



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:46 am GMT

PDB ID : 4AEZ
Title : Crystal Structure of Mitotic Checkpoint Complex
Authors : Kulkarni, K.A.; Chao, W.C.H.; Zhang, Z.; Barford, D.
Deposited on : 2012-01-13
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

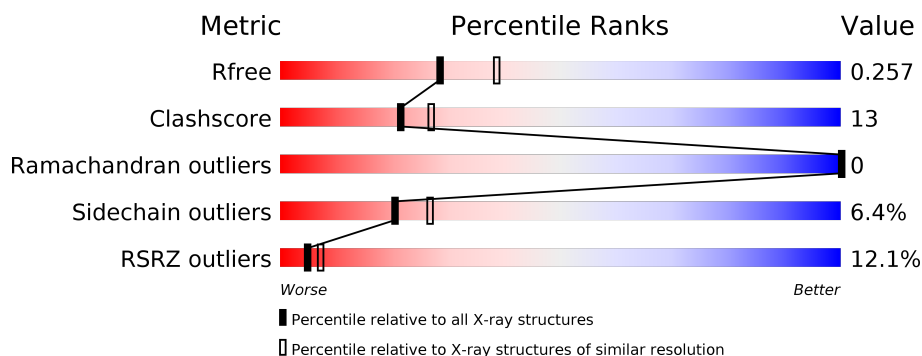
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	
1	D	401	
1	G	401	
2	B	203	
2	E	203	
2	H	203	

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Mol	Chain	Length	Quality of chain
3	C	223	<div><div></div><div>2%</div><div>77%</div><div>19%</div><div></div><div></div></div>
3	F	223	<div><div></div><div>7%</div><div>66%</div><div>19%</div><div></div><div>12%</div></div>
3	I	223	<div><div></div><div>34%</div><div>44%</div><div>34%</div><div>9%</div><div>13%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16896 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 WD REPEAT-CONTAINING PROTEIN SLP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2499	1565	445	483	6			
1	D	314	Total	C	N	O	S	0	0	0
			2406	1507	426	467	6			
1	G	317	Total	C	N	O	S	0	0	0
			2400	1502	425	467	6			

- Molecule 2 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1469	941	243	278	7			
2	E	175	Total	C	N	O	S	0	0	0
			1369	880	224	260	5			
2	H	185	Total	C	N	O	S	0	0	0
			1477	951	246	274	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
B	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417
E	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
E	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417
H	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
H	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417

- Molecule 3 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1799	1142	313	339	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	196	Total	C	N	O	S	0	0	0
			1585	1013	265	302	5			
3	I	193	Total	C	N	O	S	0	0	0
			1574	997	273	300	4			

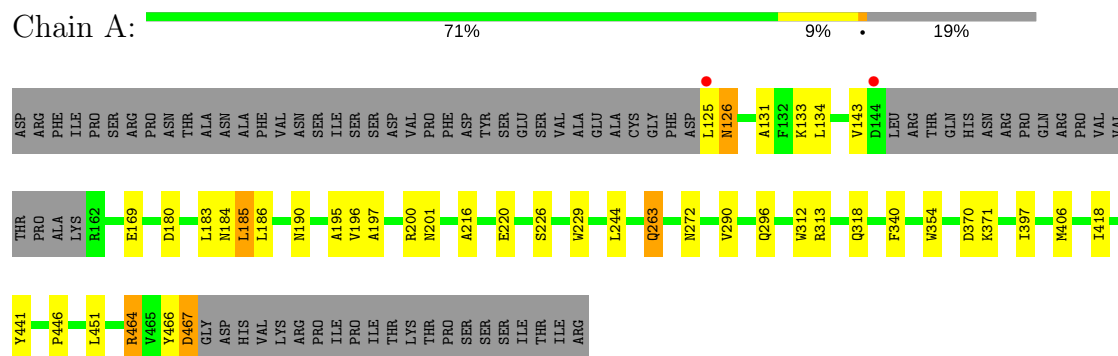
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	33	Total	O	0	0
			33	33		
4	C	33	Total	O	0	0
			33	33		
4	D	61	Total	O	0	0
			61	61		
4	E	1	Total	O	0	0
			1	1		
4	F	48	Total	O	0	0
			48	48		
4	G	21	Total	O	0	0
			21	21		
4	H	6	Total	O	0	0
			6	6		
4	I	1	Total	O	0	0
			1	1		

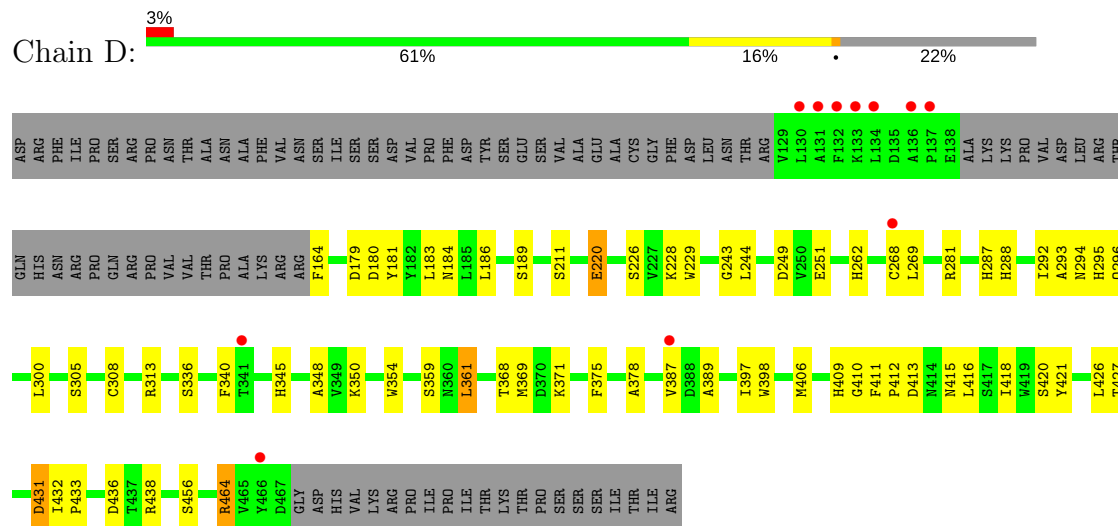
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

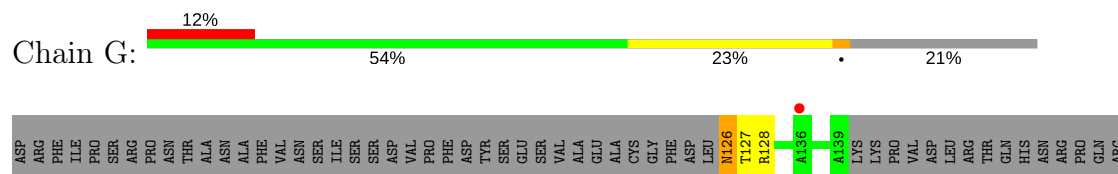
• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1

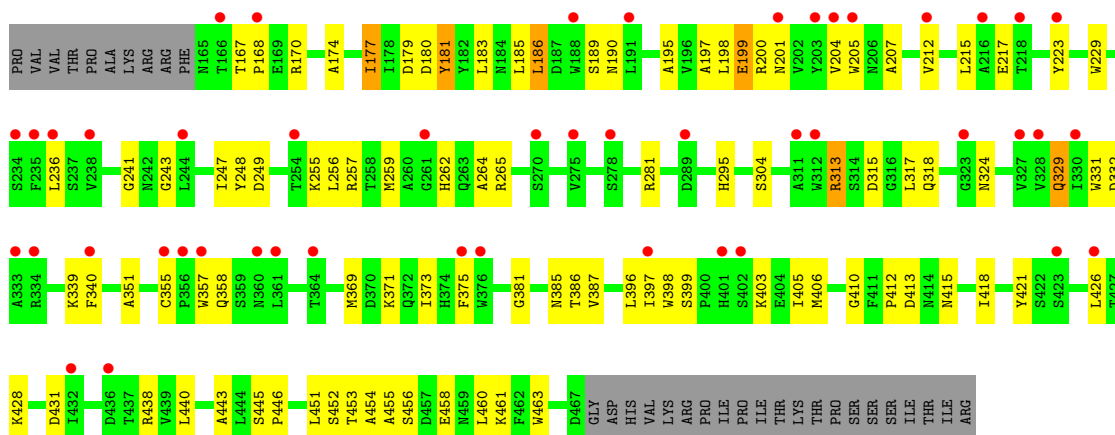


• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1



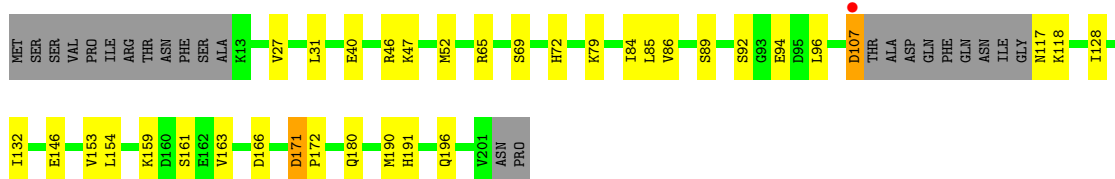
• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1





