8	PHE	CG-CD1-CE1	5.26	126.58	120.80
2	F	135	ASP	CB-CG-OD2	5.26	123.03	118.30
2	H	6	HIS	CA-CB-CG	-5.22	104.72	113.60
2	F	8	PHE	CG-CD1-CE1	5.20	126.53	120.80
2	D	8	PHE	CG-CD1-CE1	5.20	126.52	120.80
2	H	135	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	6	HIS	CA-CB-CG	-5.19	104.77	113.60
2	F	6	HIS	CA-CB-CG	-5.19	104.78	113.60
2	F	143	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	135	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	6	HIS	CA-CB-CG	-5.17	104.81	113.60
2	D	135	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	143	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	143	ASP	CB-CG-OD2	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ASP	CB-CG-OD2	5.11	122.90	118.30

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	2540	0	0	41	3
1	C	2540	0	0	53	2
1	E	2540	0	0	41	0
1	G	2540	0	0	55	0
2	B	3271	0	0	77	28
2	D	3271	0	0	84	0
2	F	3271	0	0	82	27
2	H	3271	0	0	88	0
All	All	23244	0	0	385	30

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 17.

All (385) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:51:THR:OG1	2:H:83:ARG:CD	1.77	1.32
1:E:4:SER:OG	2:H:274:SER:OG	1.52	1.27
1:C:51:THR:CB	2:D:83:ARG:NH1	1.98	1.23
1:E:51:THR:CG2	2:F:83:ARG:CG	2.14	1.22
1:A:51:THR:CG2	2:B:83:ARG:CG	2.20	1.17
1:C:51:THR:CG2	2:D:83:ARG:CG	2.21	1.16
1:G:110:PRO:CB	2:H:135:ASP:OD1	2.00	1.10
2:F:131:VAL:CG1	2:F:132:PRO:CA	2.30	1.10
2:H:131:VAL:CG1	2:H:132:PRO:CA	2.30	1.09
2:B:131:VAL:CG1	2:B:132:PRO:CA	2.30	1.09
1:G:51:THR:OG1	2:H:83:ARG:CZ	2.01	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:131:VAL:CG1	2:D:132:PRO:CA	2.30	1.08
1:G:51:THR:CB	2:H:83:ARG:NH1	2.17	1.07
2:B:142:LEU:CD1	2:B:146:LYS:CE	2.32	1.07
1:G:51:THR:OG1	2:H:83:ARG:NE	1.86	1.07
2:F:142:LEU:CD1	2:F:146:LYS:CE	2.32	1.07
2:H:142:LEU:CD1	2:H:146:LYS:CE	2.32	1.06
1:C:96:GLY:O	2:F:449:LEU:CD2	2.02	1.06
2:D:142:LEU:CD1	2:D:146:LYS:CE	2.32	1.06
2:D:272:SER:O	1:G:6:ILE:CG1	2.04	1.05
1:E:23:THR:CG2	2:H:95:VAL:CG2	2.35	1.05
2:F:126:GLN:O	2:F:131:VAL:CG2	2.05	1.05
1:C:110:PRO:CB	2:D:135:ASP:OD1	2.05	1.05
2:B:126:GLN:O	2:B:131:VAL:CG2	2.05	1.04
2:D:126:GLN:O	2:D:131:VAL:CG2	2.05	1.04
1:C:49:LEU:O	2:D:127:ALA:O	1.76	1.04
2:H:126:GLN:O	2:H:131:VAL:CG2	2.05	1.03
2:B:131:VAL:CG1	2:B:132:PRO:CB	2.39	1.01
2:H:131:VAL:CG1	2:H:132:PRO:CB	2.39	1.00
1:E:51:THR:CB	2:F:83:ARG:NH1	2.25	1.00
2:D:131:VAL:CG1	2:D:132:PRO:CB	2.39	0.99
1:C:51:THR:OG1	2:D:83:ARG:NH1	1.78	0.99
2:F:131:VAL:CG1	2:F:132:PRO:CB	2.39	0.99
2:D:274:SER:OG	1:G:4:SER:OG	1.80	0.98
1:G:51:THR:CG2	2:H:83:ARG:CG	2.40	0.98
1:E:98:THR:N	2:H:449:LEU:CD2	2.27	0.98
1:G:110:PRO:CG	2:H:135:ASP:OD1	2.12	0.98
1:A:112:LEU:CD2	2:B:76:LEU:CD2	2.40	0.97
1:C:110:PRO:CG	2:D:135:ASP:OD1	2.13	0.97
1:C:98:THR:N	2:F:449:LEU:CD2	2.27	0.97
1:G:49:LEU:O	2:H:127:ALA:O	1.83	0.96
1:C:23:THR:CG2	2:F:95:VAL:CG2	2.44	0.96
1:G:51:THR:OG1	2:H:83:ARG:NH1	2.00	0.94
2:D:126:GLN:CA	2:D:131:VAL:CG2	2.47	0.93
1:C:79:SER:OG	2:D:9:HIS:ND1	2.02	0.93
1:E:79:SER:OG	2:F:9:HIS:ND1	2.02	0.92
1:G:79:SER:OG	2:H:9:HIS:ND1	2.02	0.92
2:F:126:GLN:CA	2:F:131:VAL:CG2	2.47	0.92
1:A:79:SER:OG	2:B:9:HIS:ND1	2.02	0.92
2:B:126:GLN:CA	2:B:131:VAL:CG2	2.47	0.92
2:H:126:GLN:CA	2:H:131:VAL:CG2	2.47	0.91
1:G:112:LEU:CD1	2:H:76:LEU:CD2	2.50	0.90
1:G:51:THR:CG2	2:H:83:ARG:CD	2.51	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:126:GLN:O	2:F:131:VAL:CB	2.23	0.86
1:E:224:TYR:CE2	1:E:294:HIS:NE2	2.44	0.86
1:G:224:TYR:CE2	1:G:294:HIS:NE2	2.44	0.86
2:B:126:GLN:O	2:B:131:VAL:CB	2.23	0.86
2:H:126:GLN:O	2:H:131:VAL:CB	2.23	0.86
1:A:224:TYR:CE2	1:A:294:HIS:NE2	2.44	0.86
1:C:97:ILE:CA	2:F:449:LEU:CD2	2.53	0.85
1:C:224:TYR:CE2	1:C:294:HIS:NE2	2.44	0.85
2:D:126:GLN:O	2:D:131:VAL:CB	2.23	0.85
1:G:112:LEU:CD2	2:H:76:LEU:CD2	2.53	0.85
1:E:112:LEU:CD2	2:F:76:LEU:CD2	2.54	0.85
1:E:51:THR:OG1	2:F:83:ARG:NH1	2.02	0.83
2:D:449:LEU:CD2	1:G:98:THR:N	2.42	0.82
2:D:3:VAL:CB	2:D:4:TYR:CD2	2.62	0.82
1:C:97:ILE:C	2:F:449:LEU:CD2	2.47	0.82
1:A:51:THR:CB	2:B:83:ARG:NH1	2.43	0.82
1:G:51:THR:CB	2:H:83:ARG:CD	2.58	0.81
2:B:3:VAL:CB	2:B:4:TYR:CD2	2.63	0.81
2:F:3:VAL:CB	2:F:4:TYR:CD2	2.63	0.81
2:H:3:VAL:CB	2:H:4:TYR:CD2	2.62	0.81
2:F:126:GLN:C	2:F:131:VAL:CG2	2.49	0.80
1:G:224:TYR:CD2	1:G:294:HIS:CD2	2.69	0.80
