Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 06:47 AM EDT

PDB ID	:	2FRP
Title	:	Bacteriophage HK97 Expansion Intermediate IV
Authors	:	Gan, L.; Speir, J.A.; Conway, J.F.; Lander, G.; Cheng, N.; Firek, B.A.; Hendrix, R.W.; Duda, R.L.; Liljas, L.; Johnson, J.E.
Deposited on	:	2006-01-19
Resolution	:	7.50 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:

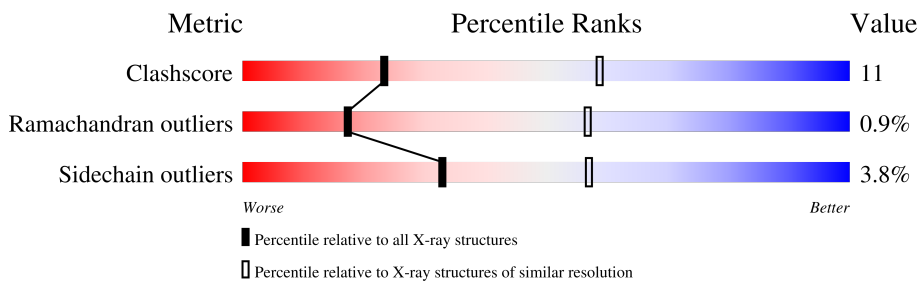|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 7.50 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0.9%
Sidechain outliers		3.8%

Worse — *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	282	70% 27% ••
1	B	282	76% 22% ••
1	C	282	79% 20% •
1	D	282	75% 22% ••
1	E	282	74% 24% ••
1	F	282	63% 26% • 9%
1	G	282	60% 23% • 14%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 14631 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.
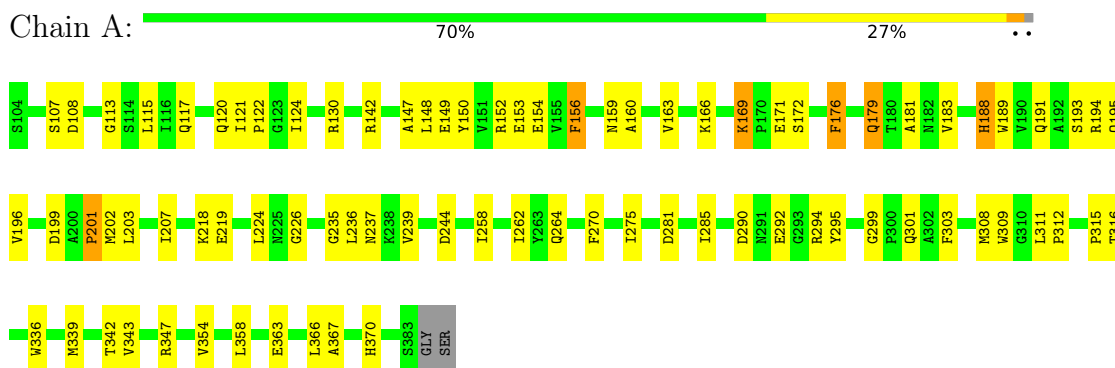
- Molecule 1 is a protein called Major capsid protein.

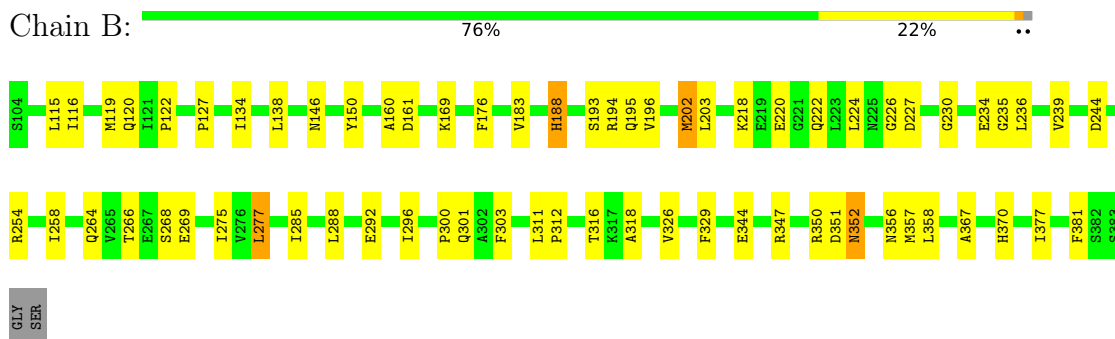| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	B	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	C	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	D	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	E	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	F	256	Total	C	N	O	S	0	0	0
			1986	1241	349	388	8			
1	G	243	Total	C	N	O	S	0	0	0
			1890	1181	333	368	8			

