



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:44 AM UTC

PDB ID : 2QLV / pdb_00002qlv
Title : Crystal structure of the heterotrimer core of the *S. cerevisiae* AMPK homolog SNF1
Authors : Amodeo, G.A.; Rudolph, M.J.; Tong, L.
Deposited on : 2007-07-13
Resolution : 2.60 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

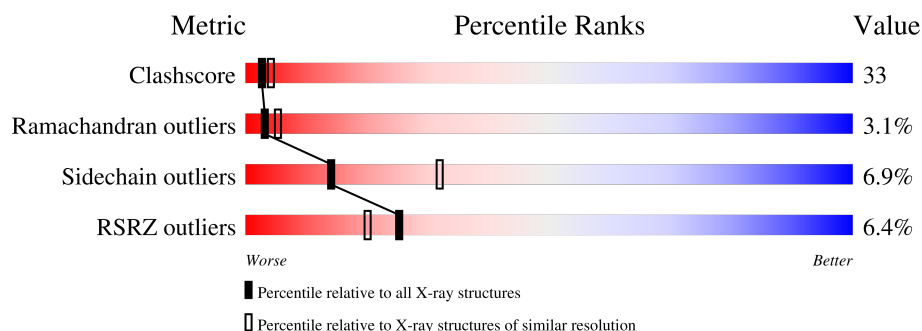
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	171	6% 34% 38% 5% • 22%
1	D	171	7% 32% 40% 6% 22%
2	B	252	4% 25% 31% 6% 38%
2	E	252	5% 30% 21% • • 44%
3	C	315	3% 50% 42% 6% •
3	F	315	7% 47% 44% 6% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9579 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 Carbon catabolite derepressing protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1079	704	177	192	6			
1	D	133	Total	C	N	O	S	0	0	0
			1079	704	177	192	6			

- Molecule 2 is a protein called Protein SIP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1264	815	219	225	5			
2	E	140	Total	C	N	O	S	0	0	0
			1131	731	198	198	4			

- Molecule 3 is a protein called Nuclear protein SNF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	310	Total	C	N	O	S	0	0	0
			2457	1570	412	465	10			
3	F	310	Total	C	N	O	S	0	0	0
			2458	1570	412	466	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	23	Total	O	0	0
			23	23		
4	C	28	Total	O	0	0
			28	28		
4	D	5	Total	O	0	0
			5	5		

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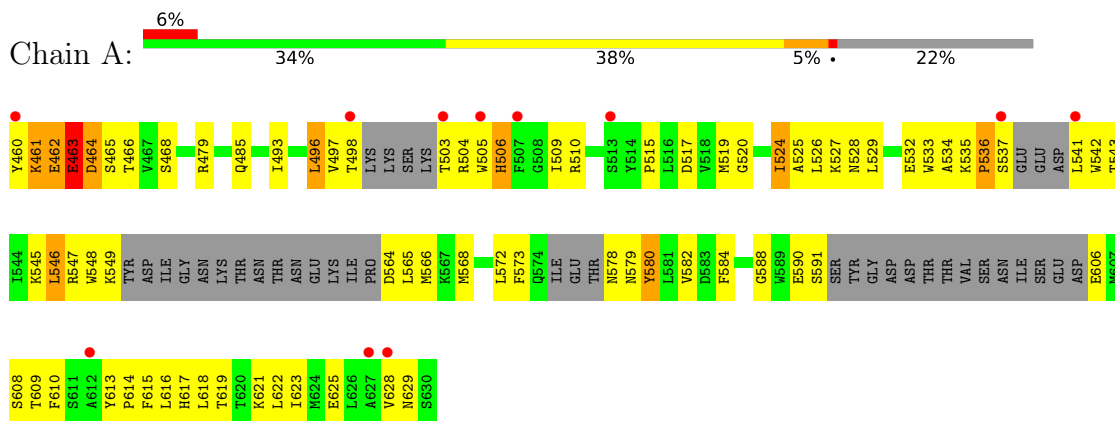
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	11	Total	O	0	0
			11	11		
4	F	29	Total	O	0	0
			29	29		

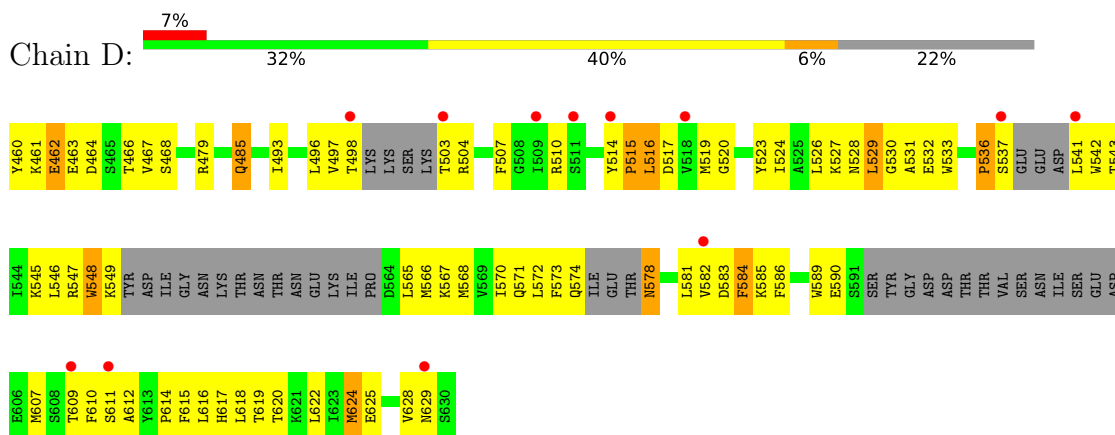
3 Residue-property plots

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.

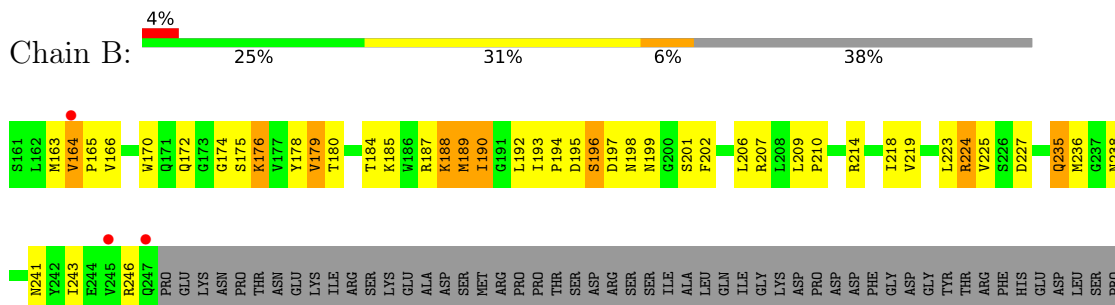
- Molecule 1: Carbon catabolite derepressing protein kinase

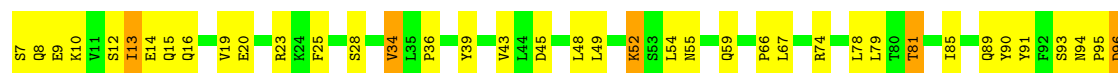


- Molecule 1: Carbon catabolite derepressing protein kinase



- Molecule 2: Protein SIP2







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.33Å 81.84Å 174.74Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	29.54 – 2.60 29.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.54-2.60) 88.0 (29.54-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.299 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.47	0/1104	0.92	6/1490 (0.4%)
1	D	0.46	0/1104	0.98	5/1490 (0.3%)
2	B	0.52	0/1295	1.00	5/1759 (0.3%)
2	E	0.52	0/1158	0.97	4/1572 (0.3%)
3	C	0.54	0/2491	0.96	4/3371 (0.1%)
3	F	0.52	0/2492	0.99	8/3371 (0.2%)
All	All	0.51	0/9644	0.97	32/13053 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	463	GLU	N-CA-C	10.46	117.35	108.78
3	F	193	ILE	N-CA-C	8.06	118.74	111.81
3	F	310	LEU	N-CA-C	-7.83	102.70	111.07
2	B	164	VAL	N-CA-C	7.27	114.88	108.63
3	C	310	LEU	N-CA-C	-6.89	103.77	111.28
2	E	235	GLN	N-CA-C	-6.64	103.14	111.11
3	F	127	HIS	CA-C-N	6.14	127.52	119.84
3	F	127	HIS	C-N-CA	6.14	127.52	119.84
2	B	174	GLY	N-CA-C	6.07	118.23	112.04
1	A	588	GLY	N-CA-C	5.94	119.30	111.52
1	A	493	ILE	N-CA-C	5.78	116.47	108.84
1	A	535	LYS	CA-C-N	5.75	127.03	119.84
1	A	535	LYS	C-N-CA	5.75	127.03	119.84
1	D	463	GLU	CB-CA-C	-5.72	108.83	117.07
3	F	36	PRO	N-CA-C	-5.65	102.94	111.41
2	E	379	ASN	N-CA-C	-5.60	98.87	110.80
1	D	493	ILE	N-CA-C	5.59	116.29	109.30
2	B	175	SER	N-CA-C	-5.53	106.46	113.43
3	C	127	HIS	CA-C-N	5.49	125.16	119.56
3	C	127	HIS	C-N-CA	5.49	125.16	119.56
2	B	224	ARG	N-CA-C	5.42	117.43	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	208	VAL	N-CA-C	5.35	115.56	110.42
3	F	97	LYS	N-CA-C	-5.35	105.02	112.03
3	F	290	ALA	N-CA-C	5.24	117.04	109.07
2	E	193	ILE	CA-C-N	5.22	125.14	119.76
2	E	193	ILE	C-N-CA	5.22	125.14	119.76
3	C	208	VAL	N-CA-C	5.16	116.51	110.62
2	B	190	ILE	N-CA-C	-5.16	100.89	108.11
1	A	468	SER	N-CA-C	5.09	115.87	108.14
1	D	463	GLU	CA-C-O	5.08	120.89	117.94
1	A	580	TYR	N-CA-C	5.07	117.38	109.52
1	D	516	LEU	N-CA-C	-5.05	108.38	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1079	0	1083	73	0
1	D	1079	0	1083	87	0
2	B	1264	0	1271	112	0
2	E	1131	0	1149	80	0
3	C	2457	0	2544	178	0
3	F	2458	0	2544	188	0
4	A	15	0	0	2	0
4	B	23	0	0	5	0
4	C	28	0	0	1	0
4	D	5	0	0	1	0
4	E	11	0	0	0	0
4	F	29	0	0	4	0
All	All	9579	0	9674	641	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 33.