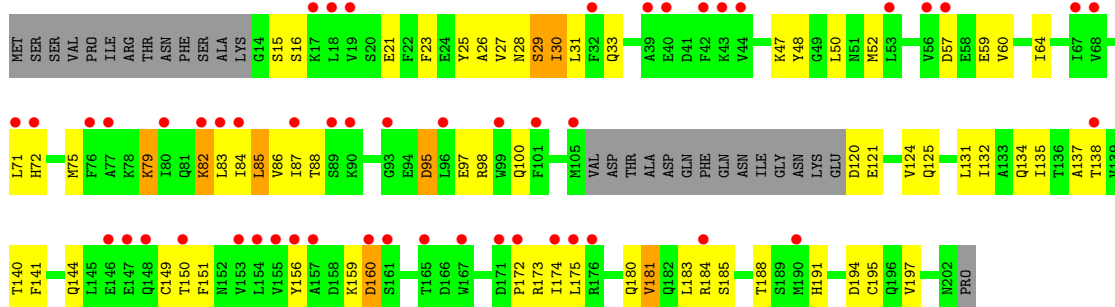
• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

Chain B: 71% 16% 11%



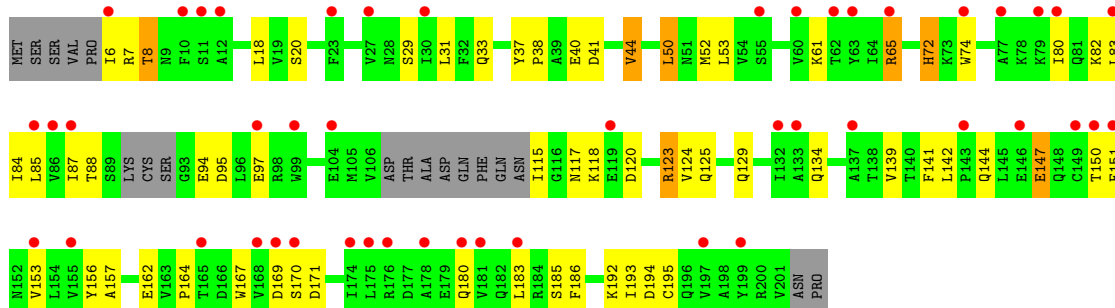
• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

Chain E: 25% 53% 30% 14%

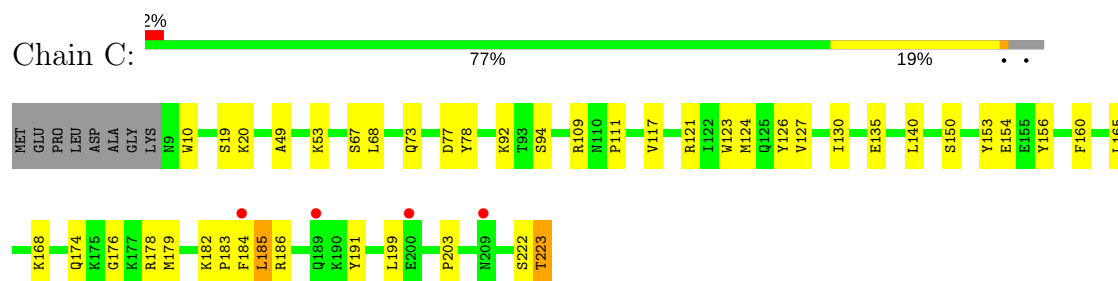


• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

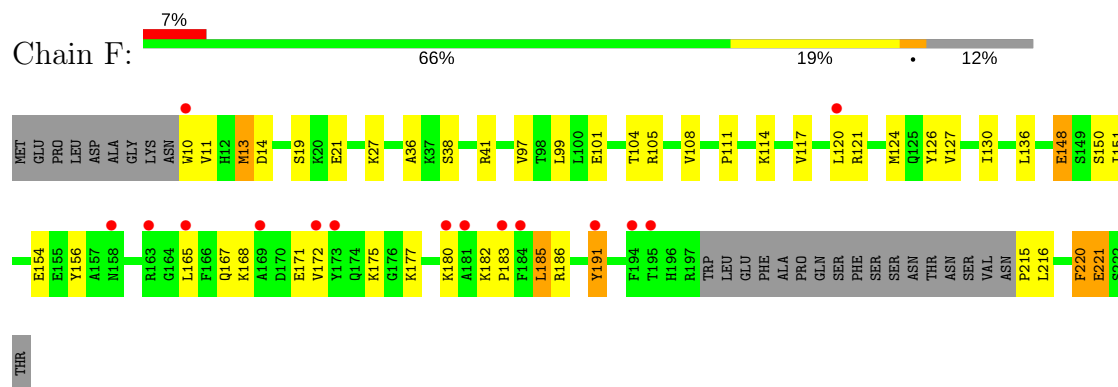
Chain H: 23% 60% 28% 9%



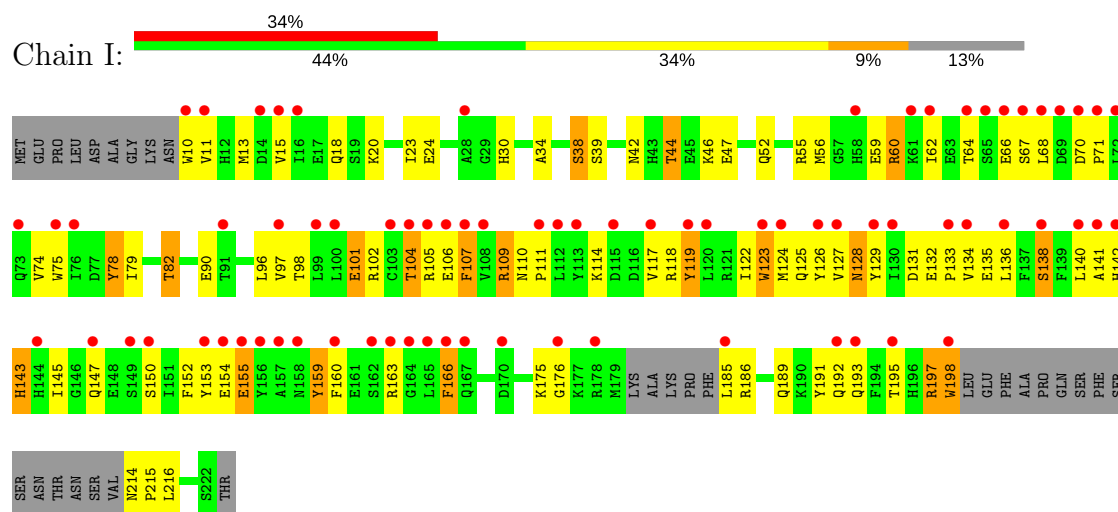
- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.81Å 286.90Å 72.01Å 90.00° 119.04° 90.00°	Depositor
Resolution (Å)	62.96 – 2.30 62.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.96-2.30) 99.8 (62.96-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.267 0.209 , 0.257	Depositor DCC
R_{free} test set	1968 reflections (1.78%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.024 for h,-k,-h-l 0.022 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16896	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/2559	0.54	0/3492
1	D	0.34	0/2465	0.56	0/3366
1	G	0.28	0/2458	0.49	0/3361
2	B	0.36	0/1494	0.50	0/2016
2	E	0.27	0/1394	0.43	0/1895
2	H	0.29	0/1502	0.46	0/2032
3	C	0.35	0/1847	0.46	0/2495
3	F	0.34	0/1625	0.48	0/2198
3	I	0.27	0/1614	0.44	0/2187
All	All	0.32	0/16958	0.50	0/23042

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	107	PHE	Peptide

5.2 Too-close contacts [i](#)

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	2499	0	2393	33	0
1	D	2406	0	2290	46	0
1	G	2400	0	2269	76	0
2	B	1469	0	1476	23	0
2	E	1369	0	1312	83	0
2	H	1477	0	1462	48	0
3	C	1799	0	1718	27	0
3	F	1585	0	1472	41	0
3	I	1574	0	1434	88	0
4	A	114	0	0	3	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	61	0	0	3	0
4	E	1	0	0	0	0
4	F	48	0	0	0	0
4	G	21	0	0	0	0
4	H	6	0	0	0	0
4	I	1	0	0	0	0
All	All	16896	0	15826	436	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 13.