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. 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. 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.
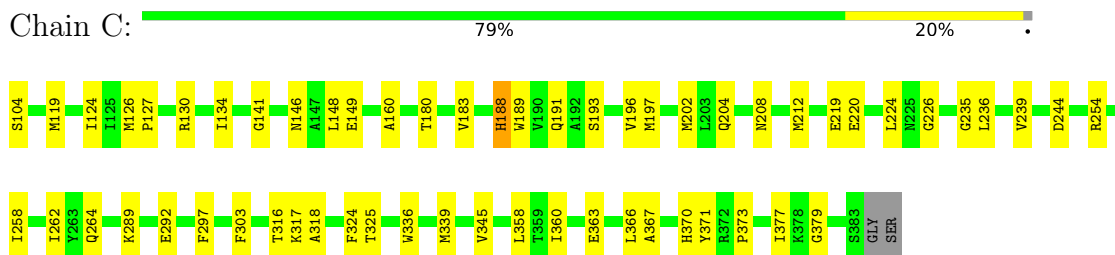
- Molecule 1: Major capsid protein
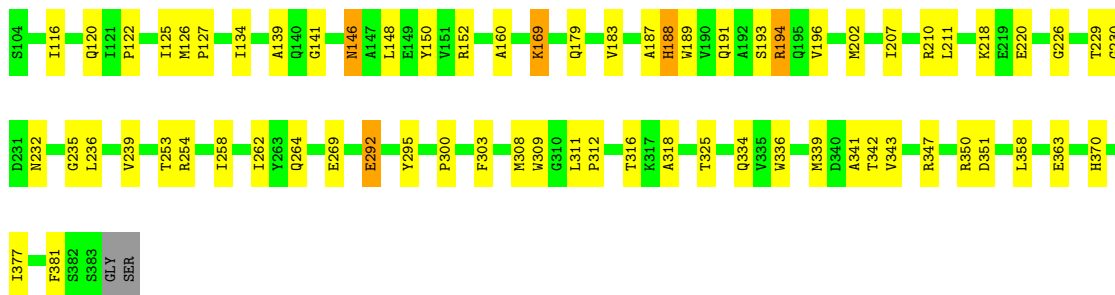
Chain A:

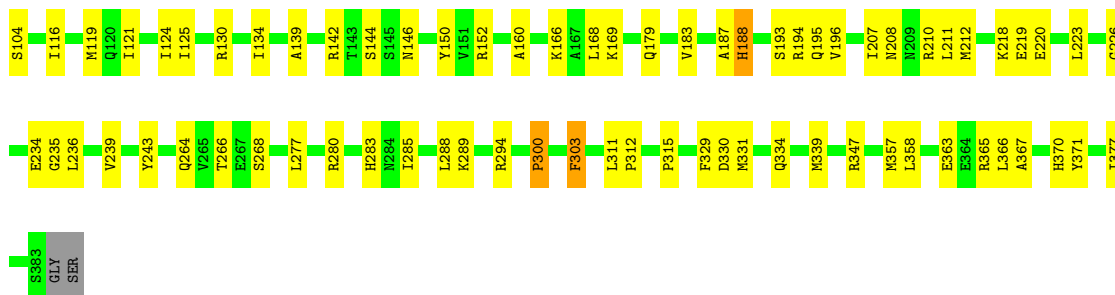- Molecule 1: Major capsid protein

Chain B:

- Molecule 1: Major capsid protein
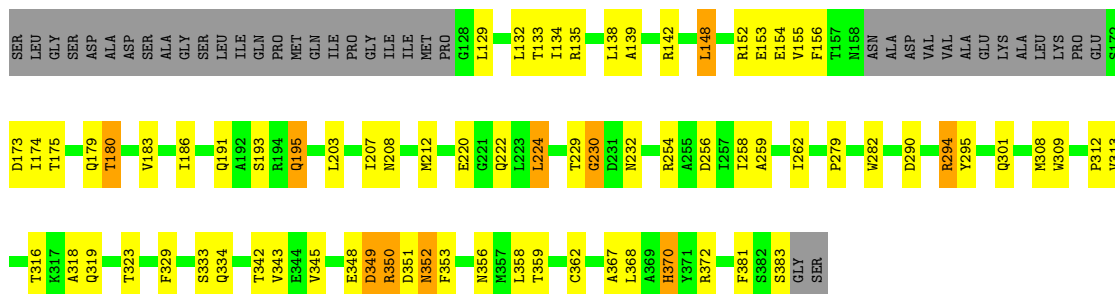
Chain C:

- Molecule 1: Major capsid protein

Chain D:

S104 I116 Q120 I121 P122 I125 M126 P127 I134 A139 Q140 G141 N146 A147 L148 E149 Y150 V151 R152 A160 K169 Q179 V183 A187 H188 W189 V190 Q191 A192 S193 R194 Q195 V196 M202 I207 R210 L211 K218 E219 E220 G226 T229 G230

D231 N232 G235 L236 V239 T253 R254 I258 I262 Y263 Q264 E269 E292 Y295 P300 F303 M308 W309 G310 L311 P312 T316 K317 A318 T325 Q334 V335 W336 M339 D340 A341 T342 V343 R347 R350 D351 L358 E363 H370

I377 F381 S382 S383 GLY SER

• Molecule 1: Major capsid protein

Chain E:

74% 24% ••

S104 I116 M119 Q120 I121 I124 I125 R130 I134 A139 R142 T143 S144 S145 N146 Y150 V151 R152 A160 K166 A167 L168 K169 Q179 V183 A187 H188 S193 R194 Q195 V196 I207 N208 N209 R210 L211 M212 K218 E219 E220 L223 G226

E234 G235 L236 V239 Y243 Q264 V265 T266 E267 S268 L277 R280 H283 N284 I285 L288 K289 R294 P300 F303 L311 P312 P315 F329 D330 M331 Q334 M339 R347 M357 L358 E363 E364 R365 L366 A367 H370 Y371 I377