All (641) 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)
2:E:189:MET:HE2	2:E:218:ILE:HD13	1.25	1.16
3:C:114:ARG:HA	3:C:119:ASP:HB3	1.34	1.09
3:F:249:ILE:HG22	3:F:250:TYR:H	1.22	1.00
2:B:189:MET:HE2	2:B:218:ILE:HD13	1.43	1.00
2:E:386:ILE:HD12	2:E:386:ILE:H	1.29	0.96
3:C:188:ILE:HD11	3:C:280:LEU:HG	1.44	0.95
3:C:82:THR:HG21	3:C:219:ARG:HH12	1.33	0.94
3:F:209:ILE:HD12	3:F:210:ASP:H	1.34	0.93
3:C:120:GLN:HG2	3:F:117:GLY:H	1.32	0.91
2:E:375:HIS:CD2	2:E:377:VAL:HG22	2.05	0.90
3:C:276:LYS:HE3	3:C:305:VAL:HG11	1.54	0.90
3:F:120:GLN:HE22	3:F:122:ASP:HB3	1.37	0.89
3:C:175:ALA:HB2	3:C:284:MET:HG3	1.55	0.89
3:C:211:VAL:HG21	3:C:257:VAL:CG1	2.04	0.87
1:D:616:LEU:HD22	2:E:393:VAL:HG13	1.56	0.87
2:E:184:THR:HG21	2:E:188:LYS:O	1.74	0.86
2:E:375:HIS:CG	2:E:376:VAL:H	1.93	0.86
2:E:189:MET:CE	2:E:218:ILE:HD13	2.05	0.85
3:F:95:PRO:O	3:F:96:ASP:HB2	1.77	0.84
2:E:375:HIS:HD2	2:E:377:VAL:HG22	1.41	0.84
2:B:184:THR:HG21	2:B:188:LYS:O	1.78	0.83
3:C:245:ILE:HA	3:C:249:ILE:HB	1.60	0.83
2:E:214:ARG:HH11	2:E:214:ARG:HB2	1.44	0.82
2:B:386:ILE:HD12	2:B:386:ILE:H	1.43	0.81
3:C:309:THR:HG22	3:C:311:SER:H	1.43	0.81
2:E:390:THR:HG21	3:F:48:LEU:HD11	1.61	0.81
3:F:165:LEU:HG	3:F:170:ILE:HD11	1.62	0.80
1:D:467:VAL:HG11	3:F:286:ASN:ND2	1.96	0.80
3:F:130:ARG:NH2	3:F:134:GLU:HG2	1.96	0.79
3:F:130:ARG:HH11	3:F:131:PRO:HD2	1.47	0.79
3:F:310:LEU:HD11	4:F:768:HOH:O	1.82	0.79
3:F:10:LYS:O	3:F:14:GLU:HG3	1.82	0.79
2:B:198:ASN:HD22	2:B:199:ASN:N	1.81	0.78
2:B:375:HIS:HD2	2:B:377:VAL:HG22	1.49	0.78
2:B:377:VAL:C	2:B:378:LEU:HD12	2.08	0.78
3:F:199:MET:HE2	3:F:304:LEU:HD21	1.66	0.77
3:C:82:THR:CG2	3:C:219:ARG:HH12	1.97	0.77
3:C:196:GLN:HE22	3:C:305:VAL:HG12	1.50	0.77
3:C:211:VAL:HG21	3:C:257:VAL:HG11	1.66	0.77
2:E:185:LYS:HD3	2:E:187:ARG:NH1	1.99	0.77
3:C:91:TYR:HB2	3:C:101:VAL:HG21	1.66	0.77
1:D:566:MET:HE2	1:D:618:LEU:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:NZ	2:B:176:LYS:HB3	2.00	0.76
3:C:127:HIS:CD2	3:C:129:SER:H	2.03	0.76
2:E:377:VAL:C	2:E:378:LEU:HD12	2.11	0.76
3:F:16:GLN:HE21	3:F:20:GLU:HG3	1.51	0.76
3:F:315:LYS:HG3	3:F:319:LEU:HD12	1.68	0.76
2:B:166:VAL:HG11	2:B:243:ILE:CD1	2.17	0.75
3:F:309:THR:HG22	3:F:311:SER:H	1.52	0.74
3:C:16:GLN:O	3:C:20:GLU:HG3	1.87	0.74
2:E:184:THR:HG23	2:E:188:LYS:HB3	1.68	0.73
2:B:376:VAL:HG23	2:B:398:ARG:HH22	1.52	0.73
2:E:375:HIS:CG	2:E:376:VAL:N	2.56	0.72
3:C:188:ILE:HD11	3:C:280:LEU:CG	2.17	0.72
3:F:188:ILE:HG13	3:F:193:ILE:HD11	1.70	0.72
3:F:152:GLN:HE21	3:F:152:GLN:HA	1.55	0.72
3:F:178:CYS:O	3:F:181:THR:HG23	1.89	0.72
2:E:184:THR:CG2	2:E:188:LYS:HB3	2.20	0.71
1:D:496:LEU:HD12	1:D:497:VAL:H	1.55	0.71
2:B:386:ILE:HG13	2:B:391:LEU:HD13	1.72	0.71
2:E:375:HIS:NE2	2:E:377:VAL:HG13	2.05	0.71
3:F:142:SER:O	3:F:144:SER:N	2.22	0.71
2:B:189:MET:CE	2:B:218:ILE:HD13	2.20	0.71
2:E:168:ILE:HD13	2:E:206:LEU:HD12	1.73	0.70
3:C:67:LEU:HD21	3:C:79:LEU:HB2	1.72	0.70
3:C:127:HIS:HD2	3:C:129:SER:H	1.36	0.70
3:F:199:MET:CE	3:F:304:LEU:HD21	2.20	0.70
2:B:178:TYR:HB3	2:B:189:MET:HB3	1.74	0.70
3:C:54:LEU:CD1	3:C:242:LEU:HD22	2.21	0.70
2:E:189:MET:HE2	2:E:218:ILE:CD1	2.15	0.70
2:E:404:VAL:HG22	3:F:39:TYR:CZ	2.27	0.70
3:F:249:ILE:HG22	3:F:250:TYR:N	2.02	0.70
2:E:386:ILE:H	2:E:386:ILE:CD1	2.05	0.69
3:C:141:GLU:HB3	3:F:118:VAL:HB	1.74	0.69
1:D:532:GLU:CD	1:D:547:ARG:HE	2.01	0.69
3:C:120:GLN:N	3:F:116:LEU:HD22	2.08	0.68
1:D:547:ARG:O	1:D:548:TRP:HB2	1.93	0.68
2:B:209:LEU:HG	2:B:210:PRO:HD2	1.75	0.68
3:F:66:PRO:HA	3:F:78:LEU:HD23	1.74	0.68
2:E:386:ILE:HD12	2:E:386:ILE:N	2.08	0.68
3:F:120:GLN:NE2	3:F:122:ASP:HB3	2.09	0.68
3:C:211:VAL:HG21	3:C:257:VAL:HG13	1.74	0.68
3:F:176:LEU:HD13	3:F:288:ARG:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:220:VAL:HG22	3:F:222:SER:H	1.58	0.68
3:F:209:ILE:HD12	3:F:210:ASP:N	2.09	0.67
3:F:209:ILE:CD1	3:F:210:ASP:H	2.07	0.67
3:C:49:LEU:HB3	3:C:52:LYS:HB2	1.77	0.67
2:B:375:HIS:CD2	2:B:377:VAL:HG22	2.28	0.67
3:C:67:LEU:HD22	3:C:106:LEU:HD13	1.77	0.67
2:B:236:MET:HE3	2:B:238:ASN:HD21	1.59	0.67
3:C:10:LYS:O	3:C:14:GLU:HG3	1.95	0.66
3:C:118:VAL:HB	3:F:116:LEU:HG	1.77	0.66
2:B:172:GLN:HE22	2:B:227:ASP:H	1.44	0.66
3:F:16:GLN:O	3:F:20:GLU:HG3	1.96	0.66
2:B:318:VAL:HA	2:B:321:ARG:HD3	1.77	0.65
3:F:124:ALA:O	3:F:148:PRO:HD2	1.97	0.65
2:B:390:THR:HG23	4:B:747:HOH:O	1.95	0.65
1:D:532:GLU:HG3	1:D:547:ARG:HB3	1.78	0.65
3:F:228:GLU:CD	3:F:228:GLU:H	2.03	0.65
3:F:245:ILE:O	3:F:247:GLY:N	2.29	0.65
3:F:128:PRO:HG3	3:F:149:LEU:HB3	1.79	0.65
3:C:118:VAL:O	3:F:116:LEU:HD21	1.97	0.65
3:F:142:SER:C	3:F:144:SER:H	2.05	0.65
3:C:77:GLY:HA2	3:C:123:THR:HG21	1.77	0.64
3:C:118:VAL:HB	3:F:116:LEU:CG	2.27	0.64
3:C:142:SER:C	3:C:144:SER:H	2.05	0.64
3:C:196:GLN:NE2	3:C:305:VAL:HG12	2.12	0.64
1:D:572:LEU:HD13	1:D:582:VAL:HG22	1.78	0.64
2:E:163:MET:HE2	2:E:207:ARG:O	1.98	0.64
3:C:196:GLN:O	3:C:199:MET:HE3	1.98	0.64
1:D:485:GLN:OE1	1:D:485:GLN:HA	1.97	0.64
3:F:309:THR:HG22	3:F:310:LEU:N	2.12	0.64
3:F:249:ILE:HG12	4:F:720:HOH:O	1.97	0.64
1:D:467:VAL:HG23	3:F:278:ASP:OD1	1.97	0.64
3:F:188:ILE:HD11	3:F:280:LEU:HG	1.80	0.64
2:B:388:HIS:C	2:B:390:THR:H	2.06	0.64
3:C:46:THR:HG22	3:C:107:ASP:HB2	1.80	0.64
1:D:566:MET:CE	1:D:618:LEU:HD12	2.28	0.63
1:D:607:MET:SD	3:F:158:ARG:NH2	2.71	0.63
1:A:590:GLU:HG3	1:A:591:SER:H	1.63	0.63
3:C:120:GLN:HG2	3:F:117:GLY:N	2.11	0.63
1:D:567:LYS:HZ2	1:D:590:GLU:CD	2.06	0.63
3:F:91:TYR:HE1	3:F:250:TYR:HB2	1.64	0.63
3:C:118:VAL:HG12	3:F:94:ASN:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:GLY:O	2:E:202:PHE:HZ	1.80	0.63
3:C:126:ILE:HD11	3:C:134:GLU:HG3	1.79	0.63
3:C:206:THR:O	3:C:257:VAL:HG22	1.99	0.63
2:E:176:LYS:HZ2	2:E:176:LYS:HB3	1.63	0.63
2:E:310:PRO:HG2	2:E:313:PHE:HD1	1.63	0.63
3:F:67:LEU:HD21	3:F:79:LEU:HB2	1.81	0.62
1:D:507:PHE:HE1	2:E:378:LEU:HD23	1.65	0.62
3:C:118:VAL:HB	3:F:116:LEU:CD1	2.29	0.62
3:F:185:LYS:HA	3:F:279:LYS:HD3	1.81	0.62
2:B:246:ARG:HH22	2:B:398:ARG:HH12	1.47	0.62
3:C:122:ASP:OD2	3:F:118:VAL:HG13	1.99	0.62
3:F:66:PRO:CA	3:F:78:LEU:HD23	2.29	0.61
3:F:114:ARG:HA	3:F:119:ASP:HB3	1.82	0.61
2:B:377:VAL:HG23	2:B:378:LEU:HD12	1.82	0.61
3:C:188:ILE:CD1	3:C:280:LEU:HG	2.25	0.61
3:C:114:ARG:CZ	3:C:121:LEU:HD11	2.30	0.61
2:B:389:ASN:HB3	3:C:52:LYS:HZ3	1.64	0.61
3:C:118:VAL:HB	3:F:116:LEU:HD11	1.81	0.61
3:C:118:VAL:C	3:F:116:LEU:HD21	2.25	0.61
3:C:142:SER:O	3:C:144:SER:N	2.34	0.61
1:D:515:PRO:O	1:D:542:TRP:HZ3	1.84	0.61
3:F:130:ARG:CZ	3:F:134:GLU:HG2	2.30	0.61
2:B:386:ILE:HD12	2:B:386:ILE:N	2.15	0.61
2:B:381:LEU:HD11	2:B:393:VAL:CG2	2.31	0.61
1:D:514:TYR:HB2	1:D:517:ASP:OD2	2.01	0.61
3:F:249:ILE:CG2	3:F:250:TYR:H	2.03	0.60
1:A:519:MET:HG2	2:B:313:PHE:CZ	2.37	0.60
2:B:376:VAL:HG23	2:B:398:ARG:NH2	2.16	0.60
3:C:208:VAL:HG11	3:C:260:ALA:HB2	1.84	0.60
3:C:276:LYS:CE	3:C:305:VAL:HG11	2.28	0.60
3:F:136:CYS:HB3	3:F:318:LEU:HD11	1.84	0.60
1:D:460:TYR:CD2	1:D:461:LYS:N	2.70	0.60
1:A:610:PHE:HA	3:C:160:ILE:HG13	1.82	0.59
2:E:410:THR:HG22	3:F:45:ASP:HB2	1.84	0.59
2:B:176:LYS:HB3	2:B:176:LYS:HZ2	1.64	0.59
2:B:307:THR:HG22	2:B:307:THR:O	2.02	0.59
1:D:585:LYS:HG3	2:E:380:HIS:CE1	2.37	0.59
