



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:36 AM EDT

PDB ID : 2FSY / pdb_00002fsy
Title : Bacteriophage HK97 Pepsin-treated 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 : 2006-01-23
Resolution : 3.80 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

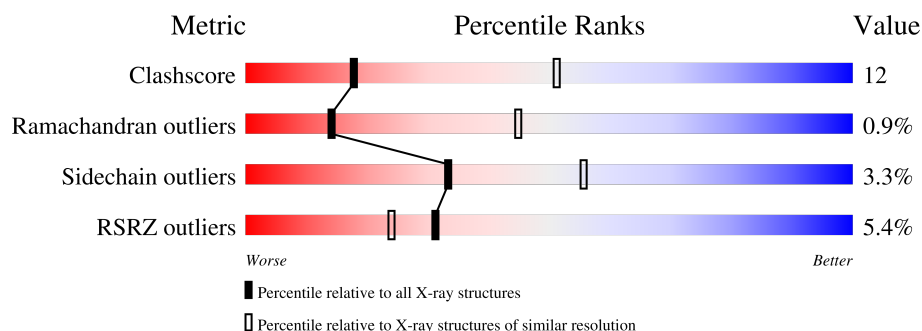
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	282	4% 68% 30% ..
1	B	282	5% 72% 26% ..
1	C	282	3% 76% 23% .
1	D	282	2% 72% 25% ..
1	E	282	2% 72% 26% ..
1	F	282	4% 60% 28% . 9%

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Mol	Chain	Length	Quality of chain
1	G	282	18% 58% 26% • 14%

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.

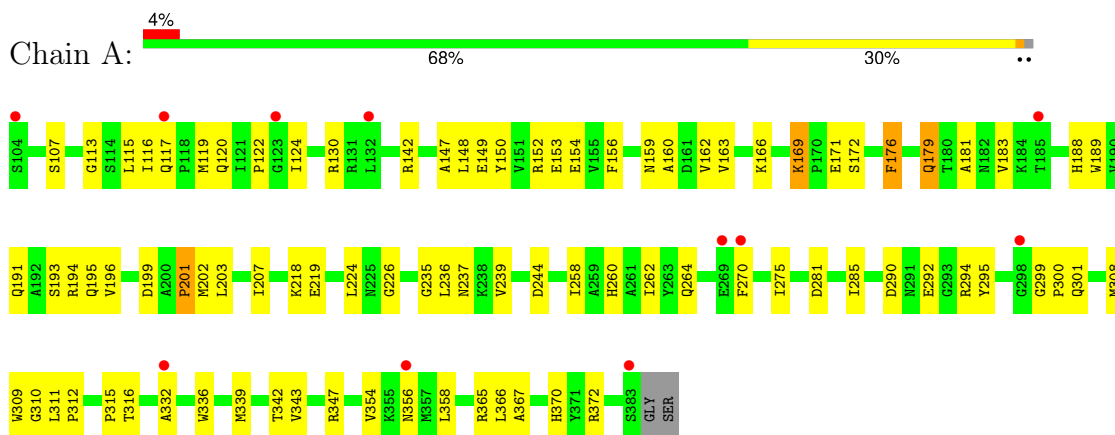
- Molecule 1 is a protein called major capsid protein.

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			

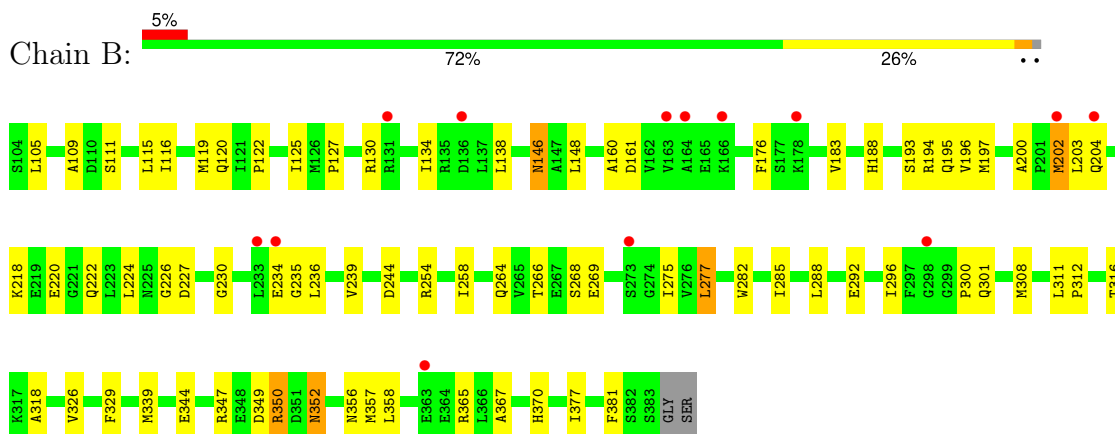
3 Residue-property plots

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 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.