1:C:112:LEU:CD1	2:D:76:LEU:CD2	2.59	0.80
1:C:224:TYR:CD2	1:C:294:HIS:CD2	2.69	0.80
1:G:79:SER:CB	2:H:9:HIS:ND1	2.45	0.80
2:B:126:GLN:C	2:B:131:VAL:CG2	2.49	0.80
1:A:79:SER:CB	2:B:9:HIS:ND1	2.45	0.80
1:E:224:TYR:CD2	1:E:294:HIS:CD2	2.69	0.80
2:H:126:GLN:C	2:H:131:VAL:CG2	2.49	0.80
1:E:79:SER:CB	2:F:9:HIS:ND1	2.45	0.80
2:D:126:GLN:C	2:D:131:VAL:CG2	2.49	0.80
1:C:79:SER:CB	2:D:9:HIS:ND1	2.45	0.80
1:A:224:TYR:CD2	1:A:294:HIS:CD2	2.69	0.79
1:G:77:ARG:NH2	2:H:16:SER:N	2.32	0.78
1:C:77:ARG:NH2	2:D:16:SER:N	2.32	0.77
1:G:224:TYR:CD2	1:G:294:HIS:NE2	2.53	0.77
1:E:224:TYR:CD2	1:E:294:HIS:NE2	2.53	0.76
1:A:77:ARG:NH2	2:B:16:SER:N	2.32	0.76
1:E:35:GLY:O	2:F:12:ILE:CG2	2.33	0.76
1:E:96:GLY:O	2:H:447:ASN:ND2	2.18	0.76
1:A:49:LEU:O	2:B:127:ALA:O	2.03	0.76
1:C:112:LEU:CD2	2:D:76:LEU:CD2	2.63	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:35:GLY:O	2:D:12:ILE:CG2	2.34	0.76
1:E:77:ARG:NH2	2:F:16:SER:N	2.32	0.76
1:C:224:TYR:CD2	1:C:294:HIS:NE2	2.53	0.76
1:A:224:TYR:CD2	1:A:294:HIS:NE2	2.53	0.76
1:E:49:LEU:O	2:F:127:ALA:O	2.03	0.76
1:G:35:GLY:O	2:H:12:ILE:CG2	2.33	0.75
1:A:35:GLY:O	2:B:12:ILE:CG2	2.33	0.75
1:A:245:LEU:CD1	2:B:68:LEU:CD2	2.26	0.74
1:E:110:PRO:CB	2:F:135:ASP:OD1	2.37	0.72
2:H:132:PRO:CG	2:H:135:ASP:CA	2.68	0.72
2:B:132:PRO:CG	2:B:135:ASP:CA	2.67	0.72
2:D:132:PRO:CG	2:D:135:ASP:CA	2.68	0.72
2:F:16:SER:O	2:F:17:THR:CG2	2.37	0.72
2:D:16:SER:O	2:D:17:THR:CG2	2.37	0.72
1:C:23:THR:CG2	2:F:95:VAL:CB	2.68	0.72
2:B:16:SER:O	2:B:17:THR:CG2	2.37	0.71
2:H:16:SER:O	2:H:17:THR:CG2	2.37	0.71
2:F:132:PRO:CG	2:F:135:ASP:CA	2.67	0.71
2:D:132:PRO:O	2:D:134:LYS:N	2.24	0.71
2:H:132:PRO:O	2:H:134:LYS:N	2.24	0.70
2:F:132:PRO:O	2:F:134:LYS:N	2.24	0.70
2:D:95:VAL:CG2	1:G:23:THR:CG2	2.68	0.70
1:A:257:THR:OG1	2:H:403:GLU:O	2.09	0.70
2:B:132:PRO:O	2:B:134:LYS:N	2.24	0.70
1:G:110:PRO:CG	2:H:135:ASP:CG	2.59	0.70
1:A:110:PRO:CB	2:B:135:ASP:OD1	2.40	0.69
1:G:112:LEU:CD2	2:H:72:MET:CG	2.71	0.69
2:B:69:ARG:NH1	2:B:133:TRP:CH2	2.62	0.68
2:H:69:ARG:NH1	2:H:133:TRP:CH2	2.62	0.68
1:G:13:THR:CG2	2:H:5:ILE:CG2	2.72	0.68
2:F:69:ARG:NH1	2:F:133:TRP:CH2	2.62	0.68
2:D:69:ARG:NH1	2:D:133:TRP:CH2	2.62	0.68
1:A:77:ARG:CD	2:B:136:LYS:NZ	2.57	0.68
1:E:13:THR:CG2	2:F:5:ILE:CG2	2.72	0.68
1:C:13:THR:CG2	2:D:5:ILE:CG2	2.72	0.68
1:A:13:THR:CG2	2:B:5:ILE:CG2	2.72	0.67
1:G:49:LEU:CB	2:H:127:ALA:CB	2.73	0.67
1:E:110:PRO:CG	2:F:135:ASP:OD1	2.43	0.67
1:A:110:PRO:CG	2:B:135:ASP:OD1	2.42	0.67
1:E:49:LEU:CD1	2:F:367:GLU:CG	2.74	0.66
2:D:3:VAL:CG2	2:D:3:VAL:O	2.44	0.65
2:H:3:VAL:CG2	2:H:3:VAL:O	2.44	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:6:ILE:CG1	2:F:272:SER:O	2.44	0.65
1:G:49:LEU:O	2:H:127:ALA:C	2.33	0.65
1:C:97:ILE:CA	2:F:449:LEU:CD1	2.75	0.65
2:B:3:VAL:O	2:B:3:VAL:CG2	2.44	0.65
2:F:3:VAL:O	2:F:3:VAL:CG2	2.44	0.64
1:C:49:LEU:CB	2:D:127:ALA:CB	2.75	0.64
1:C:219:ASP:OD1	2:D:11:VAL:CG2	2.46	0.64
1:A:219:ASP:OD1	2:B:11:VAL:CG2	2.46	0.64
1:E:219:ASP:OD1	2:F:11:VAL:CG2	2.45	0.64
1:C:110:PRO:CG	2:D:135:ASP:CG	2.67	0.63
1:G:219:ASP:OD1	2:H:11:VAL:CG2	2.46	0.63
2:F:131:VAL:CG1	2:F:132:PRO:N	2.58	0.63
1:A:158:ASN:ND2	1:A:159:ARG:N	2.47	0.62
1:G:51:THR:CG2	2:H:83:ARG:NH1	2.63	0.62
1:E:158:ASN:ND2	1:E:159:ARG:N	2.47	0.62
1:A:257:THR:CB	2:H:403:GLU:O	2.47	0.62
2:H:131:VAL:CG1	2:H:132:PRO:N	2.58	0.62
1:G:158:ASN:ND2	1:G:159:ARG:N	2.47	0.62
1:C:112:LEU:CD2	2:D:72:MET:CG	2.78	0.61
2:B:122:ALA:O	2:B:126:GLN:CG	2.49	0.61
2:D:122:ALA:O	2:D:126:GLN:CG	2.49	0.61
1:G:77:ARG:NH2	2:H:16:SER:O	2.34	0.61
2:F:122:ALA:O	2:F:126:GLN:CG	2.49	0.61
1:A:77:ARG:NH2	2:B:16:SER:O	2.34	0.61
1:C:158:ASN:ND2	1:C:159:ARG:N	2.47	0.61
1:A:51:THR:OG1	2:B:83:ARG:NH1	2.28	0.60
2:B:142:LEU:CD1	2:B:146:LYS:CG	2.77	0.60
1:E:77:ARG:NH2	2:F:16:SER:O	2.34	0.60
2:B:131:VAL:CG1	2:B:132:PRO:N	2.58	0.60
2:H:122:ALA:O	2:H:126:GLN:CG	2.49	0.60
1:C:4:SER:OG	2:F:274:SER:OG	2.20	0.60
2:D:131:VAL:CG1	2:D:132:PRO:N	2.58	0.60
1:C:77:ARG:NH2	2:D:16:SER:O	2.34	0.60
1:A:112:LEU:CD1	2:B:76:LEU:CD2	2.80	0.59
1:G:110:PRO:CB	2:H:132:PRO:CD	2.81	0.59
1:C:51:THR:CG2	2:D:83:ARG:NH1	2.65	0.59
2:H:142:LEU:CD1	2:H:146:LYS:CG	2.77	0.59
1:C:49:LEU:O	2:D:127:ALA:C	2.42	0.58
2:H:3:VAL:CA	2:H:4:TYR:CB	2.82	0.57
2:D:5:ILE:CG2	2:D:6:HIS:N	2.67	0.57