All (436) 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:A:466:TYR:O	1:A:467:ASP:HB3	1.49	1.08
3:C:222:SER:O	3:C:223:THR:HB	1.54	1.05
1:G:177:ILE:HD11	1:G:458:GLU:HA	1.42	0.99
1:D:164:PHE:HE1	1:D:432:ILE:HD11	1.25	0.97
3:I:122:ILE:HG22	3:I:126:TYR:CE1	2.01	0.95
3:I:123:TRP:HA	3:I:126:TYR:CD2	2.07	0.89
1:D:268:CYS:SG	1:D:308:CYS:O	2.31	0.88
3:I:118:ARG:O	3:I:122:ILE:HG13	1.75	0.86
3:I:109:ARG:HD3	3:I:110:ASN:H	1.41	0.85
3:I:133:PRO:O	3:I:136:LEU:HG	1.77	0.85
1:A:133:LYS:HE2	2:B:166:ASP:HA	1.59	0.84
1:D:164:PHE:CE1	1:D:432:ILE:HD11	2.10	0.84
3:I:198:TRP:HD1	3:I:198:TRP:H	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:LEU:HD11	2:H:129:GLN:HB3	1.61	0.81
2:E:87:ILE:CG2	2:E:97:GLU:HB3	2.11	0.80
3:I:127:VAL:HB	3:I:136:LEU:HD22	1.63	0.80
3:F:38:SER:O	3:F:41:ARG:HG2	1.81	0.79
3:F:220:PHE:HD1	3:F:221:GLU:N	1.80	0.78
2:E:172:PRO:HB2	2:E:174:ILE:HG13	1.64	0.77
2:E:50:LEU:HD12	2:E:52:MET:HE1	1.67	0.77
2:H:120:ASP:O	2:H:124:VAL:HG23	1.88	0.73
1:D:313:ARG:HG3	1:D:354:TRP:CD2	2.23	0.73
3:I:122:ILE:HG22	3:I:126:TYR:HE1	1.52	0.72
2:E:134:GLN:O	2:E:138:THR:HG23	1.88	0.72
2:E:87:ILE:HD12	2:E:150:THR:O	1.90	0.72
3:F:220:PHE:HD1	3:F:221:GLU:H	1.38	0.71
3:F:120:LEU:HD12	3:F:121:ARG:N	2.05	0.71
2:H:164:PRO:HB2	2:H:167:TRP:HD1	1.56	0.71
3:F:117:VAL:HA	3:F:120:LEU:HG	1.73	0.70
2:E:25:TYR:CE1	2:E:47:LYS:HD2	2.26	0.70
1:D:368:THR:HG22	1:D:369:MET:HE2	1.73	0.70
3:I:198:TRP:N	3:I:198:TRP:CD1	2.58	0.70
1:G:167:THR:HG23	1:G:168:PRO:HD2	1.73	0.70
1:A:313:ARG:HG3	1:A:354:TRP:CD2	2.26	0.70
3:I:56:MET:O	3:I:60:ARG:HD2	1.92	0.69
1:A:467:ASP:OD1	1:A:467:ASP:C	2.30	0.69
2:E:25:TYR:CZ	2:E:47:LYS:HD2	2.27	0.69
2:H:8:THR:HG23	2:H:117:ASN:HD21	1.57	0.69
1:G:180:ASP:HB3	1:G:183:LEU:HG	1.73	0.68
2:E:23:PHE:CE2	2:E:75:MET:HE3	2.28	0.68
1:G:177:ILE:HD11	1:G:458:GLU:CA	2.22	0.68
3:I:15:VAL:HG12	3:I:39:SER:HB2	1.76	0.68
2:E:138:THR:HA	2:E:141:PHE:CE2	2.27	0.67
2:H:125:GLN:O	2:H:129:GLN:HG2	1.94	0.67
1:D:413:ASP:HB3	1:D:415:ASN:OD1	1.95	0.67
1:D:369:MET:SD	2:E:140:THR:HG22	2.36	0.66
1:A:126:ASN:HD22	2:B:159:LYS:HG2	1.60	0.66
2:E:23:PHE:CD2	2:E:71:LEU:HD11	2.30	0.66
2:H:180:GLN:HB3	3:I:10:TRP:CZ3	2.31	0.65
2:E:121:GLU:O	2:E:125:GLN:HG2	1.97	0.65
1:G:177:ILE:HG23	1:G:198:LEU:CD2	2.27	0.65
1:D:415:ASN:ND2	1:D:431:ASP:OD1	2.29	0.65
3:C:174:GLN:O	3:C:178:ARG:HG3	1.96	0.64
1:A:126:ASN:O	2:B:159:LYS:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:VAL:HG13	2:E:197:VAL:HG13	1.78	0.64
1:A:126:ASN:O	1:A:126:ASN:ND2	2.30	0.64
3:C:199:LEU:O	3:C:203:PRO:HG3	1.98	0.64
2:E:88:THR:HG21	2:E:173:ARG:NH2	2.13	0.64
3:I:44:THR:HG22	3:I:47:GLU:HG3	1.80	0.63
3:I:97:VAL:HG13	3:I:98:THR:N	2.13	0.63
2:B:180:GLN:HB2	3:C:10:TRP:CZ3	2.34	0.62
2:E:87:ILE:HG22	2:E:97:GLU:HB3	1.80	0.62
2:E:120:ASP:O	2:E:124:VAL:HG23	2.00	0.62
3:C:182:LYS:HB3	3:C:183:PRO:HA	1.82	0.62
1:D:180:ASP:HB3	1:D:183:LEU:HG	1.80	0.61
3:I:78:TYR:O	3:I:82:THR:HG22	2.01	0.61
3:F:220:PHE:CD1	3:F:221:GLU:N	2.67	0.61
1:G:428:LYS:HD3	1:G:431:ASP:HB2	1.81	0.61
2:E:23:PHE:HE2	2:E:75:MET:HE3	1.65	0.61
2:E:82:LYS:HD3	2:E:100:GLN:OE1	2.01	0.61
1:G:177:ILE:CD1	1:G:458:GLU:HA	2.24	0.61
1:G:179:ASP:HB2	1:G:456:SER:CB	2.31	0.60
1:D:249:ASP:OD1	1:D:251:GLU:HG2	2.01	0.60
2:E:47:LYS:HD3	2:E:48:TYR:CE2	2.37	0.60
1:G:421:TYR:HD2	1:G:426:LEU:HD11	1.66	0.60
3:I:97:VAL:HG13	3:I:98:THR:H	1.66	0.60
3:I:66:GLU:OE1	3:I:66:GLU:N	2.34	0.60
3:C:185:LEU:HD12	3:C:186:ARG:H	1.66	0.60
1:G:249:ASP:HB2	1:G:256:LEU:HD11	1.83	0.60
2:E:26:ALA:O	2:E:30:ILE:HG23	2.02	0.60
1:D:410:GLY:HA2	1:D:438:ARG:HB3	1.84	0.59
1:G:179:ASP:HB2	1:G:456:SER:HB3	1.83	0.59
1:A:190:ASN:HA	1:A:446:PRO:HB3	1.84	0.59
2:E:82:LYS:HB2	2:E:82:LYS:HZ3	1.66	0.59
1:G:189:SER:HB3	1:G:229:TRP:CD2	2.37	0.59
1:A:406:MET:HG2	1:A:418:ILE:HG12	1.84	0.59
2:B:117:ASN:HB2	1:D:436:ASP:OD1	2.01	0.59
3:I:109:ARG:HD3	3:I:110:ASN:N	2.15	0.59
1:A:184:ASN:O	1:A:226:SER:HA	2.02	0.59
2:H:147:GLU:CD	2:H:147:GLU:H	2.05	0.59
2:B:118:LYS:NZ	1:D:433:PRO:O	2.29	0.58
3:F:127:VAL:HG23	3:F:136:LEU:HD13	1.86	0.58
2:E:79:LYS:HE3	2:E:79:LYS:HA	1.86	0.57
1:G:128:ARG:N	2:H:157:ALA:O	2.37	0.57
1:G:357:TRP:HZ3	1:G:399:SER:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:GLU:HG3	3:F:180:LYS:HB2	1.87	0.57
3:I:133:PRO:HA	3:I:136:LEU:HD23	1.86	0.57
2:E:52:MET:HE3	2:E:132:ILE:HD13	1.87	0.57
2:E:47:LYS:NZ	2:E:48:TYR:OH	2.29	0.57
1:D:268:CYS:SG	1:D:308:CYS:C	2.83	0.56
1:D:179:ASP:HB2	1:D:456:SER:HB3	1.86	0.56
3:I:90:GLU:HB2	3:I:129:TYR:HE2	1.70	0.56
2:E:85:LEU:HG	2:E:151:PHE:CZ	2.41	0.56
2:E:23:PHE:HD2	2:E:71:LEU:HD11	1.70	0.56
3:F:182:LYS:HA	3:F:183:PRO:C	2.25	0.56
2:H:8:THR:CG2	2:H:117:ASN:HD21	2.19	0.56
3:F:124:MET:O	3:F:127:VAL:HG12	2.05	0.56
1:G:397:ILE:HG23	1:G:406:MET:HB2	1.86	0.56
3:I:123:TRP:O	3:I:127:VAL:HG12	2.05	0.56
2:B:196:GLN:HB3	3:C:10:TRP:CZ3	2.41	0.55
3:F:105:ARG:O	3:F:108:VAL:HG22	2.06	0.55
3:I:150:SER:O	3:I:154:GLU:HG3	2.06	0.55
3:I:124:MET:SD	3:I:155:GLU:HG2	2.47	0.55