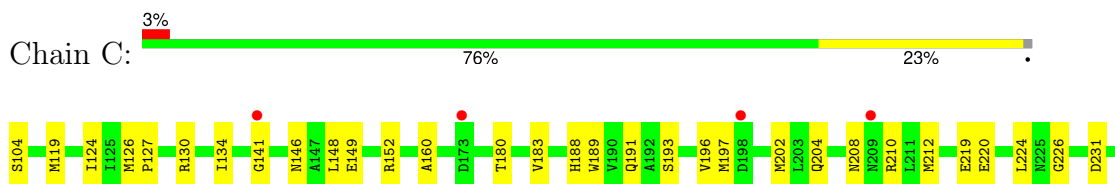
- Molecule 1: major capsid protein



- Molecule 1: major capsid protein

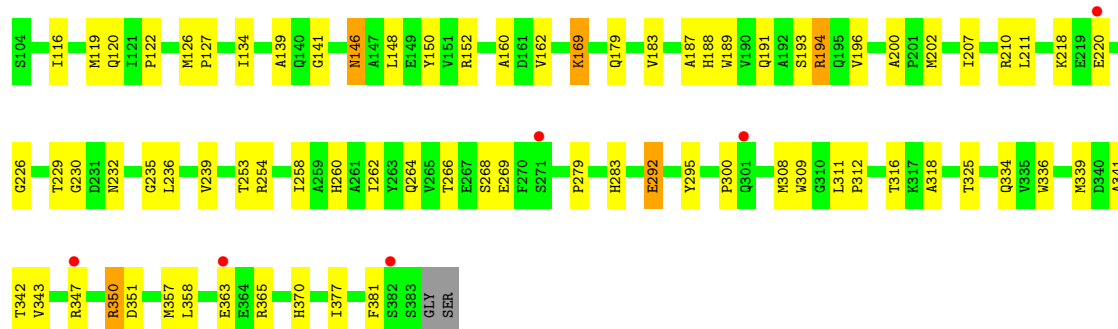


- Molecule 1: major capsid protein

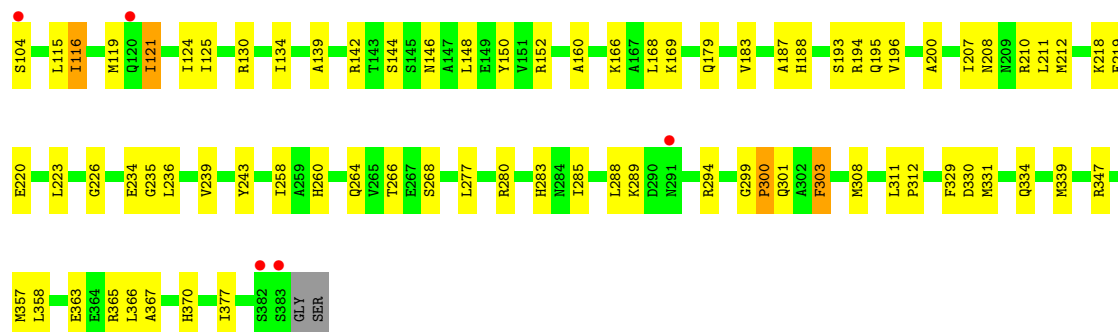




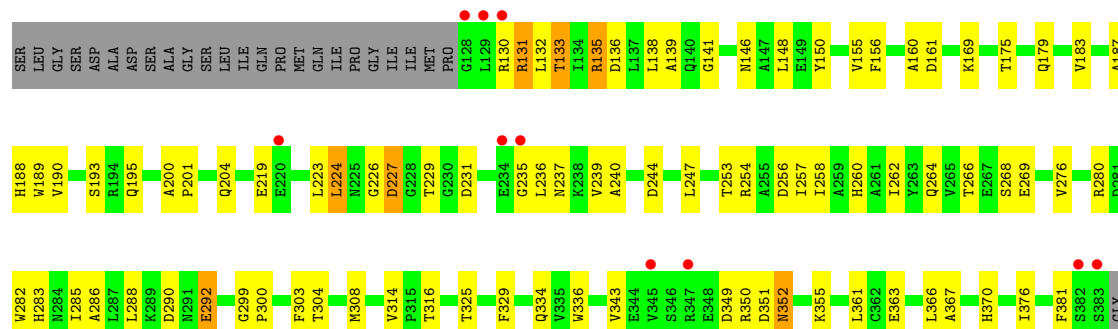
• Molecule 1: major capsid protein

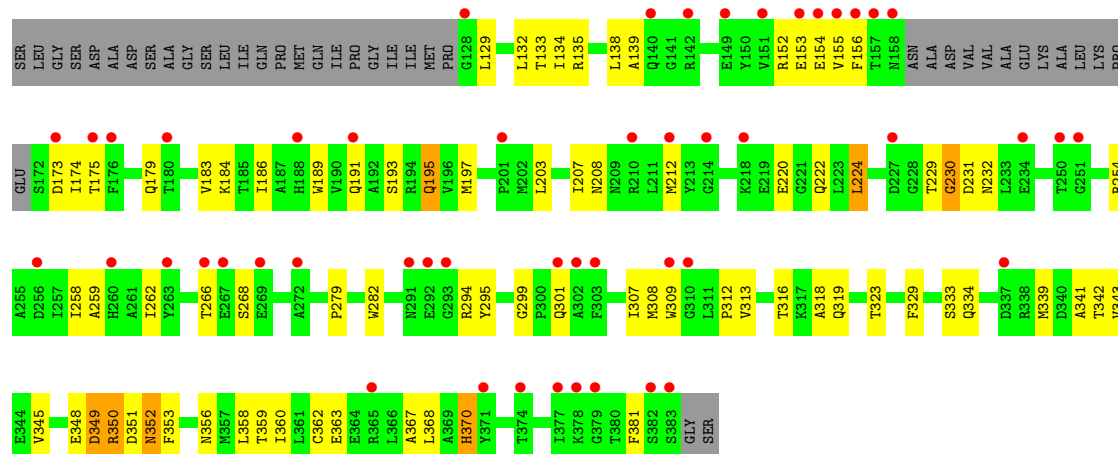


• Molecule 1: major capsid protein



• Molecule 1: major capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	1006.39Å 1006.39Å 728.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	59.9 (50.00-3.80) 60.1 (50.00-3.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.337 , (Not available) 0.327 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.28	EDS
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.32	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	B	0.36	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	C	0.33	1/2188 (0.0%)	0.82	3/2969 (0.1%)
1	D	0.34	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	E	0.31	0/2188	0.86	6/2969 (0.2%)
1	F	0.31	0/2020	0.86	4/2740 (0.1%)
1	G	0.32	0/1922	0.84	2/2605 (0.1%)
All	All	0.33	4/14882 (0.0%)	0.84	24/20190 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	ASN	CG-ND2	9.38	1.52	1.33
1	D	169	LYS	CE-NZ	7.00	1.70	1.49
1	A	356	ASN	CG-ND2	5.53	1.44	1.33
1	C	356	ASN	CG-ND2	5.16	1.44	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	GLY	CA-C-N	8.77	130.81	119.84
1	E	299	GLY	C-N-CA	8.77	130.81	119.84
1	F	200	ALA	CA-C-N	8.19	127.76	119.24
1	F	200	ALA	C-N-CA	8.19	127.76	119.24
1	D	350	ARG	CB-CA-C	-6.74	108.78	116.54
1	B	350	ARG	CB-CA-C	-6.74	108.80	116.54
1	A	372	ARG	CA-C-N	6.45	126.14	119.56
1	A	372	ARG	C-N-CA	6.45	126.14	119.56
1	A	332	ALA	N-CA-C	5.89	117.78	111.36
1	D	200	ALA	CA-C-N	5.87	125.08	118.97
1	D	200	ALA	C-N-CA	5.87	125.08	118.97
1	B	200	ALA	CA-C-N	5.73	125.20	119.24
1	B	200	ALA	C-N-CA	5.73	125.20	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	ARG	CA-C-N	5.65	125.18	119.19
1	C	372	ARG	C-N-CA	5.65	125.18	119.19
1	G	299	GLY	CA-C-N	5.58	125.25	119.56
1	G	299	GLY	C-N-CA	5.58	125.25	119.56
1	F	299	GLY	CA-C-N	5.57	126.80	119.84
1	F	299	GLY	C-N-CA	5.57	126.80	119.84
1	E	121	ILE	CA-C-N	5.50	125.82	119.93
1	E	121	ILE	C-N-CA	5.50	125.82	119.93
1	E	200	ALA	CA-C-N	5.45	125.53	119.32
1	E	200	ALA	C-N-CA	5.45	125.53	119.32
1	C	350	ARG	CB-CA-C	-5.19	110.57	116.54

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	60	0
1	B	2151	0	2119	65	0
1	C	2151	0	2119	53	0
1	D	2151	0	2119	58	0
1	E	2151	0	2119	53	0
1	F	1986	0	1951	68	0
1	G	1890	0	1851	54	0
All	All	14631	0	14397	357	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 12.