2:B:5:ILE:CG2	2:B:6:HIS:N	2.67	0.57
2:D:3:VAL:CA	2:D:4:TYR:CB	2.82	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:77:ARG:CD	2:H:136:LYS:NZ	2.68	0.57
2:H:143:ASP:O	2:H:144:ALA:CB	2.52	0.57
2:B:143:ASP:O	2:B:144:ALA:CB	2.52	0.57
2:D:143:ASP:O	2:D:144:ALA:CB	2.52	0.57
1:E:112:LEU:CD1	2:F:76:LEU:CD2	2.81	0.57
2:F:5:ILE:CG2	2:F:6:HIS:N	2.67	0.57
2:H:16:SER:O	2:H:17:THR:CB	2.53	0.57
2:B:16:SER:O	2:B:17:THR:CB	2.53	0.57
2:B:3:VAL:CA	2:B:4:TYR:CB	2.82	0.57
2:F:143:ASP:O	2:F:144:ALA:CB	2.52	0.57
1:A:281:GLU:OE1	2:B:4:TYR:CE2	2.58	0.56
2:F:3:VAL:CA	2:F:4:TYR:CB	2.82	0.56
1:E:281:GLU:OE1	2:F:4:TYR:CE2	2.58	0.56
2:H:5:ILE:CG2	2:H:6:HIS:N	2.67	0.56
1:G:281:GLU:OE1	2:H:4:TYR:CE2	2.58	0.56
2:F:16:SER:O	2:F:17:THR:CB	2.53	0.56
1:C:77:ARG:NE	2:D:136:LYS:NZ	2.54	0.56
2:D:16:SER:O	2:D:17:THR:CB	2.53	0.56
2:D:142:LEU:CD1	2:D:146:LYS:CG	2.77	0.56
1:C:281:GLU:OE1	2:D:4:TYR:CE2	2.58	0.55
2:F:142:LEU:CD1	2:F:146:LYS:CG	2.77	0.55
2:H:4:TYR:N	2:H:4:TYR:CD1	2.75	0.54
2:D:4:TYR:N	2:D:4:TYR:CD1	2.75	0.54
1:A:9:ASN:C	1:A:9:ASN:ND2	2.61	0.54
1:E:9:ASN:ND2	1:E:9:ASN:C	2.61	0.54
2:B:4:TYR:N	2:B:4:TYR:CD1	2.75	0.54
1:C:9:ASN:C	1:C:9:ASN:ND2	2.61	0.54
2:F:135:ASP:O	2:F:136:LYS:CG	2.57	0.53
2:B:135:ASP:O	2:B:136:LYS:CG	2.57	0.53
2:B:9:HIS:CE1	2:B:11:VAL:CG2	2.92	0.53
1:E:161:SER:OG	1:E:162:GLU:N	2.42	0.53
2:D:135:ASP:O	2:D:136:LYS:CG	2.57	0.53
1:G:9:ASN:C	1:G:9:ASN:ND2	2.61	0.53
2:D:9:HIS:CE1	2:D:11:VAL:CG2	2.92	0.52
2:F:4:TYR:N	2:F:4:TYR:CD1	2.75	0.52
1:C:161:SER:OG	1:C:162:GLU:N	2.42	0.52
2:H:9:HIS:CE1	2:H:11:VAL:CG2	2.92	0.52
2:H:135:ASP:O	2:H:136:LYS:CG	2.57	0.52
2:F:9:HIS:CE1	2:F:11:VAL:CG2	2.92	0.52
1:G:161:SER:OG	1:G:162:GLU:N	2.42	0.52
2:D:142:LEU:CD1	2:D:146:LYS:CD	2.88	0.52
2:D:272:SER:O	1:G:6:ILE:CD1	2.57	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:320:LEU:O	2:H:324:GLU:N	2.43	0.51
2:H:142:LEU:CD1	2:H:146:LYS:CD	2.88	0.51
2:D:69:ARG:NH1	2:D:133:TRP:CZ2	2.79	0.51
2:D:320:LEU:O	2:D:324:GLU:N	2.43	0.51
2:B:320:LEU:O	2:B:324:GLU:N	2.43	0.51
2:B:403:GLU:O	1:G:257:THR:CB	2.58	0.51
1:A:161:SER:OG	1:A:162:GLU:N	2.42	0.51
2:B:69:ARG:NH1	2:B:133:TRP:CZ2	2.79	0.51
2:F:69:ARG:NH1	2:F:133:TRP:CZ2	2.79	0.51
2:D:144:ALA:O	2:D:148:LEU:CG	2.59	0.51
2:B:142:LEU:CD1	2:B:146:LYS:CD	2.88	0.51
2:F:144:ALA:O	2:F:148:LEU:CG	2.59	0.51
2:F:142:LEU:CD1	2:F:146:LYS:CD	2.87	0.51
1:G:273:THR:CG2	1:G:274:SER:N	2.74	0.51
1:C:273:THR:CG2	1:C:274:SER:N	2.74	0.51
1:C:79:SER:CB	2:D:9:HIS:CG	2.94	0.50
2:B:144:ALA:O	2:B:148:LEU:CG	2.59	0.50
1:C:77:ARG:CD	2:D:136:LYS:NZ	2.74	0.50
2:F:133:TRP:CZ3	2:F:142:LEU:CD2	2.95	0.50
1:A:273:THR:CG2	1:A:274:SER:N	2.74	0.50
1:A:110:PRO:CB	2:B:132:PRO:CD	2.90	0.50
1:E:77:ARG:NH2	2:F:15:GLU:CB	2.75	0.50
1:G:79:SER:CB	2:H:9:HIS:CG	2.94	0.50
1:A:79:SER:CB	2:B:9:HIS:CG	2.94	0.50
2:H:69:ARG:NH1	2:H:133:TRP:CZ2	2.79	0.50
2:D:133:TRP:CZ3	2:D:142:LEU:CD2	2.95	0.50
2:H:144:ALA:O	2:H:148:LEU:CG	2.59	0.50
1:E:273:THR:CG2	1:E:274:SER:N	2.74	0.50
2:F:320:LEU:O	2:F:324:GLU:N	2.43	0.50
1:C:77:ARG:NH2	2:D:15:GLU:CB	2.75	0.50
1:A:77:ARG:NH2	2:B:15:GLU:CB	2.75	0.50
2:D:14:ASN:O	2:D:15:GLU:O	2.30	0.50
1:A:49:LEU:O	2:B:127:ALA:C	2.49	0.50
2:B:14:ASN:O	2:B:15:GLU:O	2.30	0.49
1:E:79:SER:CB	2:F:9:HIS:CG	2.94	0.49
2:H:133:TRP:CZ3	2:H:142:LEU:CD2	2.95	0.49
2:B:133:TRP:CZ3	2:B:142:LEU:CD2	2.95	0.49
1:G:77:ARG:NH2	2:H:15:GLU:CB	2.75	0.49
2:H:14:ASN:O	2:H:15:GLU:O	2.30	0.49
2:F:14:ASN:O	2:F:15:GLU:O	2.30	0.48
1:E:281:GLU:OE1	2:F:4:TYR:CZ	2.67	0.48
1:G:281:GLU:OE1	2:H:4:TYR:CZ	2.67	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:GLU:OE1	2:B:4:TYR:CZ	2.67	0.48
1:C:281:GLU:OE1	2:D:4:TYR:CZ	2.67	0.48
1:G:77:ARG:O	2:H:13:HIS:CE1	2.67	0.47
1:E:77:ARG:O	2:F:13:HIS:CE1	2.67	0.47
1:C:77:ARG:O	2:D:13:HIS:CE1	2.67	0.47
2:F:43:THR:OG1	2:F:204:ARG:NH1	2.48	0.47
2:D:43:THR:OG1	2:D:204:ARG:NH1	2.48	0.47
2:B:43:THR:OG1	2:B:204:ARG:NH1	2.48	0.47
2:D:449:LEU:CD2	1:G:96:GLY:O	2.62	0.47
2:D:126:GLN:C	2:D:131:VAL:CB	2.83	0.47
2:D:447:ASN:ND2	1:G:96:GLY:O	2.48	0.47
1:A:77:ARG:O	2:B:13:HIS:CE1	2.67	0.47
2:F:3:VAL:CA	2:F:4:TYR:CG	2.98	0.47
2:B:304:THR:O	2:B:306:SER:N	2.48	0.46
2:B:137:ASN:OD1	2:B:143:ASP:OD2	2.34	0.46
2:F:304:THR:O	2:F:306:SER:N	2.48	0.46
2:F:126:GLN:C	2:F:131:VAL:CB	2.83	0.46