2:E:181:VAL:HG13	2:E:197:VAL:CG1	2.35	0.55
2:E:15:SER:OG	2:E:188:THR:HG21	2.06	0.55
3:I:141:ALA:HA	3:I:147:GLN:NE2	2.21	0.55
3:F:150:SER:O	3:F:154:GLU:HG3	2.06	0.55
3:I:79:ILE:HA	3:I:82:THR:CG2	2.37	0.55
2:E:52:MET:CE	2:E:132:ILE:HD13	2.37	0.55
1:G:445:SER:HB2	1:G:446:PRO:HD2	1.88	0.55
2:E:184:ARG:HG3	2:E:185:SER:N	2.22	0.54
2:E:27:VAL:HG22	2:E:85:LEU:HD21	1.90	0.54
2:E:98:ARG:HH12	2:E:100:GLN:HE21	1.56	0.54
3:I:185:LEU:O	3:I:189:GLN:HG3	2.08	0.54
1:G:243:GLY:O	1:G:262:HIS:HB2	2.06	0.54
1:G:324:ASN:OD1	3:I:20:LYS:HE2	2.07	0.54
3:I:24:GLU:O	3:I:30:HIS:NE2	2.32	0.54
2:B:47:LYS:HB3	2:B:52:MET:HG3	1.90	0.54
3:I:123:TRP:HA	3:I:126:TYR:CE2	2.43	0.54
3:I:153:TYR:CZ	3:I:176:GLY:HA2	2.42	0.54
1:G:177:ILE:HG23	1:G:198:LEU:HD23	1.88	0.54
1:G:243:GLY:HA2	1:G:264:ALA:O	2.08	0.54
3:I:191:TYR:O	3:I:195:THR:HG23	2.08	0.54
3:I:52:GLN:O	3:I:56:MET:HG2	2.08	0.54
1:G:412:PRO:HG2	1:G:413:ASP:OD1	2.07	0.53
2:H:141:PHE:HB3	3:I:23:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:172:VAL:HA	3:F:175:LYS:CE	2.38	0.53
3:I:123:TRP:O	3:I:127:VAL:CG1	2.56	0.53
1:G:281:ARG:HH21	3:I:18:GLN:HB3	1.72	0.53
2:E:131:LEU:HD23	2:E:131:LEU:C	2.29	0.53
3:I:109:ARG:C	3:I:111:PRO:HD3	2.30	0.53
3:I:133:PRO:HA	3:I:136:LEU:CD2	2.39	0.53
3:I:166:PHE:HB3	3:I:197:ARG:HD3	1.91	0.52
3:F:185:LEU:HD12	3:F:186:ARG:N	2.24	0.52
2:E:172:PRO:HB2	2:E:174:ILE:CG1	2.36	0.52
2:E:84:ILE:HD12	2:E:84:ILE:N	2.24	0.52
1:G:177:ILE:HG13	1:G:456:SER:HA	1.91	0.52
3:C:124:MET:O	3:C:127:VAL:HG12	2.09	0.52
1:D:288:HIS:HA	1:D:295:HIS:O	2.10	0.52
1:G:454:ALA:HB2	1:G:460:LEU:HD13	1.89	0.52
3:I:128:ASN:ND2	3:I:128:ASN:H	2.07	0.52
1:A:185:LEU:HD22	1:A:441:TYR:CZ	2.45	0.52
2:E:48:TYR:HD2	2:E:52:MET:HE3	1.73	0.52
2:E:160:ASP:N	2:E:160:ASP:OD1	2.43	0.52
2:H:50:LEU:HD11	2:H:129:GLN:CB	2.35	0.52
2:B:107:ASP:N	2:B:107:ASP:OD1	2.42	0.52
2:H:85:LEU:N	2:H:85:LEU:HD12	2.25	0.52
1:D:340:PHE:HE2	1:D:378:ALA:O	1.93	0.51
1:G:355:CYS:SG	1:G:358:GLN:HB2	2.50	0.51
1:G:369:MET:HA	1:G:369:MET:HE2	1.92	0.51
1:D:292:ILE:HG22	1:D:294:ASN:H	1.74	0.51
2:E:21:GLU:HG2	2:E:47:LYS:NZ	2.24	0.51
2:H:31:LEU:HD21	2:H:151:PHE:CZ	2.44	0.51
3:F:177:LYS:CD	3:F:191:TYR:HE2	2.24	0.51
2:E:57:ASP:HB3	2:E:60:VAL:CG1	2.40	0.51
2:H:164:PRO:HB2	2:H:167:TRP:CD1	2.42	0.51
1:A:313:ARG:HD3	1:A:318:GLN:HB2	1.93	0.51
3:F:126:TYR:CZ	3:F:130:ILE:HD11	2.46	0.51
3:I:134:VAL:O	3:I:138:SER:OG	2.26	0.51
1:G:259:MET:HB3	1:G:295:HIS:CD2	2.46	0.51
2:E:159:LYS:HD3	2:E:159:LYS:H	1.76	0.50
3:I:71:PRO:HB2	3:I:107:PHE:HZ	1.76	0.50
3:I:122:ILE:O	3:I:125:GLN:HB2	2.11	0.50
2:B:163:VAL:HG23	2:B:163:VAL:O	2.11	0.50
2:E:23:PHE:HE2	2:E:75:MET:CE	2.24	0.50
1:G:223:TYR:CE1	1:G:241:GLY:HA3	2.46	0.50
2:H:74:TRP:HB3	2:H:80:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ILE:HG22	1:D:293:ALA:N	2.27	0.50
2:E:30:ILE:HG13	2:E:31:LEU:N	2.27	0.50
2:H:180:GLN:HB3	3:I:10:TRP:CE3	2.46	0.50
2:H:38:PRO:O	2:H:41:ASP:HB2	2.11	0.50
1:D:345:HIS:HB2	4:D:2040:HOH:O	2.11	0.50
3:F:11:VAL:HG13	3:F:36:ALA:HB2	1.94	0.50
3:F:168:LYS:O	3:F:171:GLU:HB2	2.11	0.50
3:I:123:TRP:CD1	3:I:126:TYR:HD2	2.30	0.50
1:A:201:ASN:HA	1:A:216:ALA:O	2.12	0.49
2:B:89:SER:HB2	2:B:96:LEU:HD11	1.94	0.49
3:C:183:PRO:HB2	3:C:185:LEU:CD1	2.42	0.49
1:G:247:ILE:O	1:G:256:LEU:N	2.44	0.49
3:I:127:VAL:HB	3:I:136:LEU:CD2	2.39	0.49
3:I:106:GLU:HG3	3:I:107:PHE:CD1	2.46	0.49
3:C:182:LYS:HA	3:C:183:PRO:C	2.32	0.49
2:E:86:VAL:HG22	2:E:98:ARG:HG3	1.93	0.49
1:A:467:ASP:OD1	1:A:467:ASP:O	2.30	0.49
3:F:171:GLU:O	3:F:175:LYS:HG3	2.13	0.49
1:G:315:ASP:OD2	1:G:317:LEU:HD12	2.13	0.49
1:G:415:ASN:ND2	1:G:431:ASP:OD1	2.45	0.49
3:I:140:LEU:HD12	3:I:152:PHE:CE1	2.47	0.49
1:A:169:GLU:OE2	1:A:464:ARG:HD2	2.12	0.49
1:A:131:ALA:HB2	2:B:154:LEU:HD22	1.93	0.49
1:D:300:LEU:HD21	1:D:336:SER:HA	1.95	0.49
2:E:82:LYS:HE2	2:E:156:TYR:CD2	2.48	0.49
2:E:184:ARG:HG3	2:E:185:SER:H	1.78	0.49
1:G:313:ARG:HE	1:G:318:GLN:HB2	1.77	0.49
1:G:313:ARG:HH21	1:G:318:GLN:HG3	1.78	0.49
1:G:229:TRP:CD2	1:G:236:LEU:HD13	2.48	0.48
3:I:159:TYR:CE1	3:I:163:ARG:CZ	2.96	0.48
1:A:370:ASP:O	1:A:371:LYS:HB2	2.13	0.48
3:C:73:GLN:NE2	3:C:77:ASP:OD1	2.45	0.48
2:H:185:SER:HB3	2:H:194:ASP:HB3	1.94	0.48
2:E:88:THR:HG21	2:E:173:ARG:HH21	1.77	0.48
2:H:44:VAL:HA	2:H:52:MET:O	2.12	0.48
3:I:44:THR:HG22	3:I:47:GLU:H	1.78	0.48
2:E:23:PHE:HD2	2:E:71:LEU:HD21	1.78	0.48
2:E:159:LYS:CD	2:E:159:LYS:H	2.27	0.48
3:F:165:LEU:N	3:F:165:LEU:HD12	2.28	0.48
1:D:389:ALA:HB1	1:D:409:HIS:CE1	2.49	0.48
3:F:97:VAL:O	3:F:101:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:ILE:HB	2:H:97:GLU:HB3	1.96	0.48
2:E:16:SER:HB3	2:E:75:MET:HB3	1.96	0.47
2:E:50:LEU:CD1	2:E:52:MET:HE1	2.40	0.47
1:G:329:GLN:HG2	1:G:331:TRP:CZ2	2.49	0.47
2:H:18:LEU:C	2:H:18:LEU:HD23	2.34	0.47
2:E:87:ILE:HD11	2:E:149:CYS:CB	2.44	0.47
1:G:248:TYR:CE2	1:G:255:LYS:HB2	2.49	0.47
3:I:44:THR:HG23	3:I:46:LYS:H	1.79	0.47
3:C:222:SER:O	3:C:223:THR:CB	2.40	0.47
3:F:172:VAL:HG12	3:F:175:LYS:HE3	1.97	0.47