S383 GLY SER

• Molecule 1: Major capsid protein

Chain F:

63% 26% • 9%

SER LEU GLY SER ASP ALA ASP SER ALA GLY SER LEU ILE GLN PRO MET GLN ILE PRO GLY ILE ILE MET PRO G128 L129 R130 R131 L132 T133 I134 R135 D136 L137 L138 A139 Q140 G141 N146 A147 L148 E149 Y150 V155 F156 A160 D161 K169 T175 Q179 V183 A187

H188 W189 V190 S193 R194 Q195 P201 Q204 E219 L223 L224 N225 G226 D227 G228 T229 G235 L236 N237 K238 V239 A240 D244 L247 T253 R254 A255 D256 I257 I258 A259 H260 A261 I262 Y263 Q264 E269 V276 W282 I285 A286 L287 L288 E292 P300

T304 V314 P315 T316 F324 T325 F329 Q334 V335 W336 V343 D349 R350 D351 N352 K355 L361 C362 E363 L366 A367 H370 I376 F381 S382 S383 GLY SER

• Molecule 1: Major capsid protein

Chain G:

60% 23% • 14%

SER LEU GLY SER ASP ALA ASP SER ALA GLY SER LEU ILE GLN PRO MET GLN ILE PRO GLY ILE ILE MET PRO G128 L129 L132 T133 I134 R135 L138 A139 R142 L148 R152 E153 E154 V155 F156 T157 N158 ASN ALA ASP VAL VAL ALA GLU LYS ALA LEU LYS PRO GLU S172

D173 I174 T175 Q179 T180 V183 I186 Q191 A192 S193 R194 Q195 L203 I207 N208 M212 E220 G221 Q222 L223 L224 T229 G230 D231 N232 R254 A255 D256 I257 I258 A259 I262 P279 W282 D290 R294 Y295 Q301 M308 W309 P312 V313

T316 K317 A318 Q319 T323 F329 S333 Q334 T342 V343 E344 V345 E348 D349 R350 D351 N352 F353 N356 M357 L358 T359 C362 A367 L368 A369 H370 Y371 R372 F381 S382 S383 GLY SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	1008.97Å 1008.97Å 728.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 7.50 39.94 – 7.50	Depositor EDS
% Data completeness (in resolution range)	64.7 (40.00-7.50) 65.2 (39.94-7.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 7.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.421 , (Not available) 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	152.2	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 28.9	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/2188	0.50	0/2969
1	B	0.32	1/2188 (0.0%)	0.49	0/2969
1	C	0.28	0/2188	0.48	0/2969
1	D	0.34	1/2188 (0.0%)	0.49	0/2969
1	E	0.28	0/2188	0.51	0/2969
1	F	0.28	0/2020	0.50	0/2740
1	G	0.49	1/1922 (0.1%)	0.63	4/2605 (0.2%)
All	All	0.33	3/14882 (0.0%)	0.51	4/20190 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	THR	C-N	-17.00	0.94	1.34
1	D	169	LYS	CE-NZ	8.54	1.70	1.49
1	B	356	ASN	CG-ND2	8.02	1.52	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	LEU	O-C-N	12.69	143.00	122.70
1	G	148	LEU	CA-C-N	-9.86	95.52	117.20
1	G	148	LEU	C-N-CA	-7.34	103.36	121.70
1	G	180	THR	O-C-N	-5.36	114.12	122.70