2:B:3:VAL:CA	2:B:4:TYR:CG	2.98	0.46
2:H:43:THR:OG1	2:H:204:ARG:NH1	2.48	0.46
1:E:77:ARG:CD	2:F:136:LYS:NZ	2.79	0.46
2:F:137:ASN:OD1	2:F:143:ASP:OD2	2.34	0.46
2:D:304:THR:O	2:D:306:SER:N	2.48	0.46
2:D:3:VAL:CA	2:D:4:TYR:CG	2.98	0.46
2:D:16:SER:O	2:D:17:THR:OG1	2.34	0.46
2:F:142:LEU:O	2:F:146:LYS:CB	2.64	0.46
2:H:3:VAL:CA	2:H:4:TYR:CG	2.98	0.46
2:H:142:LEU:O	2:H:146:LYS:CB	2.64	0.46
2:H:137:ASN:OD1	2:H:143:ASP:OD2	2.34	0.46
2:D:17:THR:O	2:D:18:CYS:C	2.54	0.46
2:H:14:ASN:O	2:H:15:GLU:C	2.54	0.45
2:H:16:SER:O	2:H:17:THR:OG1	2.34	0.45
2:B:17:THR:O	2:B:18:CYS:C	2.54	0.45
2:D:142:LEU:O	2:D:146:LYS:CB	2.64	0.45
2:B:142:LEU:O	2:B:146:LYS:CB	2.64	0.45
1:C:49:LEU:CD1	2:D:367:GLU:CG	2.94	0.45
2:H:304:THR:O	2:H:306:SER:N	2.48	0.45
2:F:14:ASN:N	2:F:14:ASN:ND2	2.65	0.45
2:B:14:ASN:O	2:B:15:GLU:C	2.54	0.45
2:H:132:PRO:C	2:H:134:LYS:N	2.70	0.45
2:H:14:ASN:N	2:H:14:ASN:ND2	2.64	0.45
1:G:206:SER:O	1:G:208:LEU:N	2.50	0.45
2:D:14:ASN:O	2:D:15:GLU:C	2.54	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:16:SER:O	2:B:17:THR:OG1	2.34	0.45
1:A:206:SER:O	1:A:208:LEU:N	2.50	0.45
2:F:14:ASN:O	2:F:15:GLU:C	2.54	0.44
2:B:14:ASN:N	2:B:14:ASN:ND2	2.65	0.44
2:H:125:LEU:O	2:H:129:LEU:N	2.50	0.44
2:B:326:LEU:O	2:B:333:LEU:CD1	2.66	0.44
2:H:17:THR:O	2:H:18:CYS:C	2.54	0.44
2:F:17:THR:O	2:F:18:CYS:C	2.54	0.44
2:D:14:ASN:ND2	2:D:14:ASN:N	2.65	0.44
1:C:96:GLY:C	2:F:449:LEU:CD2	2.80	0.44
2:D:137:ASN:OD1	2:D:143:ASP:OD2	2.34	0.44
2:B:125:LEU:O	2:B:129:LEU:N	2.50	0.44
2:D:132:PRO:C	2:D:134:LYS:N	2.70	0.44
1:A:129:GLU:N	1:A:129:GLU:OE1	2.51	0.44
2:F:16:SER:O	2:F:17:THR:OG1	2.34	0.44
1:C:129:GLU:OE1	1:C:129:GLU:N	2.51	0.44
1:C:206:SER:O	1:C:208:LEU:N	2.50	0.44
1:A:49:LEU:CD1	2:B:367:GLU:CG	2.96	0.44
1:E:129:GLU:N	1:E:129:GLU:OE1	2.51	0.44
2:D:125:LEU:O	2:D:129:LEU:N	2.50	0.44
1:E:206:SER:O	1:E:208:LEU:N	2.50	0.44
2:F:132:PRO:C	2:F:134:LYS:N	2.70	0.44
2:F:134:LYS:O	2:F:135:ASP:CB	2.65	0.44
2:B:134:LYS:O	2:B:135:ASP:CB	2.65	0.44
2:D:134:LYS:O	2:D:135:ASP:CB	2.65	0.44
1:G:224:TYR:CE2	1:G:294:HIS:CE1	3.06	0.44
2:F:125:LEU:O	2:F:129:LEU:N	2.50	0.44
1:G:129:GLU:OE1	1:G:129:GLU:N	2.51	0.44
2:H:326:LEU:O	2:H:333:LEU:CD1	2.66	0.44
2:F:326:LEU:O	2:F:333:LEU:CD1	2.66	0.44
2:D:326:LEU:O	2:D:333:LEU:CD1	2.66	0.44
2:H:134:LYS:O	2:H:135:ASP:CB	2.65	0.44
1:E:77:ARG:NE	2:F:136:LYS:NZ	2.66	0.44
2:B:132:PRO:C	2:B:134:LYS:N	2.70	0.44
1:C:96:GLY:CA	2:F:447:ASN:ND2	2.81	0.43
1:E:224:TYR:CE2	1:E:294:HIS:CE1	3.06	0.43
2:D:3:VAL:C	2:D:4:TYR:CG	2.92	0.43
2:B:3:VAL:C	2:B:4:TYR:CG	2.92	0.43
2:B:403:GLU:O	1:G:257:THR:OG1	2.36	0.42
1:A:77:ARG:NE	2:B:136:LYS:NZ	2.67	0.42
2:F:3:VAL:C	2:F:4:TYR:CG	2.92	0.42
2:F:222:MET:O	2:F:226:THR:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:16:SER:C	2:H:17:THR:OG1	2.58	0.42
1:A:90:ASP:OD2	1:A:91:ILE:N	2.53	0.42
2:B:222:MET:O	2:B:226:THR:N	2.53	0.42
1:E:97:ILE:CA	2:H:449:LEU:CD2	2.97	0.42
2:B:16:SER:C	2:B:17:THR:OG1	2.58	0.42
1:G:90:ASP:OD2	1:G:91:ILE:N	2.53	0.42
1:C:90:ASP:OD2	1:C:91:ILE:N	2.53	0.42
2:D:222:MET:O	2:D:226:THR:N	2.53	0.42
1:G:161:SER:O	1:G:162:GLU:CB	2.68	0.42
1:E:90:ASP:OD2	1:E:91:ILE:N	2.53	0.42
2:D:16:SER:C	2:D:17:THR:OG1	2.58	0.41
2:H:3:VAL:C	2:H:4:TYR:CG	2.92	0.41
2:D:305:GLU:O	2:D:306:SER:C	2.59	0.41
2:F:369:PRO:O	2:F:373:HIS:N	2.54	0.41
1:E:161:SER:O	1:E:162:GLU:CB	2.68	0.41
1:C:161:SER:O	1:C:162:GLU:CB	2.68	0.41
2:D:369:PRO:O	2:D:373:HIS:N	2.54	0.41
2:F:144:ALA:O	2:F:148:LEU:CD1	2.69	0.41
2:B:305:GLU:O	2:B:306:SER:C	2.59	0.41
1:A:229:THR:O	1:A:233:GLU:CG	2.69	0.41
2:H:222:MET:O	2:H:226:THR:N	2.53	0.41
2:F:16:SER:C	2:F:17:THR:OG1	2.58	0.41
1:C:224:TYR:CE2	1:C:294:HIS:CE1	3.06	0.41
2:B:144:ALA:O	2:B:148:LEU:CD1	2.69	0.41
1:G:229:THR:O	1:G:233:GLU:CG	2.69	0.41
2:B:126:GLN:C	2:B:131:VAL:CB	2.83	0.41
2:H:144:ALA:O	2:H:148:LEU:CD1	2.69	0.41
1:A:224:TYR:CE2	1:A:294:HIS:CE1	3.06	0.41
1:A:161:SER:O	1:A:162:GLU:CB	2.68	0.41
1:C:210:CYS:SG	1:C:210:CYS:O	2.79	0.41
2:H:369:PRO:O	2:H:373:HIS:N	2.54	0.41
2:H:305:GLU:O	2:H:306:SER:C	2.59	0.41
1:G:210:CYS:O	1:G:210:CYS:SG	2.79	0.41
1:E:229:THR:O	1:E:233:GLU:CG	2.69	0.41
2:H:126:GLN:C	2:H:131:VAL:CB	2.83	0.40
2:D:144:ALA:O	2:D:148:LEU:CD1	2.69	0.40
2:B:369:PRO:O	2:B:373:HIS:N	2.54	0.40
1:C:229:THR:O	1:C:233:GLU:CG	2.69	0.40