3:F:74:ARG:HH11	3:F:74:ARG:HG2	1.68	0.59
3:C:114:ARG:HA	3:C:119:ASP:CB	2.21	0.59
2:E:381:LEU:HD11	2:E:393:VAL:HG21	1.84	0.59
2:B:306:THR:HG22	2:B:308:ASP:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:ILE:HG13	2:B:391:LEU:CD1	2.33	0.59
1:D:574:GLN:HE22	1:D:578:ASN:HB3	1.66	0.59
2:B:402:LYS:NZ	3:C:32:TYR:O	2.35	0.59
1:D:497:VAL:HG12	1:D:498:THR:N	2.18	0.59
3:F:91:TYR:CE1	3:F:250:TYR:HB2	2.37	0.59
3:F:199:MET:O	3:F:199:MET:HG3	2.02	0.58
3:F:130:ARG:HD2	3:F:131:PRO:HD2	1.86	0.58
1:A:524:ILE:HG22	1:A:525:ALA:N	2.18	0.58
3:C:193:ILE:HD12	3:C:308:LEU:HD11	1.86	0.58
3:F:280:LEU:O	3:F:284:MET:HB2	2.04	0.58
2:B:190:ILE:HG21	2:B:206:LEU:HD21	1.86	0.58
3:C:142:SER:CA	3:F:118:VAL:HG12	2.34	0.58
1:D:573:PHE:HB3	2:E:343:LEU:HB2	1.86	0.58
2:E:184:THR:O	2:E:184:THR:HG22	2.03	0.58
2:B:189:MET:HE2	2:B:218:ILE:CD1	2.27	0.58
2:B:187:ARG:O	2:B:187:ARG:HG3	2.03	0.58
2:B:346:GLN:H	2:B:346:GLN:NE2	2.02	0.57
3:C:43:VAL:HG22	3:C:66:PRO:HG2	1.86	0.57
3:C:104:LEU:HD22	3:C:112:ILE:HD12	1.85	0.57
2:E:176:LYS:HB3	2:E:176:LYS:NZ	2.19	0.57
2:E:187:ARG:O	2:E:187:ARG:HG3	2.03	0.57
1:A:460:TYR:HD2	1:A:461:LYS:N	2.01	0.57
3:F:120:GLN:HE22	3:F:122:ASP:CB	2.14	0.57
2:B:386:ILE:H	2:B:386:ILE:CD1	2.15	0.57
1:D:566:MET:HG3	1:D:586:PHE:HE1	1.68	0.57
3:F:269:GLU:HG2	4:F:704:HOH:O	2.05	0.57
2:B:184:THR:HG22	2:B:184:THR:O	2.04	0.57
3:C:315:LYS:NZ	3:F:121:LEU:HB2	2.20	0.57
1:D:549:LYS:HB3	1:D:565:LEU:HG	1.85	0.57
1:A:466:THR:O	1:A:466:THR:HG22	2.06	0.56
2:E:170:TRP:CZ2	2:E:172:GLN:HB2	2.39	0.56
2:E:377:VAL:HG23	2:E:377:VAL:O	2.05	0.56
2:B:315:ASP:HB3	2:B:318:VAL:HG23	1.87	0.56
3:C:185:LYS:HA	3:C:279:LYS:HD3	1.86	0.56
2:E:187:ARG:O	2:E:188:LYS:HB2	2.06	0.56
3:C:24:LYS:HB2	3:C:24:LYS:NZ	2.21	0.56
3:C:95:PRO:O	3:C:96:ASP:HB2	2.05	0.56
1:D:543:THR:HG21	1:D:545:LYS:NZ	2.21	0.56
2:E:236:MET:HE2	2:E:238:ASN:HD21	1.71	0.56
2:B:388:HIS:C	2:B:390:THR:N	2.63	0.56
3:F:7:SER:C	3:F:9:GLU:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:ASP:O	3:F:116:LEU:HD13	2.06	0.56
3:F:16:GLN:HE21	3:F:20:GLU:CG	2.18	0.56
2:B:306:THR:CG2	2:B:308:ASP:H	2.18	0.56
3:C:142:SER:N	3:F:118:VAL:HG12	2.21	0.55
2:B:180:THR:HG22	2:B:188:LYS:O	2.06	0.55
3:C:176:LEU:HD13	3:C:288:ARG:HG3	1.86	0.55
3:F:67:LEU:HD22	3:F:106:LEU:HD13	1.88	0.55
2:B:163:MET:HB3	2:B:207:ARG:O	2.07	0.55
3:F:142:SER:C	3:F:144:SER:N	2.62	0.55
2:B:184:THR:O	2:B:184:THR:CG2	2.54	0.55
2:B:389:ASN:HB3	3:C:52:LYS:NZ	2.21	0.55
3:C:309:THR:HG22	3:C:311:SER:N	2.18	0.55
2:E:410:THR:HG22	3:F:45:ASP:CB	2.36	0.55
3:F:188:ILE:HG22	3:F:194:ILE:HD11	1.87	0.55
3:C:142:SER:C	3:C:144:SER:N	2.63	0.55
2:E:168:ILE:HG21	2:E:179:VAL:HG11	1.88	0.55
3:F:202:CYS:HB3	3:F:214:MET:HE1	1.89	0.55
3:C:197:ASP:O	3:C:198:ASN:HB2	2.07	0.55
1:D:526:LEU:HB3	1:D:531:ALA:HB3	1.87	0.55
3:F:208:VAL:HG11	3:F:260:ALA:HB2	1.87	0.55
1:D:615:PHE:O	1:D:619:THR:HG23	2.07	0.55
1:A:503:THR:HG22	1:A:504:ARG:H	1.72	0.54
3:C:54:LEU:HD11	3:C:242:LEU:HD22	1.89	0.54
2:B:311:ALA:HA	2:B:314:THR:OG1	2.07	0.54
2:B:312:VAL:HG23	4:B:725:HOH:O	2.06	0.54
3:C:78:LEU:CD1	3:C:146:ARG:HD3	2.37	0.54
3:F:209:ILE:CD1	3:F:210:ASP:N	2.69	0.54
3:C:78:LEU:HD13	3:C:146:ARG:HD3	1.89	0.54
1:A:573:PHE:HB3	2:B:343:LEU:HB2	1.90	0.54
2:B:235:GLN:HG3	4:B:717:HOH:O	2.08	0.54
1:D:496:LEU:HD11	3:F:246:LYS:NZ	2.23	0.54
3:F:7:SER:CB	3:F:10:LYS:HB3	2.37	0.54
2:B:379:ASN:O	2:B:379:ASN:ND2	2.40	0.54
2:B:402:LYS:HD2	3:C:32:TYR:CE2	2.43	0.53
3:F:143:ARG:HG3	3:F:143:ARG:O	2.09	0.53
3:F:298:VAL:HA	3:F:303:ARG:O	2.09	0.53
2:E:376:VAL:HG23	2:E:398:ARG:HH21	1.74	0.53
3:F:54:LEU:CD1	3:F:242:LEU:HD22	2.39	0.53
1:A:524:ILE:O	1:A:528:ASN:ND2	2.42	0.53
3:C:208:VAL:HG11	3:C:260:ALA:CB	2.38	0.53
1:D:624:MET:HG3	2:E:412:ILE:HG23	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HB2	3:C:263:ARG:NH2	2.24	0.53
3:F:114:ARG:O	3:F:115:ALA:C	2.52	0.53
3:F:201:SER:HB2	3:F:224:PRO:O	2.09	0.53
2:B:176:LYS:HB3	2:B:176:LYS:HZ3	1.73	0.53
1:D:566:MET:CG	1:D:586:PHE:HE1	2.22	0.53
1:A:616:LEU:HD21	2:B:395:SER:HB2	1.90	0.53
1:D:536:PRO:O	1:D:537:SER:CB	2.56	0.53
2:E:388:HIS:HB3	3:F:52:LYS:NZ	2.24	0.53
3:F:152:GLN:HA	3:F:152:GLN:NE2	2.22	0.53
3:F:268:PHE:CE2	3:F:270:GLY:HA2	2.43	0.53
3:C:251:ASN:HB2	4:C:782:HOH:O	2.09	0.52
3:C:119:ASP:N	3:F:116:LEU:HD11	2.24	0.52
1:D:536:PRO:HB3	1:D:541:LEU:HB3	1.91	0.52
2:E:307:THR:HG22	2:E:307:THR:O	2.10	0.52
2:B:170:TRP:CZ2	2:B:172:GLN:HB2	2.44	0.52
3:C:219:ARG:HB3	3:F:114:ARG:HG2	1.90	0.52
2:B:166:VAL:HG11	2:B:243:ILE:HD11	1.92	0.52
3:C:227:ASP:OD2	3:C:231:TYR:HB2	2.09	0.52
3:F:7:SER:HB2	3:F:10:LYS:HB3	1.90	0.52
3:F:211:VAL:HG21	3:F:257:VAL:CG1	2.39	0.52
2:B:179:VAL:HG22	2:B:192:LEU:CD1	2.40	0.52
3:C:180:GLU:CD	3:C:180:GLU:H	2.18	0.52
3:C:27:ASN:ND2	3:C:133:PHE:HB3	2.25	0.52
3:C:309:THR:HG22	3:C:310:LEU:N	2.24	0.52
2:E:228:PHE:O	2:E:229:LEU:HD23	2.10	0.52
3:C:54:LEU:HD23	3:C:246:LYS:O	2.10	0.52
1:D:528:ASN:C	1:D:530:GLY:H	2.17	0.52
3:C:34:VAL:O	3:C:34:VAL:CG1	2.58	0.51
3:C:100:LEU:HD12	3:C:100:LEU:O	2.08	0.51
1:D:515:PRO:O	1:D:542:TRP:CZ3	2.63	0.51
3:F:211:VAL:HG21	3:F:257:VAL:HG13	1.92	0.51
1:A:525:ALA:O	1:A:529:LEU:HG	2.10	0.51
3:F:94:ASN:HD21	3:F:116:LEU:HD12	1.75	0.51
3:F:125:SER:CB	3:F:150:ILE:HD12	2.40	0.51
1:A:527:LYS:HG3	1:A:528:ASN:N	2.25	0.51
2:B:195:ASP:O	2:B:196:SER:C	2.54	0.51
3:C:179:ARG:NH1	3:C:182:HIS:CD2	2.78	0.51
1:D:497:VAL:HG12	1:D:498:THR:H	1.75	0.51
3:F:81:THR:HG21	3:F:238:ALA:HB1	1.93	0.51
3:C:120:GLN:NE2	3:C:122:ASP:HB3	2.26	0.51
1:D:536:PRO:O	1:D:537:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HD11	1:A:622:LEU:HA	1.91	0.51
1:D:466:THR:O	3:F:274:CYS:HA	2.10	0.51
1:A:548:TRP:HD1	1:A:549:LYS:H	1.57	0.51
2:B:377:VAL:HG23	2:B:378:LEU:CD1	2.41	0.51
2:B:379:ASN:C	2:B:379:ASN:HD22	2.19	0.51
3:C:54:LEU:CD2	3:C:245:ILE:HG13	2.40	0.51
3:F:54:LEU:CD2	3:F:245:ILE:HG13	2.41	0.51
1:A:463:GLU:C	1:A:465:SER:H	2.18	0.50
1:A:606:GLU:HG3	1:A:608:SER:H	1.76	0.50
2:B:319:MET:O	2:B:322:TYR:HB3	2.11	0.50
3:C:199:MET:CE	3:C:307:VAL:HG23	2.40	0.50
2:B:184:THR:O	2:B:185:LYS:HB2	2.11	0.50
3:C:27:ASN:ND2	3:C:133:PHE:CB	2.74	0.50
3:C:315:LYS:HZ1	3:F:121:LEU:HB2	1.77	0.50
3:F:248:GLY:C	3:F:249:ILE:HG13	2.36	0.50
2:E:190:ILE:HD12	2:E:190:ILE:N	2.26	0.50
3:F:85:ILE:O	3:F:89:GLN:HG3	2.11	0.50
1:A:566:MET:HE1	1:A:615:PHE:HD1	1.77	0.50
3:C:79:LEU:HA	3:C:83:ASP:OD1	2.11	0.50
3:C:142:SER:HA	3:F:118:VAL:HG12	1.91	0.50
3:C:188:ILE:HG13	3:C:193:ILE:HD11	1.93	0.50
1:D:461:LYS:HD2	1:D:462:GLU:H	1.76	0.50
2:E:185:LYS:HD3	2:E:187:ARG:HH12	1.77	0.50
3:F:7:SER:OG	3:F:10:LYS:HB3	2.12	0.50
2:B:187:ARG:O	2:B:188:LYS:HB2	2.12	0.50
3:F:212:ILE:O	3:F:215:LEU:HB2	2.11	0.50
2:B:236:MET:O	3:C:172:LYS:HE2	2.12	0.50
3:C:82:THR:HG21	3:C:219:ARG:NH1	2.15	0.50
1:D:461:LYS:O	1:D:462:GLU:HB3	2.11	0.50
2:B:388:HIS:O	2:B:390:THR:N	2.44	0.50
3:C:79:LEU:HD12	3:C:83:ASP:OD1	2.11	0.50
3:F:245:ILE:HA	3:F:249:ILE:HD12	1.94	0.50
2:B:165:PRO:HG3	2:B:207:ARG:CG	2.42	0.50
2:B:319:MET:O	2:B:323:TYR:HD1	1.95	0.50
3:C:188:ILE:HD11	3:C:280:LEU:CD2	2.42	0.50
3:F:288:ARG:HG3	3:F:288:ARG:HH11	1.77	0.50
