



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 4AEZ / pdb_00004aez
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

<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:

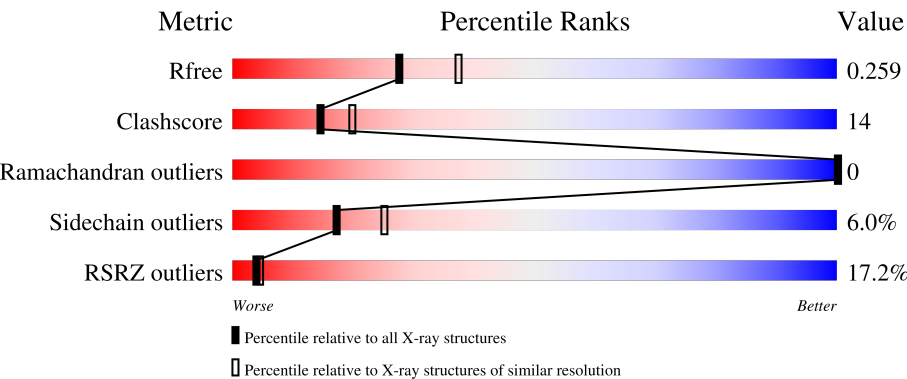
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	2% 70% 11% • 19%
1	D	401	5% 61% 16% • 22%
1	G	401	19% 54% 23% • 21%
2	B	203	2% 70% 17% • 11%
2	E	203	37% 52% 29% 5% 14%

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Mol	Chain	Length	Quality of chain
2	H	203	23%61%28%•9%
3	C	223	5%78%17%••
3	F	223	12%67%18%•12%
3	I	223	41%43%35%8%13%

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			

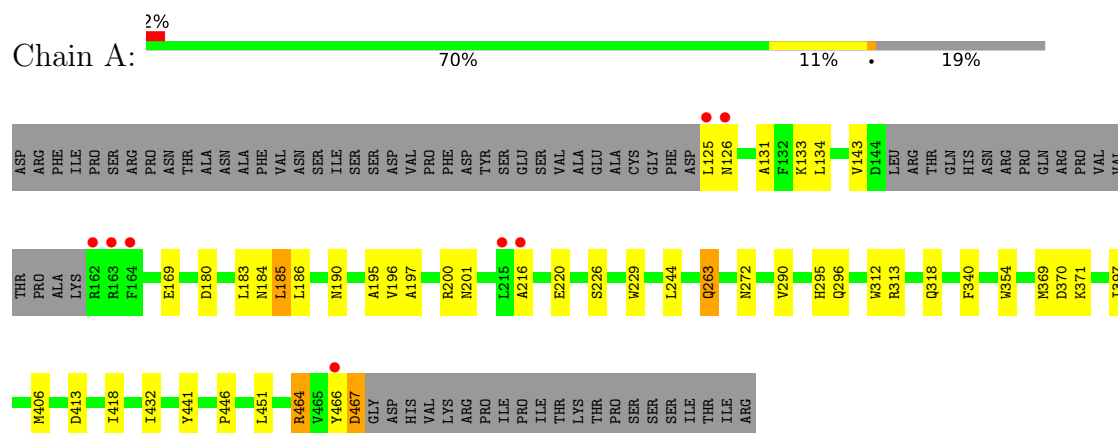
- Molecule 4 is water.

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		

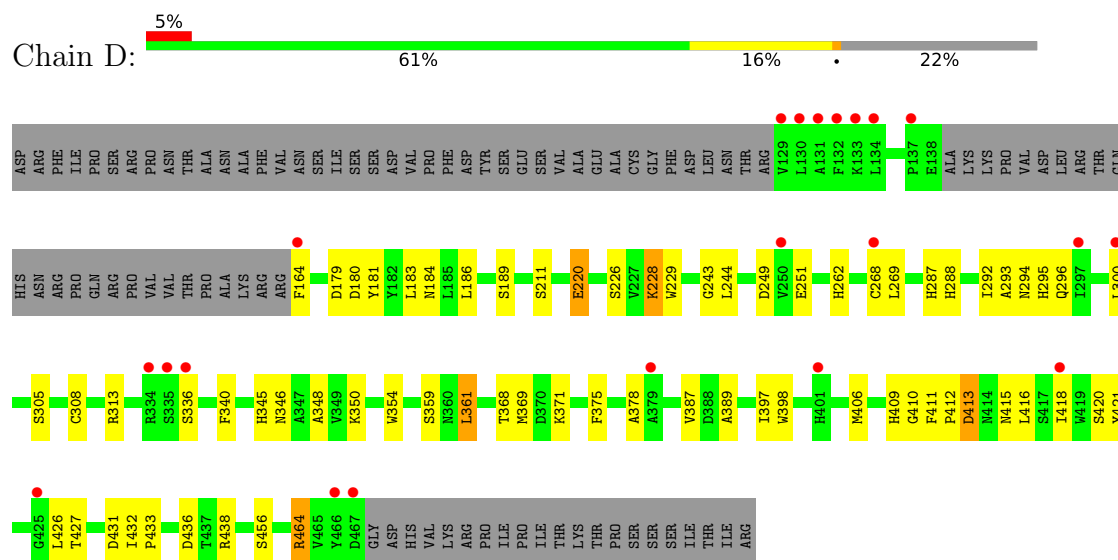
3 Residue-property plots

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.