All (30) 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)
2:B:40:GLN:NE2	2:F:40:GLN:C[8_434]	0.58	1.62
2:B:40:GLN:C	2:F:40:GLN:NE2[8_434]	0.62	1.58
2:B:40:GLN:CA	2:F:40:GLN:NE2[8_434]	1.08	1.12
2:B:40:GLN:CD	2:F:40:GLN:C[8_434]	1.11	1.09
2:B:40:GLN:NE2	2:F:40:GLN:O[8_434]	1.14	1.06
2:B:40:GLN:C	2:F:40:GLN:CD[8_434]	1.15	1.05
2:B:40:GLN:NE2	2:F:40:GLN:CA[8_434]	1.29	0.91
2:B:40:GLN:O	2:F:40:GLN:NE2[8_434]	1.36	0.84
2:B:40:GLN:CG	2:F:40:GLN:CG[8_434]	1.37	0.83
2:B:40:GLN:OE1	2:F:41:ALA:N[8_434]	1.41	0.79
2:B:41:ALA:N	2:F:40:GLN:OE1[8_434]	1.44	0.76
1:A:23:THR:CG2	2:B:95:VAL:CG2[2_545]	1.51	0.69
1:C:257:THR:OG1	2:F:403:GLU:O[3_655]	1.59	0.61
1:A:23:THR:CG2	2:B:95:VAL:CB[2_545]	1.62	0.58
2:B:40:GLN:CA	2:F:40:GLN:CD[8_434]	1.62	0.58
2:B:40:GLN:CD	2:F:40:GLN:CA[8_434]	1.72	0.48
2:B:40:GLN:CD	2:F:40:GLN:O[8_434]	1.75	0.45
2:B:41:ALA:N	2:F:40:GLN:CD[8_434]	1.75	0.45
2:B:40:GLN:CB	2:F:40:GLN:CD[8_434]	1.78	0.42
2:B:40:GLN:CD	2:F:41:ALA:N[8_434]	1.79	0.41
2:B:40:GLN:OE1	2:F:40:GLN:C[8_434]	1.79	0.41
1:C:257:THR:CB	2:F:403:GLU:O[3_655]	1.86	0.34
2:B:40:GLN:C	2:F:40:GLN:OE1[8_434]	1.87	0.33
2:B:40:GLN:CB	2:F:40:GLN:CG[8_434]	1.88	0.32
2:B:40:GLN:CD	2:F:40:GLN:CB[8_434]	1.89	0.31
2:B:41:ALA:N	2:F:40:GLN:NE2[8_434]	1.89	0.31
2:B:40:GLN:NE2	2:F:41:ALA:N[8_434]	1.90	0.30
2:B:40:GLN:O	2:F:40:GLN:CD[8_434]	1.91	0.29
1:A:98:THR:N	2:B:449:LEU:CD2[2_545]	1.92	0.28
2:B:40:GLN:CG	2:F:40:GLN:CB[8_434]	2.00	0.20

