



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:08 pm GMT

PDB ID : 5UI8
Title : structure of sigmaN-holoenzyme
Authors : Darst, S.A.; Campbell, E.A.
Deposited on : 2017-01-13
Resolution : 3.76 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

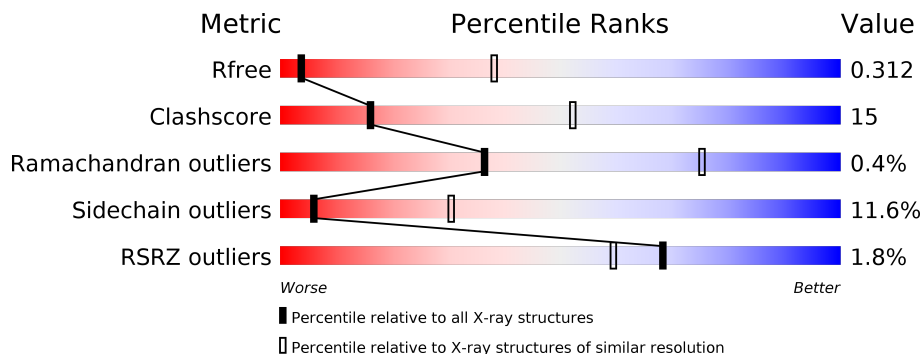
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.76 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}	111664	1140 (4.00-3.52)
Clashscore	122126	1003 (3.98-3.54)
Ramachandran outliers	120053	1172 (4.00-3.52)
Sidechain outliers	120020	1166 (4.00-3.52)
RSRZ outliers	108989	1056 (4.00-3.52)

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	G	329	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>•</div> <div>6%</div> </div> </div>
1	H	329	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>21%</div> <div>•</div> <div>35%</div> </div> </div>
2	I	1342	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>31%</div> <div>•</div> <div>9%</div> </div> </div>
3	J	1407	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>•</div> <div>5%</div> </div> </div>
4	K	91	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>26%</div> <div>7%</div> <div>13%</div> </div> </div>
5	M	477	<div> <div></div> <div> <div></div> <div>47%</div> <div>28%</div> <div>5%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27004 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	309	Total	C	N	O	S	0	0	0
			2337	1463	408	459	7			
1	H	215	Total	C	N	O	S	0	0	0
			1619	1013	279	321	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	1217	Total	C	N	O	S	0	0	0
			9382	5883	1632	1827	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	516	VAL	ASP	conflict	UNP B7MIX3

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1336	Total	C	N	O	S	0	0	0
			10148	6364	1812	1923	49			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	79	Total	C	N	O	S	0	0	0
			620	377	118	124	1			

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

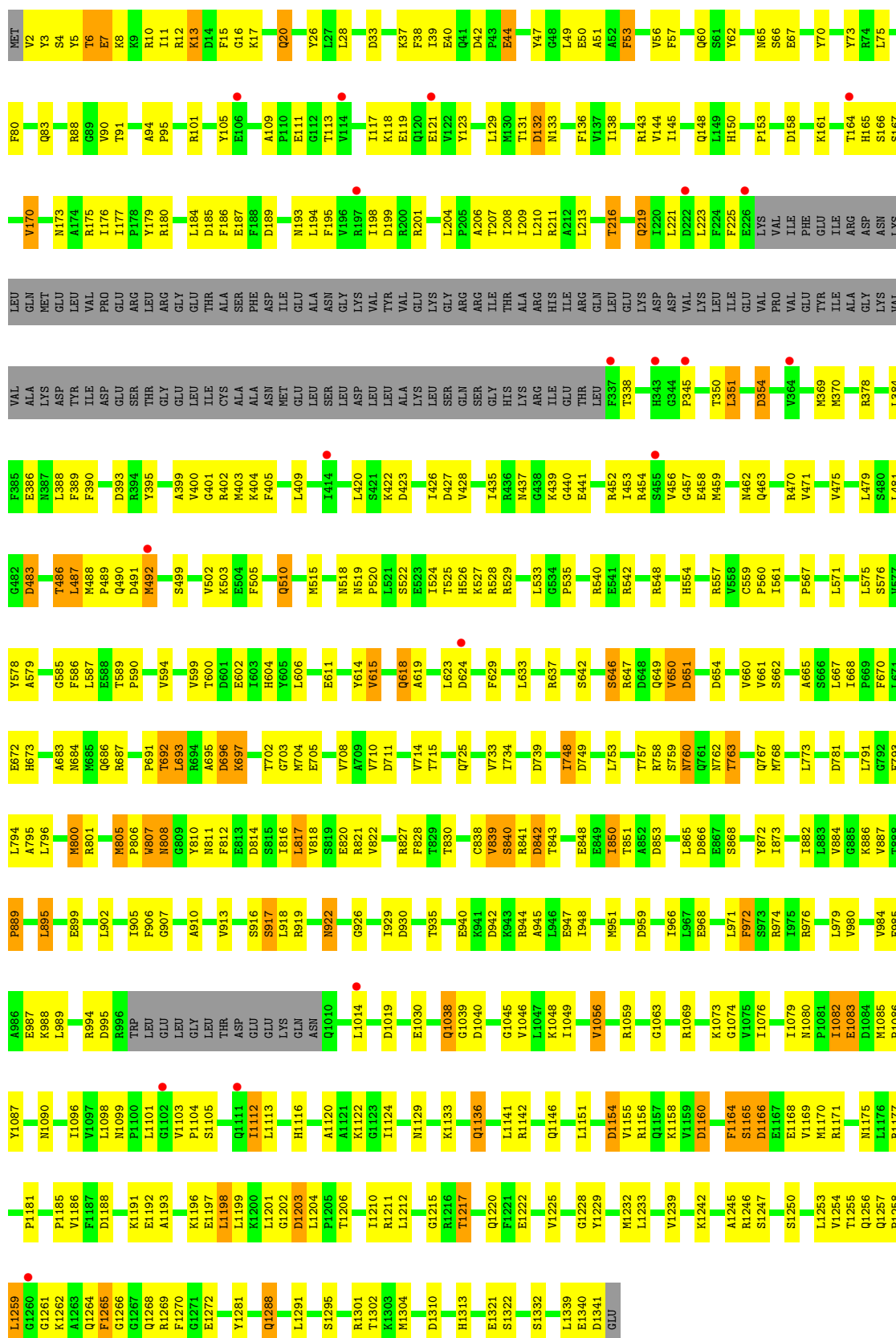
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	380	Total	C	N	O	S	0	0	0
			2895	1825	499	561	10			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		





ASP
ALA
SER
ALA
SER
LEU
ALA
GLU
LEU
LEU
ASN
ALA
GLY
LEU
GLY
GLY
SER
ASP
ASN
GLU

• Molecule 4: DNA-directed RNA polymerase subunit omega



MET A2 R3 V4 T5 V6 Q7 N15 R16 F17 V20 L21 V22 R25 R26 Q29 R30 Q31 L25 L26 K35 D36 V39 K45 T46 I49 A50 L51 R52 E53 I54 E55 E56 Q57 L58 I59 N60 M61 Q62 V66 R67 E68 R69 E76 L80 GLN ALA VAL THR ALA ILE

ALA
GLU
GLY
ARG
ARG

• Molecule 5: RNA polymerase sigma-54 factor



MET LYS GLN GLY LEU GLN LEU ARG R20 R24 L25 L26 Q27 L28 S29 L33 Q34 L37 Q38 L41 E42 E43 R44 P45 D54 E55 VAL GLU LYS VAL ASP ARG GLU SER LEU ASP THR VAL ASP ALA LEU

GLU GLN LYS MET PRO ASP GLU PRO LEU ASP ALA SER TRP ASP ILE TYR THR ALA GLY THR R20 R24 L25 L26 Q27 L28 S29 L33 Q34 L37 Q38 L41 E42 E43 R44 P45 D54 E55 VAL GLU LYS VAL ASP ARG GLU SER LEU ASP THR VAL ASP ALA LEU

D149 D150 Y153 L154 T155 T156 Q157 I158 V162 I165 D166 D167 D168 E169 I170 G171 L172 E173 E176 K180 R181 I182 Q183 R184 F185 D186 P187 V190 A191 A192 L195 R196 D197 C198 L199 L200 L201 Q202 L203 F206 A207 T210 P211 Q212 L213 A216 R217 S221

D222 H223 L224 D225 L226 L227 A228 H229 H230 ASP PHE R233 R234 L235 M236 T239 K242 E243 E244 V245 L246 I253 D257 P258 I264 H265 T266 S267 E268 P269 D275 D276 L277 V278 R279 K280 W285 T286 V287 E288 L289 N290 P295 R296 Q301 Q302 Y303 R305 R306 S307 S308 Q309 Q310 Q311 Q312 Q313 D137 R138 A139 I140 I144

SER ALA ARG ASN ASP A314 F318 I319 L333 R336 L341 R345 Q350 Q351 Q352 A353 F354 F355 Q358 E359 E360 Y361 M362 K363 P364 M365 P366 L367 A368 D369 I370 A371 V374 E375 H376 H377 E378 S379 T380 I381 S382 R383 V384 T385 T386 Q387 K388 Y389 L390 H391 S392 P393

R394 F397 E398 I399 S405 HIS VAL ASN THR GLY GLY GLY GLU ALA16 R421 V424 K425 I428 M432 S438 D439 A459 R462 L465 S466 I467 K474 GLN LEU VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.48Å 151.52Å 195.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.76 29.64 – 3.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.64-3.76) 98.4 (29.64-3.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.262 , 0.312 0.262 , 0.312	Depositor DCC
R_{free} test set	3074 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 103.3	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	27004	wwPDB-VP
Average B, all atoms (Å ²)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	G	0.27	0/2366	0.55	0/3215
1	H	0.25	0/1637	0.49	0/2224
2	I	0.28	1/9533 (0.0%)	0.49	0/12893
3	J	0.26	1/10294 (0.0%)	0.48	3/13920 (0.0%)
4	K	0.24	0/622	0.43	0/838
5	M	0.30	0/2935	0.57	4/3989 (0.1%)
All	All	0.27	2/27387 (0.0%)	0.50	7/37079 (0.0%)

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
1	G	0	1
2	I	0	5
3	J	0	4
5	M	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	109	ALA	C-N	11.59	1.56	1.34
3	J	120	LEU	C-N	6.71	1.47	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	213	LEU	CA-CB-CG	8.34	134.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	425	ARG	NE-CZ-NH2	-7.53	116.53	120.30
5	M	399	LEU	CA-CB-CG	6.10	129.34	115.30
3	J	265	LEU	N-CA-C	-5.19	97.00	111.00
3	J	78	LEU	CA-CB-CG	5.13	127.10	115.30
5	M	213	LEU	CB-CG-CD2	5.12	119.70	111.00
5	M	268	GLU	C-N-CD	-5.08	109.43	120.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	194	GLN	Peptide
2	I	1040	ASP	Peptide
2	I	1154	ASP	Peptide
2	I	1202	GLY	Peptide
2	I	1259	LEU	Peptide
2	I	889	PRO	Peptide
3	J	1296	GLY	Peptide
3	J	263	SER	Peptide
3	J	264	ASP	Peptide
3	J	320	ASN	Peptide
5	M	210	THR	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	G	2337	0	2343	75	0
1	H	1619	0	1619	54	0
2	I	9382	0	9211	315	0
3	J	10148	0	10169	325	1
4	K	620	0	621	20	0
5	M	2895	0	2828	115	1
6	J	1	0	0	0	0
7	J	2	0	0	0	0
All	All	27004	0	26791	831	1

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 15.