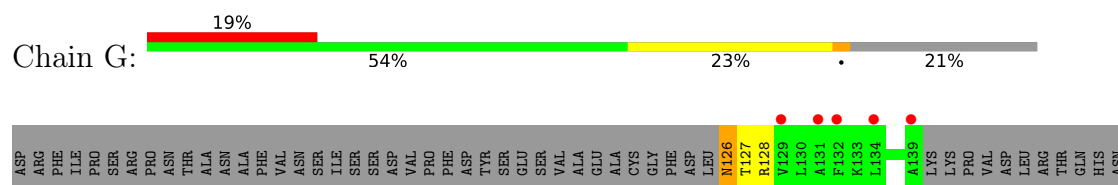
• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1

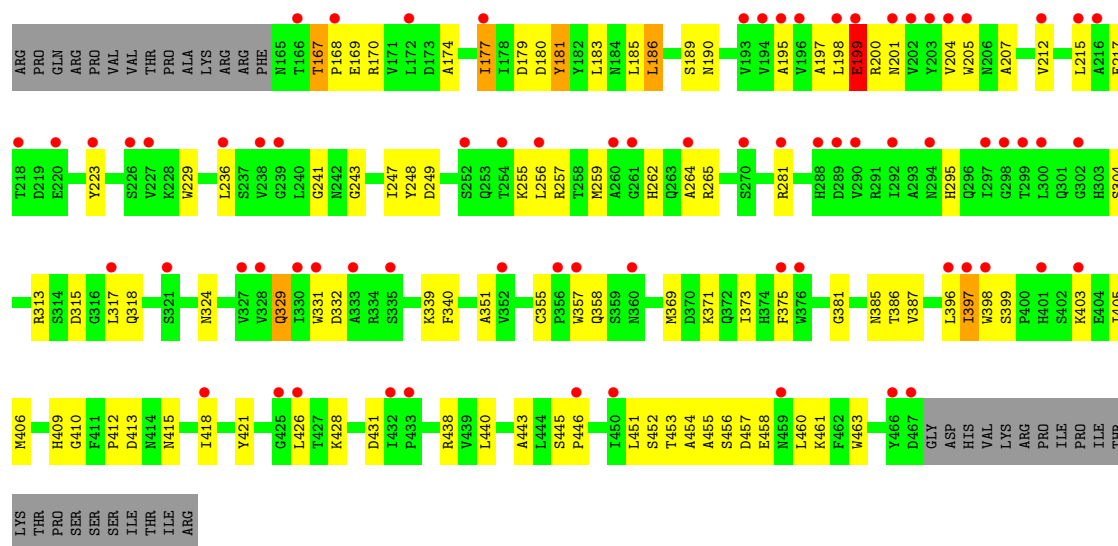


• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1

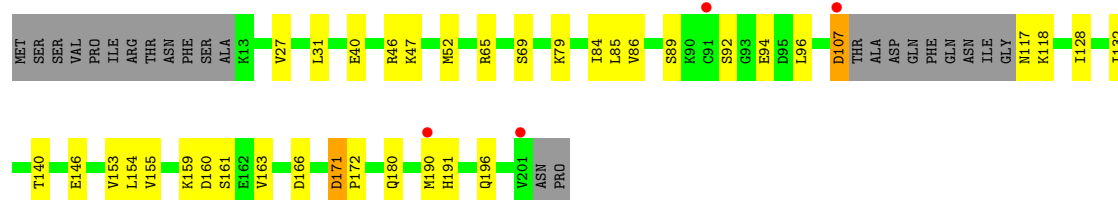


• Molecule 1: WD REPEAT-CONTAINING PROTEIN SLP1

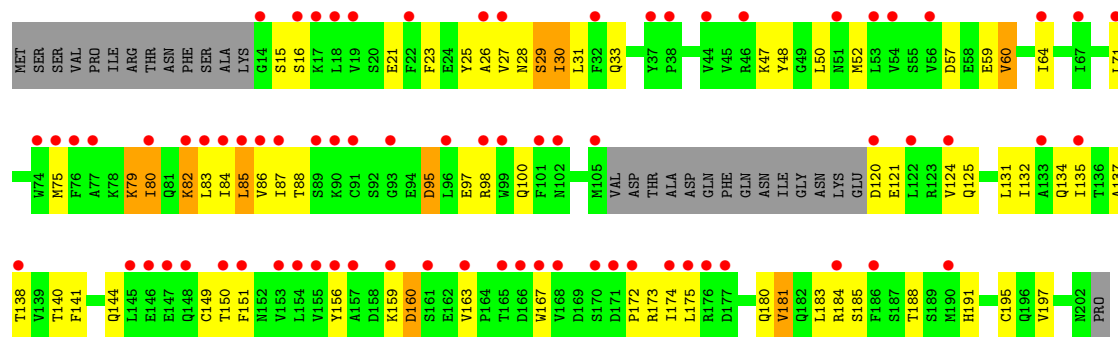




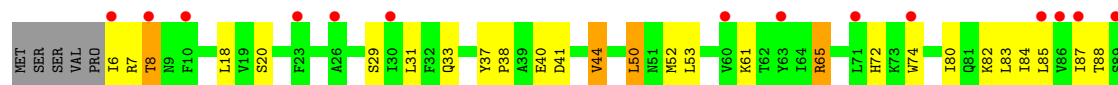
● Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2



● Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2



● Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2





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 0.213 , 0.259	Depositor DCC
R_{free} test set	1973 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	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

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	0.46	0/2559	0.84	2/3492 (0.1%)
1	D	0.43	0/2465	0.85	1/3366 (0.0%)
1	G	0.36	0/2458	0.80	2/3361 (0.1%)
2	B	0.44	0/1494	0.76	0/2016
2	E	0.33	0/1394	0.75	2/1895 (0.1%)
2	H	0.35	0/1502	0.75	0/2032
3	C	0.41	0/1847	0.77	2/2495 (0.1%)
3	F	0.43	0/1625	0.76	0/2198
3	I	0.32	0/1614	0.80	6/2187 (0.3%)
All	All	0.40	0/16958	0.80	15/23042 (0.1%)

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.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	413	ASP	N-CA-C	7.17	119.09	111.28
3	I	127	VAL	N-CA-C	6.49	117.24	110.62
3	I	112	LEU	N-CA-C	-5.89	105.86	113.16
1	A	413	ASP	N-CA-C	5.84	119.59	112.23
3	I	16	ILE	N-CA-C	5.66	115.86	110.42
1	G	409	HIS	N-CA-C	5.63	117.96	109.23
1	A	295	HIS	N-CA-C	5.63	117.42	111.28
2	E	163	VAL	N-CA-C	5.61	114.12	107.73
3	I	70	ASP	CA-C-N	5.49	125.20	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	70	ASP	C-N-CA	5.49	125.20	119.82
3	C	110	ASN	CA-C-N	5.23	124.86	119.05
3	C	110	ASN	C-N-CA	5.23	124.86	119.05
2	E	80	ILE	N-CA-C	5.10	116.04	108.23
1	G	199	GLU	CB-CA-C	-5.08	110.32	117.23
3	I	108	VAL	N-CA-C	-5.06	107.92	113.43