## 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	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	50 91

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	50	91
1	E	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	50	91
1	G	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	50	91
2	B	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	9	63
2	D	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	9	63
2	F	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	9	63
2	H	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	9	63
All	All	2972/3340 (89%)	2692 (91%)	236 (8%)	44 (2%)	15	73

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	SER
2	B	15	GLU
2	B	17	THR
1	C	206	SER
2	D	15	GLU
2	D	17	THR
1	E	206	SER
2	F	15	GLU
2	F	17	THR
1	G	206	SER
2	H	15	GLU
2	H	17	THR
2	B	4	TYR
2	B	139	THR
2	D	4	TYR
2	D	139	THR
2	F	4	TYR
2	F	139	THR
2	H	4	TYR
2	H	139	THR
2	B	144	ALA
2	B	379	GLN
2	D	144	ALA
2	D	379	GLN
2	F	144	ALA
2	F	379	GLN
2	H	144	ALA
2	H	379	GLN

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Mol	Chain	Res	Type
2	B	295	ASN
2	B	437	THR
2	D	295	ASN
2	D	437	THR
2	F	295	ASN
2	F	437	THR
2	H	295	ASN
2	H	437	THR
2	B	336	MET
2	D	336	MET
2	F	336	MET
2	H	336	MET
2	B	352	VAL
2	D	352	VAL
2	F	352	VAL
2	H	352	VAL

### 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	279/330 (84%)	265 (95%)	14 (5%)	34	79
1	C	279/330 (84%)	265 (95%)	14 (5%)	34	79
1	E	279/330 (84%)	265 (95%)	14 (5%)	34	79
1	G	279/330 (84%)	265 (95%)	14 (5%)	34	79
2	B	358/385 (93%)	340 (95%)	18 (5%)	34	79
2	D	358/385 (93%)	340 (95%)	18 (5%)	34	79
2	F	358/385 (93%)	340 (95%)	18 (5%)	34	79
2	H	358/385 (93%)	340 (95%)	18 (5%)	34	79
All	All	2548/2860 (89%)	2420 (95%)	128 (5%)	34	79

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	113	PRO
1	A	149	LYS
1	A	151	ASP
1	A	158	ASN
1	A	159	ARG
1	A	171	LEU
1	A	182	ASN
1	A	245	LEU
1	A	250	VAL
1	A	278	VAL
1	A	326	ARG
1	A	331	LEU
2	B	4	TYR
2	B	14	ASN
2	B	16	SER
2	B	17	THR
2	B	18	CYS
2	B	54	GLN
2	B	101	LEU
2	B	118	LEU
2	B	204	ARG
2	B	266	GLU
2	B	296	PHE
2	B	333	LEU
2	B	347	THR
2	B	354	GLN
2	B	368	LEU
2	B	386	ILE
2	B	417	GLU
2	B	439	LEU
1	C	9	ASN
1	C	76	LEU
1	C	113	PRO
1	C	149	LYS
1	C	151	ASP
1	C	158	ASN
1	C	159	ARG
1	C	171	LEU
1	C	182	ASN
1	C	245	LEU
1	C	250	VAL

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Mol	Chain	Res	Type
1	C	278	VAL
1	C	326	ARG
1	C	331	LEU
2	D	4	TYR
2	D	14	ASN
2	D	16	SER
2	D	17	THR
2	D	18	CYS
2	D	54	GLN
2	D	101	LEU
2	D	118	LEU
2	D	204	ARG
2	D	266	GLU
2	D	296	PHE
2	D	333	LEU
2	D	347	THR
2	D	354	GLN
2	D	368	LEU
2	D	386	ILE
2	D	417	GLU
2	D	439	LEU
1	E	9	ASN
1	E	76	LEU
1	E	113	PRO
1	E	149	LYS
1	E	151	ASP
1	E	158	ASN
1	E	159	ARG
1	E	171	LEU
1	E	182	ASN
1	E	245	LEU
1	E	250	VAL
1	E	278	VAL
1	E	326	ARG
1	E	331	LEU
2	F	4	TYR
2	F	14	ASN
2	F	16	SER
2	F	17	THR
2	F	18	CYS
2	F	54	GLN
2	F	101	LEU

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Mol	Chain	Res	Type
2	F	118	LEU
2	F	204	ARG
2	F	266	GLU
2	F	296	PHE
2	F	333	LEU
2	F	347	THR
2	F	354	GLN
2	F	368	LEU
2	F	386	ILE
2	F	417	GLU
2	F	439	LEU
1	G	9	ASN
1	G	76	LEU
1	G	113	PRO
1	G	149	LYS
1	G	151	ASP
1	G	158	ASN
1	G	159	ARG
1	G	171	LEU
1	G	182	ASN
1	G	245	LEU
1	G	250	VAL
1	G	278	VAL
1	G	326	ARG
1	G	331	LEU
2	H	4	TYR
2	H	14	ASN
2	H	16	SER
2	H	17	THR
2	H	18	CYS
2	H	54	GLN
2	H	101	LEU
2	H	118	LEU
2	H	204	ARG
2	H	266	GLU
2	H	296	PHE
2	H	333	LEU
2	H	347	THR
2	H	354	GLN
2	H	368	LEU
2	H	386	ILE
2	H	417	GLU

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Mol	Chain	Res	Type
2	H	439	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	330/383 (86%)	0.64	38 (11%) 5 9	177, 273, 376, 684	0
1	C	330/383 (86%)	0.63	44 (13%) 4 7	200, 315, 406, 568	0
1	E	330/383 (86%)	0.68	39 (11%) 5 9	236, 314, 400, 518	0
1	G	330/383 (86%)	0.65	47 (14%) 3 6	240, 337, 443, 633	0
2	B	423/452 (93%)	0.94	58 (13%) 4 6	131, 273, 412, 537	1 (0%)
2	D	423/452 (93%)	1.02	93 (21%) 1 3	225, 360, 512, 725	1 (0%)
2	F	423/452 (93%)	0.97	71 (16%) 2 4	180, 285, 429, 757	1 (0%)
2	H	423/452 (93%)	1.26	92 (21%) 1 3	212, 357, 521, 686	1 (0%)
All	All	3012/3340 (90%)	0.87	482 (16%) 3 5	131, 317, 467, 757	4 (0%)

All (482) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	179	PHE	15.6
2	H	244	ALA	14.4
2	H	178	VAL	13.7
2	H	243	LEU	13.6
2	D	202	LEU	11.4
2	H	416	PRO	10.6
1	G	95	GLY	9.6
2	H	373	HIS	9.0
2	H	202	LEU	8.2
2	D	245	PHE	8.1
1	G	96	GLY	7.9
2	H	177	GLY	7.8
2	H	301	VAL	7.6
2	H	190	PHE	7.1
2	H	203	PRO	7.0
2	H	133	TRP	7.0