All (357) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:VAL:HB	1:G:358:LEU:HD21	1.56	0.88
1:B:349:ASP:OD2	1:B:350:ARG:HG2	1.75	0.85
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:G:319:GLN:HE21	1:G:323:THR:HB	1.43	0.83
1:A:218:LYS:HE2	1:B:161:ASP:OD1	1.80	0.82
1:A:130:ARG:HA	1:B:269:GLU:HG2	1.62	0.82
1:G:229:THR:HG23	1:G:230:GLY:H	1.44	0.81
1:B:218:LYS:HE3	1:B:222:GLN:NE2	1.95	0.81
1:E:130:ARG:HA	1:F:269:GLU:HG2	1.63	0.80
1:E:218:LYS:HE2	1:F:161:ASP:OD1	1.84	0.76
1:B:339:MET:HE2	1:B:365:ARG:HG3	1.66	0.76
1:E:121:ILE:HD12	1:F:150:TYR:HB3	1.69	0.75
1:G:368:LEU:HG	1:G:370:HIS:HE1	1.52	0.74
1:A:153:GLU:HA	1:A:176:PHE:HB3	1.71	0.73
1:F:133:THR:HG22	1:F:136:ASP:H	1.54	0.72
1:C:219:GLU:HG3	1:C:366:LEU:HD11	1.70	0.72
1:E:194:ARG:HH12	1:E:347:ARG:NE	1.86	0.72
1:D:316:THR:HG22	1:D:318:ALA:H	1.54	0.71
1:B:349:ASP:O	1:B:350:ARG:HG3	1.90	0.70
1:C:149:GLU:HG2	1:C:180:THR:HG22	1.72	0.70
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.72	0.70
1:D:127:PRO:HD2	1:D:210:ARG:HH21	1.57	0.70
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.55	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
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.59	0.68
1:E:119:MET:HB3	1:F:148:LEU:HD23	1.77	0.66
1:A:339:MET:HE2	1:A:365:ARG:HG3	1.78	0.66
1:B:226:GLY:H	1:B:235:GLY:HA3	1.61	0.66
1:C:339:MET:HE2	1:C:365:ARG:HG3	1.76	0.66
1:G:368:LEU:HG	1:G:370:HIS:CE1	2.31	0.65
1:A:244:ASP:HB2	1:A:264:GLN:NE2	2.11	0.65
1:C:130:ARG:HA	1:D:269:GLU:HG2	1.80	0.64
1:F:130:ARG:C	1:F:132:LEU:H	2.05	0.64
1:G:193:SER:HB2	1:G:195:GLN:NE2	2.13	0.64
1:F:133:THR:HG23	1:F:135:ARG:HB3	1.79	0.63
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.81	0.63
1:B:218:LYS:HE3	1:B:222:GLN:HE21	1.63	0.63
1:B:349:ASP:C	1:B:350:ARG:CG	2.71	0.62
1:C:189:TRP:HZ3	1:C:191:GLN:HB2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.65	0.61
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.35	0.61
1:B:349:ASP:O	1:B:350:ARG:CG	2.48	0.61
1:B:349:ASP:C	1:B:350:ARG:HG2	2.26	0.61
1:B:218:LYS:CE	1:B:222:GLN:NE2	2.64	0.60
1:F:286:ALA:HB1	1:F:304:THR:HG21	1.84	0.60
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.36	0.60
1:B:275:ILE:HG23	1:B:326:VAL:HG22	1.82	0.60
1:A:236:LEU:HD23	1:A:370:HIS:HE1	1.66	0.60
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.65	0.60
1:F:244:ASP:HB2	1:F:264:GLN:NE2	2.17	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	1.67	0.59
1:B:301:GLN:HE22	1:C:297:PHE:HA	1.67	0.59
1:G:189:TRP:CD1	1:G:189:TRP:H	2.19	0.59
1:B:316:THR:HG22	1:B:318:ALA:H	1.68	0.59
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.38	0.59
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.85	0.59
1:E:210:ARG:HB3	1:F:156:PHE:HE2	1.67	0.58
1:G:254:ARG:HB3	1:G:381:PHE:HZ	1.68	0.58
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.68	0.58
1:B:197:MET:HE1	1:B:204:GLN:HA	1.84	0.58
1:G:134:ILE:HD12	1:G:220:GLU:HG2	1.84	0.58
1:D:189:TRP:HZ3	1:D:191:GLN:HB2	1.67	0.58
1:D:339:MET:HE2	1:D:365:ARG:HG3	1.84	0.58
1:B:347:ARG:HB3	1:B:358:LEU:HD12	1.85	0.58
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.86	0.58
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.84	0.58
1:F:138:LEU:HD23	1:F:329:PHE:HB3	1.86	0.58
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.85	0.58
1:C:226:GLY:HA3	1:C:235:GLY:H	1.69	0.58
1:A:189:TRP:HZ3	1:A:191:GLN:HB2	1.68	0.57
1:A:336:TRP:HB2	1:A:367:ALA:HB3	1.86	0.57
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.85	0.57
1:F:133:THR:CG2	1:F:136:ASP:H	2.17	0.57
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.40	0.57
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.70	0.57
1:D:146:ASN:O	1:D:183:VAL:HG12	2.04	0.57
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:TYR:HA	1:E:264:GLN:HE22	1.70	0.56
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.88	0.56
1:C:316:THR:HG22	1:C:318:ALA:H	1.69	0.56
1:E:187:ALA:HB2	1:E:363:GLU:HA	1.87	0.56