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

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	35	0
1	D	2406	0	2290	47	0
1	G	2400	0	2269	80	0
2	B	1469	0	1476	27	0
2	E	1369	0	1312	90	0
2	H	1477	0	1462	48	0
3	C	1799	0	1718	28	0
3	F	1585	0	1472	42	0
3	I	1574	0	1434	90	0
4	A	114	0	0	2	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	454	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 (454) 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:H	3:I:198:TRP:HD1	1.26	0.82
2:H:50:LEU:HD11	2:H:129:GLN:HB3	1.61	0.81
2:E:48:TYR:HD2	2:E:52:MET:HE3	1.45	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
2:E:52:MET:HE1	2:E:132:ILE:HD13	1.62	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
1:D:369:MET:HE2	1:D:369:MET:HA	1.65	0.77
3:I:198:TRP:H	3:I:198:TRP:CD1	2.01	0.77
2:E:50:LEU:HB2	2:E:52:MET:HE2	1.69	0.74
1:A:467:ASP:C	1:A:467:ASP:OD1	2.30	0.74
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
3:I:198:TRP:CD1	3:I:198:TRP:N	2.58	0.70
2:E:75:MET:HE2	2:E:80:ILE:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:368:THR:HG22	1:D:369:MET:HE3	1.76	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:G:369:MET:HE2	1:G:369:MET:HA	1.77	0.66
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:E:82:LYS:HZ3	2:E:82:LYS:HB2	1.60	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
2:H:147:GLU:CD	2:H:147:GLU:H	2.05	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
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:A:369:MET:HE3	2:B:140:THR:HG22	1.81	0.61
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
1:D:268:CYS:SG	1:D:308:CYS:C	2.83	0.61
2:E:138:THR:HG22	3:F:13:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:21:GLU:HG2	2:E:47:LYS:HZ1	1.66	0.61
3:F:182:LYS:HA	3:F:183:PRO:C	2.25	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
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: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
2:E:131:LEU:C	2:E:131:LEU:HD23	2.29	0.57
3:I:109:ARG:C	3:I:111:PRO:HD3	2.30	0.57
1:G:128:ARG:N	2:H:157:ALA:O	2.37	0.57
3:C:124:MET:HA	3:C:124:MET:HE2	1.87	0.57
1:G:357:TRP:HZ3	1:G:399:SER:O	1.87	0.57
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
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
2:E:21:GLU:CG	2:E:47:LYS:HZ1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:445:SER:HB2	1:G:446:PRO:HD2	1.88	0.55
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
2:E:184:ARG:HG3	2:E:185:SER:N	2.22	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:C:182:LYS:HA	3:C:183:PRO:C	2.32	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
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:83:LEU:C	2:E:84:ILE:HD12	2.34	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:84:ILE:HD12	2:E:84:ILE:N	2.24	0.52
2:E:172:PRO:HB2	2:E:174:ILE:CG1	2.36	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:H	3:I:128:ASN:ND2	2.07	0.52
1:A:185:LEU:HD22	1:A:441:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:134:VAL:O	3:I:138:SER:OG	2.26	0.52
2:E:160:ASP:OD1	2:E:160:ASP:N	2.43	0.52
2:H:50:LEU:HD11	2:H:129:GLN:CB	2.35	0.52
2:B:107:ASP:OD1	2:B:107:ASP:N	2.42	0.52
2:H:18:LEU:C	2:H:18:LEU:HD23	2.34	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: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:50:LEU:HD12	2:E:52:MET:HE1	1.91	0.51
2:B:85:LEU:HD23	2:B:85:LEU:C	2.36	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
2:E:23:PHE:CE2	2:E:75:MET:HE3	2.46	0.51
3:F:126:TYR:CZ	3:F:130:ILE:HD11	2.46	0.51
3:F:168:LYS:HA	3:F:171:GLU:CD	2.36	0.51
1:G:259:MET:HB3	1:G:295:HIS:CD2	2.46	0.51
2:E:159:LYS:H	2:E:159:LYS:HD3	1.76	0.50
2:H:83:LEU:C	2:H:84:ILE:HD13	2.36	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:O	2:B:163:VAL:HG23	2.11	0.50
2:E:21:GLU:CD	2:E:47:LYS:HZ1	2.19	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
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:38:PRO:O	2:H:41:ASP:HB2	2.11	0.50
2:H:180:GLN:HB3	3:I:10:TRP:CE3	2.46	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
2:E:137:ALA:HB3	3:F:13:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:LEU:HD13	3:I:70:ASP:C	2.37	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
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
2:H:192:LYS:C	2:H:193:ILE:HD12	2.37	0.49
3:I:140:LEU:HD12	3:I:152:PHE:CE1	2.47	0.49
1:A:131:ALA:HB2	2:B:154:LEU:HD22	1.93	0.49
1:A:169:GLU:OE2	1:A:464:ARG:HD2	2.12	0.49
1:D:300:LEU:HD21	1:D:336:SER:HA	1.95	0.49
1:A:184:ASN:C	1:A:185:LEU:HD13	2.38	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
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:52:MET:CE	2:E:132:ILE:HD13	2.37	0.48