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	2151	0	2119	56	0
1	B	2151	0	2119	52	0
1	C	2151	0	2119	49	0
1	D	2151	0	2119	53	0
1	E	2151	0	2119	52	0
1	F	1986	0	1951	61	0
1	G	1890	0	1850	52	0
All	All	14631	0	14396	328	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 11.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LYS:CE	1:D:169:LYS:NZ	1.70	1.50
1:F:224:LEU:HD11	1:F:276:VAL:HG11	1.53	0.89
1:G:345:VAL:HB	1:G:358:LEU:HD21	1.56	0.88
1:G:316:THR:HG22	1:G:318:ALA:H	1.41	0.85
1:G:138:LEU:HD23	1:G:329:PHE:HB3	1.56	0.84
1:A:218:LYS:HE2	1:B:161:ASP:OD1	1.77	0.83
1:G:319:GLN:HE21	1:G:323:THR:HB	1.43	0.83
1:B:218:LYS:HE3	1:B:222:GLN:NE2	1.95	0.81
1:G:229:THR:HG23	1:G:230:GLY:H	1.45	0.81
1:G:368:LEU:HG	1:G:370:HIS:HE1	1.52	0.74
1:A:153:GLU:HA	1:A:176:PHE:HB3	1.70	0.73
1:F:133:THR:HG22	1:F:136:ASP:H	1.53	0.73
1:E:194:ARG:HH12	1:E:347:ARG:NE	1.86	0.72
1:C:219:GLU:HG3	1:C:366:LEU:HD11	1.70	0.72
1:E:218:LYS:HE2	1:F:161:ASP:OD1	1.89	0.72
1:D:316:THR:HG22	1:D:318:ALA:H	1.54	0.71
1:E:121:ILE:HD12	1:F:150:TYR:HB3	1.73	0.71
1:C:149:GLU:HG2	1:C:180:THR:HG22	1.72	0.71
1:G:148:LEU:O	1:G:180:THR:HA	1.90	0.70
1:E:130:ARG:HA	1:F:269:GLU:HG2	1.72	0.70
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.55	0.70
1:D:127:PRO:HD2	1:D:210:ARG:HH21	1.57	0.70
1:A:347:ARG:HB3	1:A:358:LEU:HD12	1.74	0.68
1:F:236:LEU:HD23	1:F:370:HIS:HE1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.59	0.68
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.60	0.66
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.10	0.66
1:B:226:GLY:H	1:B:235:GLY:HA3	1.61	0.66
1:G:368:LEU:HG	1:G:370:HIS:CE1	2.31	0.66
1:A:244:ASP:HB2	1:A:264:GLN:NE2	2.11	0.65
1:A:130:ARG:HA	1:B:269:GLU:HG2	1.79	0.65
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.80	0.64
1:G:193:SER:HB2	1:G:195:GLN:NE2	2.13	0.64
1:B:301:GLN:HE22	1:C:297:PHE:HA	1.62	0.63
1:F:133:THR:HG23	1:F:135:ARG:HB3	1.79	0.63
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.14	0.63
1:B:218:LYS:HE3	1:B:222:GLN:HE21	1.63	0.63
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.81	0.63
1:C:189:TRP:HZ3	1:C:191:GLN:HB2	1.65	0.62
1:G:183:VAL:HG22	1:G:367:ALA:HB2	1.81	0.62
1:E:193:SER:HB3	1:E:196:VAL:HG23	1.81	0.61
1:A:226:GLY:H	1:A:235:GLY:HA3	1.64	0.61
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.36	0.61
1:B:218:LYS:CE	1:B:222:GLN:NE2	2.64	0.61
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.36	0.60
1:F:286:ALA:HB1	1:F:304:THR:HG21	1.84	0.60
1:A:236:LEU:HD23	1:A:370:HIS:HE1	1.66	0.60
1:B:275:ILE:HG23	1:B:326:VAL:HG22	1.82	0.60
1:F:244:ASP:HB3	1:F:247:LEU:HG	1.83	0.60
1:D:229:THR:HG22	1:D:232:ASN:HD22	1.66	0.60
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.65	0.59
1:F:244:ASP:HB2	1:F:264:GLN:NE2	2.17	0.59
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.38	0.59
1:F:130:ARG:C	1:F:132:LEU:H	2.05	0.59
1:B:316:THR:HG22	1:B:318:ALA:H	1.68	0.59
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.85	0.59
1:G:134:ILE:HD12	1:G:220:GLU:HG2	1.84	0.58
1:G:254:ARG:HB3	1:G:381:PHE:HZ	1.68	0.58
1:B:347:ARG:HB3	1:B:358:LEU:HD12	1.85	0.58
1:D:189:TRP:HZ3	1:D:191:GLN:HB2	1.67	0.58
1:C:226:GLY:HA3	1:C:235:GLY:H	1.69	0.58
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.84	0.58
1:C:104:SER:HB3	1:E:166:LYS:NZ	2.18	0.58
1:F:138:LEU:HD23	1:F:329:PHE:HB3	1.86	0.58
1:C:130:ARG:HA	1:D:269:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.84	0.57
1:F:133:THR:CG2	1:F:136:ASP:H	2.17	0.57
1:A:336:TRP:HB2	1:A:367:ALA:HB3	1.87	0.57
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.86	0.57
1:A:189:TRP:HZ3	1:A:191:GLN:HB2	1.69	0.57
1:E:119:MET:HB3	1:F:148:LEU:HD23	1.87	0.57
1:A:189:TRP:CD1	1:B:169:LYS:HB2	2.38	0.57
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.40	0.57
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.69	0.56
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.70	0.56
1:D:146:ASN:O	1:D:183:VAL:HG12	2.04	0.56
1:E:243:TYR:HA	1:E:264:GLN:HE22	1.70	0.56
1:C:316:THR:HG22	1:C:318:ALA:H	1.68	0.56
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.88	0.56
1:E:116:ILE:HD12	1:F:146:ASN:HB2	1.86	0.56
1:E:187:ALA:HB2	1:E:363:GLU:HA	1.87	0.55
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.41	0.55
1:G:156:PHE:CD1	1:G:174:ILE:HG12	2.41	0.55
1:A:188:HIS:CE1	1:B:160:ALA:HB2	2.42	0.55
1:D:139:ALA:HB3	1:D:334:GLN:HB2	1.88	0.55
1:B:193:SER:HB3	1:B:196:VAL:HG23	1.89	0.55
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.41	0.55
1:C:141:GLY:O	1:C:336:TRP:HA	2.07	0.55
1:F:227:ASP:HB3	1:F:229:THR:HG22	1.88	0.55
1:F:350:ARG:HG3	1:F:351:ASP:H	1.72	0.55
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.22	0.54
1:B:264:GLN:HB3	1:B:377:ILE:HD13	1.90	0.54
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.23	0.54
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.89	0.54
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.90	0.54
1:B:244:ASP:HB2	1:B:264:GLN:NE2	2.23	0.54
1:E:210:ARG:HB3	1:F:156:PHE:HE2	1.73	0.53
1:A:142:ARG:NH1	1:A:142:ARG:HB3	2.23	0.53
1:B:218:LYS:CE	1:B:222:GLN:HE21	2.21	0.53
1:A:107:SER:O	1:A:113:GLY:HA3	2.07	0.53
1:G:132:LEU:HD13	1:G:312:PRO:HB3	1.90	0.53
1:F:201:PRO:O	1:F:204:GLN:HB3	2.08	0.53
1:B:352:ASN:HA	1:B:357:MET:HB2	1.91	0.53
1:D:141:GLY:O	1:D:336:TRP:HA	2.08	0.53
1:F:236:LEU:HD23	1:F:370:HIS:CE1	2.42	0.53