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:B:193:SER:HB3	1:B:196:VAL:HG23	1.89	0.55
1:D:139:ALA:HB3	1:D:334:GLN:HB2	1.88	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:B:264:GLN:HB3	1:B:377:ILE:HD13	1.90	0.54
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.89	0.54
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.22	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:D:339:MET:HE1	1:D:363:GLU:HG3	1.90	0.54
1:A:309:TRP:O	1:F:303:PHE:HB3	2.08	0.54
1:G:132:LEU:HD13	1:G:312:PRO:HB3	1.90	0.54
1:A:142:ARG:NH1	1:A:142:ARG:HB3	2.23	0.53
1:F:236:LEU:HD23	1:F:370:HIS:CE1	2.42	0.53
1:A:107:SER:O	1:A:113:GLY:HA3	2.07	0.53
1:B:352:ASN:HA	1:B:357:MET:HB2	1.90	0.53
1:B:218:LYS:CE	1:B:222:GLN:HE21	2.22	0.53
1:F:201:PRO:O	1:F:204:GLN:HB3	2.08	0.53
1:D:141:GLY:O	1:D:336:TRP:HA	2.08	0.53
1:F:224:LEU:HD23	1:F:237:ASN:ND2	2.23	0.53
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.43	0.53
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.44	0.52
1:E:266:THR:C	1:E:268:SER:H	2.17	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:D:229:THR:CG2	1:D:232:ASN:HD22	2.22	0.52
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:D:226:GLY:H	1:D:235:GLY:HA3	1.75	0.51
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.25	0.51
1:C:292:GLU:HG2	1:D:292:GLU:OE2	2.10	0.51
1:A:224:LEU:HD13	1:A:237:ASN:HD22	1.76	0.51
1:E:258:ILE:HD12	1:E:308:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:MET:HE2	1:G:360:ILE:HD11	1.92	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	1.92	0.51
1:F:343:VAL:HA	1:F:361:LEU:O	2.11	0.51
1:D:193:SER:HB3	1:D:196:VAL:HG23	1.93	0.50
1:E:236:LEU:HD12	1:E:370:HIS:HE1	1.76	0.50
1:A:116:ILE:HG21	1:B:146:ASN:HB3	1.94	0.50
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.27	0.50
1:D:187:ALA:HB3	1:E:169:LYS:HE2	1.93	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:A:160:ALA:HB2	1:F:188:HIS:ND1	2.27	0.50
1:A:172:SER:O	1:F:190:VAL:HG22	2.12	0.50
1:A:218:LYS:O	1:A:218:LYS:HG3	2.12	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: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:B:349:ASP:CG	1:B:350:ARG:HG2	2.36	0.49
1:B:282:TRP:HZ3	1:B:308:MET:HE2	1.78	0.49
1:E:130:ARG:HA	1:F:269:GLU:CG	2.38	0.49
1:A:163:VAL:HG21	1:A:169:LYS:HG3	1.95	0.49
1:D:120:GLN:O	1:D:122:PRO:HD3	2.12	0.49
1:C:119:MET:HB3	1:D:148:LEU:HD23	1.93	0.49
1:C:124:ILE:N	1:C:124:ILE:HD12	2.27	0.49
1:G:191:GLN:OE1	1:G:350:ARG:NH1	2.45	0.49
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.48	0.49
1:E:168:LEU:HD23	1:E:169:LYS:N	2.27	0.49
1:E:226:GLY:H	1:E:235:GLY:HA3	1.77	0.49
1:G:133:THR:HG22	1:G:135:ARG:H	1.76	0.49
1:B:115:LEU:N	1:B:115:LEU:HD12	2.27	0.49
1:E:139:ALA:O	1:E:334:GLN:HG3	2.12	0.49
1:D:188:HIS:CE1	1:E:160:ALA:HB2	2.48	0.49
1:D:189:TRP:CZ3	1:D:191:GLN:HB2	2.48	0.49
1:B:116:ILE:HG21	1:C:146:ASN:HB2	1.95	0.49
1:D:347:ARG:HG2	1:D:358:LEU:CD1	2.43	0.49
1:C:345:VAL:HG12	1:C:360:ILE:HG12	1.94	0.49
1:F:132:LEU:HB3	1:F:314:VAL:HG12	1.94	0.49
1:A:120:GLN:O	1:A:122:PRO:HD3	2.12	0.48
1:A:194:ARG:CZ	1:A:347:ARG:NH1	2.76	0.48
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:O	1:B:296:ILE:HG12	2.14	0.48
1:D:254:ARG:O	1:D:258:ILE:HD12	2.13	0.48
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.94	0.48
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.94	0.48
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.28	0.48
1:G:186:ILE:HG21	1:G:222:GLN:HG3	1.95	0.48
1:E:124:ILE:HG22	1:E:125:ILE:N	2.28	0.48
1:A:166:LYS:HE3	1:E:104:SER:HB2	1.96	0.48
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.94	0.48
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.62	0.47
1:C:130:ARG:HD2	1:C:317:LYS:HB2	1.96	0.47
1:D:218:LYS:O	1:D:218:LYS:HG3	2.14	0.47
1:D:283:HIS:NE2	1:E:260:HIS:HA	2.29	0.47
1:E:187:ALA:HB3	1:F:169:LYS:HE2	1.96	0.47
1:G:139:ALA:HB3	1:G:334:GLN:HB2	1.96	0.47