2:E:159:LYS:H	2:E:159:LYS:CD	2.27	0.48
3:F:165:LEU:HD12	3:F:165:LEU:N	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
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
1:G:329:GLN:HG2	1:G:331:TRP:CZ2	2.49	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
1:A:370:ASP:O	1:A:371:LYS:HB2	2.13	0.47
3:C:222:SER:O	3:C:223:THR:CB	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ARG:NH2	3:F:21:GLU:O	2.47	0.47
3:F:172:VAL:HG12	3:F:175:LYS:HE3	1.97	0.47
2:E:167:TRP:H	2:E:167:TRP:CD1	2.32	0.47
3:I:114:LYS:NZ	3:I:143:HIS:O	2.48	0.47
3:I:119:TYR:CE2	3:I:123:TRP:HZ3	2.31	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
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
3:I:68:LEU:HD11	3:I:71:PRO:HA	1.96	0.47
3:I:119:TYR:CE2	3:I:123:TRP:CZ3	3.02	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
3:I:136:LEU:C	3:I:136:LEU:HD12	2.40	0.47
2:B:27:VAL:O	2:B:31:LEU:HG	2.15	0.46
2:B:171:ASP:HB2	2:B:172:PRO:HD2	1.97	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:E:71:LEU:C	2:E:71:LEU:HD23	2.41	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
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:79:LYS:NZ	2:B:160:ASP:OD1	2.47	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
2:H:84:ILE:C	2:H:85:LEU:HD12	2.40	0.45
2:E:71:LEU:HD21	2:E:75:MET:HE3	1.98	0.45
1:G:127:THR:HG23	2:H:156:TYR:HB3	1.98	0.45
2:E:23:PHE:HE2	2:E:75:MET:HE3	1.81	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
2:H:186:PHE:CD1	2:H:186:PHE:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:E:50:LEU:HD12	2:E:52:MET:CE	2.48	0.44
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: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
3:C:124:MET:HE2	3:C:124:MET:CA	2.47	0.44
1:G:201:ASN:OD1	1:G:217:GLU:HG2	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:LYS:HZ3	2:E:82:LYS:CB	2.25	0.44
2:E:86:VAL:HG13	2:E:95:ASP:HB3	2.00	0.44
2:E:159:LYS:HD3	2:E:159:LYS:N	2.32	0.44
1:G:126:ASN:N	1:G:126:ASN:HD22	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:87:ILE:HD11	2:E:149:CYS:HB2	2.01	0.43
2:E:180:GLN:HB3	3:F:10:TRP:CH2	2.53	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
2:E:137:ALA:O	2:E:140:THR:OG1	2.30	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
2:E:137:ALA:HB3	3:F:13:MET:CE	2.49	0.43
3:F:111:PRO:HA	3:F:114:LYS:HD3	2.01	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:186:LEU:HD11	1:G:460:LEU:HD11	2.01	0.43
1:G:190:ASN:HA	1:G:446:PRO:HB3	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
1:G:455:ALA:C	1:G:457:ASP:N	2.76	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
1:A:340:PHE:CE1	1:D:211:SER:HB2	2.55	0.42
1:D:179:ASP:HB2	1:D:456:SER:CB	2.50	0.42
1:G:443:ALA:O	1:G:451:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:52:MET:HE1	2:E:132:ILE:CD1	2.43	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
2:B:117:ASN:HB2	1:D:436:ASP:CG	2.45	0.42
1:G:181:TYR:CD1	1:G:181:TYR:C	2.97	0.42
1:G:453:THR:O	1:G:460:LEU:HD12	2.20	0.42
2:E:23:PHE:CD2	2:E:71:LEU:HD21	2.55	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
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: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
1:A:185:LEU:HD13	1:A:185:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:LEU:HD12	3:I:68:LEU:C	2.46	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:H	1:D:220:GLU:HG3	1.60	0.41
1:G:406:MET:HG2	1:G:418:ILE:HG12	2.03	0.41
2:H:156:TYR:N	2:H:156:TYR:HD1	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:O	1:A:290:VAL:HG12	2.20	0.41
2:B:180:GLN:HB2	3:C:10:TRP:CE3	2.55	0.41
1:G:205:TRP:HD1	1:G:212:VAL:HG22	1.86	0.41
1:G:249:ASP:HB2	1:G:256:LEU:HD21	2.03	0.41
1:G:456:SER:C	1:G:458:GLU:N	2.79	0.41
2:H:37:TYR:HB3	2:H:38:PRO:HD2	2.02	0.41
3:I:59:GLU:O	3:I:62:ILE:HG22	2.21	0.41
3:I:106:GLU:OE1	3:I:106:GLU:HA	2.19	0.41
3:I:143:HIS:HB3	3:I:145:ILE:HG13	2.02	0.41
1:D:361:LEU:HD11	1:D:421:TYR:CZ	2.56	0.41
2:E:47:LYS:NZ	2:E:48:TYR:CZ	2.86	0.41
2:E:87:ILE:HD11	2:E:149:CYS:HB3	2.03	0.41
1:G:456:SER:C	1:G:458:GLU:H	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:126:ASN:C	2:B:159:LYS:HG2	2.46	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 [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	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%)	33	50
1	D	259/340 (76%)	248 (96%)	11 (4%)	26	40
1	G	255/340 (75%)	242 (95%)	13 (5%)	21	32
2	B	166/187 (89%)	157 (95%)	9 (5%)	20	29
2	E	145/187 (78%)	135 (93%)	10 (7%)	14	20
2	H	160/187 (86%)	151 (94%)	9 (6%)	19	28
3	C	196/203 (97%)	185 (94%)	11 (6%)	19	28
3	F	163/203 (80%)	155 (95%)	8 (5%)	22	34
3	I	162/203 (80%)	135 (83%)	27 (17%)	2	2
All	All	1775/2190 (81%)	1668 (94%)	107 (6%)	17	25