3:F:292:VAL:HG11	3:F:295:PHE:CZ	2.46	0.50
2:B:163:MET:HE2	2:B:207:ARG:O	2.12	0.49
2:B:198:ASN:HD22	2:B:198:ASN:C	2.17	0.49
3:C:185:LYS:HD3	3:C:185:LYS:N	2.26	0.49
3:F:91:TYR:HE1	3:F:250:TYR:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:MET:HG2	2:B:209:LEU:HD12	1.93	0.49
2:E:342:GLN:O	2:E:344:PRO:HD3	2.12	0.49
2:B:342:GLN:O	2:B:344:PRO:HD3	2.12	0.49
3:C:283:ILE:HG23	3:C:295:PHE:CE1	2.47	0.49
3:C:227:ASP:O	3:C:228:GLU:C	2.54	0.49
1:D:616:LEU:HD21	2:E:395:SER:HB2	1.93	0.49
1:A:497:VAL:O	1:A:498:THR:C	2.56	0.49
1:A:506:HIS:CD2	1:A:510:ARG:HE	2.30	0.49
2:B:376:VAL:HG22	2:B:376:VAL:O	2.13	0.49
3:C:136:CYS:HA	3:C:139:MET:HE3	1.94	0.49
3:C:148:PRO:HA	3:C:164:VAL:HA	1.94	0.49
1:D:510:ARG:HG2	1:D:510:ARG:HH11	1.78	0.49
1:D:584:PHE:N	1:D:584:PHE:CD1	2.80	0.49
2:E:390:THR:CG2	3:F:48:LEU:HD11	2.37	0.49
3:F:90:TYR:O	3:F:94:ASN:HB2	2.12	0.49
3:C:91:TYR:O	3:C:91:TYR:CD2	2.66	0.49
1:D:507:PHE:CE1	2:E:378:LEU:HD23	2.47	0.49
1:D:612:ALA:CB	2:E:406:GLN:HE21	2.26	0.49
3:F:250:TYR:O	3:F:251:ASN:C	2.55	0.49
3:F:309:THR:HG22	3:F:311:SER:N	2.25	0.49
2:B:236:MET:HG2	3:C:176:LEU:HD21	1.95	0.48
1:D:549:LYS:CB	1:D:565:LEU:HG	2.43	0.48
3:F:54:LEU:HD11	3:F:242:LEU:HD22	1.95	0.48
1:A:506:HIS:NE2	1:A:510:ARG:NE	2.57	0.48
1:A:617:HIS:CE1	1:A:621:LYS:HD2	2.48	0.48
1:D:519:MET:O	1:D:523:TYR:HD1	1.96	0.48
1:D:532:GLU:OE1	1:D:547:ARG:NH2	2.46	0.48
1:D:612:ALA:CB	2:E:406:GLN:NE2	2.76	0.48
3:C:37:VAL:HG12	3:C:37:VAL:O	2.12	0.48
3:C:112:ILE:O	3:C:115:ALA:HB3	2.13	0.48
3:C:185:LYS:CA	3:C:279:LYS:HD3	2.43	0.48
3:F:112:ILE:O	3:F:115:ALA:HB3	2.11	0.48
2:B:179:VAL:HG22	2:B:192:LEU:HD11	1.94	0.48
3:F:309:THR:CG2	3:F:310:LEU:N	2.75	0.48
1:A:628:VAL:HG23	1:A:629:ASN:N	2.27	0.48
3:C:120:GLN:HE22	3:C:122:ASP:HB3	1.78	0.48
2:E:187:ARG:O	2:E:188:LYS:CB	2.62	0.48
2:E:234:ASP:OD2	2:E:238:ASN:HB2	2.13	0.48
3:C:118:VAL:HG23	3:F:116:LEU:HD21	1.96	0.48
3:C:196:GLN:NE2	3:C:305:VAL:O	2.39	0.48
1:D:589:TRP:HE1	1:D:611:SER:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:225:ILE:CD1	3:F:261:LEU:HD11	2.44	0.48
3:C:114:ARG:NE	3:C:119:ASP:OD1	2.46	0.48
3:C:134:GLU:OE2	3:C:138:LYS:HE2	2.13	0.48
3:C:212:ILE:O	3:C:215:LEU:HB2	2.13	0.48
2:E:233:THR:HA	2:E:238:ASN:O	2.13	0.48
1:A:526:LEU:O	1:A:529:LEU:N	2.42	0.48
1:A:613:TYR:HB2	1:A:614:PRO:HD3	1.95	0.48
3:F:7:SER:O	3:F:9:GLU:N	2.47	0.48
3:C:18:ALA:HB1	3:C:180:GLU:HB2	1.95	0.48
3:C:217:GLN:C	3:C:219:ARG:H	2.22	0.48
3:C:275:THR:HG22	3:C:298:VAL:O	2.14	0.47
2:E:247:GLN:OE1	2:E:247:GLN:HA	2.14	0.47
3:F:151:ASP:OD1	3:F:152:GLN:N	2.44	0.47
1:A:463:GLU:HB3	1:A:464:ASP:H	1.42	0.47
2:B:310:PRO:HG2	2:B:313:PHE:HD1	1.79	0.47
3:C:12:SER:HA	3:C:186:ILE:HD11	1.97	0.47
3:F:201:SER:HB3	3:F:224:PRO:HG2	1.95	0.47
2:B:386:ILE:CG2	2:B:412:ILE:HD11	2.44	0.47
3:C:208:VAL:HG22	3:C:255:LEU:O	2.15	0.47
2:E:381:LEU:HD11	2:E:393:VAL:CG2	2.44	0.47
3:F:188:ILE:HD11	3:F:280:LEU:CG	2.42	0.47
1:A:547:ARG:NE	1:A:565:LEU:HD13	2.30	0.47
1:D:524:ILE:O	1:D:527:LYS:HG2	2.14	0.47
1:D:546:LEU:HD11	1:D:568:MET:HB2	1.96	0.47
1:A:625:GLU:O	1:A:628:VAL:HG22	2.14	0.47
2:B:187:ARG:O	2:B:188:LYS:CB	2.62	0.47
2:B:243:ILE:O	2:B:243:ILE:HG13	2.15	0.47
1:D:617:HIS:O	1:D:620:THR:HB	2.14	0.47
1:A:520:GLY:HA3	4:A:791:HOH:O	2.14	0.47
1:A:609:THR:HG23	2:B:397:VAL:HG11	1.97	0.47
2:B:198:ASN:HD22	2:B:199:ASN:H	1.55	0.47
3:C:31:SER:HA	3:C:132:LEU:HD13	1.96	0.47
3:C:106:LEU:O	3:C:109:LEU:HB2	2.13	0.47
1:D:460:TYR:HD2	1:D:461:LYS:N	2.12	0.47
2:E:178:TYR:CB	2:E:189:MET:HB2	2.44	0.47
3:F:130:ARG:HH11	3:F:131:PRO:CD	2.21	0.47
2:B:219:VAL:HB	2:B:224:ARG:HH11	1.79	0.47
3:C:263:ARG:HH11	3:C:263:ARG:HG2	1.79	0.47
1:A:461:LYS:O	1:A:461:LYS:HG2	2.14	0.47
1:A:497:VAL:HG12	1:A:498:THR:N	2.29	0.47
3:C:238:ALA:O	3:C:241:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:114:ARG:O	3:F:115:ALA:O	2.32	0.47
2:B:384:SER:OG	2:B:392:CYS:HB3	2.16	0.47
3:C:175:ALA:CB	3:C:284:MET:HG3	2.36	0.47
3:F:85:ILE:HG23	3:F:212:ILE:HG23	1.96	0.47
3:F:197:ASP:CG	3:F:198:ASN:H	2.23	0.47
3:C:245:ILE:HA	3:C:249:ILE:CB	2.39	0.46
1:D:496:LEU:HD11	3:F:246:LYS:HZ3	1.80	0.46
1:A:515:PRO:HB2	1:A:542:TRP:CZ3	2.50	0.46
2:B:184:THR:HG23	2:B:188:LYS:HB3	1.96	0.46
2:E:378:LEU:HD12	2:E:378:LEU:N	2.29	0.46
3:F:228:GLU:CD	3:F:228:GLU:N	2.73	0.46
1:A:613:TYR:O	1:A:614:PRO:C	2.55	0.46
1:A:619:THR:O	1:A:623:ILE:HG13	2.14	0.46
3:C:119:ASP:C	3:F:116:LEU:HD22	2.40	0.46
3:F:25:PHE:CD1	3:F:178:CYS:SG	3.08	0.46
3:F:318:LEU:O	3:F:319:LEU:HD23	2.15	0.46
2:B:410:THR:HG22	2:B:411:PRO:HD2	1.97	0.46
3:C:104:LEU:CD2	3:C:112:ILE:HD12	2.46	0.46
2:E:193:ILE:N	2:E:193:ILE:HD12	2.30	0.46
1:A:590:GLU:CG	1:A:591:SER:H	2.27	0.46
1:D:628:VAL:HG23	1:D:629:ASN:N	2.29	0.46
1:A:461:LYS:O	1:A:462:GLU:HG2	2.15	0.46
1:D:548:TRP:HD1	1:D:549:LYS:N	2.14	0.46
1:D:611:SER:C	1:D:614:PRO:HD2	2.41	0.46
3:F:9:GLU:O	3:F:13:ILE:HB	2.15	0.46
3:F:19:VAL:HG12	3:F:23:ARG:HH21	1.80	0.46
1:A:547:ARG:CZ	1:A:565:LEU:HD13	2.46	0.46
1:D:529:LEU:HD11	1:D:622:LEU:HA	1.97	0.46
3:F:54:LEU:HD21	3:F:245:ILE:HG13	1.96	0.46
1:A:534:ALA:O	1:A:536:PRO:HD3	2.16	0.46
3:F:227:ASP:OD1	3:F:227:ASP:C	2.59	0.46
2:E:182:SER:C	2:E:184:THR:H	2.24	0.46
2:E:214:ARG:HB2	2:E:214:ARG:NH1	2.22	0.46
3:F:220:VAL:HG22	3:F:221:SER:N	2.31	0.46
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.81	0.45
1:A:536:PRO:O	1:A:537:SER:HB3	2.17	0.45
3:C:188:ILE:CG2	3:C:194:ILE:HD11	2.46	0.45
1:D:496:LEU:HD13	3:F:263:ARG:NH2	2.31	0.45
1:A:505:TRP:HH2	3:C:40:ARG:HE	1.64	0.45
2:B:324:TYR:OH	2:B:328:ARG:NH2	2.48	0.45
2:B:389:ASN:O	2:B:389:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:VAL:HG12	2:B:398:ARG:N	2.30	0.45
1:D:571:GLN:O	1:D:582:VAL:HA	2.16	0.45
1:A:517:ASP:HA	4:A:791:HOH:O	2.16	0.45
1:A:549:LYS:CB	1:A:565:LEU:HD23	2.46	0.45
3:F:7:SER:C	3:F:9:GLU:N	2.73	0.45
1:A:524:ILE:O	1:A:527:LYS:HG2	2.16	0.45
1:A:527:LYS:HB3	1:A:533:TRP:HH2	1.81	0.45
2:B:165:PRO:HG3	2:B:207:ARG:HG3	1.98	0.45
2:B:390:THR:HG21	3:C:48:LEU:HD11	1.97	0.45
3:C:293:HIS:O	3:C:294:ARG:HB3	2.15	0.45
3:F:296:PHE:CD2	3:F:307:VAL:HG13	2.52	0.45
1:A:462:GLU:OE1	1:A:462:GLU:HA	2.16	0.45
2:B:195:ASP:O	2:B:197:ASP:N	2.50	0.45
1:A:548:TRP:CD2	1:A:618:LEU:HD13	2.51	0.45
1:D:514:TYR:C	1:D:516:LEU:H	2.24	0.45
1:D:547:ARG:HG2	1:D:548:TRP:H	1.82	0.45
3:F:12:SER:HA	3:F:186:ILE:HD11	1.98	0.45
3:F:55:ASN:O	3:F:59:GLN:HB2	2.16	0.45
3:C:234:ASN:OD1	3:C:235:VAL:N	2.41	0.45
3:F:197:ASP:O	3:F:198:ASN:HB2	2.16	0.45
2:B:317:SER:O	2:B:321:ARG:HG3	2.16	0.45
2:B:406:GLN:HB3	4:B:808:HOH:O	2.17	0.45
2:E:202:PHE:N	2:E:202:PHE:CD1	2.85	0.45
1:A:506:HIS:CD2	1:A:510:ARG:NE	2.85	0.45
1:A:527:LYS:HE3	1:A:528:ASN:OD1	2.16	0.45
1:D:625:GLU:O	1:D:628:VAL:HG22	2.17	0.45
2:E:410:THR:CG2	3:F:45:ASP:HB2	2.46	0.45
2:B:246:ARG:HH22	2:B:398:ARG:NH1	2.14	0.44
3:C:114:ARG:HH21	3:F:93:SER:HA	1.82	0.44
3:C:115:ALA:O	3:C:116:LEU:C	2.59	0.44
3:C:120:GLN:OE1	3:C:122:ASP:HB3	2.17	0.44
3:F:199:MET:HE1	3:F:304:LEU:HD11	1.99	0.44
3:F:314:LEU:O	3:F:318:LEU:HG	2.17	0.44
1:D:581:LEU:C	1:D:581:LEU:HD23	2.42	0.44
2:E:178:TYR:HB3	2:E:189:MET:HB2	2.00	0.44
3:F:130:ARG:HH12	3:F:134:GLU:HB2	1.82	0.44