1:B:119:MET:HB3	1:C:148:LEU:HD23	1.95	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:E:130:ARG:CA	1:F:269:GLU:HG2	2.40	0.47
1:A:310:GLY:HA3	1:F:303:PHE:HD2	1.80	0.47
1:D:350:ARG:HB3	1:D:351:ASP:H	1.44	0.46
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.31	0.46
1:F:133:THR:CG2	1:F:135:ARG:HB3	2.43	0.46
1:A:300:PRO:HG2	1:B:296:ILE:HG21	1.97	0.46
1:B:282:TRP:CZ3	1:B:308:MET:HE2	2.50	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:B:236:LEU:HD23	1:B:370:HIS:CE1	2.49	0.46
1:D:258:ILE:O	1:D:262:ILE:HG13	2.16	0.46
1:F:258:ILE:O	1:F:262:ILE:HG13	2.16	0.46
1:G:258:ILE:O	1:G:262:ILE:HG13	2.15	0.46
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.31	0.46
1:D:341:ALA:HA	1:D:363:GLU:O	2.16	0.46
1:F:139:ALA:O	1:F:334:GLN:HG3	2.16	0.46
1:G:229:THR:HG23	1:G:230:GLY:N	2.21	0.46
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.81	0.46
1:B:266:THR:C	1:B:268:SER:H	2.23	0.46
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.50	0.46
1:D:342:THR:HG22	1:D:343:VAL:N	2.30	0.46
1:G:229:THR:CG2	1:G:232:ASN:HD22	2.29	0.46
1:A:150:TYR:HE2	1:A:181:ALA:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:HA	1:F:283:HIS:NE2	2.31	0.46
1:F:285:ILE:O	1:F:288:LEU:HG	2.16	0.46
1:B:138:LEU:HD23	1:B:329:PHE:HB3	1.99	0.45
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.31	0.45
1:G:350:ARG:HG2	1:G:350:ARG:H	1.47	0.45
1:D:236:LEU:HD23	1:D:370:HIS:CE1	2.48	0.45
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.98	0.45
1:F:155:VAL:H	1:F:175:THR:HB	1.81	0.45
1:E:285:ILE:O	1:E:288:LEU:HG	2.16	0.45
1:G:155:VAL:H	1:G:175:THR:HB	1.81	0.45
1:E:234:GLU:HG2	1:E:239:VAL:CG2	2.46	0.45
1:C:325:THR:HA	1:C:377:ILE:O	2.16	0.45
1:A:119:MET:HB3	1:B:148:LEU:CD2	2.46	0.45
1:E:329:PHE:C	1:E:331:MET:H	2.24	0.45
1:F:156:PHE:CD1	1:F:156:PHE:C	2.95	0.45
1:A:154:GLU:H	1:A:176:PHE:HA	1.82	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:G:339:MET:HE1	1:G:363:GLU:HG3	1.99	0.45
1:C:124:ILE:HD12	1:C:124:ILE:H	1.81	0.45
1:A:156:PHE:C	1:A:156:PHE:CD1	2.94	0.44
1:B:134:ILE:HD12	1:B:220:GLU:CG	2.47	0.44
1:D:266:THR:C	1:D:268:SER:H	2.25	0.44
1:F:258:ILE:HD12	1:F:308:MET:HE1	1.99	0.44
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.98	0.44
1:B:120:GLN:O	1:B:122:PRO:HD3	2.17	0.44
1:D:229:THR:HG23	1:D:230:GLY:N	2.32	0.44
1:A:130:ARG:HA	1:B:269:GLU:CG	2.42	0.44
1:A:290:ASP:OD2	1:A:294:ARG:HB2	2.17	0.44
1:B:134:ILE:HD12	1:B:220:GLU:HG2	1.98	0.44
1:B:285:ILE:O	1:B:288:LEU:HG	2.17	0.44
1:G:282:TRP:CE3	1:G:313:VAL:HG11	2.53	0.44
1:C:226:GLY:H	1:C:235:GLY:HA3	1.81	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:F:349:ASP:O	1:F:352:ASN:HB2	2.18	0.44
1:A:347:ARG:HB3	1:A:358:LEU:CD1	2.46	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	0.44
1:C:191:GLN:HG2	1:C:357:MET:HE3	2.00	0.44
1:D:191:GLN:HG2	1:D:357:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:HD2	1:B:347:ARG:NH1	2.32	0.44
1:C:104:SER:HB3	1:E:166:LYS:NZ	2.32	0.44
1:F:266:THR:C	1:F:268:SER:H	2.25	0.44
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:F:130:ARG:C	1:F:132:LEU:N	2.73	0.43
1:G:266:THR:C	1:G:268:SER:H	2.26	0.43
1:E:116:ILE:HD12	1:F:146:ASN:HB2	2.01	0.43
1:G:203:LEU:O	1:G:207:ILE:HG13	2.17	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:F:244:ASP:HB2	1:F:264:GLN:HE22	1.83	0.43
1:G:352:ASN:O	1:G:356:ASN:N	2.51	0.43
1:D:325:THR:HA	1:D:377:ILE:O	2.18	0.43
1:A:152:ARG:CZ	1:A:179:GLN:HG3	2.48	0.43
1:B:125:ILE:HB	1:C:152:ARG:HB2	2.00	0.43
1:E:116:ILE:H	1:E:116:ILE:HG12	1.71	0.43
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.01	0.43
1:G:138:LEU:HD22	1:G:333:SER:O	2.18	0.43
1:G:279:PRO:HD3	1:G:316:THR:O	2.19	0.43
1:C:239:VAL:HG12	1:C:373:PRO:HB3	2.01	0.43
1:A:199:ASP:O	1:A:201:PRO:HD3	2.19	0.43
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.47	0.43
1:A:292:GLU:HG3	1:B:292:GLU:HG2	2.00	0.43
1:B:125:ILE:HB	1:C:152:ARG:CB	2.48	0.43
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.48	0.43
1:A:342:THR:HG22	1:A:343:VAL:N	2.34	0.43