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	143	VAL
1	A	185	LEU
1	A	186	LEU
1	A	244	LEU
1	A	263	GLN
1	A	432	ILE
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	86	VAL
2	B	107	ASP
2	B	153	VAL
2	B	155	VAL
2	B	171	ASP

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Mol	Chain	Res	Type
3	C	19	SER
3	C	66	GLU
3	C	67	SER
3	C	68	LEU
3	C	74	VAL
3	C	94	SER
3	C	135	GLU
3	C	179	MET
3	C	184	PHE
3	C	185	LEU
3	C	223	THR
1	D	186	LEU
1	D	220	GLU
1	D	228	LYS
1	D	244	LEU
1	D	346	ASN
1	D	359	SER
1	D	361	LEU
1	D	371	LYS
1	D	397	ILE
1	D	416	LEU
1	D	464	ARG
2	E	29	SER
2	E	30	ILE
2	E	60	VAL
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
3	F	13	MET
3	F	19	SER
3	F	99	LEU
3	F	148	GLU
3	F	165	LEU
3	F	172	VAL
3	F	185	LEU
3	F	221	GLU
1	G	126	ASN
1	G	167	THR

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Mol	Chain	Res	Type
1	G	169	GLU
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	329	GLN
1	G	371	LYS
1	G	397	ILE
2	H	6	ILE
2	H	8	THR
2	H	44	VAL
2	H	50	LEU
2	H	65	ARG
2	H	94	GLU
2	H	147	GLU
2	H	150	THR
2	H	153	VAL
3	I	11	VAL
3	I	38	SER
3	I	42	ASN
3	I	44	THR
3	I	62	ILE
3	I	74	VAL
3	I	82	THR
3	I	101	GLU
3	I	104	THR
3	I	108	VAL
3	I	109	ARG
3	I	117	VAL
3	I	123	TRP
3	I	127	VAL
3	I	128	ASN
3	I	131	ASP
3	I	132	GLU
3	I	134	VAL
3	I	138	SER
3	I	142	HIS
3	I	143	HIS
3	I	151	ILE

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Mol	Chain	Res	Type
3	I	155	GLU
3	I	175	LYS
3	I	186	ARG
3	I	197	ARG
3	I	198	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
3	C	192	GLN
1	D	190	ASN
1	D	344	ASN
1	D	360	ASN
1	D	459	ASN
2	E	28	ASN
2	E	70	GLN
2	E	125	GLN
1	G	126	ASN
1	G	360	ASN
2	H	70	GLN
2	H	117	ASN
3	I	128	ASN
3	I	193	GLN