1:A:541:LEU:HG	1:A:543:THR:H	1.82	0.44
1:A:566:MET:CE	1:A:615:PHE:HD1	2.30	0.44
1:D:624:MET:CG	2:E:412:ILE:HG23	2.47	0.44
3:C:294:ARG:HD2	3:C:296:PHE:CE1	2.52	0.44
3:C:309:THR:CG2	3:C:310:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ARG:HG3	3:F:262:MET:CE	2.47	0.44
3:F:171:LEU:HD12	3:F:310:LEU:HD22	2.00	0.44
3:F:296:PHE:CE2	3:F:307:VAL:HG13	2.52	0.44
3:C:120:GLN:CA	3:F:116:LEU:HD22	2.48	0.44
1:D:583:ASP:OD1	2:E:380:HIS:HB3	2.17	0.44
2:E:375:HIS:CE1	2:E:376:VAL:HG12	2.52	0.44
3:F:43:VAL:HG22	3:F:66:PRO:HG2	2.00	0.44
3:F:106:LEU:O	3:F:109:LEU:HB2	2.18	0.44
1:A:532:GLU:OE2	1:A:547:ARG:NH2	2.47	0.44
3:C:227:ASP:OD1	3:C:227:ASP:C	2.60	0.44
1:D:514:TYR:CD1	1:D:514:TYR:N	2.86	0.44
1:A:466:THR:HB	3:C:278:ASP:OD1	2.18	0.44
2:B:176:LYS:NZ	2:B:176:LYS:CB	2.72	0.44
2:B:195:ASP:OD1	2:B:201:SER:HB3	2.17	0.44
3:C:212:ILE:HA	3:C:215:LEU:HD12	2.00	0.44
1:D:529:LEU:CD1	1:D:622:LEU:HA	2.48	0.44
2:E:213:HIS:O	2:E:242:TYR:HA	2.17	0.44
3:F:85:ILE:HG23	3:F:212:ILE:CG2	2.47	0.44
1:D:572:LEU:HD12	1:D:581:LEU:O	2.18	0.43
2:B:312:VAL:HG12	2:B:312:VAL:O	2.17	0.43
3:C:39:TYR:OH	3:C:162:VAL:HG12	2.17	0.43
3:C:109:LEU:HD12	3:C:109:LEU:HA	1.77	0.43
3:F:199:MET:SD	3:F:306:GLY:HA2	2.58	0.43
2:B:386:ILE:HG21	2:B:412:ILE:HD11	2.00	0.43
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.33	0.43
3:C:217:GLN:C	3:C:219:ARG:N	2.76	0.43
3:F:34:VAL:CG1	3:F:34:VAL:O	2.66	0.43
2:B:346:GLN:H	2:B:346:GLN:HE21	1.66	0.43
3:C:120:GLN:CD	3:F:117:GLY:HA2	2.44	0.43
1:D:497:VAL:HA	4:D:734:HOH:O	2.18	0.43
1:A:548:TRP:HD1	1:A:549:LYS:N	2.16	0.43
3:C:159:GLU:O	3:C:160:ILE:HG12	2.19	0.43
3:C:165:LEU:HD21	3:C:170:ILE:HD11	1.99	0.43
3:C:209:ILE:HD12	3:C:210:ASP:H	1.83	0.43
3:F:15:GLN:OE1	3:F:184:LEU:HA	2.18	0.43
3:F:180:GLU:H	3:F:180:GLU:CD	2.27	0.43
3:F:182:HIS:O	3:F:182:HIS:ND1	2.51	0.43
3:C:196:GLN:O	3:C:197:ASP:C	2.62	0.43
1:D:543:THR:HG21	1:D:545:LYS:HZ2	1.83	0.43
3:F:126:ILE:HD12	3:F:138:LYS:HD2	2.01	0.43
1:A:526:LEU:O	1:A:527:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:CD1	1:A:582:VAL:HG22	2.49	0.43
3:C:199:MET:HE1	3:C:306:GLY:HA2	2.00	0.43
1:D:570:ILE:HG22	1:D:582:VAL:HG12	2.00	0.43
2:B:198:ASN:C	2:B:198:ASN:ND2	2.77	0.43
3:C:192:ASN:C	3:C:192:ASN:HD22	2.27	0.43
1:A:610:PHE:CE2	3:C:152:GLN:C	2.97	0.43
3:C:178:CYS:O	3:C:181:THR:HG23	2.19	0.43
3:C:251:ASN:C	3:C:253:LEU:N	2.77	0.43
1:A:590:GLU:HG3	1:A:591:SER:N	2.32	0.42
1:D:527:LYS:HB3	1:D:533:TRP:HH2	1.83	0.42
2:E:174:GLY:O	2:E:202:PHE:CZ	2.66	0.42
1:A:580:TYR:CD1	1:A:580:TYR:N	2.86	0.42
3:C:118:VAL:C	3:F:116:LEU:HD11	2.44	0.42
3:C:127:HIS:CD2	3:C:129:SER:HB2	2.55	0.42
2:B:404:VAL:HG22	3:C:39:TYR:CZ	2.55	0.42
3:C:49:LEU:O	3:C:52:LYS:N	2.50	0.42
3:C:251:ASN:C	3:C:253:LEU:H	2.27	0.42
1:D:609:THR:C	1:D:611:SER:N	2.76	0.42
1:D:610:PHE:N	1:D:610:PHE:CD2	2.88	0.42
2:E:171:GLN:HG3	2:E:228:PHE:CD1	2.54	0.42
2:E:376:VAL:HG22	2:E:376:VAL:O	2.19	0.42
2:E:389:ASN:HD22	2:E:389:ASN:HA	1.55	0.42
3:F:111:ASP:O	3:F:115:ALA:HB2	2.20	0.42
1:A:479:ARG:HG3	3:C:262:MET:HE2	2.01	0.42
1:A:519:MET:HB3	2:B:313:PHE:CD2	2.54	0.42
1:A:548:TRP:O	1:A:566:MET:N	2.42	0.42
1:D:520:GLY:O	1:D:524:ILE:HG13	2.18	0.42
3:F:25:PHE:HD1	3:F:178:CYS:SG	2.43	0.42
3:F:139:MET:HE1	3:F:170:ILE:HG13	2.02	0.42
3:C:283:ILE:HD13	3:C:308:LEU:HD23	2.02	0.42
1:D:503:THR:HG22	1:D:504:ARG:HG2	2.00	0.42
1:D:609:THR:C	1:D:611:SER:H	2.27	0.42
3:F:172:LYS:O	3:F:176:LEU:HB2	2.19	0.42
3:F:188:ILE:CD1	3:F:280:LEU:HG	2.48	0.42
3:C:196:GLN:O	3:C:197:ASP:O	2.37	0.42
1:D:479:ARG:HG3	3:F:262:MET:HE3	2.00	0.42
1:D:536:PRO:HA	1:D:541:LEU:HD23	2.01	0.42
3:F:263:ARG:O	3:F:264:ARG:C	2.62	0.42
3:C:75:PHE:HB3	3:C:159:GLU:OE1	2.20	0.42
1:A:549:LYS:HB3	1:A:565:LEU:HD23	2.01	0.42
2:B:163:MET:HG2	2:B:209:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ILE:HG22	3:C:250:TYR:N	2.35	0.42
1:D:514:TYR:HD1	1:D:514:TYR:H	1.67	0.42
3:F:293:HIS:CE1	4:F:768:HOH:O	2.73	0.42
1:A:463:GLU:C	1:A:465:SER:N	2.78	0.42
1:A:609:THR:HA	2:B:397:VAL:HG11	2.01	0.42
3:C:179:ARG:C	3:C:181:THR:H	2.27	0.42
1:A:519:MET:HG2	2:B:313:PHE:CE2	2.55	0.41
2:B:225:VAL:HG13	2:B:241:ASN:CG	2.45	0.41
2:B:408:LEU:HG	4:B:757:HOH:O	2.19	0.41
3:C:143:ARG:HE	3:F:114:ARG:NH2	2.18	0.41
1:A:509:ILE:HD12	1:A:584:PHE:HZ	1.84	0.41
3:F:138:LYS:O	3:F:141:GLU:HB2	2.20	0.41
3:F:140:LEU:HA	3:F:140:LEU:HD23	1.77	0.41
1:A:546:LEU:HG	1:A:568:MET:HB3	2.02	0.41
2:B:164:VAL:HA	2:B:165:PRO:HD3	1.84	0.41
2:B:198:ASN:ND2	2:B:199:ASN:N	2.59	0.41
3:C:199:MET:HE1	3:C:307:VAL:HG23	2.02	0.41
1:D:514:TYR:O	1:D:516:LEU:N	2.40	0.41
1:D:533:TRP:HA	1:D:546:LEU:HA	2.02	0.41
1:A:527:LYS:CG	1:A:528:ASN:N	2.84	0.41
2:B:193:ILE:HG23	2:B:194:PRO:HD2	2.02	0.41
1:A:566:MET:HE1	1:A:615:PHE:HA	2.03	0.41
3:C:120:GLN:CD	3:C:122:ASP:HB3	2.45	0.41
2:E:174:GLY:HA2	2:E:220:ASP:OD2	2.20	0.41
3:C:37:VAL:O	3:C:37:VAL:CG1	2.69	0.41
3:C:179:ARG:O	3:C:181:THR:N	2.54	0.41
2:E:170:TRP:CD1	2:E:172:GLN:H	2.39	0.41
2:B:377:VAL:CG2	2:B:378:LEU:HD12	2.48	0.41
3:C:27:ASN:HD22	3:C:27:ASN:HA	1.51	0.41
3:C:27:ASN:HD22	3:C:133:PHE:HB3	1.84	0.41
3:C:245:ILE:O	3:C:246:LYS:C	2.63	0.41
1:D:612:ALA:HB3	2:E:406:GLN:NE2	2.35	0.41
2:E:340:PRO:HA	2:E:341:PRO:HD2	1.88	0.41
3:F:122:ASP:OD1	3:F:122:ASP:C	2.63	0.41
3:F:293:HIS:O	3:F:294:ARG:HB3	2.19	0.41
3:C:15:GLN:OE1	3:C:184:LEU:HA	2.21	0.41
3:C:146:ARG:HA	3:C:165:LEU:O	2.21	0.41
1:D:543:THR:HG21	1:D:545:LYS:HZ3	1.85	0.41
2:E:235:GLN:H	2:E:235:GLN:HG2	1.69	0.41
2:B:192:LEU:HB3	2:B:202:PHE:HB3	2.03	0.41
2:B:380:HIS:ND1	2:B:380:HIS:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:GLN:HE22	3:C:216:THR:CB	2.34	0.41
3:C:141:GLU:CB	3:F:118:VAL:HB	2.44	0.41
1:D:568:MET:HE3	1:D:584:PHE:HB3	2.03	0.41
3:C:309:THR:O	3:C:313:ILE:HG13	2.20	0.41
2:E:201:SER:C	2:E:202:PHE:CD1	2.99	0.41
1:D:464:ASP:O	1:D:464:ASP:OD1	2.37	0.40
3:F:137:LEU:HA	3:F:137:LEU:HD23	1.86	0.40
3:F:166:THR:O	3:F:170:ILE:HG12	2.21	0.40
3:F:188:ILE:CG2	3:F:194:ILE:HD11	2.51	0.40
2:B:377:VAL:O	2:B:378:LEU:HD12	2.20	0.40
3:C:64:SER:HA	3:C:79:LEU:O	2.21	0.40
3:C:120:GLN:OE1	3:C:120:GLN:C	2.64	0.40
3:F:119:ASP:OD1	3:F:121:LEU:HD11	2.21	0.40
3:C:273:THR:HA	3:C:296:PHE:O	2.21	0.40
2:E:375:HIS:HB3	2:E:378:LEU:HD13	2.03	0.40
1:A:578:ASN:CG	1:A:579:ASN:H	2.30	0.40
3:C:179:ARG:NH1	3:C:182:HIS:CG	2.90	0.40
3:F:19:VAL:HG12	3:F:23:ARG:NH2	2.35	0.40
3:F:123:THR:O	3:F:123:THR:HG22	2.22	0.40
3:F:197:ASP:CG	3:F:198:ASN:N	2.78	0.40
3:F:299:ASP:OD1	3:F:303:ARG:HB2	2.21	0.40
2:B:189:MET:HG2	2:B:218:ILE:HD13	2.02	0.40
3:F:127:HIS:HA	3:F:128:PRO:HD3	1.86	0.40
3:F:141:GLU:OE1	3:F:141:GLU:HA	2.20	0.40
3:F:318:LEU:C	3:F:319:LEU:HG	2.46	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	121/171 (71%)	105 (87%)	13 (11%)	3 (2%)	4 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	121/171 (71%)	105 (87%)	11 (9%)	5 (4%)	2	3
2	B	147/252 (58%)	125 (85%)	17 (12%)	5 (3%)	3	4
2	E	132/252 (52%)	115 (87%)	11 (8%)	6 (4%)	2	2
3	C	306/315 (97%)	265 (87%)	32 (10%)	9 (3%)	3	6
3	F	306/315 (97%)	272 (89%)	27 (9%)	7 (2%)	5	9
All	All	1133/1476 (77%)	987 (87%)	111 (10%)	35 (3%)	3	5