1:C:208:ASN:C	1:C:210:ARG:H	2.27	0.43
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.54	0.42
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.84	0.42
1:A:153:GLU:CA	1:A:176:PHE:HB3	2.46	0.42
1:C:189:TRP:CZ3	1:C:191:GLN:HB2	2.51	0.42
1:C:193:SER:HB3	1:C:196:VAL:HG23	2.01	0.42
1:C:258:ILE:O	1:C:262:ILE:HG13	2.19	0.42
1:C:264:GLN:HB3	1:C:377:ILE:CD1	2.49	0.42
1:A:171:GLU:HB2	1:F:189:TRP:CZ2	2.54	0.42
1:B:311:LEU:HA	1:B:312:PRO:HD3	1.89	0.42
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.42
1:G:152:ARG:HB3	1:G:153:GLU:H	1.60	0.42
1:D:295:TYR:HE1	1:D:300:PRO:HG3	1.84	0.42
1:E:264:GLN:HE21	1:E:377:ILE:HG12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ARG:NE	1:G:179:GLN:HG3	2.35	0.42
1:B:277:LEU:HD12	1:B:277:LEU:N	2.34	0.42
1:D:308:MET:HG2	1:D:309:TRP:CD1	2.54	0.42
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.55	0.42
1:F:350:ARG:HG3	1:F:351:ASP:N	2.34	0.42
1:A:159:ASN:H	1:A:172:SER:HB3	1.84	0.42
1:G:308:MET:HG2	1:G:309:TRP:CD1	2.55	0.42
1:B:254:ARG:O	1:B:258:ILE:HD13	2.19	0.42
1:C:371:TYR:CD1	1:C:371:TYR:N	2.88	0.42
1:D:311:LEU:HA	1:D:312:PRO:HD3	1.91	0.42
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.02	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	2.19	0.42
1:A:162:VAL:HG11	1:F:231:ASP:O	2.20	0.42
1:A:300:PRO:HG2	1:B:296:ILE:CG2	2.49	0.42
1:G:212:MET:HE1	1:G:341:ALA:HB3	2.00	0.42
1:G:319:GLN:NE2	1:G:323:THR:HB	2.24	0.42
1:C:283:HIS:NE2	1:D:260:HIS:HA	2.35	0.41
1:A:119:MET:HB3	1:B:148:LEU:HD23	2.00	0.41
1:D:119:MET:HB3	1:E:148:LEU:HD23	2.02	0.41
1:E:339:MET:HB3	1:E:365:ARG:HG3	2.02	0.41
1:G:203:LEU:HD21	1:G:207:ILE:HD11	2.02	0.41
1:G:259:ALA:HA	1:G:262:ILE:HD12	2.02	0.41
1:G:348:GLU:H	1:G:348:GLU:HG2	1.75	0.41
1:A:203:LEU:O	1:A:207:ILE:HG13	2.20	0.41
1:A:308:MET:HG2	1:A:309:TRP:CD1	2.55	0.41
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.91	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:C:231:ASP:O	1:D:162:VAL:HG11	2.21	0.41
1:C:371:TYR:H	1:C:371:TYR:HD1	1.69	0.41
1:F:276:VAL:HB	1:F:325:THR:HB	2.03	0.41
1:B:109:ALA:C	1:B:111:SER:H	2.29	0.41
1:C:126:MET:HA	1:C:127:PRO:HD3	1.90	0.41
1:G:135:ARG:HG3	1:G:135:ARG:HH11	1.86	0.41
1:A:281:ASP:O	1:A:285:ILE:HG13	2.20	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:E:207:ILE:O	1:E:211:LEU:HD13	2.21	0.41
1:E:234:GLU:HG2	1:E:239:VAL:HG22	2.01	0.41
1:F:133:THR:HG22	1:F:136:ASP:CG	2.46	0.41
1:F:223:LEU:O	1:F:236:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:THR:OG1	1:F:256:ASP:HB2	2.21	0.41
1:G:342:THR:HG22	1:G:343:VAL:N	2.35	0.41
1:E:194:ARG:NH1	1:E:347:ARG:NE	2.63	0.41
1:F:236:LEU:HD22	1:F:376:ILE:HD13	2.03	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:193:SER:HB2	1:G:195:GLN:HE21	1.86	0.41
1:G:294:ARG:HD3	1:G:295:TYR:H	1.86	0.41
1:G:351:ASP:O	1:G:353:PHE:N	2.54	0.41
1:A:258:ILE:N	1:A:258:ILE:HD12	2.36	0.41
1:B:130:ARG:HA	1:C:269:GLU:CG	2.51	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.93	0.41
1:A:147:ALA:HA	1:A:183:VAL:HG23	2.04	0.40
1:A:176:PHE:CD1	1:A:176:PHE:N	2.89	0.40
1:D:226:GLY:N	1:D:235:GLY:HA3	2.35	0.40
1:B:234:GLU:HG2	1:B:239:VAL:HG23	2.03	0.40
1:C:197:MET:CE	1:C:204:GLN:HB2	2.45	0.40
1:G:358:LEU:HD23	1:G:359:THR:N	2.36	0.40
1:A:295:TYR:HB2	1:A:299:GLY:HA2	2.03	0.40
1:B:202:MET:HG2	1:B:203:LEU:N	2.37	0.40
1:E:289:LYS:HA	1:E:294:ARG:O	2.21	0.40
1:G:184:LYS:HD3	1:G:231:ASP:C	2.46	0.40
1:G:343:VAL:HG22	1:G:362:CYS:SG	2.61	0.40
1:C:183:VAL:HG13	1:C:366:LEU:O	2.22	0.40
1:E:194:ARG:HH22	1:E:347:ARG:CZ	2.34	0.40
1:F:141:GLY:O	1:F:336:TRP:HA	2.22	0.40
1:F:290:ASP:C	1:F:292:GLU:H	2.29	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%)	18	51
1	B	278/282 (99%)	252 (91%)	22 (8%)	4 (1%)	9	37
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%)	11	41
1	F	254/282 (90%)	229 (90%)	21 (8%)	4 (2%)	7	35
1	G	239/282 (85%)	209 (87%)	26 (11%)	4 (2%)	7	34
All	All	1883/1974 (95%)	1699 (90%)	167 (9%)	17 (1%)	14	45

