



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:53 AM UTC

PDB ID : 1OHG / pdb_00001ohg
Title : STRUCTURE OF THE DSDNA BACTERIOPHAGE HK97 MATURE
EMPTY CAPSID
Authors : Helgstrand, C.; Wikoff, W.R.; Duda, R.L.; Hendrix, R.W.; Johnson, J.E.;
Liljas, L.
Deposited on : 2003-05-26
Resolution : 3.45 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

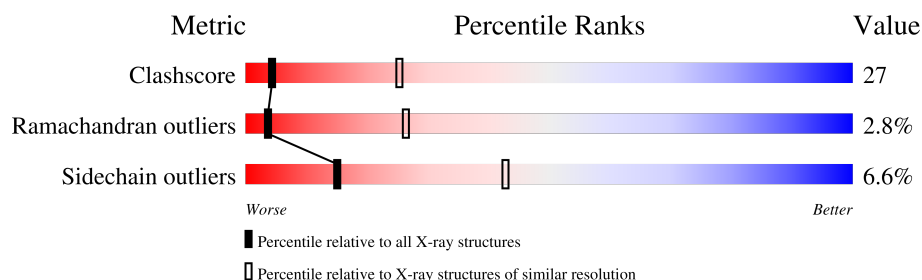
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	282	54% 38% 7%
1	B	282	55% 40% 5%
1	C	282	55% 37% 8%
1	D	282	52% 42% 5%
1	E	282	52% 40% 6% •
1	F	282	54% 40% 6%
1	G	282	55% 39% 6%

2 Entry composition [i](#)

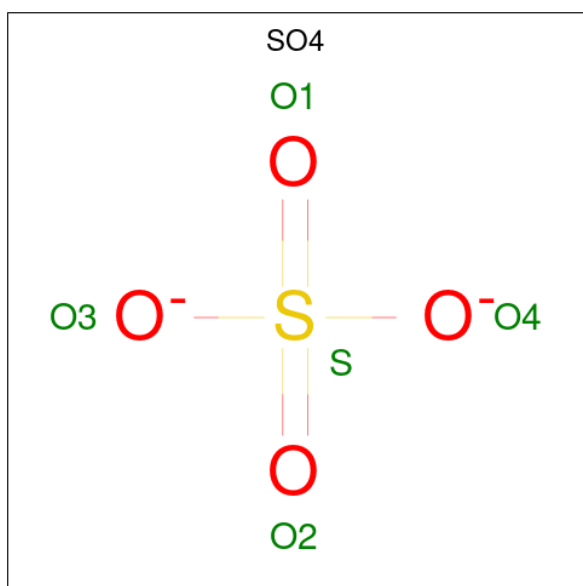
There are 3 unique types of molecules in this entry. The entry contains 15070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	B	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	C	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	D	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	E	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	F	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	G	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

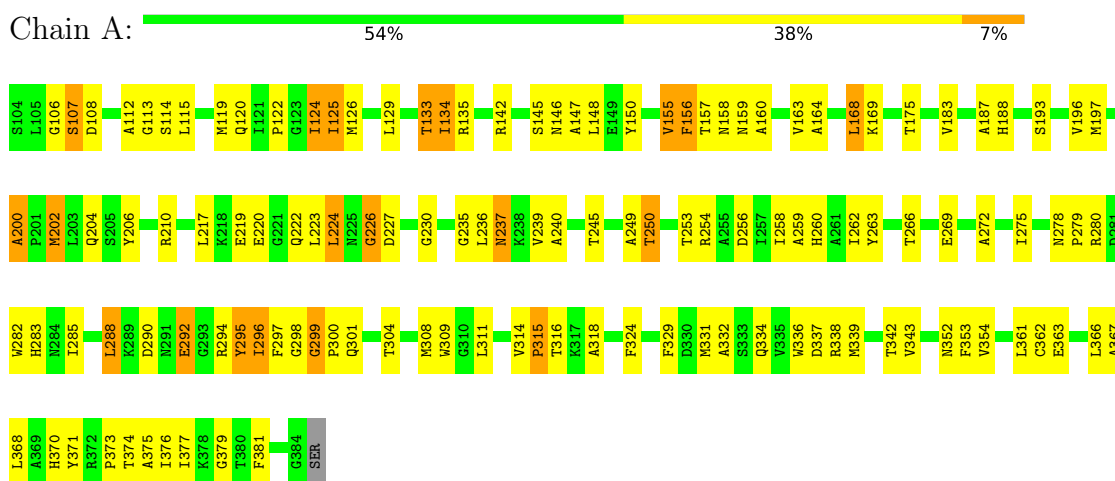
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

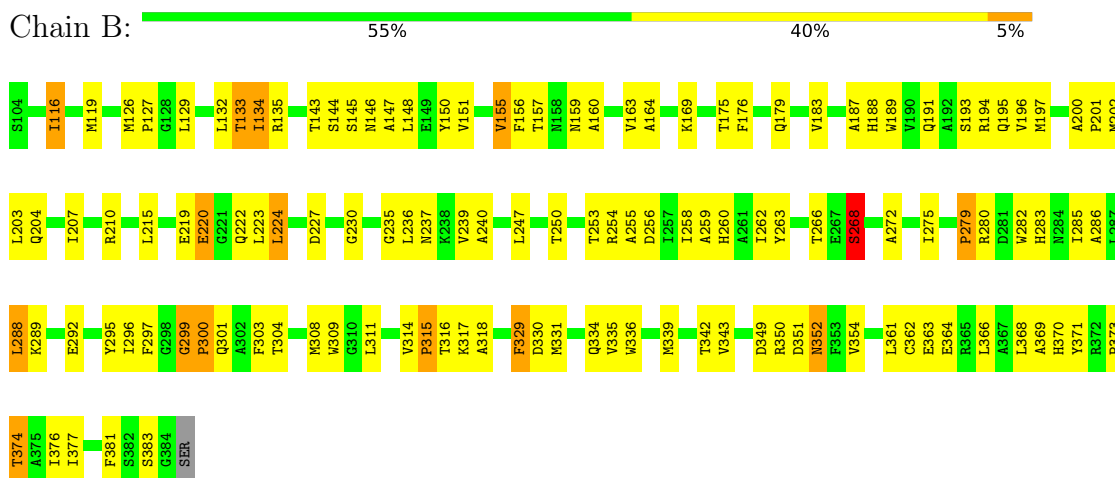
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS failed to run properly.