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.91	0.52
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.44	0.52
1:F:224:LEU:HD23	1:F:237:ASN:ND2	2.23	0.52
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.22	0.52
1:G:153:GLU:HG3	1:G:372:ARG:NH1	2.25	0.52
1:G:254:ARG:HB3	1:G:381:PHE:CZ	2.44	0.52
1:C:134:ILE:HB	1:C:220:GLU:HG3	1.91	0.52
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.91	0.51
1:C:208:ASN:O	1:C:212:MET:HG2	2.10	0.51
1:G:208:ASN:O	1:G:212:MET:HG2	2.10	0.51
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.25	0.51
1:D:226:GLY:H	1:D:235:GLY:HA3	1.76	0.51
1:A:166:LYS:HE3	1:E:104:SER:HB2	1.92	0.51
1:A:224:LEU:HD13	1:A:237:ASN:HD22	1.76	0.51
1:E:223:LEU:O	1:E:236:LEU:HD13	2.11	0.51
1:G:154:GLU:HB2	1:G:175:THR:HB	1.93	0.51
1:C:339:MET:HE3	1:C:363:GLU:HG3	1.92	0.51
1:D:193:SER:HB3	1:D:196:VAL:HG23	1.93	0.50
1:F:343:VAL:HA	1:F:361:LEU:O	2.12	0.50
1:E:236:LEU:HD12	1:E:370:HIS:HE1	1.77	0.50
1:F:282:TRP:O	1:F:285:ILE:HB	2.11	0.50
1:A:258:ILE:O	1:A:262:ILE:HG13	2.12	0.50
1:F:351:ASP:HB3	1:F:355:LYS:HD3	1.93	0.50
1:B:188:HIS:HB3	1:C:160:ALA:HA	1.94	0.50
1:D:139:ALA:HB3	1:D:334:GLN:CB	2.41	0.50
1:F:226:GLY:H	1:F:235:GLY:HA3	1.75	0.50
1:A:218:LYS:O	1:A:218:LYS:HG3	2.12	0.50
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.27	0.50
1:E:226:GLY:H	1:E:235:GLY:HA3	1.77	0.49
1:A:163:VAL:HG21	1:A:169:LYS:HG3	1.95	0.49
1:C:124:ILE:N	1:C:124:ILE:HD12	2.27	0.49
1:E:168:LEU:HD23	1:E:169:LYS:N	2.27	0.49
1:G:191:GLN:OE1	1:G:350:ARG:NH1	2.45	0.49
1:B:115:LEU:N	1:B:115:LEU:HD12	2.27	0.49
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.93	0.49
1:D:120:GLN:O	1:D:122:PRO:HD3	2.12	0.49
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.48	0.49
1:D:189:TRP:CZ3	1:D:191:GLN:HB2	2.48	0.49
1:G:133:THR:HG22	1:G:135:ARG:H	1.76	0.49
1:E:139:ALA:O	1:E:334:GLN:HG3	2.13	0.49
1:A:120:GLN:O	1:A:122:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:HG2	1:D:358:LEU:CD1	2.43	0.49
1:F:132:LEU:HB3	1:F:314:VAL:HG12	1.94	0.49
1:C:119:MET:HB3	1:D:148:LEU:HD23	1.94	0.49
1:C:292:GLU:HG2	1:D:292:GLU:OE2	2.13	0.48
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.42	0.48
1:A:194:ARG:CZ	1:A:347:ARG:NH1	2.76	0.48
1:G:186:ILE:HG21	1:G:222:GLN:HG3	1.95	0.48
1:B:288:LEU:O	1:B:296:ILE:HG12	2.14	0.48
1:C:345:VAL:HG12	1:C:360:ILE:HG12	1.94	0.48
1:D:254:ARG:O	1:D:258:ILE:HD12	2.13	0.48
1:A:169:LYS:HB3	1:F:189:TRP:HD1	1.77	0.48
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.94	0.48
1:D:188:HIS:ND1	1:E:160:ALA:HB2	2.28	0.48
1:E:124:ILE:HG22	1:E:125:ILE:N	2.28	0.48
1:E:266:THR:C	1:E:268:SER:H	2.17	0.48
1:A:121:ILE:HG13	1:B:150:TYR:HB3	1.95	0.48
1:C:104:SER:HB3	1:E:166:LYS:HZ2	1.78	0.48
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.94	0.48
1:B:119:MET:HB3	1:C:148:LEU:HD23	1.96	0.48
1:D:218:LYS:O	1:D:218:LYS:HG3	2.14	0.48
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.28	0.48
1:C:130:ARG:HD2	1:C:317:LYS:HB2	1.96	0.47
1:D:188:HIS:CE1	1:E:160:ALA:HB2	2.49	0.47
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.62	0.47
1:G:153:GLU:HG3	1:G:372:ARG:CZ	2.44	0.47
1:G:139:ALA:HB3	1:G:334:GLN:HB2	1.96	0.47
1:G:349:ASP:OD1	1:G:350:ARG:HG2	2.15	0.47
1:B:218:LYS:NZ	1:B:222:GLN:NE2	2.62	0.47
1:A:160:ALA:HA	1:F:188:HIS:HB3	1.97	0.47
1:C:197:MET:CE	1:C:204:GLN:HB2	2.45	0.46
1:F:133:THR:CG2	1:F:135:ARG:HB3	2.43	0.46
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.95	0.46
1:D:350:ARG:HB3	1:D:351:ASP:H	1.44	0.46
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.98	0.46
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.30	0.46
1:G:229:THR:HG23	1:G:230:GLY:N	2.21	0.46
1:G:258:ILE:O	1:G:262:ILE:HG13	2.15	0.46
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.81	0.46
1:D:258:ILE:O	1:D:262:ILE:HG13	2.16	0.46
1:D:342:THR:HG22	1:D:343:VAL:N	2.30	0.46
1:F:139:ALA:O	1:F:334:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD23	1:B:370:HIS:CE1	2.49	0.46
1:F:258:ILE:O	1:F:262:ILE:HG13	2.16	0.46
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.50	0.46
1:D:341:ALA:HA	1:D:363:GLU:O	2.16	0.46
1:F:285:ILE:O	1:F:288:LEU:HG	2.16	0.46
1:A:150:TYR:HE2	1:A:181:ALA:HB2	1.80	0.46
1:G:229:THR:CG2	1:G:232:ASN:HD22	2.29	0.46
1:A:172:SER:O	1:F:190:VAL:HG22	2.15	0.46
1:F:155:VAL:H	1:F:175:THR:HB	1.81	0.45
1:B:138:LEU:HD23	1:B:329:PHE:HB3	1.99	0.45
1:G:350:ARG:HG2	1:G:350:ARG:H	1.47	0.45
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.98	0.45
1:E:234:GLU:HG2	1:E:239:VAL:CG2	2.46	0.45
1:G:155:VAL:H	1:G:175:THR:HB	1.81	0.45
1:B:116:ILE:HG21	1:C:146:ASN:HB2	1.98	0.45
1:D:236:LEU:HD23	1:D:370:HIS:CE1	2.48	0.45
1:E:285:ILE:O	1:E:288:LEU:HG	2.16	0.45
1:C:325:THR:HA	1:C:377:ILE:O	2.16	0.45
1:D:295:TYR:CE1	1:D:300:PRO:HG3	2.51	0.45
1:D:207:ILE:O	1:D:211:LEU:HD23	2.17	0.45
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.98	0.45
1:B:134:ILE:HD12	1:B:220:GLU:CG	2.47	0.45
1:A:154:GLU:H	1:A:176:PHE:HA	1.82	0.44
1:B:120:GLN:O	1:B:122:PRO:HD3	2.17	0.44
1:C:124:ILE:HD12	1:C:124:ILE:H	1.81	0.44
1:D:229:THR:HG23	1:D:230:GLY:N	2.32	0.44
1:B:134:ILE:HD12	1:B:220:GLU:HG2	1.98	0.44
1:A:347:ARG:HB3	1:A:358:LEU:CD1	2.46	0.44
1:C:254:ARG:O	1:C:258:ILE:HD13	2.17	0.44
1:F:193:SER:OG	1:F:195:GLN:HG2	2.18	0.44
1:G:282:TRP:CE3	1:G:313:VAL:HG11	2.53	0.44
1:B:194:ARG:HD2	1:B:347:ARG:NH1	2.32	0.44