1:D:438:ARG:NH2	3:F:21:GLU:O	2.47	0.47
2:E:83:LEU:C	2:E:84:ILE:HD12	2.34	0.47
3:I:119:TYR:CE2	3:I:123:TRP:HZ3	2.31	0.47
1:G:375:PHE:HB2	1:G:385:ASN:HB2	1.97	0.47
2:H:20:SER:OG	2:H:72:HIS:HA	2.15	0.47
1:A:196:VAL:HG11	3:I:216:LEU:HD11	1.97	0.47
2:B:190:MET:HG2	2:B:191:HIS:CE1	2.50	0.47
1:G:177:ILE:CD1	1:G:455:ALA:O	2.63	0.47
3:I:119:TYR:CE2	3:I:123:TRP:CZ3	3.02	0.47
3:I:68:LEU:HD11	3:I:71:PRO:HA	1.96	0.47
2:H:183:LEU:HB2	2:H:195:CYS:O	2.14	0.47
1:G:215:LEU:HD23	1:G:236:LEU:HD23	1.95	0.47
2:B:171:ASP:HB2	2:B:172:PRO:HD2	1.97	0.46
2:B:27:VAL:O	2:B:31:LEU:HG	2.15	0.46
3:C:126:TYR:CZ	3:C:130:ILE:HD11	2.50	0.46
3:I:166:PHE:CB	3:I:197:ARG:HD3	2.45	0.46
2:B:85:LEU:HD23	2:B:85:LEU:C	2.36	0.46
1:G:177:ILE:CG2	1:G:198:LEU:HD23	2.46	0.46
3:I:111:PRO:O	3:I:114:LYS:HG2	2.15	0.46
3:C:160:PHE:HD1	3:C:165:LEU:HD12	1.81	0.46
3:F:168:LYS:HA	3:F:171:GLU:CD	2.36	0.46
2:E:29:SER:O	2:E:33:GLN:HG3	2.15	0.46
3:I:104:THR:OG1	3:I:126:TYR:CD2	2.63	0.46
1:A:466:TYR:O	1:A:467:ASP:CB	2.35	0.46
3:C:49:ALA:O	3:C:53:LYS:HD3	2.15	0.46
1:G:205:TRP:CZ3	1:G:207:ALA:HA	2.51	0.46
1:D:361:LEU:HD13	1:D:398:TRP:CH2	2.50	0.46
3:F:104:THR:O	3:F:108:VAL:HG13	2.16	0.46
1:A:263:GLN:NE2	4:A:2042:HOH:O	2.49	0.45
2:B:146:GLU:HG3	3:C:186:ARG:HH12	1.81	0.45
1:G:410:GLY:HA2	1:G:438:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:C	2:H:84:ILE:HD13	2.36	0.45
3:I:68:LEU:HD13	3:I:70:ASP:C	2.37	0.45
1:G:127:THR:HG23	2:H:156:TYR:HB3	1.98	0.45
2:E:30:ILE:HD11	2:E:151:PHE:CE1	2.52	0.45
3:F:185:LEU:HD12	3:F:186:ARG:H	1.81	0.45
1:D:243:GLY:O	1:D:262:HIS:HB2	2.17	0.45
1:D:420:SER:OG	1:D:427:THR:HB	2.16	0.45
2:H:87:ILE:HD12	2:H:97:GLU:HB3	1.98	0.45
3:I:101:GLU:OE1	3:I:102:ARG:HG3	2.16	0.45
3:I:106:GLU:HG3	3:I:107:PHE:CE1	2.52	0.45
1:A:180:ASP:HB3	1:A:183:LEU:HG	1.98	0.45
3:C:109:ARG:O	3:C:111:PRO:HD3	2.17	0.45
1:D:369:MET:HA	1:D:369:MET:CE	2.46	0.45
1:G:174:ALA:CB	1:G:177:ILE:HD13	2.47	0.45
3:I:97:VAL:CG1	3:I:98:THR:N	2.80	0.45
3:C:183:PRO:HB2	3:C:185:LEU:HD11	1.99	0.45
2:H:38:PRO:HB2	2:H:40:GLU:HG2	1.99	0.45
1:D:411:PHE:HA	1:D:412:PRO:HA	1.62	0.45
1:G:357:TRP:CZ3	1:G:399:SER:O	2.68	0.45
3:I:56:MET:HA	3:I:59:GLU:CG	2.47	0.45
3:F:120:LEU:HD13	3:F:151:ILE:HG21	1.98	0.44
3:F:148:GLU:OE2	3:F:180:LYS:CG	2.65	0.44
1:G:340:PHE:CE1	1:G:381:GLY:HA3	2.52	0.44
1:G:351:ALA:HB1	1:G:396:LEU:HG	1.99	0.44
2:H:170:SER:OG	2:H:171:ASP:N	2.50	0.44
2:H:192:LYS:C	2:H:193:ILE:HD12	2.37	0.44
2:B:84:ILE:HB	2:B:154:LEU:HB2	1.99	0.44
1:D:184:ASN:O	1:D:226:SER:HA	2.17	0.44
2:E:134:GLN:O	2:E:137:ALA:HB3	2.17	0.44
1:G:256:LEU:O	1:G:257:ARG:HB3	2.18	0.44
3:I:123:TRP:CD1	3:I:126:TYR:CD2	3.05	0.44
1:G:201:ASN:OD1	1:G:217:GLU:HG2	2.17	0.44
1:A:184:ASN:C	1:A:185:LEU:HD13	2.38	0.44
1:D:305:SER:HB2	4:D:2037:HOH:O	2.17	0.44
2:H:156:TYR:CD1	2:H:156:TYR:N	2.86	0.44
1:D:181:TYR:CZ	1:D:350:LYS:HB2	2.52	0.44
1:D:348:ALA:HB3	3:F:21:GLU:HG3	1.99	0.44
1:G:195:ALA:HB2	1:G:229:TRP:CZ2	2.52	0.44
2:H:120:ASP:O	2:H:123:ARG:HG3	2.18	0.44
3:I:62:ILE:HD11	3:I:75:TRP:CZ2	2.53	0.44
3:F:167:GLN:O	3:F:171:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:SER:O	2:H:33:GLN:HG3	2.17	0.44
3:F:117:VAL:HG23	3:F:120:LEU:HD11	2.00	0.44
1:G:398:TRP:CD2	1:G:405:ILE:HD12	2.52	0.44
1:G:421:TYR:CD2	1:G:426:LEU:HD11	2.49	0.44
2:H:82:LYS:HD2	2:H:156:TYR:CD2	2.52	0.44
3:I:34:ALA:O	3:I:38:SER:OG	2.34	0.44
3:C:168:LYS:HB3	3:C:168:LYS:HE3	1.74	0.44
1:D:287:HIS:O	1:D:296:GLN:HA	2.18	0.44
1:D:464:ARG:NH2	4:D:2060:HOH:O	2.49	0.44
2:E:159:LYS:N	2:E:159:LYS:HD3	2.32	0.44
2:E:86:VAL:HG13	2:E:95:ASP:HB3	2.00	0.44
1:G:126:ASN:HD22	1:G:126:ASN:N	2.16	0.43
1:G:387:VAL:CG1	1:G:426:LEU:HB2	2.47	0.43
2:E:180:GLN:HB3	3:F:10:TRP:CZ3	2.53	0.43
3:F:172:VAL:HA	3:F:175:LYS:HE3	2.00	0.43
2:E:180:GLN:HB3	3:F:10:TRP:CH2	2.53	0.43
2:E:87:ILE:HD11	2:E:149:CYS:HB2	2.01	0.43
3:C:153:TYR:OH	3:C:179:MET:HG3	2.18	0.43
1:D:228:LYS:HG3	1:D:269:LEU:O	2.18	0.43
1:A:131:ALA:HB2	2:B:154:LEU:CD2	2.48	0.43
1:A:185:LEU:HG	1:A:197:ALA:HB3	2.01	0.43
1:A:296:GLN:NE2	4:A:2039:HOH:O	2.42	0.43
1:G:451:LEU:O	1:G:463:TRP:HD1	2.01	0.43
3:I:104:THR:HG22	3:I:105:ARG:N	2.33	0.43
1:D:415:ASN:HB2	1:D:432:ILE:O	2.19	0.43
1:D:189:SER:HB3	1:D:229:TRP:CD2	2.54	0.43
2:E:84:ILE:HG12	2:E:98:ARG:NH2	2.33	0.43
3:I:55:ARG:O	3:I:59:GLU:HG2	2.18	0.43
1:D:340:PHE:CE2	1:D:378:ALA:O	2.71	0.43
3:F:111:PRO:HA	3:F:114:LYS:HD3	2.01	0.43
2:E:137:ALA:HB3	3:F:13:MET:CE	2.49	0.43
3:I:64:THR:HG22	3:I:67:SER:HB2	2.01	0.43
1:A:195:ALA:HB2	1:A:229:TRP:CZ2	2.54	0.43
3:C:176:GLY:HA2	3:C:179:MET:HB2	2.00	0.43
1:G:177:ILE:H	1:G:177:ILE:HG12	1.66	0.43
1:G:190:ASN:HA	1:G:446:PRO:HB3	2.01	0.43
1:G:186:LEU:HD11	1:G:460:LEU:HD11	2.01	0.43
2:H:88:THR:HG23	2:H:95:ASP:N	2.34	0.43
1:G:387:VAL:HG11	1:G:426:LEU:HB2	2.00	0.42
2:E:28:ASN:HD21	2:E:64:ILE:CD1	2.32	0.42
2:H:7:ARG:HB2	2:H:115:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:HB2	1:D:456:SER:CB	2.50	0.42
1:A:340:PHE:CE1	1:D:211:SER:HB2	2.55	0.42
1:G:443:ALA:O	1:G:451:LEU:HD12	2.19	0.42