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 oligosaccharides 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%)	-0.14	8 (2%) 58 60	17, 33, 64, 116	0
1	D	314/401 (78%)	0.28	21 (6%) 24 26	19, 42, 84, 116	0
1	G	317/401 (79%)	1.41	78 (24%) 2 2	43, 72, 103, 124	0
2	B	180/203 (88%)	0.08	4 (2%) 62 64	25, 44, 69, 109	0
2	E	175/203 (86%)	1.94	75 (42%) 0 0	40, 85, 127, 150	0
2	H	185/203 (91%)	1.52	46 (24%) 2 2	47, 70, 117, 139	0
3	C	215/223 (96%)	0.38	12 (5%) 30 32	19, 46, 80, 118	0
3	F	196/223 (87%)	0.66	26 (13%) 7 8	21, 53, 115, 149	0
3	I	193/223 (86%)	2.09	92 (47%) 0 0	40, 97, 133, 147	0
All	All	2101/2481 (84%)	0.83	362 (17%) 4 4	17, 56, 111, 150	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	153	VAL	8.2
2	H	151	PHE	8.2
3	I	103	CYS	6.8
2	H	30	ILE	6.1
2	E	96	LEU	5.8
3	I	108	VAL	5.6
1	G	467	ASP	5.5
2	E	155	VAL	5.4
3	F	180	LYS	5.3
2	E	53	LEU	5.3
3	I	123	TRP	5.3
1	D	134	LEU	5.1
2	E	18	LEU	5.0
2	H	106	VAL	5.0
1	A	125	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
3	I	107	PHE	4.9
3	I	185	LEU	4.9
3	F	184	PHE	4.8
3	I	117	VAL	4.8
3	I	112	LEU	4.7
3	I	120	LEU	4.7
2	H	137	ALA	4.7
3	I	134	VAL	4.5
3	I	127	VAL	4.4
3	F	185	LEU	4.4
3	I	10	TRP	4.3
3	I	140	LEU	4.3
1	D	268	CYS	4.3
2	H	177	ASP	4.2
3	I	139	PHE	4.2
3	I	198	TRP	4.2
3	I	179	MET	4.2
3	I	150	SER	4.2
3	I	153	TYR	4.2
2	E	91	CYS	4.1
3	I	156	TYR	4.1
2	E	154	LEU	4.1
3	I	111	PRO	4.1
3	F	181	ALA	4.1
3	I	72	LEU	4.1
3	I	195	THR	4.1
3	I	141	ALA	4.0
3	I	76	ILE	4.0
2	E	83	LEU	4.0
3	F	197	ARG	4.0
2	H	115	ILE	4.0
3	I	160	PHE	4.0
1	G	139	ALA	3.9
3	I	75	TRP	3.9
3	I	157	ALA	3.9
2	E	101	PHE	3.9
2	H	149	CYS	3.8
2	E	80	ILE	3.8
1	D	130	LEU	3.8
3	F	165	LEU	3.8
3	F	195	THR	3.8
2	E	163	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
3	I	100	LEU	3.8
2	E	172	PRO	3.8
3	I	28	ALA	3.7
3	I	130	ILE	3.7
2	E	124	VAL	3.7
3	I	129	TYR	3.7
2	E	77	ALA	3.7
2	E	54	VAL	3.7
1	D	132	PHE	3.6
3	I	15	VAL	3.6
2	H	26	ALA	3.6
3	I	119	TYR	3.6
3	C	200	GLU	3.6
3	I	133	PRO	3.6
3	I	126	TYR	3.6
2	H	201	VAL	3.5
1	G	290	VAL	3.5
3	F	183	PRO	3.5
2	H	153	VAL	3.5
3	I	166	PHE	3.5
1	D	131	ALA	3.4
3	I	99	LEU	3.4
3	I	165	LEU	3.4
3	F	10	TRP	3.4
2	H	148	GLN	3.4
3	I	158	ASN	3.4
3	I	62	ILE	3.3
1	G	357	TRP	3.3
2	H	86	VAL	3.3
1	G	375	PHE	3.3
2	E	151	PHE	3.3
3	I	64	THR	3.3
3	I	104	THR	3.3
2	H	99	TRP	3.3
2	H	171	ASP	3.3
3	I	69	ASP	3.3
2	H	10	PHE	3.3
2	E	84	ILE	3.3