1:B:285:ILE:O	1:B:288:LEU:HG	2.17	0.44
1:E:130:ARG:HA	1:F:269:GLU:CG	2.44	0.44
1:A:290:ASP:OD2	1:A:294:ARG:HB2	2.17	0.44
1:C:226:GLY:H	1:C:235:GLY:HA3	1.81	0.44
1:F:349:ASP:O	1:F:352:ASN:HB2	2.18	0.44
1:B:234:GLU:HG2	1:B:239:VAL:CG2	2.48	0.44
1:B:275:ILE:HG22	1:B:277:LEU:HD11	1.99	0.43
1:G:203:LEU:O	1:G:207:ILE:HG13	2.17	0.43
1:B:301:GLN:NE2	1:C:297:PHE:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ASN:O	1:E:212:MET:HG2	2.18	0.43
1:E:303:PHE:HD2	1:E:303:PHE:HA	1.70	0.43
1:G:352:ASN:O	1:G:356:ASN:N	2.51	0.43
1:D:254:ARG:HH21	1:D:381:PHE:HB3	1.83	0.43
1:F:131:ARG:HH21	1:F:316:THR:HA	1.84	0.43
1:A:152:ARG:CZ	1:A:179:GLN:HG3	2.48	0.43
1:F:244:ASP:HB2	1:F:264:GLN:HE22	1.83	0.43
1:G:279:PRO:HD3	1:G:316:THR:O	2.18	0.43
1:D:325:THR:HA	1:D:377:ILE:O	2.18	0.43
1:G:138:LEU:HD22	1:G:333:SER:O	2.18	0.43
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.49	0.43
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.01	0.43
1:B:119:MET:HB3	1:C:148:LEU:CD2	2.49	0.43
1:A:153:GLU:CA	1:A:176:PHE:HB3	2.45	0.43
1:A:199:ASP:O	1:A:201:PRO:HD3	2.19	0.43
1:C:239:VAL:HG12	1:C:373:PRO:HB3	2.01	0.43
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.48	0.43
1:D:339:MET:HE3	1:D:363:GLU:HG3	2.01	0.43
1:G:152:ARG:HB3	1:G:153:GLU:H	1.60	0.43
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.54	0.43
1:E:116:ILE:H	1:E:116:ILE:HG12	1.71	0.43
1:A:342:THR:HG22	1:A:343:VAL:N	2.34	0.42
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.84	0.42
1:C:189:TRP:CZ3	1:C:191:GLN:HB2	2.51	0.42
1:C:258:ILE:O	1:C:262:ILE:HG13	2.19	0.42
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.35	0.42
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.42
1:C:193:SER:HB3	1:C:196:VAL:HG23	2.01	0.42
1:E:264:GLN:HE21	1:E:377:ILE:HG12	1.83	0.42
1:C:264:GLN:HB3	1:C:377:ILE:CD1	2.49	0.42
1:D:187:ALA:HB3	1:E:169:LYS:HE2	2.02	0.42
1:G:152:ARG:HG2	1:G:370:HIS:O	2.19	0.42
1:B:350:ARG:HB3	1:B:351:ASP:H	1.47	0.42
1:D:295:TYR:HE1	1:D:300:PRO:HG3	1.84	0.42
1:D:308:MET:HG2	1:D:309:TRP:CD1	2.54	0.42
1:D:311:LEU:HA	1:D:312:PRO:HD3	1.91	0.42
1:G:319:GLN:NE2	1:G:323:THR:HB	2.24	0.42
1:B:311:LEU:HA	1:B:312:PRO:HD3	1.89	0.42
1:G:152:ARG:NE	1:G:179:GLN:HG3	2.35	0.42
1:A:159:ASN:H	1:A:172:SER:HB3	1.84	0.42
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:ARG:HG3	1:F:351:ASP:N	2.35	0.42
1:A:171:GLU:HB2	1:F:189:TRP:CZ2	2.55	0.42
1:B:254:ARG:O	1:B:258:ILE:HD13	2.19	0.42
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.02	0.42
1:C:371:TYR:CD1	1:C:371:TYR:N	2.88	0.42
1:G:139:ALA:O	1:G:334:GLN:HB2	2.20	0.42
1:G:224:LEU:HD21	1:G:319:GLN:OE1	2.20	0.42
1:G:259:ALA:HA	1:G:262:ILE:HD12	2.02	0.42
1:G:308:MET:HG2	1:G:309:TRP:CD1	2.55	0.42
1:B:277:LEU:HD12	1:B:277:LEU:N	2.34	0.41
1:G:348:GLU:H	1:G:348:GLU:HG2	1.75	0.41
1:G:135:ARG:HG3	1:G:135:ARG:HH11	1.85	0.41
1:A:339:MET:HE3	1:A:363:GLU:HG3	2.02	0.41
1:B:266:THR:C	1:B:268:SER:H	2.22	0.41
1:C:126:MET:HA	1:C:127:PRO:HD3	1.90	0.41
1:A:203:LEU:O	1:A:207:ILE:HG13	2.20	0.41
1:G:203:LEU:HD21	1:G:207:ILE:HD11	2.02	0.41
1:A:308:MET:HG2	1:A:309:TRP:CD1	2.55	0.41
1:C:197:MET:HG3	1:C:358:LEU:HD23	2.02	0.41
1:E:311:LEU:HA	1:E:312:PRO:HD3	1.92	0.41
1:E:339:MET:HB3	1:E:365:ARG:HG3	2.02	0.41
1:A:281:ASP:O	1:A:285:ILE:HG13	2.20	0.41
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.91	0.41
1:E:207:ILE:O	1:E:211:LEU:HD13	2.21	0.41
1:F:276:VAL:HB	1:F:325:THR:HB	2.03	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:C:371:TYR:H	1:C:371:TYR:HD1	1.69	0.41
1:E:234:GLU:HG2	1:E:239:VAL:HG22	2.01	0.41
1:F:253:THR:OG1	1:F:256:ASP:HB2	2.21	0.41
1:G:193:SER:HB2	1:G:195:GLN:HE21	1.85	0.41
1:G:294:ARG:HD3	1:G:295:TYR:H	1.85	0.41
1:G:342:THR:HG22	1:G:343:VAL:N	2.36	0.41
1:A:156:PHE:C	1:A:156:PHE:CD1	2.94	0.41
1:F:223:LEU:O	1:F:236:LEU:HG	2.20	0.41
1:F:236:LEU:HD22	1:F:376:ILE:HD13	2.03	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.93	0.41
1:E:357:MET:HG3	1:E:358:LEU:H	1.85	0.41
1:F:257:ILE:O	1:F:260:HIS:HB2	2.21	0.41
1:G:351:ASP:O	1:G:353:PHE:N	2.54	0.41
1:A:147:ALA:HA	1:A:183:VAL:HG23	2.03	0.40
1:A:176:PHE:CD1	1:A:176:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:MET:HG2	1:B:203:LEU:N	2.36	0.40
1:E:187:ALA:HB3	1:F:169:LYS:HE2	2.03	0.40
1:E:194:ARG:NH1	1:E:347:ARG:NE	2.63	0.40
1:A:258:ILE:N	1:A:258:ILE:HD12	2.36	0.40
1:A:295:TYR:HB2	1:A:299:GLY:HA2	2.03	0.40
1:B:234:GLU:HG2	1:B:239:VAL:HG23	2.03	0.40
1:D:125:ILE:HD13	1:E:371:TYR:HB3	2.04	0.40
1:D:226:GLY:N	1:D:235:GLY:HA3	2.35	0.40
1:E:289:LYS:HA	1:E:294:ARG:O	2.21	0.40
1:C:183:VAL:HG13	1:C:366:LEU:O	2.22	0.40
1:E:329:PHE:C	1:E:331:MET:H	2.24	0.40
1:F:141:GLY:O	1:F:336:TRP:HA	2.22	0.40
1:G:358:LEU:HD23	1:G:359:THR:N	2.36	0.40
1:E:277:LEU:O	1:E:315:PRO:HA	2.22	0.40
1:F:147:ALA:HA	1:F:183:VAL:HG23	2.02	0.40
1:F:324:PHE:HB3	1:F:381:PHE:HE1	1.84	0.40
1:G:343:VAL:HG22	1:G:362:CYS:SG	2.61	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	278/282 (99%)	249 (90%)	27 (10%)	2 (1%)	22	63
1	B	278/282 (99%)	252 (91%)	22 (8%)	4 (1%)	11	46
1	C	278/282 (99%)	258 (93%)	20 (7%)	0	100	100
1	D	278/282 (99%)	256 (92%)	22 (8%)	0	100	100
1	E	278/282 (99%)	246 (88%)	29 (10%)	3 (1%)	14	52
1	F	254/282 (90%)	229 (90%)	21 (8%)	4 (2%)	9	44
1	G	239/282 (85%)	208 (87%)	27 (11%)	4 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1883/1974 (95%)	1698 (90%)	168 (9%)	17 (1%)	17 57