All (831) 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:I:49:LEU:O	2:I:53:PHE:HB2	1.68	0.93
1:G:43:LEU:O	1:G:47:LEU:HB2	1.74	0.88
5:M:216:ALA:HB1	5:M:253:ILE:HD11	1.56	0.87
3:J:289:ASP:O	3:J:293:ARG:HB2	1.77	0.84
5:M:127:GLN:HE22	5:M:182:ILE:HA	1.45	0.82
2:I:1154:ASP:HB3	2:I:1155:VAL:HG22	1.60	0.81
2:I:1245:ALA:HB2	3:J:372:MET:HG3	1.62	0.81
5:M:26:LEU:O	5:M:388:LYS:NZ	2.14	0.81
3:J:265:LEU:O	3:J:268:LEU:N	2.14	0.80
5:M:425:LYS:HB2	5:M:465:LEU:HD11	1.63	0.80
5:M:158:ILE:HD11	5:M:176:GLU:HG2	1.64	0.80
2:I:101:ARG:HG3	2:I:118:LYS:HB2	1.65	0.79
5:M:45:PRO:O	5:M:301:GLN:NE2	2.16	0.79
1:H:50:SER:HA	1:H:151:GLY:HA2	1.64	0.79
1:H:71:LYS:HA	1:H:72:GLU:HB2	1.65	0.78
2:I:8:LYS:HE3	2:I:1171:ARG:HH22	1.46	0.78
5:M:351:GLN:NE2	5:M:363:LYS:O	2.17	0.78
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.48	0.78
2:I:1262:LYS:HG2	2:I:1268:GLN:HE22	1.47	0.77
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.18	0.76
5:M:285:TRP:HZ3	5:M:352:GLN:HG3	1.49	0.76
1:H:109:PRO:HA	1:H:133:LEU:H	1.51	0.76
1:G:309:SER:O	5:M:184:ARG:NH1	2.19	0.76
5:M:439:ASP:OD2	5:M:462:ARG:NH2	2.19	0.76
1:H:60:GLU:HG2	1:H:143:ARG:H	1.52	0.75
2:I:1268:GLN:HG3	3:J:352:ARG:HG3	1.67	0.75
2:I:211:ARG:HH21	2:I:351:LEU:HD21	1.52	0.75
5:M:127:GLN:HB2	5:M:185:PHE:CD2	2.22	0.74
2:I:886:LYS:HB3	2:I:917:SER:HA	1.69	0.74
2:I:971:LEU:HD11	2:I:1014:LEU:HD11	1.70	0.74
2:I:499:SER:O	2:I:503:LYS:HB2	1.88	0.74
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.71	0.73
3:J:154:LEU:H	3:J:154:LEU:HD12	1.53	0.73
2:I:907:GLY:O	2:I:910:ALA:HA	1.88	0.73
2:I:1268:GLN:HE21	3:J:352:ARG:HE	1.37	0.72
1:G:47:LEU:HB3	1:G:183:ILE:HD13	1.71	0.72
2:I:1191:LYS:HD3	2:I:1192:GLU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1345:ARG:O	3:J:1350:ASN:ND2	2.24	0.71
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.72	0.71
3:J:425:ARG:HG2	3:J:427:PRO:HD2	1.73	0.70
3:J:4:LEU:O	3:J:8:LEU:CB	2.39	0.70
5:M:37:LEU:O	5:M:41:LEU:N	2.22	0.70
3:J:341:ASN:HB3	3:J:1352:ILE:HG23	1.73	0.70
3:J:797:THR:HB	3:J:924:GLY:HA3	1.74	0.69
2:I:17:LYS:HA	2:I:1155:VAL:HG23	1.73	0.69
3:J:56:LEU:HB3	3:J:250:ARG:HH12	1.58	0.69
5:M:128:VAL:O	5:M:138:ARG:NH1	2.26	0.69
3:J:108:ALA:HB2	3:J:280:LYS:HG2	1.73	0.69
3:J:1:MET:N	3:J:1:MET:SD	2.60	0.69
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.75	0.69
5:M:222:ASP:HB3	5:M:224:LEU:HG	1.75	0.69
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.73	0.69
2:I:3:TYR:HB3	2:I:7:GLU:HB2	1.75	0.69
3:J:262:THR:HG21	3:J:270:ARG:HE	1.57	0.69
2:I:1262:LYS:HD3	3:J:352:ARG:HB2	1.75	0.68
5:M:185:PHE:HD1	5:M:186:ASP:N	1.91	0.68
5:M:227:LEU:HA	5:M:229:ASN:H	1.57	0.68
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.75	0.68
3:J:278:ARG:NH1	3:J:295:GLU:OE1	2.24	0.68
3:J:253:VAL:O	3:J:260:PHE:N	2.26	0.68
5:M:360:GLU:OE2	5:M:361:TYR:N	2.27	0.68
2:I:1258:PRO:HB2	3:J:346:ARG:HB2	1.75	0.68
2:I:1105:SER:HB2	3:J:731:ARG:HG3	1.74	0.68
3:J:886:VAL:HA	3:J:1258:ARG:HG3	1.75	0.67
3:J:816:THR:HB	3:J:889:ASP:HB2	1.77	0.67
2:I:702:THR:HG23	2:I:704:MET:H	1.60	0.67
3:J:863:LEU:HD11	3:J:901:ARG:HD3	1.76	0.66
2:I:816:ILE:HG12	2:I:1098:LEU:HD21	1.78	0.66
1:H:109:PRO:HB3	1:H:132:HIS:HA	1.77	0.66
2:I:576:SER:HB2	2:I:579:ALA:HB2	1.77	0.66
2:I:132:ASP:N	2:I:132:ASP:OD1	2.28	0.66
3:J:431:ARG:HG2	3:J:493:PRO:HG3	1.78	0.66
5:M:165:ILE:HG21	5:M:170:ILE:HG21	1.77	0.66
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.60	0.65
5:M:367:LEU:H	5:M:367:LEU:HD23	1.62	0.65
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.79	0.65
1:G:25:LYS:HG2	1:G:204:GLU:HA	1.78	0.65
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:LEU:HD21	1:G:278:ILE:HD12	1.78	0.65
2:I:165:HIS:O	2:I:167:SER:N	2.30	0.65
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.78	0.65
2:I:980:VAL:HG13	2:I:984:VAL:HB	1.79	0.65
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.79	0.65
3:J:1266:ILE:HG22	3:J:1268:ASN:H	1.62	0.64
3:J:1261:LEU:HB3	3:J:1304:ARG:HD3	1.78	0.64
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.78	0.64
2:I:1261:GLY:HA2	3:J:346:ARG:HH12	1.62	0.64
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.79	0.64
1:G:46:ILE:HD11	1:H:38:THR:HG21	1.79	0.64
3:J:930:LEU:HD23	3:J:1138:LEU:HB2	1.78	0.64
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.80	0.64
5:M:462:ARG:HG3	5:M:467:ILE:HG23	1.80	0.64
2:I:138:ILE:HD13	2:I:143:ARG:HD2	1.80	0.63
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.62	0.63
3:J:1286:LYS:O	3:J:1290:ARG:HB2	1.99	0.63
3:J:582:ILE:HD13	3:J:627:THR:HG21	1.81	0.63
1:H:73:GLY:O	1:H:133:LEU:HA	1.99	0.63
5:M:38:GLN:O	5:M:42:GLU:HG2	1.98	0.63
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.31	0.63
4:K:3:ARG:NH1	4:K:5:THR:O	2.32	0.63
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.80	0.63
3:J:1231:ARG:O	3:J:1235:ASN:HB2	1.99	0.62
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.81	0.62
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.81	0.62
2:I:40:GLU:O	2:I:73:TYR:OH	2.18	0.62
3:J:388:ARG:NH2	3:J:414:GLU:OE1	2.30	0.62
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.80	0.62
3:J:857:LEU:HD23	3:J:857:LEU:H	1.65	0.62
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.82	0.62
1:G:109:PRO:HA	1:G:132:HIS:HA	1.82	0.62
3:J:901:ARG:HB2	3:J:908:ILE:HA	1.81	0.62
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	1.82	0.61
2:I:691:PRO:HD2	2:I:763:THR:HG21	1.81	0.61
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.82	0.61
3:J:844:THR:OG1	3:J:860:ARG:O	2.16	0.61
5:M:242:LYS:O	5:M:245:VAL:HG12	2.00	0.61
3:J:338:PHE:HA	3:J:342:LEU:HB3	1.83	0.61
5:M:200:LEU:HD21	5:M:221:SER:HB3	1.82	0.61
2:I:929:ILE:HG13	2:I:930:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:478:LEU:HD22	4:K:20:VAL:HA	1.81	0.61
4:K:29:GLN:HB3	4:K:35:LYS:HD3	1.82	0.61
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.83	0.61
2:I:1253:LEU:HB3	5:M:115:GLU:HB2	1.81	0.61
2:I:158:ASP:HB3	2:I:173:ASN:HD21	1.64	0.61
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.65	0.61
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.64	0.60
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.82	0.60
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.84	0.60
1:G:304:LYS:HG2	1:G:314:LEU:HD11	1.84	0.60
2:I:401:GLY:O	2:I:405:PHE:HB2	2.01	0.60
3:J:826:ILE:H	3:J:831:VAL:HG23	1.65	0.60
3:J:85:CYS:SG	3:J:87:LYS:N	2.74	0.60
3:J:123:ARG:HH12	3:J:223:LEU:HD11	1.66	0.60
1:H:44:ARG:HG3	1:H:183:ILE:HB	1.84	0.60
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.65	0.60
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.84	0.59
2:I:808:ASN:ND2	3:J:630:ALA:HA	2.17	0.59
3:J:203:GLU:O	3:J:207:GLU:HG2	2.02	0.59
5:M:285:TRP:CH2	5:M:355:PHE:HB3	2.38	0.59
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.35	0.59
2:I:758:ARG:NH2	2:I:762:ASN:OD1	2.36	0.59
2:I:338:THR:HG23	2:I:345:PRO:HG3	1.84	0.59
2:I:670:PHE:HB3	2:I:673:HIS:HD2	1.67	0.59
2:I:968:GLU:O	2:I:972:PHE:HB2	2.03	0.59
2:I:1164:PHE:O	2:I:1168:GLU:HB3	2.03	0.59
2:I:161:LYS:HA	2:I:170:VAL:HA	1.84	0.59
5:M:278:VAL:HG12	5:M:287:VAL:HG23	1.84	0.59
2:I:483:ASP:OD1	2:I:486:THR:OG1	2.20	0.59
2:I:980:VAL:HA	2:I:984:VAL:HA	1.84	0.59
3:J:1322:ALA:HA	3:J:1326:GLN:HE22	1.67	0.59
3:J:1347:LEU:H	3:J:1347:LEU:HD12	1.66	0.59
2:I:1105:SER:O	3:J:736:GLN:NE2	2.36	0.59
3:J:755:ILE:HG22	3:J:757:THR:H	1.66	0.59
5:M:192:ALA:HB1	5:M:197:ASP:HB3	1.84	0.59
1:G:192:VAL:O	1:G:194:GLN:HB2	2.03	0.58
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.58
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.85	0.58
2:I:895:LEU:O	2:I:899:GLU:HB2	2.03	0.58
2:I:423:ASP:O	2:I:427:ASP:HB2	2.03	0.58
2:I:807:TRP:O	2:I:808:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1261:GLY:HA2	3:J:346:ARG:NH1	2.18	0.58
3:J:576:ARG:HD3	3:J:593:ASN:HA	1.84	0.58
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.86	0.58
2:I:1262:LYS:HG2	2:I:1268:GLN:NE2	2.18	0.58
3:J:232:ASN:OD1	3:J:232:ASN:N	2.36	0.58
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.85	0.58
5:M:128:VAL:HA	5:M:133:PHE:HE2	1.67	0.58
3:J:1361:THR:HG23	4:K:21:LEU:HD11	1.85	0.58
2:I:1099:ASN:OD1	2:I:1101:LEU:N	2.36	0.58
2:I:882:ILE:HG13	2:I:919:ARG:HG2	1.85	0.58
3:J:1181:ASP:N	3:J:1181:ASP:OD1	2.37	0.58
2:I:1262:LYS:HZ3	3:J:352:ARG:HD2	1.68	0.58
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.86	0.58
3:J:116:PHE:HB3	3:J:123:ARG:HB2	1.85	0.58
3:J:418:GLU:O	3:J:481:ARG:NH2	2.36	0.58
4:K:4:VAL:HG22	4:K:5:THR:HG22	1.86	0.58
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.87	0.57
2:I:206:ALA:O	2:I:209:ILE:HG22	2.05	0.57
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.87	0.57
1:H:19:VAL:HB	1:H:23:HIS:HB3	1.86	0.57
3:J:1238:GLN:O	3:J:1242:ARG:HB3	2.04	0.57
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.04	0.57
3:J:606:ASN:OD1	3:J:610:ARG:NH1	2.38	0.57
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.87	0.57
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.87	0.57
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.85	0.57
5:M:115:GLU:N	5:M:115:GLU:OE1	2.34	0.57
3:J:198:CYS:HA	3:J:221:ILE:HD11	1.87	0.57
5:M:358:GLY:O	5:M:394:ARG:NH1	2.38	0.57
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.87	0.56
5:M:213:LEU:HA	5:M:216:ALA:HB3	1.87	0.56
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.05	0.56
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.70	0.56
3:J:416:ILE:HG21	3:J:441:LEU:HD21	1.88	0.56
3:J:1319:PHE:HD2	3:J:1342:ASP:HB2	1.71	0.56
3:J:398:LYS:HA	3:J:401:VAL:HG22	1.88	0.56
1:G:172:LEU:HD12	1:G:172:LEU:H	1.70	0.56
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.87	0.56
2:I:696:ASP:OD1	2:I:696:ASP:N	2.38	0.56
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.87	0.56