3:I:114:LYS:NZ	3:I:143:HIS:O	2.48	0.42
3:I:97:VAL:CG1	3:I:98:THR:H	2.32	0.42
2:B:79:LYS:HB3	2:B:161:SER:OG	2.19	0.42
2:E:28:ASN:HD21	2:E:64:ILE:HD12	1.84	0.42
2:H:8:THR:O	2:H:8:THR:OG1	2.35	0.42
3:I:96:LEU:HD23	3:I:129:TYR:OH	2.19	0.42
3:I:155:GLU:OE1	3:I:155:GLU:HA	2.18	0.42
2:E:57:ASP:OD2	2:E:60:VAL:HG12	2.19	0.42
1:G:339:LYS:HG2	1:G:340:PHE:CD2	2.54	0.42
3:C:117:VAL:O	3:C:121:ARG:HG3	2.19	0.42
3:C:123:TRP:CD2	3:C:140:LEU:HD21	2.54	0.42
2:E:52:MET:HE3	2:E:132:ILE:CD1	2.49	0.42
3:I:90:GLU:CB	3:I:129:TYR:HE2	2.33	0.42
2:B:128:ILE:O	2:B:132:ILE:HG12	2.19	0.42
2:E:188:THR:N	2:E:191:HIS:O	2.53	0.42
3:F:215:PRO:O	3:F:216:LEU:HB2	2.19	0.42
1:G:205:TRP:CH2	1:G:207:ALA:HA	2.55	0.42
1:G:452:SER:HA	1:G:461:LYS:O	2.19	0.42
2:H:139:VAL:HA	2:H:142:LEU:HD12	2.01	0.42
2:H:162:GLU:O	2:H:164:PRO:HD3	2.19	0.42
1:G:453:THR:O	1:G:460:LEU:HD12	2.20	0.42
3:I:136:LEU:HD12	3:I:136:LEU:C	2.40	0.42
2:E:135:ILE:HA	2:E:138:THR:HG23	2.02	0.42
2:E:183:LEU:HB2	2:E:195:CYS:O	2.19	0.42
2:E:23:PHE:CD2	2:E:71:LEU:HD21	2.55	0.42
3:F:27:LYS:HE2	3:F:27:LYS:HB3	1.74	0.42
1:G:398:TRP:CE2	1:G:405:ILE:HD12	2.55	0.42
3:I:56:MET:O	3:I:59:GLU:HG3	2.19	0.42
1:G:181:TYR:HA	1:G:440:LEU:HD22	2.02	0.42
1:G:373:ILE:O	1:G:386:THR:HA	2.19	0.42
2:E:71:LEU:HD23	2:E:71:LEU:C	2.41	0.41
2:E:84:ILE:HG22	2:E:86:VAL:HG23	2.00	0.41
1:G:185:LEU:HD22	1:G:197:ALA:HB3	2.02	0.41
3:I:197:ARG:O	3:I:197:ARG:HG3	2.18	0.41
1:A:200:ARG:HD3	1:A:220:GLU:HA	2.01	0.41
1:D:406:MET:HG2	1:D:418:ILE:HG12	2.02	0.41
1:G:199:GLU:HB3	1:G:200:ARG:H	1.48	0.41
3:I:106:GLU:HA	3:I:106:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:N	1:A:185:LEU:HD13	2.36	0.41
1:D:313:ARG:HG3	1:D:354:TRP:CG	2.54	0.41
2:E:30:ILE:HG12	2:E:85:LEU:HD23	2.02	0.41
1:G:167:THR:HG23	1:G:168:PRO:CD	2.47	0.41
2:H:61:LYS:O	2:H:65:ARG:HD2	2.20	0.41
2:H:84:ILE:C	2:H:85:LEU:HD12	2.40	0.41
2:H:134:GLN:HB2	3:I:13:MET:HG2	2.02	0.41
1:D:375:PHE:CZ	1:D:426:LEU:HD21	2.55	0.41
1:D:387:VAL:HG11	1:D:426:LEU:HB2	2.03	0.41
3:I:122:ILE:HG22	3:I:126:TYR:CZ	2.52	0.41
2:E:95:ASP:HB2	2:E:175:LEU:HD21	2.02	0.41
2:H:61:LYS:O	2:H:65:ARG:HB2	2.20	0.41
3:I:136:LEU:O	3:I:140:LEU:HB2	2.20	0.41
3:I:189:GLN:O	3:I:193:GLN:HG3	2.19	0.41
3:C:123:TRP:CE2	3:C:140:LEU:HD21	2.56	0.41
1:D:220:GLU:HG3	1:D:220:GLU:H	1.60	0.41
2:E:21:GLU:HG2	2:E:47:LYS:HZ1	1.85	0.41
1:G:406:MET:HG2	1:G:418:ILE:HG12	2.03	0.41
2:H:156:TYR:HD1	2:H:156:TYR:N	2.18	0.41
3:I:107:PHE:HE1	3:I:109:ARG:NH1	2.19	0.41
3:I:192:GLN:O	3:I:195:THR:OG1	2.36	0.41
3:F:172:VAL:HA	3:F:175:LYS:HE2	2.02	0.41
1:A:133:LYS:HG3	1:A:134:LEU:HD23	2.02	0.41
1:A:290:VAL:HG12	1:A:290:VAL:O	2.20	0.41
1:G:205:TRP:HD1	1:G:212:VAL:HG22	1.86	0.41
2:H:37:TYR:HB3	2:H:38:PRO:HD2	2.02	0.41
3:I:143:HIS:HB3	3:I:145:ILE:HG13	2.02	0.41
2:B:180:GLN:HB2	3:C:10:TRP:CE3	2.55	0.41
2:E:137:ALA:HB3	3:F:13:MET:HE3	2.03	0.41
2:E:21:GLU:CG	2:E:47:LYS:HZ1	2.33	0.41
1:G:249:ASP:HB2	1:G:256:LEU:HD21	2.03	0.41
3:I:59:GLU:O	3:I:62:ILE:HG22	2.21	0.41
1:D:361:LEU:HD11	1:D:421:TYR:CZ	2.56	0.41
2:E:87:ILE:HD11	2:E:149:CYS:HB3	2.03	0.41
2:E:47:LYS:NZ	2:E:48:TYR:CZ	2.86	0.41
1:A:397:ILE:HD12	1:A:451:LEU:HD11	2.04	0.40
2:B:92:SER:OG	2:B:94:GLU:HG2	2.21	0.40
3:C:150:SER:O	3:C:154:GLU:HG3	2.21	0.40
2:E:85:LEU:HG	2:E:151:PHE:CE1	2.56	0.40
2:E:134:GLN:NE2	3:F:14:ASP:OD1	2.51	0.40
1:G:265:ARG:NH2	1:G:281:ARG:NH1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:PHE:CD1	2:H:186:PHE:C	2.94	0.40
2:H:53:LEU:N	2:H:53:LEU:HD22	2.36	0.40
3:I:214:ASN:HA	3:I:215:PRO:HD2	1.90	0.40
2:E:87:ILE:CG2	2:E:97:GLU:CB	2.93	0.40
2:H:120:ASP:OD1	2:H:123:ARG:NE	2.49	0.40
1:A:272:ASN:HB2	1:A:312:TRP:CG	2.57	0.40
4:A:2068:HOH:O	3:C:20:LYS:NZ	2.53	0.40
1:G:332:ASP:OD1	1:G:339:LYS:HD2	2.21	0.40
3:I:134:VAL:HG12	3:I:135:GLU:N	2.36	0.40
2:E:59:GLU:N	2:E:59:GLU:OE1	2.55	0.40
1:G:357:TRP:CH2	1:G:403:LYS:HA	2.56	0.40
3:I:119:TYR:CD2	3:I:123:TRP:HZ3	2.39	0.40
2:H:144:GLN:O	2:H:144:GLN:HG3	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	322/401 (80%)	318 (99%)	4 (1%)	0	100	100
1	D	310/401 (77%)	303 (98%)	7 (2%)	0	100	100
1	G	313/401 (78%)	306 (98%)	7 (2%)	0	100	100
2	B	176/203 (87%)	176 (100%)	0	0	100	100
2	E	171/203 (84%)	169 (99%)	2 (1%)	0	100	100
2	H	179/203 (88%)	178 (99%)	1 (1%)	0	100	100
3	C	213/223 (96%)	213 (100%)	0	0	100	100
3	F	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
3	I	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
All	All	2063/2481 (83%)	2039 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	269/340 (79%)	260 (97%)	9 (3%)	43	59
1	D	259/340 (76%)	248 (96%)	11 (4%)	34	47
1	G	255/340 (75%)	244 (96%)	11 (4%)	33	45
2	B	166/187 (89%)	157 (95%)	9 (5%)	26	35
2	E	145/187 (78%)	134 (92%)	11 (8%)	15	19
2	H	160/187 (86%)	147 (92%)	13 (8%)	14	17
3	C	196/203 (97%)	184 (94%)	12 (6%)	22	29
3	F	163/203 (80%)	154 (94%)	9 (6%)	25	34
3	I	162/203 (80%)	134 (83%)	28 (17%)	2	2
All	All	1775/2190 (81%)	1662 (94%)	113 (6%)	20	27