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	300	PRO
1	F	352	ASN
1	G	352	ASN
1	E	330	ASP
1	G	224	LEU
1	A	201	PRO
1	B	127	PRO
1	B	230	GLY
1	F	131	ARG
1	G	349	ASP
1	B	352	ASN
1	E	144	SER
1	F	240	ALA
1	F	300	PRO
1	G	230	GLY
1	A	315	PRO
1	B	300	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	230/231 (100%)	214 (93%)	16 (7%)	15	40
1	B	230/231 (100%)	221 (96%)	9 (4%)	32	56
1	C	230/231 (100%)	226 (98%)	4 (2%)	60	78
1	D	230/231 (100%)	223 (97%)	7 (3%)	41	63
1	E	230/231 (100%)	223 (97%)	7 (3%)	41	63
1	F	211/231 (91%)	205 (97%)	6 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	201/231 (87%)	190 (94%)	11 (6%)	21	47
All	All	1562/1617 (97%)	1502 (96%)	60 (4%)	33	57

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	115	LEU
1	A	117	GLN
1	A	148	LEU
1	A	149	GLU
1	A	156	PHE
1	A	169	LYS
1	A	176	PHE
1	A	179	GLN
1	A	188	HIS
1	A	195	GLN
1	A	202	MET
1	A	270	PHE
1	A	301	GLN
1	A	303	PHE
1	A	316	THR
1	B	146	ASN
1	B	188	HIS
1	B	195	GLN
1	B	202	MET
1	B	224	LEU
1	B	227	ASP
1	B	277	LEU
1	B	303	PHE
1	B	344	GLU
1	C	188	HIS
1	C	202	MET
1	C	224	LEU
1	C	303	PHE
1	D	146	ASN
1	D	152	ARG
1	D	188	HIS
1	D	194	ARG
1	D	202	MET
1	D	292	GLU
1	D	303	PHE