1:G:15:ASP:OD1	1:G:15:ASP:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:THR:HG23	2:I:138:ILE:HA	1.88	0.56
2:I:193:ASN:HB3	2:I:350:THR:HG23	1.87	0.56
5:M:235:LEU:O	5:M:239:THR:N	2.28	0.56
1:G:125:LYS:HE2	1:G:128:HIS:CG	2.40	0.56
3:J:84:ILE:HG13	3:J:85:CYS:H	1.69	0.56
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.87	0.56
2:I:926:GLY:HA2	2:I:1056:VAL:HG13	1.87	0.56
3:J:424:ASN:O	3:J:466:MET:HG3	2.06	0.56
5:M:170:ILE:HD12	5:M:171:GLY:N	2.21	0.56
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.72	0.55
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	1.88	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.41	0.55
3:J:218:THR:HA	3:J:221:ILE:HG22	1.88	0.55
5:M:366:VAL:HG12	5:M:368:ALA:H	1.71	0.55
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.88	0.55
2:I:684:ASN:OD1	2:I:687:ARG:NH2	2.39	0.55
2:I:976:ARG:HG3	2:I:989:LEU:HD23	1.88	0.55
5:M:149:ASP:OD1	5:M:150:ASP:N	2.39	0.55
5:M:428:ILE:O	5:M:432:ASN:ND2	2.40	0.55
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.87	0.55
2:I:703:GLY:N	2:I:705:GLU:OE2	2.40	0.55
5:M:127:GLN:NE2	5:M:182:ILE:HA	2.19	0.55
5:M:153:TYR:OH	5:M:258:PRO:O	2.23	0.55
3:J:1067:ARG:HB2	3:J:1072:LYS:HG3	1.89	0.55
3:J:548:VAL:HG21	3:J:574:VAL:HG23	1.89	0.55
2:I:510:GLN:HG3	2:I:535:PRO:HD3	1.89	0.55
2:I:60:GLN:HA	2:I:67:GLU:HA	1.89	0.55
2:I:974:ARG:HG2	2:I:1014:LEU:HD21	1.89	0.55
3:J:1026:PRO:HB3	3:J:1120:THR:HG22	1.89	0.55
5:M:341:LEU:O	5:M:345:ARG:HG3	2.07	0.55
2:I:686:GLN:HE21	2:I:796:LEU:HD13	1.72	0.55
2:I:942:ASP:N	2:I:942:ASP:OD1	2.40	0.55
3:J:952:VAL:HG21	3:J:984:LEU:HD13	1.89	0.55
2:I:889:PRO:HA	2:I:913:VAL:HG12	1.89	0.54
1:G:56:VAL:HG13	1:G:173:VAL:HG21	1.88	0.54
2:I:16:GLY:HA3	2:I:1188:ASP:O	2.07	0.54
1:G:51:MET:HB3	1:G:179:PRO:HD2	1.89	0.54
1:H:134:THR:HG22	1:H:135:ASP:H	1.73	0.54
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.71	0.54
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.43	0.54
3:J:352:ARG:HG2	3:J:467:ALA:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:27:GLN:HB3	5:M:383:ARG:HB3	1.89	0.54
2:I:1322:SER:OG	3:J:341:ASN:ND2	2.41	0.54
3:J:1138:LEU:HG	3:J:1139:PRO:HD3	1.89	0.54
3:J:848:VAL:HG11	3:J:880:VAL:HG22	1.90	0.54
2:I:725:GLN:N	2:I:733:VAL:O	2.38	0.54
3:J:17:PHE:HZ	3:J:1353:VAL:HG21	1.72	0.54
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.89	0.54
5:M:374:VAL:HG13	5:M:376:MET:HG2	1.90	0.54
2:I:223:LEU:HD13	2:I:426:ILE:HG21	1.89	0.54
2:I:518:ASN:N	2:I:518:ASN:OD1	2.41	0.54
3:J:371:LYS:HZ2	3:J:371:LYS:HB2	1.72	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
2:I:800:MET:O	2:I:1229:TYR:HA	2.06	0.54
2:I:524:ILE:HD12	2:I:708:VAL:HG13	1.90	0.54
3:J:356:THR:OG1	3:J:357:VAL:N	2.41	0.54
1:G:27:THR:HA	1:G:201:LEU:O	2.08	0.53
2:I:985:GLU:O	2:I:989:LEU:HB2	2.08	0.53
3:J:422:LEU:HB2	3:J:469:HIS:HB2	1.90	0.53
2:I:499:SER:HA	2:I:502:VAL:HG12	1.90	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.56	0.53
3:J:194:LEU:HD21	3:J:224:LEU:HD22	1.90	0.53
5:M:167:ASP:OD2	5:M:168:ASP:N	2.42	0.53
3:J:395:LYS:HD2	5:M:186:ASP:H	1.74	0.53
5:M:276:VAL:HG13	5:M:277:LEU:N	2.23	0.53
1:G:275:ILE:HG21	1:G:281:LEU:HD12	1.90	0.53
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.88	0.53
4:K:39:VAL:HG21	4:K:56:GLU:HG3	1.91	0.53
3:J:357:VAL:HG13	3:J:461:PHE:HE1	1.73	0.53
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.89	0.53
3:J:70:CYS:HB3	3:J:73:GLY:H	1.73	0.53
1:G:207:THR:HG22	1:G:209:GLY:H	1.72	0.53
2:I:619:ALA:HB2	2:I:654:ASP:HB2	1.90	0.53
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.53
5:M:236:MET:SD	5:M:243:GLU:HA	2.48	0.53
2:I:1142:ARG:CZ	2:I:1165:SER:HB2	2.39	0.53
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.42	0.53
2:I:153:PRO:HA	2:I:177:ILE:O	2.09	0.53
2:I:117:ILE:HG21	2:I:488:MET:HG2	1.89	0.53
2:I:850:ILE:HD11	2:I:1048:LYS:HD2	1.91	0.53
3:J:96:LYS:O	3:J:99:ARG:HG2	2.08	0.53
1:G:312:LEU:HA	5:M:181:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1129:ASN:O	2:I:1133:LYS:N	2.38	0.53
2:I:1257:GLN:HE22	3:J:340:GLN:HB3	1.73	0.53
2:I:133:ASN:OD1	2:I:527:LYS:NZ	2.41	0.53
3:J:948:SER:OG	3:J:949:SER:N	2.42	0.53
2:I:841:ARG:HA	2:I:848:GLU:HB2	1.91	0.53
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.20	0.53
1:G:228:LEU:O	1:G:232:VAL:HG23	2.09	0.53
1:G:82:LEU:HD11	1:G:171:LEU:HG	1.91	0.53
5:M:187:PRO:HG2	5:M:190:VAL:HB	1.91	0.52
2:I:1211:ARG:HE	2:I:1220:GLN:HE22	1.57	0.52
2:I:88:ARG:NE	2:I:1039:GLY:O	2.38	0.52
5:M:198:CYS:O	5:M:202:GLN:HB2	2.09	0.52
5:M:381:ILE:HA	5:M:384:VAL:HG12	1.90	0.52
3:J:930:LEU:HA	3:J:1244:GLN:HE22	1.74	0.52
2:I:886:LYS:CE	2:I:916:SER:HB3	2.40	0.52
3:J:85:CYS:SG	3:J:86:GLU:N	2.82	0.52
1:H:149:GLY:HA2	1:H:177:TYR:CG	2.45	0.52
2:I:1142:ARG:HH22	2:I:1166:ASP:CG	2.13	0.52
1:H:41:ASN:ND2	2:I:1217:THR:O	2.42	0.52
2:I:409:LEU:HD11	2:I:428:VAL:HG22	1.92	0.52
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.74	0.52
2:I:947:GLU:O	2:I:951:MET:HB2	2.10	0.52
3:J:68:TYR:CD2	3:J:78:LEU:HB3	2.45	0.52
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.92	0.52
2:I:667:LEU:HA	2:I:702:THR:HG21	1.91	0.52
2:I:916:SER:HA	5:M:264:ILE:HG21	1.92	0.52
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.92	0.52
1:G:314:LEU:HD12	1:G:314:LEU:H	1.74	0.52
2:I:1268:GLN:NE2	3:J:352:ARG:HE	2.05	0.52
3:J:616:PRO:O	3:J:620:PHE:CB	2.58	0.52
3:J:903:LEU:HG	3:J:904:ALA:H	1.75	0.52
1:H:48:LEU:HD11	3:J:539:SER:HB3	1.91	0.52
2:I:820:GLU:N	2:I:1080:ASN:O	2.42	0.52
2:I:758:ARG:HG2	2:I:759:SER:H	1.75	0.52
3:J:1172:LYS:HB3	3:J:1189:MET:HB3	1.92	0.52
3:J:526:VAL:HA	3:J:549:LYS:O	2.10	0.52
2:I:808:ASN:N	3:J:633:ALA:HB2	2.25	0.51
5:M:113:GLN:O	5:M:113:GLN:NE2	2.43	0.51
5:M:227:LEU:HA	5:M:229:ASN:N	2.24	0.51
2:I:1160:ASP:N	2:I:1160:ASP:OD1	2.30	0.51
2:I:180:ARG:NH2	2:I:393:ASP:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:471:PRO:O	3:J:477:GLN:HG2	2.11	0.51
5:M:336:ARG:HH21	5:M:388:LYS:HE2	1.74	0.51
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.93	0.51
2:I:734:ILE:HB	2:I:749:ASP:HB2	1.93	0.51
3:J:355:ILE:CG2	3:J:466:MET:HB2	2.40	0.51
5:M:124:LEU:O	5:M:127:GLN:HB3	2.10	0.51
5:M:288:GLU:OE1	5:M:289:LEU:N	2.43	0.51
1:G:61:ILE:HB	1:G:64:VAL:HB	1.92	0.51
1:H:73:GLY:O	1:H:134:THR:N	2.40	0.51
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.46	0.51
2:I:810:TYR:HB3	2:I:817:LEU:HD23	1.91	0.51
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.46	0.51
3:J:154:LEU:HD23	3:J:160:LEU:HD21	1.93	0.51
5:M:367:LEU:HB2	5:M:381:ILE:HD11	1.92	0.51
1:G:151:GLY:O	1:G:177:TYR:HB2	2.09	0.51
2:I:886:LYS:HE3	2:I:916:SER:O	2.10	0.51
3:J:144:TYR:HA	3:J:180:MET:HB3	1.93	0.51
3:J:557:LYS:HA	3:J:563:LEU:HA	1.92	0.51
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.92	0.51
3:J:761:ALA:H	3:J:771:GLN:HE22	1.59	0.51
5:M:354:PHE:HB2	5:M:362:MET:HG2	1.91	0.51
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.92	0.51
3:J:110:PRO:HD2	3:J:183:GLU:HG2	1.92	0.51
5:M:113:GLN:HB2	5:M:115:GLU:OE1	2.11	0.51
1:G:100:LEU:HD23	1:G:115:ILE:HD13	1.93	0.51
1:H:149:GLY:HA2	1:H:177:TYR:CD1	2.46	0.51
2:I:1262:LYS:NZ	3:J:352:ARG:HD2	2.26	0.51
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.93	0.51
2:I:705:GLU:HB2	2:I:794:LEU:H	1.76	0.51
5:M:432:ASN:OD1	5:M:432:ASN:N	2.44	0.51
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.46	0.50
3:J:826:ILE:HA	3:J:831:VAL:HA	1.92	0.50
3:J:1034:PHE:HA	3:J:1114:GLN:HA	1.93	0.50
3:J:643:ASP:O	3:J:720:ASN:ND2	2.45	0.50
1:G:89:ALA:H	1:G:125:LYS:HD3	1.76	0.50
2:I:458:GLU:O	2:I:462:ASN:ND2	2.44	0.50
1:G:218:ARG:NH1	1:H:231:PHE:O	2.44	0.50
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.77	0.50
3:J:1176:VAL:HG13	3:J:1187:GLU:HG2	1.92	0.50
5:M:278:VAL:HG22	5:M:392:SER:HA	1.92	0.50
1:G:182:ARG:HG2	1:G:183:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.93	0.50
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.47	0.50
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.94	0.50
2:I:972:PHE:HZ	2:I:994:ARG:O	1.94	0.50
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.77	0.50
3:J:674:THR:O	3:J:678:ARG:HB3	2.12	0.50
5:M:275:ASP:O	5:M:276:VAL:HG12	2.12	0.50
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.94	0.50
2:I:594:VAL:HG22	2:I:599:VAL:HG13	1.94	0.50
2:I:839:VAL:HG21	2:I:1046:VAL:HG13	1.94	0.50
3:J:320:ASN:CB	3:J:321:LYS:HA	2.42	0.50
4:K:60:ASN:ND2	4:K:62:GLN:H	2.09	0.50
2:I:487:LEU:HD23	2:I:487:LEU:H	1.76	0.49
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.09	0.49
3:J:1159:ILE:HG12	3:J:1160:SER:H	1.77	0.49
3:J:957:SER:N	3:J:985:ILE:O	2.45	0.49
5:M:154:LEU:HD23	5:M:156:ILE:HD11	1.94	0.49
1:G:166:ARG:N	1:G:167:PRO:HD2	2.26	0.49
2:I:1191:LYS:HD3	2:I:1192:GLU:HG2	1.93	0.49
5:M:38:GLN:NE2	5:M:42:GLU:OE2	2.45	0.49
3:J:480:ALA:HA	3:J:484:MET:HB2	1.93	0.49
1:H:60:GLU:HG2	1:H:143:ARG:N	2.24	0.49
5:M:196:ARG:O	5:M:200:LEU:N	2.29	0.49
2:I:839:VAL:HB	2:I:1049:ILE:HA	1.94	0.49
3:J:478:LEU:HB3	4:K:20:VAL:HG13	1.95	0.49
5:M:186:ASP:HA	5:M:187:PRO:C	2.31	0.49
2:I:557:ARG:HD3	2:I:587:LEU:HB3	1.94	0.49
1:G:19:VAL:HG13	1:G:20:SER:H	1.78	0.49
2:I:204:LEU:HD11	2:I:369:MET:HG3	1.95	0.49
2:I:75:LEU:HD12	2:I:94:ALA:HB3	1.95	0.49
3:J:1140:ARG:O	3:J:1144:LEU:HG	2.13	0.49
1:G:203:ILE:HG22	1:G:205:MET:H	1.78	0.49
2:I:1258:PRO:HD3	2:I:1295:SER:HB2	1.93	0.48
3:J:338:PHE:HB3	3:J:342:LEU:HD23	1.94	0.48
3:J:338:PHE:N	3:J:338:PHE:CD1	2.79	0.48
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.95	0.48
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.47	0.48
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.14	0.48
2:I:1281:TYR:HB3	3:J:483:LEU:HD12	1.96	0.48
2:I:905:ILE:HG13	2:I:906:PHE:N	2.28	0.48
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1171:ARG:O	2:I:1175:ASN:ND2	2.47	0.48
2:I:459:MET:HA	2:I:462:ASN:HD22	1.77	0.48