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	126	ASN
1	A	143	VAL
1	A	185	LEU
1	A	186	LEU
1	A	244	LEU
1	A	263	GLN
1	A	464	ARG
1	A	467	ASP
2	B	40	GLU
2	B	46	ARG
2	B	65	ARG
2	B	69	SER
2	B	72	HIS
2	B	86	VAL

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Mol	Chain	Res	Type
2	B	107	ASP
2	B	153	VAL
2	B	171	ASP
3	C	19	SER
3	C	67	SER
3	C	68	LEU
3	C	78	TYR
3	C	92	LYS
3	C	94	SER
3	C	135	GLU
3	C	156	TYR
3	C	184	PHE
3	C	185	LEU
3	C	191	TYR
3	C	223	THR
1	D	186	LEU
1	D	220	GLU
1	D	244	LEU
1	D	281	ARG
1	D	359	SER
1	D	361	LEU
1	D	371	LYS
1	D	397	ILE
1	D	416	LEU
1	D	431	ASP
1	D	464	ARG
2	E	29	SER
2	E	30	ILE
2	E	72	HIS
2	E	79	LYS
2	E	82	LYS
2	E	85	LEU
2	E	95	ASP
2	E	144	GLN
2	E	160	ASP
2	E	181	VAL
2	E	194	ASP
3	F	13	MET
3	F	19	SER
3	F	99	LEU
3	F	148	GLU
3	F	156	TYR