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	F	131	ARG
1	G	224	LEU
1	A	201	PRO
1	B	127	PRO
1	B	230	GLY
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%)	218 (95%)	12 (5%)	21	46
1	B	230/231 (100%)	222 (96%)	8 (4%)	32	54
1	C	230/231 (100%)	228 (99%)	2 (1%)	70	74
1	D	230/231 (100%)	224 (97%)	6 (3%)	40	60
1	E	230/231 (100%)	220 (96%)	10 (4%)	26	50
1	F	211/231 (91%)	205 (97%)	6 (3%)	38	58
1	G	201/231 (87%)	194 (96%)	7 (4%)	32	54
All	All	1562/1617 (97%)	1511 (97%)	51 (3%)	33	56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	117	GLN
1	A	148	LEU
1	A	149	GLU
1	A	169	LYS
1	A	176	PHE
1	A	179	GLN
1	A	195	GLN
1	A	202	MET
1	A	270	PHE
1	A	301	GLN
1	A	316	THR
1	B	105	LEU
1	B	146	ASN
1	B	195	GLN
1	B	202	MET
1	B	224	LEU
1	B	227	ASP
1	B	277	LEU
1	B	344	GLU
1	C	202	MET
1	C	224	LEU
1	D	146	ASN
1	D	152	ARG
1	D	194	ARG
1	D	202	MET
1	D	279	PRO
1	D	292	GLU
1	E	115	LEU