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.96	0.48
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.94	0.48
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.28	0.48
2:I:158:ASP:HB3	2:I:173:ASN:ND2	2.28	0.48
3:J:186:GLN:HA	3:J:238:ILE:HG13	1.95	0.48
3:J:848:VAL:HG22	3:J:858:VAL:HG22	1.96	0.48
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.95	0.48
2:I:1112:ILE:HG22	2:I:1113:LEU:HD12	1.95	0.48
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.95	0.48
5:M:280:LYS:HB3	5:M:285:TRP:CD1	2.49	0.48
1:G:10:LYS:O	1:G:30:PRO:HB2	2.13	0.48
2:I:399:ALA:O	2:I:403:MET:HB2	2.13	0.48
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.95	0.48
3:J:1279:GLN:HB2	3:J:1282:TYR:HB2	1.96	0.48
5:M:128:VAL:HA	5:M:133:PHE:CE2	2.47	0.48
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.95	0.48
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.79	0.48
2:I:492:MET:H	2:I:492:MET:HG3	1.50	0.48
3:J:1081:VAL:HG12	3:J:1087:ASP:HA	1.96	0.48
3:J:519:ASN:CG	3:J:709:ARG:HD3	2.34	0.48
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.94	0.48
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.95	0.48
1:G:284:ARG:HB3	1:G:289:LEU:CD2	2.43	0.48
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.14	0.48
2:I:118:LYS:HE2	2:I:118:LYS:HB3	1.71	0.48
2:I:38:PHE:HB2	2:I:457:GLY:CA	2.43	0.48
2:I:53:PHE:HD1	2:I:70:TYR:CE1	2.31	0.48
2:I:801:ARG:HD2	2:I:1229:TYR:CE1	2.48	0.48
2:I:985:GLU:HB3	2:I:988:LYS:HG3	1.95	0.48
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.14	0.48
3:J:72:CYS:N	3:J:88:CYS:SG	2.87	0.48
4:K:22:VAL:HG11	4:K:60:ASN:HA	1.95	0.48
2:I:708:VAL:HG11	2:I:794:LEU:HD22	1.94	0.47
2:I:95:PRO:HB3	2:I:123:TYR:HE1	1.79	0.47
3:J:678:ARG:NH1	3:J:756:GLU:OE2	2.47	0.47
1:H:182:ARG:O	1:H:205:MET:HG3	2.14	0.47
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.48	0.47
5:M:140:ILE:O	5:M:144:ILE:HG13	2.14	0.47
5:M:287:VAL:HG11	5:M:345:ARG:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284:ARG:O	1:G:314:LEU:HB3	2.14	0.47
1:G:57:THR:HG22	1:G:58:GLU:HG3	1.96	0.47
2:I:1242:LYS:HD3	3:J:465:GLN:NE2	2.29	0.47
3:J:163:GLU:O	3:J:167:ASP:HB3	2.13	0.47
3:J:395:LYS:HB2	5:M:185:PHE:CE1	2.49	0.47
1:H:51:MET:HB3	1:H:178:SER:HA	1.95	0.47
1:G:182:ARG:NH1	2:I:1090:ASN:OD1	2.47	0.47
2:I:1339:LEU:HB3	3:J:17:PHE:HD1	1.79	0.47
2:I:637:ARG:HG2	2:I:642:SER:HB3	1.96	0.47
2:I:670:PHE:HB3	2:I:673:HIS:CD2	2.48	0.47
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.47	0.47
3:J:579:LEU:HA	3:J:582:ILE:HD12	1.97	0.47
3:J:650:LYS:HE3	3:J:654:ILE:HD11	1.95	0.47
5:M:203:LEU:HA	5:M:206:PHE:HB3	1.96	0.47
1:G:284:ARG:HB3	1:G:289:LEU:HD21	1.96	0.47
1:G:295:LEU:HD23	1:G:295:LEU:HA	1.77	0.47
2:I:1083:GLU:O	2:I:1215:GLY:HA3	2.14	0.47
2:I:1247:SER:HB3	3:J:375:GLU:O	2.14	0.47
3:J:437:PHE:CZ	3:J:453:VAL:HG21	2.50	0.47
4:K:4:VAL:HG13	4:K:5:THR:H	1.80	0.47
3:J:789:LYS:HD2	3:J:1138:LEU:CD2	2.44	0.47
3:J:870:ASP:O	3:J:874:GLU:HG2	2.14	0.47
5:M:381:ILE:HG13	5:M:382:SER:N	2.29	0.47
5:M:390:LEU:N	5:M:397:PHE:O	2.43	0.47
3:J:122:SER:O	3:J:126:LEU:HB3	2.15	0.47
3:J:271:ARG:HH22	3:J:315:ALA:HB1	1.79	0.47
3:J:321:LYS:HE3	3:J:321:LYS:H	1.77	0.47
3:J:62:PHE:O	3:J:101:ARG:HD2	2.15	0.47
5:M:217:ARG:O	5:M:221:SER:OG	2.27	0.47
5:M:399:LEU:HD12	5:M:399:LEU:O	2.15	0.47
2:I:198:ILE:HD13	2:I:388:LEU:HD13	1.96	0.47
2:I:817:LEU:HD11	2:I:1080:ASN:HB2	1.96	0.47
2:I:90:VAL:HG12	2:I:91:THR:H	1.80	0.47
3:J:958:ILE:HG12	3:J:1011:VAL:HG21	1.96	0.47
2:I:388:LEU:O	2:I:395:TYR:HB2	2.15	0.47
3:J:735:ALA:HA	3:J:738:ARG:NH1	2.30	0.47
3:J:485:MET:HB3	3:J:488:ASN:HD22	1.80	0.47
3:J:973:LEU:HB3	3:J:1003:LEU:HB2	1.97	0.47
1:G:74:VAL:HG22	1:G:76:GLU:H	1.80	0.47
2:I:173:ASN:HA	2:I:186:PHE:O	2.15	0.47
5:M:180:LYS:O	5:M:184:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:VAL:HG11	1:G:183:ILE:HD11	1.96	0.46
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.96	0.46
2:I:370:MET:HE2	2:I:384:LEU:HD11	1.96	0.46
3:J:47:ARG:NE	3:J:47:ARG:O	2.41	0.46
3:J:513:MET:SD	3:J:544:LEU:HD11	2.55	0.46
5:M:377:HIS:O	5:M:381:ILE:HG23	2.15	0.46
1:G:158:ARG:CZ	1:G:172:LEU:HD23	2.46	0.46
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.31	0.46
2:I:851:THR:C	2:I:853:ASP:H	2.19	0.46
3:J:1090:ILE:HG13	3:J:1097:ALA:HB2	1.98	0.46
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.49	0.46
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.97	0.46
3:J:628:GLY:O	3:J:632:ALA:HB2	2.15	0.46
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.49	0.46
5:M:125:MET:HE3	5:M:125:MET:HA	1.97	0.46
1:H:102:LEU:HD11	1:H:110:VAL:HG11	1.97	0.46
2:I:522:SER:O	2:I:526:HIS:HB2	2.16	0.46
2:I:739:ASP:N	2:I:739:ASP:OD1	2.40	0.46
2:I:922:ASN:OD1	2:I:922:ASN:N	2.47	0.46
3:J:123:ARG:HH21	3:J:1334:GLU:HG2	1.80	0.46
3:J:485:MET:HG3	3:J:486:SER:H	1.80	0.46
3:J:709:ARG:HD2	3:J:710:ASP:N	2.30	0.46
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.97	0.46
2:I:945:ALA:HA	2:I:948:ILE:HD12	1.97	0.46
3:J:1011:VAL:HG12	3:J:1012:ALA:H	1.81	0.46
3:J:194:LEU:HD13	3:J:224:LEU:HB3	1.96	0.46
3:J:888:CYS:SG	3:J:890:THR:HG22	2.56	0.46
3:J:19:ALA:HA	3:J:1342:ASP:O	2.16	0.46
3:J:84:ILE:HA	3:J:91:GLU:HA	1.97	0.46
1:H:13:LEU:HB2	1:H:28:LEU:HD12	1.97	0.46
1:H:102:LEU:HD22	1:H:140:ILE:HG12	1.98	0.46
2:I:138:ILE:HB	2:I:143:ARG:CZ	2.46	0.46
3:J:490:ILE:HG13	3:J:491:LEU:HG	1.97	0.46
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.97	0.46
1:G:150:ARG:NH2	1:H:32:GLU:OE1	2.49	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.16	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.46
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.98	0.46
5:M:296:ARG:HD2	5:M:296:ARG:HA	1.73	0.46
1:G:255:ARG:NE	1:G:259:ASP:OD2	2.44	0.46
2:I:842:ASP:HB2	2:I:1045:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:221:LEU:H	2:I:221:LEU:HD12	1.79	0.46
1:G:320:ASN:O	1:G:321:TRP:CD2	2.69	0.45
2:I:805:MET:O	2:I:811:ASN:ND2	2.49	0.45
3:J:381:ILE:HD11	3:J:412:LEU:HD12	1.98	0.45
3:J:395:LYS:HG3	5:M:186:ASP:HB3	1.99	0.45
3:J:422:LEU:O	3:J:468:VAL:HA	2.16	0.45
1:G:28:LEU:HD21	1:H:231:PHE:HE1	1.80	0.45
1:H:46:ILE:HD12	1:H:224:LEU:HB2	1.97	0.45
2:I:806:PRO:O	3:J:633:ALA:HA	2.16	0.45
2:I:822:VAL:HG13	2:I:827:ARG:HD3	1.99	0.45
3:J:371:LYS:HZ3	3:J:445:LYS:HE2	1.81	0.45
5:M:382:SER:O	5:M:386:THR:HG23	2.17	0.45
5:M:398:GLU:O	5:M:399:LEU:HB3	2.15	0.45
2:I:1142:ARG:NH1	2:I:1165:SER:HB2	2.32	0.45
2:I:38:PHE:HB2	2:I:457:GLY:HA2	1.98	0.45
2:I:1341:ASP:HB3	3:J:18:ASP:HB3	1.98	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.17	0.45
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.97	0.45
3:J:961:SER:OG	3:J:983:LYS:HD2	2.16	0.45
1:G:14:VAL:HG22	1:G:15:ASP:H	1.81	0.45
2:I:1124:ILE:HD11	2:I:1201:LEU:HB3	1.97	0.45
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.98	0.45
3:J:357:VAL:C	3:J:359:PRO:HD3	2.36	0.45
3:J:616:PRO:O	3:J:620:PHE:HB2	2.17	0.45
3:J:789:LYS:HE3	3:J:931:THR:O	2.15	0.45
1:H:72:GLU:HA	1:H:72:GLU:OE2	2.16	0.45
2:I:2:VAL:HG11	2:I:1158:LYS:NZ	2.31	0.45
3:J:183:GLU:OE1	3:J:296:LYS:NZ	2.48	0.45
5:M:341:LEU:HD21	5:M:345:ARG:HH21	1.82	0.45
5:M:459:ALA:HA	5:M:462:ARG:NH2	2.31	0.45
3:J:22:ILE:HG22	3:J:1340:LYS:O	2.17	0.45
3:J:347:VAL:HG12	3:J:348:ASP:O	2.17	0.45
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.45
5:M:381:ILE:O	5:M:385:THR:OG1	2.19	0.45
2:I:1258:PRO:CB	3:J:346:ARG:HB2	2.46	0.45
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.81	0.45
3:J:614:LEU:O	3:J:617:THR:HG22	2.17	0.45
3:J:1150:PRO:HG2	3:J:1153:PRO:HB3	1.98	0.45
3:J:860:ARG:NH1	3:J:861:ASN:HD22	2.15	0.45
1:G:28:LEU:HD13	1:G:201:LEU:HD22	1.98	0.45
3:J:332:LYS:O	3:J:336:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:495:ASN:HD22	3:J:497:GLU:HB2	1.81	0.45
2:I:801:ARG:HA	2:I:1228:GLY:O	2.16	0.45
2:I:1288:GLN:HB2	2:I:1288:GLN:HE21	1.57	0.45
2:I:710:VAL:HA	2:I:715:THR:HG21	1.98	0.45
3:J:1:MET:HG2	3:J:2:LYS:H	1.81	0.45
3:J:116:PHE:CD2	3:J:237:MET:HG2	2.52	0.45
2:I:808:ASN:HD21	3:J:630:ALA:HA	1.81	0.45
2:I:1321:GLU:OE2	3:J:99:ARG:NH1	2.50	0.45
2:I:1069:ARG:HG3	2:I:1233:LEU:HD21	1.99	0.44
2:I:807:TRP:N	2:I:811:ASN:HD21	2.14	0.44
3:J:709:ARG:HG3	3:J:710:ASP:OD2	2.16	0.44
5:M:279:ARG:O	5:M:285:TRP:HD1	2.00	0.44
2:I:1203:ASP:O	2:I:1204:LEU:HG	2.17	0.44
2:I:522:SER:HA	2:I:525:THR:HG22	1.98	0.44
3:J:370:LYS:HG3	3:J:441:LEU:HD12	1.99	0.44
1:G:8:PHE:C	1:G:9:LEU:HG	2.38	0.44
2:I:814:ASP:O	2:I:1074:GLY:HA2	2.17	0.44
3:J:958:ILE:HD12	3:J:982:LEU:HG	1.98	0.44
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.99	0.44
2:I:13:LYS:HE2	2:I:15:PHE:CE2	2.52	0.44
2:I:489:PRO:O	2:I:490:GLN:HB3	2.17	0.44
3:J:1146:GLU:HA	3:J:1309:ILE:HG12	1.97	0.44
3:J:201:LEU:O	3:J:217:LEU:HD11	2.17	0.44
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.99	0.44
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.44	0.44
3:J:184:ALA:O	3:J:188:LEU:HB2	2.17	0.44
1:G:11:PRO:HG2	1:H:227:GLN:O	2.18	0.44
2:I:1142:ARG:HE	2:I:1142:ARG:HB2	1.42	0.44
2:I:1246:ARG:HD2	2:I:1266:GLY:C	2.38	0.44
2:I:187:GLU:O	2:I:195:PHE:HB2	2.18	0.44
2:I:840:SER:CB	2:I:886:LYS:HZ3	2.30	0.44
3:J:710:ASP:CG	3:J:711:GLY:H	2.18	0.44
2:I:1264:GLN:N	2:I:1264:GLN:OE1	2.50	0.44
3:J:128:LEU:HB3	3:J:157:GLN:NE2	2.33	0.44
3:J:707:ILE:HD11	3:J:716:GLN:HG2	2.00	0.44
5:M:197:ASP:O	5:M:201:ILE:N	2.28	0.44
5:M:424:VAL:O	5:M:428:ILE:HG22	2.17	0.44
1:H:31:LEU:HD12	1:H:35:PHE:HB3	1.99	0.44
2:I:440:GLY:HA3	2:I:441:GLU:CD	2.38	0.44
2:I:692:THR:OG1	2:I:693:LEU:N	2.51	0.44
2:I:929:ILE:HG13	2:I:930:ASP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1269:ARG:HA	3:J:346:ARG:HA	1.98	0.44
2:I:559:CYS:HB2	2:I:662:SER:HB3	2.00	0.44
2:I:697:LYS:H	2:I:697:LYS:HD3	1.83	0.44
3:J:1262:ARG:NH2	3:J:1312:ALA:O	2.51	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.98	0.44
3:J:836:ARG:HG3	3:J:869:CYS:SG	2.58	0.44