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	188	LYS
2	B	379	ASN
3	C	197	ASP
3	C	246	LYS
2	E	188	LYS
2	E	379	ASN
2	E	387	LYS
2	E	388	HIS
3	F	115	ALA
3	F	246	LYS
1	A	536	PRO
2	B	196	SER
3	C	143	ARG
3	C	180	GLU
3	C	217	GLN
3	C	229	ASN
1	D	548	TRP
3	F	8	GLN
3	F	143	ARG
3	F	250	TYR
2	B	389	ASN
3	C	250	TYR
1	D	462	GLU
1	D	529	LEU
1	D	536	PRO
2	E	386	ILE
3	F	96	ASP
3	C	124	ALA
3	C	216	THR
1	D	515	PRO

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Mol	Chain	Res	Type
3	F	217	GLN
1	A	463	GLU
1	A	464	ASP
2	B	345	PRO
2	E	341	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/155 (77%)	109 (92%)	10 (8%)	10	23
1	D	119/155 (77%)	114 (96%)	5 (4%)	26	52
2	B	145/234 (62%)	135 (93%)	10 (7%)	14	32
2	E	130/234 (56%)	119 (92%)	11 (8%)	10	22
3	C	285/290 (98%)	265 (93%)	20 (7%)	14	31
3	F	285/290 (98%)	266 (93%)	19 (7%)	15	33
All	All	1083/1358 (80%)	1008 (93%)	75 (7%)	14	32