1	G	196	VAL	3.3
1	G	426	LEU	3.2
2	E	22	PHE	3.2
2	E	99	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	175	LEU	3.2
1	G	397	ILE	3.2
1	G	205	TRP	3.2
3	F	215	PRO	3.2
2	E	76	PHE	3.2
1	G	212	VAL	3.2
2	E	148	GLN	3.2
2	H	89	SER	3.1
2	H	97	GLU	3.1
2	H	93	GLY	3.1
2	E	19	VAL	3.1
3	I	70	ASP	3.1
3	I	147	GLN	3.1
2	B	201	VAL	3.1
2	E	156	TYR	3.1
3	F	120	LEU	3.1
2	E	138	THR	3.1
3	F	166	PHE	3.1
2	E	14	GLY	3.1
2	E	64	ILE	3.1
2	H	150	THR	3.0
3	F	196	HIS	3.0
1	D	164	PHE	3.0
1	A	216	ALA	3.0
2	E	26	ALA	3.0
1	G	134	LEU	3.0
3	I	16	ILE	3.0
2	H	170	SER	3.0
3	I	187	PHE	3.0
2	E	67	ILE	3.0
1	G	195	ALA	3.0
1	G	202	VAL	3.0
3	C	184	PHE	2.9
1	D	401	HIS	2.9
1	A	126	ASN	2.9
3	I	124	MET	2.9
1	A	162	ARG	2.9
3	F	127	VAL	2.9
2	E	89	SER	2.9
2	E	146	GLU	2.9
2	H	63	TYR	2.9
2	H	104	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	163	ARG	2.9
1	D	133	LYS	2.9
2	E	82	LYS	2.9
3	I	143	HIS	2.9
1	G	131	ALA	2.9
2	E	105	MET	2.9
3	F	179	MET	2.9
1	G	466	TYR	2.8
3	I	109	ARG	2.8
3	C	185	LEU	2.8
2	H	162	GLU	2.8
1	G	252	SER	2.8
1	G	298	GLY	2.8
1	G	425	GLY	2.8
2	E	147	GLU	2.8
2	H	155	VAL	2.8
3	F	167	GLN	2.8
3	I	174	GLN	2.8
1	G	166	THR	2.8
1	G	288	HIS	2.8
2	H	6	ILE	2.8
1	D	335	SER	2.8
2	H	164	PRO	2.8
2	H	23	PHE	2.8
1	G	194	VAL	2.8
3	I	97	VAL	2.8
3	C	211	ASN	2.7
2	E	71	LEU	2.7
1	G	223	TYR	2.7
3	F	194	PHE	2.7
1	D	129	VAL	2.7
1	G	227	VAL	2.7
2	E	168	VAL	2.7
1	G	330	ILE	2.7
1	D	250	VAL	2.7
1	G	204	VAL	2.7
3	I	144	HIS	2.6
3	I	73	GLN	2.6
3	I	132	GLU	2.6
3	I	172	VAL	2.6
3	F	163	ARG	2.6
1	G	398	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	220	GLU	2.6
1	G	261	GLY	2.6
3	I	149	SER	2.6
2	H	85	LEU	2.6
2	H	145	LEU	2.6
2	E	167	TRP	2.6
1	D	466	TYR	2.6
1	G	226	SER	2.6
3	I	93	THR	2.6
1	G	418	ILE	2.6
2	E	170	SER	2.6
3	I	65	SER	2.6
3	I	145	ILE	2.6
1	G	172	LEU	2.5
2	E	122	LEU	2.5
3	I	67	SER	2.5
2	E	85	LEU	2.5
1	G	459	ASN	2.5
1	G	446	PRO	2.5
2	E	93	GLY	2.5
1	G	129	VAL	2.5
2	H	161	SER	2.5
1	G	256	LEU	2.5
2	E	157	ALA	2.5
1	G	302	GLY	2.5
2	H	74	TRP	2.5
3	I	105	ARG	2.5
1	G	317	LEU	2.5
2	H	154	LEU	2.5
2	E	159	LYS	2.5
1	G	201	ASN	2.5
3	C	181	ALA	2.5
1	G	254	THR	2.4
3	I	106	GLU	2.4
3	I	175	LYS	2.4
3	C	9	ASN	2.4
1	G	333	ALA	2.4
2	H	165	THR	2.4
2	E	174	ILE	2.4
2	H	168	VAL	2.4
3	I	152	PHE	2.4
1	G	403	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	190	MET	2.4
3	C	10	TRP	2.4
1	G	203	TYR	2.4
1	G	289	ASP	2.4
2	H	200	ARG	2.4
3	F	222	SER	2.4