5:M:171:GLY:C	5:M:173:GLU:H	2.20	0.44
5:M:26:LEU:HD12	5:M:27:GLN:N	2.33	0.44
2:I:20:GLN:HG2	2:I:20:GLN:H	1.63	0.43
3:J:785:ASP:O	3:J:789:LYS:HG2	2.17	0.43
3:J:872:LEU:HD22	3:J:877:VAL:HG11	2.00	0.43
3:J:885:VAL:HG12	3:J:899:TYR:HA	2.00	0.43
4:K:15:ASN:C	4:K:17:PHE:H	2.22	0.43
5:M:223:HIS:C	5:M:225:ASP:H	2.20	0.43
1:G:256:PRO:O	1:G:259:ASP:HB2	2.17	0.43
1:H:62:ASP:HB3	1:H:141:SER:O	2.17	0.43
2:I:827:ARG:HG3	2:I:828:PHE:HD1	1.84	0.43
3:J:1215:GLU:HB2	3:J:1220:ILE:HD11	2.00	0.43
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.53	0.43
3:J:850:LYS:HG3	3:J:857:LEU:HD22	2.00	0.43
1:H:73:GLY:O	1:H:133:LEU:HD12	2.18	0.43
1:H:192:VAL:O	1:H:195:ARG:HB2	2.18	0.43
2:I:1120:ALA:HB1	2:I:1198:LEU:HD12	2.00	0.43
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.48	0.43
3:J:190:LYS:HA	3:J:235:GLU:HG3	2.00	0.43
3:J:432:LEU:HD11	3:J:492:SER:HA	2.01	0.43
1:H:76:GLU:H	1:H:76:GLU:CD	2.22	0.43
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.83	0.43
3:J:57:PHE:CD1	3:J:247:PRO:HB3	2.53	0.43
2:I:1313:HIS:CD2	3:J:477:GLN:HE22	2.36	0.43
2:I:1272:GLU:OE1	3:J:798:ARG:NH2	2.51	0.43
2:I:33:ASP:O	2:I:37:LYS:HG2	2.19	0.43
2:I:979:LEU:HD11	2:I:989:LEU:HD22	1.98	0.43
2:I:1339:LEU:HD23	3:J:17:PHE:CD1	2.53	0.43
2:I:1247:SER:O	3:J:348:ASP:HB3	2.18	0.43
4:K:31:GLN:HE21	4:K:46:THR:HG21	1.84	0.43
5:M:25:LEU:O	5:M:33:LEU:HD12	2.17	0.43
2:I:760:ASN:OD1	2:I:760:ASN:N	2.51	0.43
3:J:1355:ARG:HE	3:J:1355:ARG:HB3	1.59	0.43
3:J:186:GLN:HB2	3:J:238:ILE:HG21	2.01	0.43
1:H:190:ALA:HB3	1:H:198:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.25	0.43
3:J:1111:ASP:OD1	3:J:1112:GLY:N	2.52	0.43
2:I:145:ILE:HB	2:I:456:VAL:HG22	2.00	0.43
2:I:695:ALA:HB1	2:I:795:ALA:HB3	2.01	0.43
3:J:807:LEU:HD11	3:J:1258:ARG:NH1	2.34	0.43
2:I:1268:GLN:CG	3:J:352:ARG:HG3	2.41	0.43
5:M:368:ALA:HA	5:M:371:ALA:HB3	2.00	0.43
1:G:302:GLU:O	1:G:306:VAL:HG23	2.19	0.43
3:J:1234:VAL:O	3:J:1238:GLN:HB2	2.19	0.43
3:J:554:GLU:HB3	3:J:589:TYR:HB2	2.01	0.43
3:J:746:LEU:HD23	3:J:758:PRO:HG3	2.00	0.43
5:M:170:ILE:H	5:M:170:ILE:HG13	1.60	0.43
5:M:235:LEU:O	5:M:239:THR:HG22	2.18	0.43
5:M:351:GLN:CD	5:M:362:MET:HB3	2.39	0.43
1:H:219:ARG:O	1:H:223:ILE:HG13	2.19	0.43
2:I:1250:SER:O	2:I:1259:LEU:HD13	2.19	0.43
3:J:220:ARG:O	3:J:224:LEU:HG	2.19	0.43
3:J:224:LEU:O	3:J:228:VAL:HG23	2.19	0.43
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.53	0.42
2:I:808:ASN:HD22	2:I:808:ASN:HA	1.66	0.42
2:I:884:VAL:HG22	2:I:918:LEU:HD23	2.00	0.42
3:J:858:VAL:HG12	3:J:868:TRP:CE3	2.54	0.42
5:M:127:GLN:HB2	5:M:185:PHE:HD2	1.78	0.42
2:I:189:ASP:N	2:I:189:ASP:OD1	2.52	0.42
3:J:1316:THR:HG22	3:J:1318:SER:H	1.84	0.42
1:G:125:LYS:HB2	1:G:128:HIS:HB2	2.00	0.42
2:I:1212:LEU:HB2	2:I:1225:VAL:HG21	2.01	0.42
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.83	0.42
2:I:1332:SER:HA	3:J:243:PRO:HB2	2.02	0.42
3:J:532:GLU:HG2	3:J:536:LEU:HD23	2.02	0.42
3:J:853:THR:HG22	3:J:854:ALA:H	1.82	0.42
2:I:1270:PHE:O	3:J:343:LEU:O	2.37	0.42
2:I:216:THR:H	2:I:219:GLN:NE2	2.18	0.42
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.00	0.42
2:I:972:PHE:CZ	2:I:994:ARG:HB3	2.54	0.42
2:I:979:LEU:HD21	2:I:989:LEU:HD21	2.01	0.42
3:J:623:GLN:O	3:J:627:THR:HG22	2.20	0.42
3:J:634:ARG:NH1	3:J:634:ARG:HB3	2.35	0.42
3:J:971:GLY:C	3:J:972:LYS:HG2	2.40	0.42
5:M:24:ARG:O	5:M:28:LEU:HG	2.20	0.42
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:ARG:HG3	3:J:387:LEU:HD11	2.02	0.42
2:I:557:ARG:NH2	2:I:611:GLU:OE1	2.53	0.42
2:I:866:ASP:HA	2:I:872:TYR:CZ	2.54	0.42
3:J:553:THR:HG23	3:J:566:LYS:O	2.20	0.42
2:I:615:VAL:HG13	2:I:651:ASP:HB2	2.00	0.42
2:I:753:LEU:HB3	2:I:767:GLN:HB2	2.01	0.42
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.52	0.42
5:M:130:LEU:HD12	5:M:131:THR:N	2.34	0.42
5:M:264:ILE:HG13	5:M:265:HIS:O	2.20	0.42
5:M:365:MET:HE2	5:M:365:MET:HB3	1.83	0.42
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.84	0.42
5:M:34:GLN:HA	5:M:37:LEU:HG	2.01	0.42
2:I:1046:VAL:HG11	2:I:1049:ILE:HD11	2.01	0.42
2:I:1136:GLN:HE21	2:I:1136:GLN:HB3	1.52	0.42
2:I:207:THR:HG21	2:I:354:ASP:HB2	2.02	0.42
3:J:844:THR:HG22	3:J:880:VAL:HG11	2.02	0.42
2:I:435:ILE:HA	2:I:439:LYS:O	2.20	0.42
3:J:1297:LYS:NZ	3:J:1299:GLY:HA3	2.35	0.42
3:J:418:GLU:H	4:K:45:LYS:HZ3	1.67	0.42
3:J:814:CYS:HB3	3:J:890:THR:HB	2.01	0.42
5:M:295:PRO:HG2	5:M:333:LEU:HD21	2.01	0.42
1:G:12:ARG:H	1:G:30:PRO:HD2	1.85	0.42
1:G:25:LYS:HA	1:G:203:ILE:O	2.20	0.42
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.85	0.42
1:H:82:LEU:O	1:H:86:LYS:HG3	2.20	0.42
2:I:529:ARG:HH21	2:I:687:ARG:NH1	2.18	0.42
3:J:1251:LYS:O	3:J:1255:VAL:HG13	2.19	0.42
3:J:169:LEU:HD23	3:J:173:GLY:HA2	2.02	0.42
3:J:987:GLU:HG3	3:J:987:GLU:H	1.52	0.42
5:M:167:ASP:OD2	5:M:169:GLU:N	2.41	0.42
2:I:1098:LEU:HA	2:I:1098:LEU:HD23	1.65	0.41
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	2.02	0.41
2:I:1254:VAL:HG22	2:I:1255:THR:HG23	2.01	0.41
2:I:47:TYR:HA	2:I:51:ALA:HB2	2.02	0.41
2:I:542:ARG:HB3	2:I:542:ARG:HE	1.73	0.41
2:I:865:LEU:HD21	2:I:882:ILE:O	2.20	0.41
3:J:1081:VAL:HA	3:J:1088:VAL:HG23	2.01	0.41
3:J:1219:ASP:OD1	3:J:1222:ARG:NH2	2.52	0.41
1:H:78:ILE:O	1:H:82:LEU:HB2	2.20	0.41
2:I:401:GLY:O	2:I:405:PHE:CB	2.68	0.41
2:I:471:VAL:O	2:I:475:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.34	0.41
3:J:353:SER:HB3	3:J:447:ILE:HG13	2.02	0.41
1:G:154:PRO:HB2	2:I:1059:ARG:HH22	1.84	0.41
2:I:148:GLN:O	2:I:453:ILE:HA	2.20	0.41
2:I:452:ARG:HG3	2:I:585:GLY:HA3	2.01	0.41
2:I:56:VAL:HG13	2:I:57:PHE:CD2	2.55	0.41
3:J:123:ARG:HD3	3:J:123:ARG:HA	1.91	0.41
1:H:222:THR:HG1	1:H:222:THR:H	1.62	0.41
2:I:548:ARG:NH2	2:I:567:PRO:O	2.54	0.41
3:J:265:LEU:O	3:J:267:ASP:N	2.54	0.41
3:J:418:GLU:H	4:K:45:LYS:NZ	2.18	0.41
5:M:162:VAL:HG22	5:M:170:ILE:HD13	2.01	0.41
1:G:104:LYS:HG3	1:G:105:SER:N	2.34	0.41
1:G:299:SER:O	1:G:303:ILE:HG22	2.21	0.41
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.86	0.41
2:I:42:ASP:OD2	2:I:44:GLU:HG2	2.19	0.41
2:I:179:TYR:HE1	2:I:454:ARG:HH11	1.68	0.41
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.85	0.41
2:I:817:LEU:HA	2:I:817:LEU:HD22	1.90	0.41
2:I:841:ARG:HA	2:I:848:GLU:CB	2.51	0.41
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.53	0.41
3:J:34:SER:HG	3:J:104:HIS:CG	2.37	0.41
3:J:45:ASN:HB3	3:J:48:THR:O	2.21	0.41
5:M:127:GLN:HB2	5:M:185:PHE:CE2	2.54	0.41
1:G:14:VAL:HG22	1:G:15:ASP:OD1	2.20	0.41
1:H:44:ARG:HD3	1:H:185:TYR:HE2	1.85	0.41
1:H:74:VAL:HG11	1:H:131:CYS:HB2	2.03	0.41
2:I:101:ARG:HA	2:I:118:LYS:HA	2.03	0.41
2:I:175:ARG:HG3	2:I:184:LEU:O	2.20	0.41
2:I:528:ARG:NH2	2:I:575:LEU:HB3	2.36	0.41
5:M:133:PHE:HB3	5:M:137:ASP:HB2	2.03	0.41
2:I:843:THR:HG22	5:M:269:PRO:HD2	2.02	0.41
1:G:182:ARG:O	1:G:183:ILE:HG13	2.20	0.41
1:H:151:GLY:O	1:H:177:TYR:HB2	2.21	0.41
2:I:204:LEU:HD13	2:I:208:ILE:HD13	2.01	0.41
2:I:66:SER:HB3	2:I:479:LEU:HD22	2.02	0.41
3:J:364:HIS:NE2	3:J:438:GLU:OE1	2.44	0.41
3:J:71:LEU:HD22	3:J:71:LEU:HA	1.94	0.41
3:J:740:LEU:HD12	3:J:763:PHE:HB2	2.01	0.41
3:J:418:GLU:HB2	4:K:45:LYS:HG3	2.02	0.41
1:G:211:ILE:HA	1:G:211:ILE:HD13	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:VAL:HG21	1:H:69:SER:CB	2.51	0.41
2:I:1085:MET:HA	2:I:1085:MET:HE2	2.01	0.41
2:I:1086:PRO:HB2	2:I:1212:LEU:HD23	2.03	0.41
2:I:1340:GLU:HB2	3:J:19:ALA:O	2.21	0.41
2:I:575:LEU:HG	2:I:576:SER:H	1.86	0.41
3:J:51:PRO:HB2	3:J:57:PHE:O	2.20	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.20	0.41
3:J:98:ARG:O	3:J:247:PRO:HD2	2.20	0.41
4:K:26:ARG:NH2	4:K:36:ASP:O	2.54	0.41
5:M:354:PHE:CD1	5:M:359:GLU:HA	2.56	0.41
2:I:748:ILE:HD12	2:I:966:ILE:HD12	2.03	0.41
3:J:1067:ARG:NH1	3:J:1074:LEU:O	2.54	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.95	0.41
3:J:660:GLU:HB2	3:J:685:ILE:HD12	2.02	0.41
5:M:203:LEU:O	5:M:207:ALA:N	2.54	0.41
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.96	0.41
3:J:702:GLN:O	3:J:718:SER:N	2.51	0.41
3:J:739:GLN:NE2	3:J:744:ARG:HB2	2.36	0.41
5:M:289:LEU:CB	5:M:290:ASN:HA	2.51	0.41
1:G:14:VAL:HG12	1:G:27:THR:O	2.20	0.41
2:I:150:HIS:HE1	2:I:153:PRO:HD3	1.86	0.41
2:I:207:THR:OG1	2:I:354:ASP:OD1	2.39	0.41
2:I:606:LEU:HD21	2:I:614:TYR:HD1	1.86	0.41
3:J:263:SER:O	3:J:265:LEU:N	2.54	0.41
3:J:371:LYS:NZ	3:J:445:LYS:HE2	2.36	0.41
3:J:45:ASN:O	3:J:46:TYR:HB2	2.20	0.41
3:J:537:TYR:CE2	3:J:544:LEU:HD13	2.55	0.41
3:J:653:ILE:HG12	3:J:692:ARG:NH2	2.36	0.41
3:J:654:ILE:O	3:J:658:GLU:HB2	2.21	0.41
5:M:367:LEU:CB	5:M:381:ILE:HD11	2.50	0.41
1:G:231:PHE:HE2	1:H:217:ILE:HG22	1.86	0.40
2:I:13:LYS:HE2	2:I:15:PHE:CZ	2.56	0.40
2:I:209:ILE:HG23	2:I:210:LEU:N	2.37	0.40
3:J:416:ILE:HG21	3:J:441:LEU:CD2	2.50	0.40
3:J:394:ILE:HG21	5:M:130:LEU:HD21	2.03	0.40
2:I:560:PRO:HB3	3:J:776:THR:HG21	2.03	0.40
2:I:629:PHE:O	2:I:647:ARG:NH2	2.53	0.40
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.30	0.40
3:J:133:ARG:NH1	3:J:136:GLU:OE1	2.54	0.40
3:J:265:LEU:C	3:J:267:ASP:N	2.72	0.40
3:J:805:GLN:HA	3:J:917:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:80:PHE:HZ	2:I:1038:GLN:HE22	1.69	0.40
2:I:404:LYS:HD3	2:I:586:PHE:HZ	1.86	0.40
2:I:841:ARG:HA	2:I:848:GLU:H	1.86	0.40
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	2.04	0.40
3:J:1264:ALA:N	3:J:1278:GLU:O	2.50	0.40
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.77	0.40
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.92	0.40
3:J:552:ILE:HD11	3:J:570:LYS:HG3	2.04	0.40
1:G:193:GLU:HA	1:G:194:GLN:HB2	2.03	0.40
1:H:148:ARG:HD3	1:H:148:ARG:HA	1.81	0.40
2:I:1063:GLY:HA3	2:I:1239:VAL:HG11	2.03	0.40
2:I:1264:GLN:HA	2:I:1265:PHE:HA	1.84	0.40
3:J:983:LYS:HD3	3:J:991:THR:HG21	2.02	0.40
5:M:192:ALA:HB3	5:M:198:CYS:HB2	2.04	0.40
5:M:285:TRP:CZ3	5:M:352:GLN:HG3	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:82:GLY:O	5:M:438:SER:OG[3_745]	2.18	0.02