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	LYS
1	A	462	GLU
1	A	463	GLU
1	A	485	GLN
1	A	496	LEU
1	A	506	HIS
1	A	524	ILE
1	A	545	LYS
1	A	546	LEU
1	A	564	ASP
2	B	176	LYS
2	B	179	VAL
2	B	189	MET

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Mol	Chain	Res	Type
2	B	214	ARG
2	B	223	LEU
2	B	235	GLN
2	B	318	VAL
2	B	346	GLN
2	B	380	HIS
2	B	410	THR
3	C	19	VAL
3	C	24	LYS
3	C	27	ASN
3	C	52	LYS
3	C	81	THR
3	C	120	GLN
3	C	179	ARG
3	C	185	LYS
3	C	188	ILE
3	C	209	ILE
3	C	246	LYS
3	C	257	VAL
3	C	264	ARG
3	C	281	SER
3	C	288	ARG
3	C	291	ARG
3	C	292	VAL
3	C	300	ASP
3	C	301	VAL
3	C	307	VAL
1	D	468	SER
1	D	485	GLN
1	D	578	ASN
1	D	584	PHE
1	D	624	MET
2	E	176	LYS
2	E	179	VAL
2	E	180	THR
2	E	214	ARG
2	E	223	LEU
2	E	235	GLN
2	E	243	ILE
2	E	386	ILE
2	E	389	ASN
2	E	391	LEU