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Mol	Chain	Res	Type
1	E	142	ARG
1	E	152	ARG
1	E	188	HIS
1	E	195	GLN
1	E	280	ARG
1	E	300	PRO
1	E	303	PHE
1	F	133	THR
1	F	135	ARG
1	F	156	PHE
1	F	188	HIS
1	F	227	ASP
1	F	292	GLU
1	G	129	LEU
1	G	142	ARG
1	G	173	ASP
1	G	195	GLN
1	G	256	ASP
1	G	290	ASP
1	G	294	ARG
1	G	301	GLN
1	G	350	ARG
1	G	370	HIS
1	G	383	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	204	GLN
1	A	225	ASN
1	A	237	ASN
1	A	334	GLN
1	B	191	GLN
1	B	222	GLN
1	B	301	GLN
1	B	334	GLN
1	B	352	ASN
1	C	159	ASN
1	C	191	GLN
1	C	222	GLN
1	C	334	GLN

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Mol	Chain	Res	Type
1	C	352	ASN
1	D	191	GLN
1	D	222	GLN
1	D	232	ASN
1	D	334	GLN
1	D	352	ASN
1	E	191	GLN
1	E	204	GLN
1	E	208	ASN
1	E	237	ASN
1	E	291	ASN
1	E	334	GLN
1	E	352	ASN
1	F	222	GLN
1	F	260	HIS
1	F	334	GLN
1	G	195	GLN
1	G	232	ASN
1	G	237	ASN
1	G	260	HIS
1	G	319	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 monosaccharides 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	180:THR	C	181:ALA	N	0.94

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.