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	G	305/329 (93%)	270 (88%)	33 (11%)	2 (1%)	24 65
1	H	211/329 (64%)	191 (90%)	20 (10%)	0	100 100
2	I	1211/1342 (90%)	1094 (90%)	110 (9%)	7 (1%)	27 67
3	J	1326/1407 (94%)	1198 (90%)	125 (9%)	3 (0%)	49 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	77/91 (85%)	71 (92%)	6 (8%)	0	100	100
5	M	370/477 (78%)	345 (93%)	22 (6%)	3 (1%)	21	62
All	All	3500/3975 (88%)	3169 (90%)	316 (9%)	15 (0%)	36	75

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	166	SER
3	J	266	ASN
5	M	276	VAL
2	I	170	VAL
2	I	437	ASN
3	J	265	LEU
2	I	808	ASN
5	M	211	PRO
2	I	164	THR
1	G	313	SER
5	M	386	THR
2	I	201	ARG
2	I	1186	VAL
1	G	30	PRO
3	J	826	ILE

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	G	252/286 (88%)	229 (91%)	23 (9%)	10	40
1	H	175/286 (61%)	158 (90%)	17 (10%)	9	37
2	I	999/1157 (86%)	884 (88%)	115 (12%)	6	31
3	J	1058/1168 (91%)	934 (88%)	124 (12%)	6	30
4	K	65/75 (87%)	55 (85%)	10 (15%)	3	20
5	M	306/423 (72%)	265 (87%)	41 (13%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2855/3395 (84%)	2525 (88%)	330 (12%)	6 30