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Mol	Chain	Res	Type	RSRZ
2	H	417	GLU	6.9
2	D	203	PRO	6.9
2	H	222	MET	6.9
2	D	201	VAL	6.7
2	D	362	LEU	6.5
2	F	416	PRO	6.4
1	E	308	LEU	6.4
2	D	179	PHE	6.1
2	H	390	GLU	6.1
2	F	362	LEU	5.9
2	D	178	VAL	5.9
2	H	110	LEU	5.9
2	H	194	LEU	5.9
2	D	172	LEU	5.8
2	H	172	LEU	5.7
2	H	234	LEU	5.5
2	D	113	LEU	5.4
2	H	180	THR	5.3
2	H	245	PHE	5.3
2	D	176	VAL	5.3
1	G	308	LEU	5.2
2	B	373	HIS	5.2
2	D	133	TRP	5.2
1	G	217	LEU	5.2
2	H	403	GLU	5.1
2	H	113	LEU	5.1
2	H	221	PHE	5.1
2	H	362	LEU	5.1
1	E	239	LEU	5.0
2	D	442	LEU	5.0
2	H	447	ASN	5.0
2	F	255	MET	5.0
2	D	244	ALA	4.9
2	H	129	LEU	4.9
2	F	367	GLU	4.9
2	F	447	ASN	4.9
2	F	373	HIS	4.9
2	H	176	VAL	4.8
2	D	44	SER	4.7
2	H	116	GLY	4.7
2	F	301	VAL	4.7
2	D	226	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	110	LEU	4.7
1	E	96	GLY	4.7
1	G	94	VAL	4.6
1	G	97	ILE	4.6
2	H	174	THR	4.6
2	D	243	LEU	4.6
2	H	370	ALA	4.6
1	E	95	GLY	4.5
1	G	133	GLY	4.4
2	D	373	HIS	4.4
2	D	357	TYR	4.4
2	H	389	GLY	4.4
2	F	129	LEU	4.4
2	D	386	ILE	4.4
2	D	222	MET	4.3
1	C	171	LEU	4.3
1	C	239	LEU	4.3
1	G	32	PHE	4.3
1	G	218	VAL	4.3
2	B	129	LEU	4.3
2	D	349	PRO	4.2
2	H	388	VAL	4.2
2	H	448	PRO	4.2
2	B	362	LEU	4.2
2	F	399	LEU	4.2
2	D	43	THR	4.2
1	G	171	LEU	4.1
2	D	301	VAL	4.1
2	H	369	PRO	4.1
1	C	133	GLY	4.1
2	F	286	PHE	4.1
1	A	132	ILE	4.1
2	H	186	LEU	4.1
2	F	351	LEU	4.1
2	D	367	GLU	4.1
2	H	300	GLN	4.1
2	D	46	VAL	4.0
2	H	147	VAL	4.0
2	B	386	ILE	4.0
2	D	299	THR	4.0
1	E	97	ILE	4.0
1	A	171	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	255	MET	3.9
2	H	381	LEU	3.9
2	H	309	LEU	3.9
2	B	255	MET	3.9
2	H	158	LEU	3.9
1	E	151	ASP	3.9
2	H	218	ILE	3.8
1	E	139	PHE	3.8
2	F	133	TRP	3.8
2	F	300	GLN	3.8
1	E	32	PHE	3.8
1	C	270	TYR	3.8
2	B	172	LEU	3.8
1	E	327	ILE	3.8
1	E	196	ILE	3.8
2	D	175	VAL	3.8
2	H	191	VAL	3.8
1	C	235	LEU	3.8
2	H	363	LEU	3.8
2	B	158	LEU	3.8
2	D	129	LEU	3.7
2	B	339	LEU	3.7
1	E	142	ILE	3.7
2	B	245	PHE	3.7
2	D	399	LEU	3.7
2	D	128	ILE	3.6
2	D	234	LEU	3.6
2	F	334	ASN	3.6
1	E	312	PHE	3.6
2	H	204	ARG	3.6
2	F	243	LEU	3.6
2	H	311	LEU	3.6
1	C	95	GLY	3.6
1	G	19	ILE	3.6
2	H	312	ILE	3.6
2	H	299	THR	3.6
2	F	363	LEU	3.6
2	D	441	PHE	3.6
2	F	350	GLN	3.6
2	D	388	VAL	3.6
2	H	242	THR	3.6
2	D	186	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	303	PHE	3.5
2	H	399	LEU	3.5
1	E	76	LEU	3.5
2	F	113	LEU	3.5
1	E	329	PHE	3.5
2	D	427	PHE	3.5
2	F	178	VAL	3.5
2	B	403	GLU	3.5
2	D	363	LEU	3.5
1	G	40	TRP	3.5
2	B	447	ASN	3.4
2	B	312	ILE	3.4
2	D	174	THR	3.4
2	B	416	PRO	3.4
1	C	203	VAL	3.4
1	C	32	PHE	3.4
2	B	180	THR	3.4
2	F	303	PHE	3.4
2	F	446	ALA	3.4
2	F	312	ILE	3.3
2	B	202	LEU	3.3
2	D	430	ALA	3.3
1	E	218	VAL	3.3
1	A	76	LEU	3.3
1	E	150	GLU	3.3
2	F	386	ILE	3.3
2	B	301	VAL	3.3
2	B	303	PHE	3.3
2	F	158	LEU	3.3
2	D	221	PHE	3.3
1	E	138	ILE	3.3
1	A	239	LEU	3.3
2	D	101	LEU	3.2
2	H	339	LEU	3.2
1	C	21	ILE	3.2
2	F	339	LEU	3.2
2	D	352	VAL	3.2
2	H	441	PHE	3.2
2	F	245	PHE	3.2
2	D	200	VAL	3.2
1	E	83	VAL	3.2
1	E	171	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	105	GLU	3.2
2	H	255	MET	3.2
2	D	190	PHE	3.2
2	D	381	LEU	3.2
2	D	109	THR	3.2
2	F	287	GLN	3.2
2	B	243	LEU	3.2
2	F	176	VAL	3.1
2	D	397	PHE	3.1
2	B	207	ASP	3.1
2	F	128	ILE	3.1
1	G	329	PHE	3.1
1	E	293	ILE	3.1
2	D	84	ILE	3.1
1	C	308	LEU	3.1
1	G	92	ILE	3.1
2	D	348	MET	3.1
1	G	116	LEU	3.1
2	B	133	TRP	3.0
2	H	165	ASP	3.0
2	D	180	THR	3.0
1	G	148	LEU	3.0
2	F	202	LEU	3.0
1	C	155	PHE	3.0
2	B	179	PHE	3.0
1	E	208	LEU	3.0
1	E	148	LEU	3.0
2	B	197	TYR	3.0
2	B	363	LEU	3.0
2	H	151	LEU	3.0
2	B	128	ILE	3.0
2	B	430	ALA	3.0
2	D	429	PHE	3.0
1	C	40	TRP	3.0
2	F	311	LEU	3.0
2	B	113	LEU	3.0
2	H	351	LEU	3.0
2	H	395	ILE	3.0
2	B	399	LEU	3.0
2	D	225	VAL	3.0
2	D	309	LEU	2.9
1	C	134	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	403	GLU	2.9
2	D	448	PRO	2.9
1	A	263	PHE	2.9
2	F	448	PRO	2.9
2	H	107	PHE	2.9
2	H	303	PHE	2.9
2	B	176	VAL	2.9
1	C	243	LYS	2.9
1	G	55	TYR	2.9
2	F	431	VAL	2.9
2	D	177	GLY	2.9
1	G	76	LEU	2.9
2	F	349	PRO	2.9
2	D	158	LEU	2.9
2	F	159	VAL	2.9
1	E	92	ILE	2.9
2	D	100	VAL	2.9
1	A	125	MET	2.9
1	A	32	PHE	2.9
1	E	121	GLY	2.9
1	E	125	MET	2.8
1	A	14	GLN	2.8
1	G	172	GLY	2.8