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Mol	Chain	Res	Type
1	E	116	ILE
1	E	142	ARG
1	E	152	ARG
1	E	195	GLN
1	E	277	LEU
1	E	280	ARG
1	E	300	PRO
1	E	301	GLN
1	E	303	PHE
1	F	133	THR
1	F	135	ARG
1	F	224	LEU
1	F	227	ASP
1	F	280	ARG
1	F	292	GLU
1	G	129	LEU
1	G	173	ASP
1	G	195	GLN
1	G	301	GLN
1	G	307	ILE
1	G	350	ARG
1	G	370	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	158	ASN
1	A	179	GLN
1	A	204	GLN
1	A	225	ASN
1	A	301	GLN
1	A	334	GLN
1	A	356	ASN
1	B	158	ASN
1	B	191	GLN
1	B	222	GLN
1	B	301	GLN
1	B	334	GLN
1	B	352	ASN
1	C	140	GLN
1	C	158	ASN

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Mol	Chain	Res	Type
1	C	222	GLN
1	C	291	ASN
1	C	334	GLN
1	D	158	ASN
1	D	195	GLN
1	D	222	GLN
1	D	232	ASN
1	D	334	GLN
1	E	117	GLN
1	E	158	ASN
1	E	191	GLN
1	E	208	ASN
1	E	291	ASN
1	E	306	ASN
1	E	352	ASN
1	F	146	ASN
1	F	158	ASN
1	F	222	GLN
1	F	237	ASN
1	F	260	HIS
1	F	306	ASN
1	F	334	GLN
1	G	195	GLN
1	G	232	ASN
1	G	260	HIS
1	G	264	GLN
1	G	283	HIS
1	G	306	ASN
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 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	280/282 (99%)	0.24	11 (3%) 43 31	43, 89, 136, 236	0
1	B	280/282 (99%)	0.37	13 (4%) 37 27	39, 79, 127, 147	0
1	C	280/282 (99%)	0.26	8 (2%) 53 37	39, 80, 128, 182	0
1	D	280/282 (99%)	0.26	6 (2%) 63 44	44, 80, 123, 162	0
1	E	280/282 (99%)	0.24	5 (1%) 67 46	40, 79, 121, 169	0
1	F	256/282 (90%)	0.18	10 (3%) 43 31	47, 87, 147, 208	0
1	G	243/282 (86%)	1.14	50 (20%) 2 4	81, 167, 255, 321	0
All	All	1899/1974 (96%)	0.37	103 (5%) 31 24	39, 86, 182, 321	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	382	SER	8.1
1	E	383	SER	7.0
1	F	128	GLY	5.2
1	A	269	GLU	5.0
1	G	378	LYS	4.8
1	B	234	GLU	4.7
1	C	383	SER	4.7
1	G	175	THR	4.7
1	G	154	GLU	4.5
1	G	383	SER	4.4
1	G	140	GLN	4.4
1	F	383	SER	4.4
1	G	155	VAL	4.3
1	C	173	ASP	4.2
1	G	302	ALA	4.0
1	D	301	GLN	3.8
1	G	371	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	157	THR	3.6
1	G	266	THR	3.6
1	G	151	VAL	3.6
1	F	345	VAL	3.6
1	G	153	GLU	3.5
1	G	218	LYS	3.5
1	A	383	SER	3.5
1	E	291	ASN	3.5
1	B	166	LYS	3.4
1	G	158	ASN	3.4
1	E	120	GLN	3.3
1	D	347	ARG	3.3
1	G	156	PHE	3.3
1	G	269	GLU	3.2
1	G	310	GLY	3.2
1	G	260	HIS	3.2
1	B	363	GLU	3.1
1	B	136	ASP	3.1
1	G	292	GLU	3.0
1	G	251	GLY	3.0
1	B	131	ARG	2.9
1	G	149	GLU	2.9
1	G	377	ILE	2.9
1	G	291	ASN	2.8
1	G	382	SER	2.8
1	F	235	GLY	2.8
1	A	270	PHE	2.8
1	E	104	SER	2.8
1	G	256	ASP	2.7
1	G	176	PHE	2.7
1	F	234	GLU	2.7
1	G	309	TRP	2.7
1	G	301	GLN	2.7
1	D	382	SER	2.7
1	A	185	THR	2.6
1	G	214	GLY	2.6
1	G	180	THR	2.6
1	A	356	ASN	2.6
1	A	123	GLY	2.6
1	B	204	GLN	2.6
1	B	178	LYS	2.5
1	G	374	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	289	LYS	2.5
1	G	267	GLU	2.5
1	F	130	ARG	2.4
1	C	141	GLY	2.4
1	C	198	ASP	2.4
1	G	365	ARG	2.4
1	G	337	ASP	2.4
1	G	173	ASP	2.4
1	G	263	TYR	2.4
1	F	347	ARG	2.4
1	C	209	ASN	2.4
1	F	129	LEU	2.4
1	G	379	GLY	2.4
1	G	188	HIS	2.3
1	A	332	ALA	2.3
1	D	363	GLU	2.3
1	G	212	MET	2.3
1	B	202	MET	2.3
1	A	104	SER	2.3
1	G	250	THR	2.2
1	C	292	GLU	2.2
1	G	128	GLY	2.2
1	C	241	THR	2.2
1	D	271	SER	2.2
1	D	220	GLU	2.2
1	G	303	PHE	2.2
1	A	298	GLY	2.2
1	B	164	ALA	2.1
1	B	273	SER	2.1
1	G	210	ARG	2.1
1	A	117	GLN	2.1
1	G	191	GLN	2.1
1	G	272	ALA	2.1
1	B	298	GLY	2.1
1	F	220	GLU	2.1
1	B	163	VAL	2.1
1	G	227	ASP	2.1
1	G	234	GLU	2.1
1	B	233	LEU	2.1
1	F	382	SER	2.1
1	A	132	LEU	2.1
1	G	293	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	142	ARG	2.0
1	G	201	PRO	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.