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	9	LEU
1	G	15	ASP
1	G	23	HIS
1	G	39	LEU
1	G	72	GLU
1	G	79	LEU
1	G	102	LEU
1	G	127	GLN
1	G	171	LEU
1	G	172	LEU
1	G	195	ARG
1	G	197	ASP
1	G	201	LEU
1	G	228	LEU
1	G	229	GLU
1	G	233	ASP
1	G	254	LEU
1	G	257	VAL
1	G	268	ASN
1	G	295	LEU
1	G	314	LEU
1	G	318	LEU
1	G	320	ASN
1	H	13	LEU
1	H	16	ILE
1	H	43	LEU
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	77	ASP
1	H	82	LEU
1	H	91	ARG
1	H	132	HIS
1	H	134	THR
1	H	176	CYS
1	H	183	ILE

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Mol	Chain	Res	Type
1	H	191	ARG
1	H	222	THR
1	H	232	VAL
2	I	4	SER
2	I	5	TYR
2	I	6	THR
2	I	7	GLU
2	I	11	ILE
2	I	13	LYS
2	I	20	GLN
2	I	39	ILE
2	I	44	GLU
2	I	53	PHE
2	I	62	TYR
2	I	83	GLN
2	I	111	GLU
2	I	113	THR
2	I	119	GLU
2	I	121	GLU
2	I	131	THR
2	I	132	ASP
2	I	185	ASP
2	I	194	LEU
2	I	199	ASP
2	I	216	THR
2	I	219	GLN
2	I	351	LEU
2	I	354	ASP
2	I	378	ARG
2	I	400	VAL
2	I	402	ARG
2	I	470	ARG
2	I	481	LEU
2	I	483	ASP
2	I	486	THR
2	I	487	LEU
2	I	491	ASP
2	I	492	MET
2	I	510	GLN
2	I	540	ARG
2	I	554	HIS
2	I	561	ILE