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Mol	Chain	Res	Type
2	E	393	VAL
3	F	13	ILE
3	F	28	SER
3	F	34	VAL
3	F	49	LEU
3	F	52	LYS
3	F	81	THR
3	F	120	GLN
3	F	200	LYS
3	F	209	ILE
3	F	228	GLU
3	F	241	VAL
3	F	246	LYS
3	F	257	VAL
3	F	264	ARG
3	F	284	MET
3	F	300	ASP
3	F	301	VAL
3	F	303	ARG
3	F	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN
1	A	578	ASN
1	A	617	HIS
2	B	172	GLN
2	B	198	ASN
2	B	221	ASN
2	B	235	GLN
2	B	238	ASN
2	B	346	GLN
2	B	375	HIS
2	B	389	ASN
2	B	406	GLN
3	C	27	ASN
3	C	59	GLN
3	C	94	ASN
3	C	105	GLN
3	C	127	HIS
3	C	152	GLN

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Mol	Chain	Res	Type
3	C	192	ASN
3	C	213	GLN
3	C	217	GLN
1	D	478	HIS
1	D	506	HIS
1	D	571	GLN
1	D	574	GLN
1	D	617	HIS
2	E	172	GLN
2	E	198	ASN
2	E	235	GLN
2	E	238	ASN
2	E	346	GLN
2	E	375	HIS
2	E	389	ASN
2	E	406	GLN
3	F	16	GLN
3	F	60	ASN
3	F	127	HIS
3	F	152	GLN
3	F	192	ASN
3	F	196	GLN
3	F	217	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	133/171 (77%)	0.74	11 (8%)	17 13	38, 75, 96, 99	0
1	D	133/171 (77%)	0.80	12 (9%)	15 11	40, 81, 100, 102	0
2	B	155/252 (61%)	0.41	9 (5%)	29 23	37, 65, 97, 101	0
2	E	140/252 (55%)	0.53	13 (9%)	14 11	39, 62, 101, 102	0
3	C	310/315 (98%)	0.22	10 (3%)	50 44	37, 57, 93, 102	0
3	F	310/315 (98%)	0.38	21 (6%)	23 19	35, 59, 93, 102	0
All	All	1181/1476 (80%)	0.45	76 (6%)	25 20	35, 63, 97, 102	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	250	TYR	5.8
3	F	152	GLN	4.6
2	E	314	THR	4.4
1	A	503	THR	3.9
1	A	537	SER	3.8
3	C	116	LEU	3.8
2	E	312	VAL	3.7
3	F	99	GLU	3.6
3	C	143	ARG	3.6
3	C	134	GLU	3.5
3	F	249	ILE	3.4
1	A	612	ALA	3.4
2	E	307	THR	3.3
3	F	159	GLU	3.3
2	E	389	ASN	3.2
3	F	119	ASP	3.2
1	D	514	TYR	3.2
1	A	541	LEU	3.1
1	D	509	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	266	ASP	3.0
3	F	114	ARG	3.0
1	D	541	LEU	3.0
1	D	609	THR	2.8
2	E	162	LEU	2.8
2	E	344	PRO	2.8
1	D	582	VAL	2.8
2	B	322	TYR	2.8
1	D	611	SER	2.8
3	F	160	ILE	2.7
3	F	121	LEU	2.7
2	E	311	ALA	2.6
2	E	340	PRO	2.6
1	D	503	THR	2.6
2	E	345	PRO	2.6
2	B	389	ASN	2.6
3	F	116	LEU	2.5
3	C	250	TYR	2.5
3	F	143	ARG	2.5
3	F	158	ARG	2.5
3	C	158	ARG	2.4
2	B	377	VAL	2.4
1	D	629	ASN	2.4
1	A	505	TRP	2.4
3	C	228	GLU	2.4
1	A	628	VAL	2.4
3	C	123	THR	2.4
3	F	198	ASN	2.4
2	B	344	PRO	2.4
1	A	627	ALA	2.4
2	B	343	LEU	2.3
3	F	123	THR	2.3
1	A	498	THR	2.3
1	D	498	THR	2.3
3	F	118	VAL	2.3
2	E	199	ASN	2.3
2	B	340	PRO	2.2
2	B	247	GLN	2.2
1	A	460	TYR	2.2
1	D	511	SER	2.2
1	A	513	SER	2.2
1	D	537	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	507	PHE	2.2
3	F	120	GLN	2.2
3	C	100	LEU	2.2
1	D	518	VAL	2.2
2	E	161	SER	2.2
3	C	249	ILE	2.1
3	F	107	ASP	2.1
3	F	228	GLU	2.1
2	B	164	VAL	2.1
2	E	342	GLN	2.0
3	F	144	SER	2.0
2	E	341	PRO	2.0
3	F	191	LEU	2.0
3	C	251	ASN	2.0
2	B	245	VAL	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.