1	E	80	THR	2.8
1	E	94	VAL	2.8
2	H	348	MET	2.8
1	A	265	LEU	2.8
1	C	263	PHE	2.8
1	C	42	PRO	2.8
2	D	45	PRO	2.8
1	C	261	ILE	2.8
2	D	311	LEU	2.8
1	E	295	ALA	2.8
2	D	111	ALA	2.8
1	C	92	ILE	2.8
2	H	248	TYR	2.8
2	B	208	PHE	2.8
2	H	225	VAL	2.7
2	B	337	LYS	2.7
2	H	211	LEU	2.7
1	G	142	ILE	2.7
2	H	357	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	103	PHE	2.7
1	A	270	TYR	2.7
2	D	327	THR	2.7
1	C	246	PHE	2.7
2	B	309	LEU	2.7
2	F	352	VAL	2.7
1	G	134	ARG	2.7
1	C	218	VAL	2.7
2	D	344	ILE	2.7
2	H	175	VAL	2.7
2	D	231	GLY	2.7
2	D	107	PHE	2.7
2	B	327	THR	2.7
2	D	387	ARG	2.7
1	G	312	PHE	2.7
1	C	19	ILE	2.7
1	E	40	TRP	2.7
1	E	277	TYR	2.7
2	B	83	ARG	2.7
2	H	226	THR	2.7
1	G	122	VAL	2.7
2	D	114	TYR	2.6
2	B	110	LEU	2.6
2	B	194	LEU	2.6
2	F	172	LEU	2.6
2	H	55	LEU	2.6
2	H	442	LEU	2.6
2	D	247	THR	2.6
1	G	265	LEU	2.6
2	B	203	PRO	2.6
1	G	119	PHE	2.6
2	D	208	PHE	2.6
2	D	449	LEU	2.6
1	G	123	VAL	2.6
1	A	118	GLU	2.6
2	D	312	ILE	2.6
2	F	397	PHE	2.6
1	C	132	ILE	2.6
2	D	59	ALA	2.6
1	C	293	ILE	2.6
2	F	444	ARG	2.6
2	B	80	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	41	VAL	2.5
1	E	155	PHE	2.5
1	A	272	LEU	2.5
2	D	351	LEU	2.5
2	B	426	PRO	2.5
1	C	125	MET	2.5
2	F	366	ALA	2.5
2	D	328	PHE	2.5
2	D	428	LEU	2.5
1	C	83	VAL	2.5
1	E	132	ILE	2.5
2	D	8	PHE	2.5
1	A	293	ILE	2.5
1	G	196	ILE	2.5
1	C	123	VAL	2.5
1	C	322	ARG	2.5
2	B	234	LEU	2.5
2	H	440	HIS	2.5
2	H	201	VAL	2.5
2	H	439	LEU	2.4
2	H	431	VAL	2.4
1	G	216	ALA	2.4
1	A	196	ILE	2.4
1	C	142	ILE	2.4
2	B	211	LEU	2.4
1	C	153	PHE	2.4
2	H	337	LYS	2.4
2	B	444	ARG	2.4
2	F	179	PHE	2.4
2	H	111	ALA	2.4
2	D	333	LEU	2.4
1	E	298	ILE	2.4
1	A	235	LEU	2.4
1	C	94	VAL	2.4
1	G	270	TYR	2.4
2	F	194	LEU	2.4
2	F	84	ILE	2.4
1	E	235	LEU	2.4
2	B	431	VAL	2.4
2	D	285	THR	2.4
2	D	359	LEU	2.4
2	H	428	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	245	LEU	2.4
2	B	186	LEU	2.4
2	F	337	LYS	2.4
1	C	298	ILE	2.3
2	F	381	LEU	2.3
2	H	200	VAL	2.3
1	A	142	ILE	2.3
1	A	208	LEU	2.3
2	B	84	ILE	2.3
2	H	287	GLN	2.3
1	C	76	LEU	2.3
1	A	312	PHE	2.3
2	D	296	PHE	2.3
2	F	80	LEU	2.3
2	F	296	PHE	2.3
2	F	309	LEU	2.3
2	F	357	TYR	2.3
2	B	178	VAL	2.3
2	B	206	LEU	2.3
1	A	155	PHE	2.3
2	H	359	LEU	2.3
2	D	72	MET	2.3
2	F	5	ILE	2.3
1	A	21	ILE	2.3
2	H	346	LEU	2.3
1	G	125	MET	2.3
2	F	222	MET	2.3
2	F	55	LEU	2.3
2	D	204	ARG	2.3
2	H	43	THR	2.3
1	A	198	MET	2.3
2	H	328	PHE	2.3
2	F	348	MET	2.3
1	G	293	ILE	2.3
1	A	87	LEU	2.3
2	F	147	VAL	2.3
2	D	346	LEU	2.3
2	D	248	TYR	2.2
1	A	218	VAL	2.2
2	F	110	LEU	2.2
2	B	287	GLN	2.2
1	G	239	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	VAL	2.2
1	G	261	ILE	2.2
1	G	225	ILE	2.2
2	H	251	PHE	2.2
1	A	92	ILE	2.2
1	C	225	ILE	2.2
1	E	302	THR	2.2
1	G	138	ILE	2.2
2	F	441	PHE	2.2
1	A	308	LEU	2.2
1	G	83	VAL	2.2
2	B	381	LEU	2.2
2	D	439	LEU	2.2
2	F	186	LEU	2.2
1	A	261	ILE	2.2
1	C	148	LEU	2.2
2	F	258	PHE	2.2
2	F	449	LEU	2.2
1	A	306	TRP	2.2
2	D	334	ASN	2.2
2	F	388	VAL	2.2
1	C	116	LEU	2.2
1	C	97	ILE	2.2
1	G	203	VAL	2.2
2	B	442	LEU	2.2
1	C	151	ASP	2.2
2	H	128	ILE	2.2
1	A	83	VAL	2.2
1	G	104	GLY	2.2
2	B	159	VAL	2.2
2	F	155	GLN	2.1
2	D	237	ALA	2.1
1	A	138	ILE	2.1
1	G	39	VAL	2.1
2	D	191	VAL	2.1
1	A	78	TYR	2.1
1	A	39	VAL	2.1
1	C	312	PHE	2.1
2	B	167	GLN	2.1
1	G	235	LEU	2.1
2	H	125	LEU	2.1
2	B	351	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	6	HIS	2.1
1	C	145	GLN	2.1
2	H	233	SER	2.1
1	A	40	TRP	2.1
1	A	258	LEU	2.1
2	H	84	ILE	2.1
2	F	436	ALA	2.1
2	B	313	GLN	2.1
1	A	116	LEU	2.1
2	F	234	LEU	2.1
1	C	236	MET	2.1
1	C	74	LEU	2.1
1	A	329	PHE	2.1
1	E	225	ILE	2.1
2	D	151	LEU	2.1
1	E	263	PHE	2.1
2	B	328	PHE	2.1
2	H	189	PRO	2.1
2	D	194	LEU	2.1
2	B	73	VAL	2.1
1	G	132	ILE	2.1
1	E	265	LEU	2.1
2	B	427	PHE	2.1
2	D	431	VAL	2.1
2	F	170	LEU	2.1
1	G	114	PHE	2.1
2	B	296	PHE	2.1
1	A	302	THR	2.1
2	H	349	PRO	2.1
2	F	346	LEU	2.0
1	G	155	PHE	2.0
2	F	440	HIS	2.0
1	C	139	PHE	2.0
2	F	184	LEU	2.0
2	F	439	LEU	2.0
1	E	123	VAL	2.0
1	G	99	VAL	2.0
2	F	175	VAL	2.0
2	H	36	PRO	2.0
2	D	440	HIS	2.0
2	B	170	LEU	2.0
1	G	5	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	429	PHE	2.0
1	C	118	GLU	2.0
2	F	299	THR	2.0
2	H	334	ASN	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.