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Mol	Chain	Res	Type
2	I	589	THR
2	I	600	THR
2	I	602	GLU
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	624	ASP
2	I	633	LEU
2	I	646	SER
2	I	650	VAL
2	I	651	ASP
2	I	672	GLU
2	I	692	THR
2	I	693	LEU
2	I	696	ASP
2	I	697	LYS
2	I	711	ASP
2	I	748	ILE
2	I	757	THR
2	I	760	ASN
2	I	763	THR
2	I	768	MET
2	I	773	LEU
2	I	791	LEU
2	I	800	MET
2	I	805	MET
2	I	807	TRP
2	I	817	LEU
2	I	830	THR
2	I	838	CYS
2	I	839	VAL
2	I	840	SER
2	I	842	ASP
2	I	850	ILE
2	I	868	SER
2	I	887	VAL
2	I	895	LEU
2	I	902	LEU
2	I	917	SER
2	I	922	ASN
2	I	935	THR

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Mol	Chain	Res	Type
2	I	940	GLU
2	I	959	ASP
2	I	972	PHE
2	I	987	GLU
2	I	995	ASP
2	I	1019	ASP
2	I	1030	GLU
2	I	1038	GLN
2	I	1056	VAL
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1112	ILE
2	I	1136	GLN
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1160	ASP
2	I	1164	PHE
2	I	1165	SER
2	I	1166	ASP
2	I	1170	MET
2	I	1198	LEU
2	I	1203	ASP
2	I	1217	THR
2	I	1222	GLU
2	I	1232	MET
2	I	1265	PHE
2	I	1288	GLN
2	I	1291	LEU
2	I	1302	THR
2	I	1304	MET
2	I	1310	ASP
3	J	1	MET
3	J	5	LEU
3	J	14	THR
3	J	17	PHE
3	J	33	TRP
3	J	43	THR
3	J	48	THR
3	J	53	ARG

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Mol	Chain	Res	Type
3	J	65	VAL
3	J	70	CYS
3	J	71	LEU
3	J	80	HIS
3	J	87	LYS
3	J	92	VAL
3	J	93	THR
3	J	115	TRP
3	J	126	LEU
3	J	134	ASP
3	J	136	GLU
3	J	140	TYR
3	J	154	LEU
3	J	167	ASP
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	195	GLU
3	J	208	THR
3	J	219	LYS
3	J	232	ASN
3	J	241	VAL
3	J	250	ARG
3	J	265	LEU
3	J	266	ASN
3	J	271	ARG
3	J	279	LEU
3	J	297	ARG
3	J	321	LYS
3	J	322	ARG
3	J	324	LEU
3	J	337	ARG
3	J	338	PHE
3	J	341	ASN
3	J	345	LYS
3	J	356	THR
3	J	357	VAL
3	J	363	LEU
3	J	378	LYS
3	J	395	LYS
3	J	412	LEU
3	J	415	VAL

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Mol	Chain	Res	Type
3	J	453	VAL
3	J	478	LEU
3	J	483	LEU
3	J	504	GLN
3	J	506	VAL
3	J	516	ASP
3	J	517	CYS
3	J	536	LEU
3	J	538	ARG
3	J	545	HIS
3	J	548	VAL
3	J	554	GLU
3	J	558	ASP
3	J	596	LEU
3	J	617	THR
3	J	641	ILE
3	J	642	ASP
3	J	644	MET
3	J	678	ARG
3	J	681	LYS
3	J	705	THR
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	739	GLN
3	J	746	LEU
3	J	749	LYS
3	J	769	VAL
3	J	772	TYR
3	J	788	LEU
3	J	810	THR
3	J	817	HIS
3	J	843	VAL
3	J	846	GLU
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	860	ARG
3	J	866	GLU
3	J	869	CYS
3	J	891	ASP

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Mol	Chain	Res	Type
3	J	894	VAL
3	J	895	CYS
3	J	897	HIS
3	J	898	CYS
3	J	907	HIS
3	J	908	ILE
3	J	918	ILE
3	J	955	LYS
3	J	987	GLU
3	J	1017	VAL
3	J	1019	ASN
3	J	1056	LEU
3	J	1063	ASP
3	J	1073	ASP
3	J	1082	ASP
3	J	1094	ASP
3	J	1138	LEU
3	J	1146	GLU
3	J	1155	ILE
3	J	1208	ASP
3	J	1215	GLU
3	J	1221	LEU
3	J	1223	LEU
3	J	1258	ARG
3	J	1275	LEU
3	J	1283	SER
3	J	1293	GLU
3	J	1305	ASP
3	J	1319	PHE
3	J	1326	GLN
3	J	1348	LYS
3	J	1371	ARG
4	K	3	ARG
4	K	4	VAL
4	K	5	THR
4	K	25	ARG
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
4	K	67	ARG
4	K	68	GLU

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Mol	Chain	Res	Type
5	M	27	GLN
5	M	29	SER
5	M	44	ASN
5	M	113	GLN
5	M	115	GLU
5	M	125	MET
5	M	185	PHE
5	M	186	ASP
5	M	195	LEU
5	M	197	ASP
5	M	200	LEU
5	M	202	GLN
5	M	203	LEU
5	M	213	LEU
5	M	226	LEU
5	M	236	MET
5	M	244	GLU
5	M	246	LEU
5	M	257	ASP
5	M	265	HIS
5	M	276	VAL
5	M	285	TRP
5	M	288	GLU
5	M	302	GLN
5	M	303	TYR
5	M	318	PHE
5	M	319	ILE
5	M	350	GLN
5	M	354	PHE
5	M	360	GLU
5	M	365	MET
5	M	367	LEU
5	M	370	ILE
5	M	377	HIS
5	M	378	GLU
5	M	379	SER
5	M	381	ILE
5	M	387	GLN
5	M	399	LEU
5	M	421	ARG
5	M	432	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	18	GLN
1	G	23	HIS
1	G	75	GLN
1	G	84	ASN
1	G	132	HIS
1	G	194	GLN
1	G	320	ASN
1	H	23	HIS
1	H	147	GLN
2	I	20	GLN
2	I	173	ASN
2	I	219	GLN
2	I	450	ASN
2	I	462	ASN
2	I	463	GLN
2	I	510	GLN
2	I	613	ASN
2	I	620	ASN
2	I	808	ASN
2	I	811	ASN
2	I	1116	HIS
2	I	1136	GLN
2	I	1175	ASN
2	I	1220	GLN
2	I	1268	GLN
2	I	1288	GLN
2	I	1313	HIS
3	J	157	GLN
3	J	277	ASN
3	J	341	ASN
3	J	488	ASN
3	J	495	ASN
3	J	593	ASN
3	J	702	GLN
3	J	739	GLN
3	J	861	ASN
3	J	1114	GLN
3	J	1268	ASN
3	J	1326	GLN
4	K	60	ASN
4	K	61	ASN
5	M	27	GLN

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Mol	Chain	Res	Type
5	M	113	GLN
5	M	127	GLN
5	M	202	GLN
5	M	254	GLN
5	M	322	ASN
5	M	350	GLN
5	M	352	GLN
5	M	449	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	G	309/329 (93%)	-0.22	3 (0%) 82 75	115, 174, 216, 248	0
1	H	215/329 (65%)	0.16	7 (3%) 46 36	144, 209, 239, 261	0
2	I	1217/1342 (90%)	-0.07	19 (1%) 72 62	97, 179, 242, 273	0
3	J	1336/1407 (94%)	0.00	33 (2%) 57 46	88, 182, 243, 270	0
4	K	79/91 (86%)	-0.16	1 (1%) 77 69	131, 168, 207, 230	0
5	M	380/477 (79%)	-0.34	2 (0%) 90 87	103, 150, 191, 226	0
All	All	3536/3975 (88%)	-0.07	65 (1%) 68 59	88, 177, 239, 273	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	4.8
2	I	197	ARG	4.0
3	J	1108	GLN	4.0
3	J	1099	TYR	3.9
2	I	106	GLU	3.6
2	I	164	THR	3.6
3	J	150	GLY	3.4
2	I	624	ASP	3.4
3	J	928	THR	3.4
1	H	25	LYS	3.3
2	I	414	ILE	3.3
1	G	263	THR	3.2
1	H	234	LEU	3.2
2	I	114	VAL	3.2
1	G	160	HIS	3.1
3	J	1097	ALA	3.1
3	J	1045	THR	3.1
3	J	1214	PRO	3.0
3	J	1066	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	J	829	GLY	3.0
2	I	492	MET	2.9
2	I	222	ASP	2.9
3	J	1044	GLN	2.9
3	J	958	ILE	2.9
5	M	266	THR	2.9
2	I	226	GLU	2.8
2	I	343	HIS	2.8
4	K	76	GLU	2.8
3	J	682	VAL	2.6
2	I	455	SER	2.6
3	J	1107	VAL	2.6
3	J	960	LEU	2.6
3	J	1201	GLY	2.6
3	J	1068	THR	2.5
2	I	345	PRO	2.5
3	J	638	SER	2.4
2	I	1260	GLY	2.4
5	M	54	ASP	2.4
3	J	1065	ALA	2.4
3	J	830	ASP	2.4
2	I	337	PHE	2.3
3	J	1077	ALA	2.3
3	J	1069	ALA	2.2
3	J	318	GLY	2.2
3	J	1014	GLY	2.2
1	G	311	GLY	2.2
2	I	1102	GLY	2.2
1	H	24	ALA	2.2
2	I	1111	GLN	2.2
2	I	1014	LEU	2.2
3	J	998	PRO	2.2
3	J	1152	GLU	2.2
3	J	969	SER	2.2
3	J	677	GLU	2.2
1	H	66	HIS	2.1
1	H	147	GLN	2.1
2	I	121	GLU	2.1
1	H	95	LYS	2.1
3	J	319	SER	2.0
3	J	983	LYS	2.0
1	H	233	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	I	364	VAL	2.0
3	J	1017	VAL	2.0
3	J	1114	GLN	2.0
3	J	1083	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	J	1503	1/1	0.93	0.16	179,179,179,179	0
6	MG	J	1501	1/1	0.94	0.15	192,192,192,192	0
7	ZN	J	1502	1/1	0.98	0.20	225,225,225,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.