2	E	27	VAL	2.4
1	G	198	LEU	2.4
2	E	171	ASP	2.4
3	I	131	ASP	2.4
2	E	161	SER	2.4
2	B	107	ASP	2.3
1	G	239	GLY	2.3
1	G	216	ALA	2.3
3	I	142	HIS	2.3
1	D	300	LEU	2.3
1	G	433	PRO	2.3
1	D	379	ALA	2.3
2	E	165	THR	2.3
2	E	16	SER	2.3
3	I	39	SER	2.3
1	D	297	ILE	2.3
1	A	164	PHE	2.3
1	G	132	PHE	2.3
1	G	238	VAL	2.3
2	E	120	ASP	2.3
1	G	331	TRP	2.3
1	G	376	TRP	2.3
1	G	335	SER	2.3
1	G	199	GLU	2.3
3	I	23	ILE	2.3
1	G	328	VAL	2.3
2	E	51	ASN	2.3
3	C	209	ASN	2.3
1	G	260	ALA	2.3
1	G	299	THR	2.3
1	G	177	ILE	2.3
3	F	182	LYS	2.3
3	I	51	LEU	2.2
3	I	194	PHE	2.2
1	G	401	HIS	2.2
2	E	135	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	215	LEU	2.2
1	G	327	VAL	2.2
2	H	60	VAL	2.2
3	I	96	LEU	2.2
1	G	294	ASN	2.2
1	D	137	PRO	2.2
1	D	334	ARG	2.2
3	F	190	LYS	2.2
3	I	113	TYR	2.2
1	G	236	LEU	2.2
2	H	71	LEU	2.2
1	G	352	VAL	2.2
2	E	86	VAL	2.2
2	H	163	VAL	2.2
3	F	137	PHE	2.2
3	I	14	ASP	2.2
3	I	197	ARG	2.2
1	G	168	PRO	2.2
2	E	190	MET	2.2
2	E	17	LYS	2.2
3	I	58	HIS	2.2
3	I	196	HIS	2.2
3	I	44	THR	2.2
3	I	49	ALA	2.2
1	G	321	SER	2.2
1	A	215	LEU	2.2
3	C	130	ILE	2.2
3	I	79	ILE	2.2
2	H	197	VAL	2.2
2	H	141	PHE	2.2
3	F	128	ASN	2.2
3	I	48	VAL	2.2
2	B	91	CYS	2.2
2	E	150	THR	2.2
3	C	223	THR	2.2
3	I	159	TYR	2.1
3	I	173	TYR	2.1
2	H	135	ILE	2.1
2	H	174	ILE	2.1
2	E	74	TRP	2.1
2	E	177	ASP	2.1
3	I	11	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	32	PHE	2.1
1	G	218	THR	2.1
1	G	264	ALA	2.1
1	G	270	SER	2.1
1	G	432	ILE	2.1
2	E	87	ILE	2.1
1	G	360	ASN	2.1
3	I	66	GLU	2.1
1	D	336	SER	2.1
1	G	292	ILE	2.1
3	F	216	LEU	2.1
3	I	68	LEU	2.1
2	E	166	ASP	2.1
2	H	199	TYR	2.1
2	E	44	VAL	2.1
2	E	56	VAL	2.1
2	E	184	ARG	2.1
2	H	8	THR	2.1
2	H	198	ALA	2.1
3	I	61	LYS	2.1
2	E	145	LEU	2.1
3	F	112	LEU	2.1
1	G	297	ILE	2.1
2	E	102	ASN	2.1
2	E	38	PRO	2.1
3	F	191	TYR	2.1
1	G	193	VAL	2.1
2	E	186	PHE	2.1
2	E	46	ARG	2.1
2	E	98	ARG	2.1
2	E	90	LYS	2.0
3	I	98	THR	2.0
2	E	133	ALA	2.0
3	I	52	GLN	2.0
1	D	467	ASP	2.0
1	G	396	LEU	2.0
2	H	87	ILE	2.0
3	I	122	ILE	2.0
3	I	151	ILE	2.0
1	A	466	TYR	2.0
2	E	37	TYR	2.0
1	G	281	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	425	GLY	2.0
2	E	75	MET	2.0
3	C	67	SER	2.0
3	C	212	SER	2.0
1	G	300	LEU	2.0
3	I	136	LEU	2.0
1	D	418	ILE	2.0
1	G	356	PRO	2.0
1	G	450	ILE	2.0
2	E	176	ARG	2.0
3	I	163	ARG	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 oligosaccharides 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.