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Mol	Chain	Res	Type
3	F	185	LEU
3	F	191	TYR
3	F	220	PHE
3	F	221	GLU
1	G	126	ASN
1	G	170	ARG
1	G	177	ILE
1	G	181	TYR
1	G	186	LEU
1	G	199	GLU
1	G	204	VAL
1	G	304	SER
1	G	313	ARG
1	G	329	GLN
1	G	371	LYS
2	H	6	ILE
2	H	8	THR
2	H	44	VAL
2	H	50	LEU
2	H	65	ARG
2	H	72	HIS
2	H	94	GLU
2	H	118	LYS
2	H	123	ARG
2	H	147	GLU
2	H	150	THR
2	H	153	VAL
2	H	169	ASP
3	I	11	VAL
3	I	38	SER
3	I	42	ASN
3	I	44	THR
3	I	60	ARG
3	I	74	VAL
3	I	78	TYR
3	I	82	THR
3	I	101	GLU
3	I	104	THR
3	I	109	ARG
3	I	117	VAL
3	I	119	TYR
3	I	123	TRP

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Mol	Chain	Res	Type
3	I	128	ASN
3	I	131	ASP
3	I	132	GLU
3	I	138	SER
3	I	142	HIS
3	I	143	HIS
3	I	155	GLU
3	I	159	TYR
3	I	160	PHE
3	I	166	PHE
3	I	175	LYS
3	I	186	ARG
3	I	197	ARG
3	I	198	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	429	GLN
2	E	70	GLN
2	H	70	GLN
2	H	117	ASN
3	I	128	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/401 (81%)	0.38	2 (0%) 89 92	17, 33, 64, 116	0
1	D	314/401 (78%)	0.51	11 (3%) 44 51	19, 42, 84, 116	0
1	G	317/401 (79%)	1.06	48 (15%) 3 4	43, 72, 103, 124	0
2	B	180/203 (88%)	0.33	1 (0%) 89 92	25, 44, 69, 109	0
2	E	175/203 (86%)	1.53	51 (29%) 1 1	40, 85, 127, 150	0
2	H	185/203 (91%)	1.36	47 (25%) 1 1	47, 70, 117, 139	0
3	C	215/223 (96%)	0.41	4 (1%) 67 73	19, 46, 81, 118	0
3	F	196/223 (87%)	0.62	15 (7%) 14 19	21, 53, 115, 149	0
3	I	193/223 (86%)	1.92	76 (39%) 0 0	40, 97, 133, 147	0
All	All	2101/2481 (84%)	0.85	255 (12%) 5 7	17, 56, 111, 150	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	151	PHE	9.2
2	E	153	VAL	8.3
3	I	117	VAL	7.9
3	I	141	ALA	7.9
3	I	158	ASN	7.8
2	E	155	VAL	7.4
3	I	115	ASP	7.0
3	I	134	VAL	6.9
3	I	103	CYS	6.9
3	I	107	PHE	6.9
3	F	165	LEU	6.7
2	H	87	ILE	6.5
3	I	69	ASP	6.4
3	I	133	PRO	6.3
1	D	131	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	134	LEU	5.6
3	I	100	LEU	5.5
1	D	133	LYS	5.5
3	I	198	TRP	5.4
2	H	85	LEU	5.3
3	I	108	VAL	5.2
2	E	93	GLY	5.2
3	I	123	TRP	5.2
1	G	334	ARG	5.2
1	G	375	PHE	5.1
2	E	147	GLU	5.0
2	E	96	LEU	5.0
2	E	80	ILE	4.9
2	H	97	GLU	4.9
2	E	68	VAL	4.8
3	I	70	ASP	4.7
3	I	120	LEU	4.7
2	H	30	ILE	4.6
2	E	82	LYS	4.6
3	F	10	TRP	4.5
2	E	53	LEU	4.5
1	G	376	TRP	4.4
3	I	156	TYR	4.4
3	F	194	PHE	4.4
2	E	172	PRO	4.4
3	I	10	TRP	4.3
2	H	63	TYR	4.3
3	I	166	PHE	4.3
3	I	157	ALA	4.3
2	E	83	LEU	4.1
2	E	72	HIS	4.1
3	I	111	PRO	4.1
3	I	142	HIS	4.1
1	D	130	LEU	4.0
2	E	160	ASP	4.0
2	E	42	PHE	4.0
2	H	137	ALA	4.0
3	I	127	VAL	4.0
2	E	17	LYS	4.0
3	I	126	TYR	3.9
1	G	397	ILE	3.9
1	G	191	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
3	I	76	ILE	3.9
3	F	163	ARG	3.9
1	D	136	ALA	3.8
3	I	58	HIS	3.8
2	H	146	GLU	3.8
1	G	261	GLY	3.8
2	E	77	ALA	3.7
3	I	150	SER	3.7
3	I	97	VAL	3.7
2	E	101	PHE	3.6
2	H	197	VAL	3.6
3	I	112	LEU	3.6
3	I	185	LEU	3.6
3	I	15	VAL	3.6
1	G	423	SER	3.6
3	I	99	LEU	3.6
3	F	183	PRO	3.6
2	E	56	VAL	3.5
3	F	195	THR	3.5
3	I	178	ARG	3.5
2	H	6	ILE	3.5
3	F	120	LEU	3.5
1	G	201	ASN	3.4
3	I	154	GLU	3.4
3	I	105	ARG	3.4
2	B	107	ASP	3.4
2	H	175	LEU	3.4
3	C	184	PHE	3.4
1	D	137	PRO	3.4
3	I	140	LEU	3.4
3	I	104	THR	3.4
2	H	83	LEU	3.4
2	E	146	GLU	3.3
3	I	72	LEU	3.3
3	I	155	GLU	3.3
1	G	357	TRP	3.3
3	I	75	TRP	3.3
2	H	150	THR	3.3
1	G	401	HIS	3.3
2	E	18	LEU	3.3
1	G	289	ASP	3.3
1	G	136	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	I	147	GLN	3.2
2	E	150	THR	3.1
2	H	174	ILE	3.1
3	I	16	ILE	3.1
3	I	162	SER	3.1
3	I	106	GLU	3.1
1	G	356	PRO	3.1
1	G	244	LEU	3.1
2	E	43	LYS	3.1
3	I	153	TYR	3.1
3	I	68	LEU	3.1
2	H	143	PRO	3.1
3	I	160	PHE	3.1
2	H	149	CYS	3.0
2	E	87	ILE	3.0
2	H	80	ILE	3.0
3	I	62	ILE	3.0
2	H	10	PHE	3.0
2	E	156	TYR	3.0
3	C	200	GLU	3.0
2	E	175	LEU	3.0
2	H	55	SER	2.9
3	I	64	THR	2.9
2	H	62	THR	2.8
1	G	323	GLY	2.8
2	H	99	TRP	2.8
3	I	170	ASP	2.8
2	H	168	VAL	2.8
3	F	191	TYR	2.8
1	G	327	VAL	2.8
3	I	61	LYS	2.8
2	H	181	VAL	2.7
3	I	165	LEU	2.7
2	E	84	ILE	2.7
2	H	133	ALA	2.7
2	E	44	VAL	2.7
3	F	184	PHE	2.7
1	G	205	TRP	2.7
3	I	66	GLU	2.7
2	H	170	SER	2.7
3	I	28	ALA	2.7
3	C	209	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	361	LEU	2.7
1	G	311	ALA	2.7
2	H	86	VAL	2.7
2	H	155	VAL	2.7
3	I	149	SER	2.6
1	G	216	ALA	2.6
1	G	235	PHE	2.6
3	I	91	THR	2.6
1	D	466	TYR	2.6
1	G	364	THR	2.6
3	I	65	SER	2.6
2	E	105	MET	2.6
2	H	178	ALA	2.6
1	G	203	TYR	2.6
2	H	77	ALA	2.6
2	E	184	ARG	2.5
2	E	76	PHE	2.5
3	I	164	GLY	2.5
1	G	254	THR	2.5
3	I	144	HIS	2.5
1	G	328	VAL	2.5
2	E	99	TRP	2.5
3	I	67	SER	2.5
1	D	268	CYS	2.5
3	I	176	GLY	2.5
1	G	270	SER	2.5
1	G	436	ASP	2.5
1	G	312	TRP	2.5
3	I	113	TYR	2.4
3	I	138	SER	2.4
1	D	132	PHE	2.4
1	G	168	PRO	2.4
1	G	234	SER	2.4
1	G	204	VAL	2.4
2	E	19	VAL	2.4
2	H	60	VAL	2.4
2	E	40	GLU	2.4
1	G	330	ILE	2.4
3	I	130	ILE	2.4
1	G	426	LEU	2.4
3	I	193	GLN	2.4
2	H	183	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	11	VAL	2.4
2	H	153	VAL	2.4
3	F	169	ALA	2.3
3	C	189	GLN	2.3
1	G	340	PHE	2.3
1	G	360	ASN	2.3
3	F	172	VAL	2.3
2	E	157	ALA	2.3
3	I	124	MET	2.3
1	G	278	SER	2.3
2	H	180	GLN	2.3
3	I	73	GLN	2.3
3	I	71	PRO	2.3
2	H	199	TYR	2.3
2	H	79	LYS	2.3
1	G	238	VAL	2.3
2	E	67	ILE	2.3
2	E	174	ILE	2.3
2	H	11	SER	2.3
2	H	12	ALA	2.3
1	A	144	ASP	2.3
2	E	154	LEU	2.2
3	F	173	TYR	2.2
1	G	402	SER	2.2
1	G	333	ALA	2.2
2	E	71	LEU	2.2
1	G	223	TYR	2.2
1	G	355	CYS	2.2
2	E	176	ARG	2.2
2	E	165	THR	2.2
1	G	188	TRP	2.2
3	I	167	GLN	2.2
3	I	119	TYR	2.2
1	G	212	VAL	2.2
2	E	161	SER	2.2
2	H	104	GLU	2.2
1	D	341	THR	2.2
1	G	166	THR	2.2
1	A	125	LEU	2.2
2	E	39	ALA	2.2
2	H	165	THR	2.2
1	G	236	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	136	LEU	2.2
1	D	387	VAL	2.1
3	F	180	LYS	2.1
3	I	14	ASP	2.1
2	E	89	SER	2.1
3	F	158	ASN	2.1
2	E	32	PHE	2.1
2	E	171	ASP	2.1
2	H	23	PHE	2.1
2	H	176	ARG	2.1
3	I	192	GLN	2.1
1	G	218	THR	2.1
2	E	167	TRP	2.1
2	H	65	ARG	2.1
2	H	119	GLU	2.1
2	H	169	ASP	2.1
2	E	190	MET	2.1
2	H	132	ILE	2.0
2	E	138	THR	2.0
3	F	181	ALA	2.0
2	H	74	TRP	2.0
2	E	90	LYS	2.0
3	I	195	THR	2.0
1	G	275	VAL	2.0
2	H	27	VAL	2.0
3	I	129	TYR	2.0
1	G	432	ILE	2.0
2	E	148	GLN	2.0
2	E	57	ASP	2.0
3	I	163	ARG	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.