• Molecule 1: MAJOR CAPSID PROTEIN

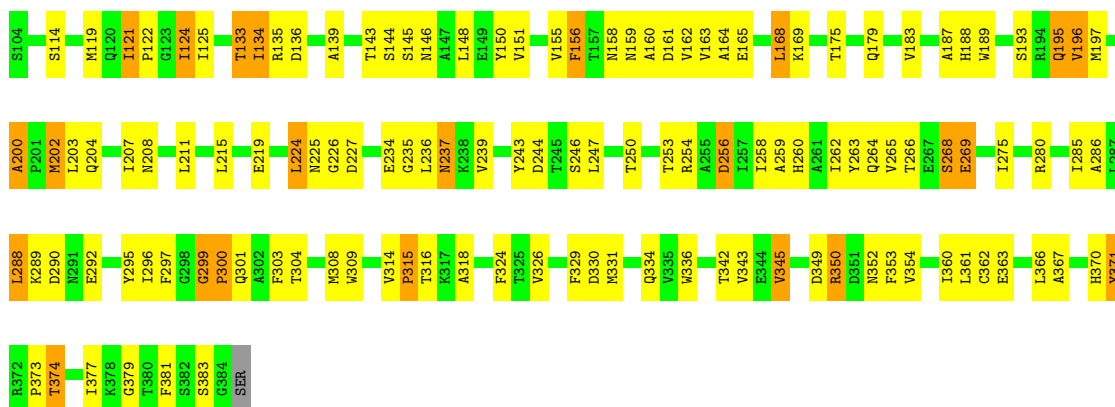


• Molecule 1: MAJOR CAPSID PROTEIN



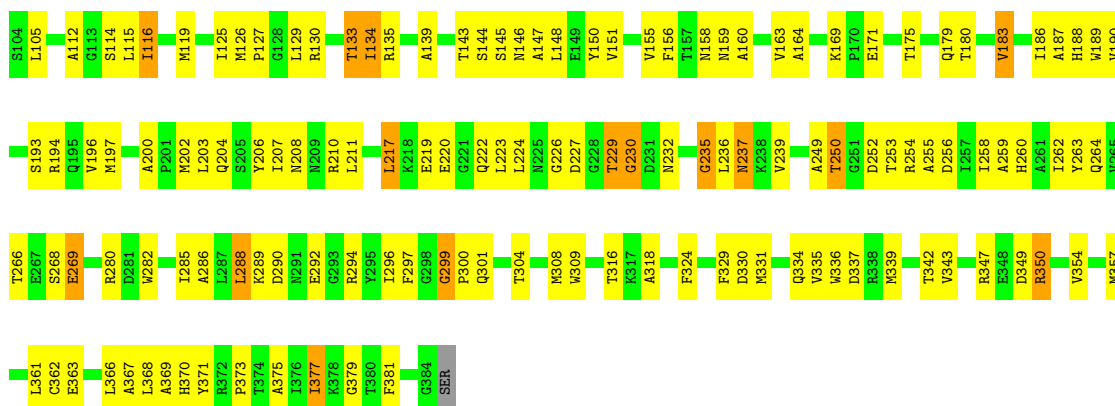
• Molecule 1: MAJOR CAPSID PROTEIN





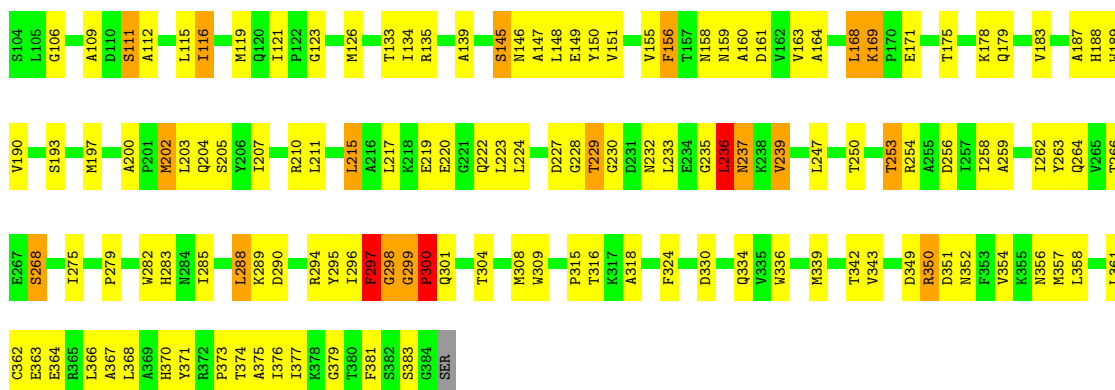
• Molecule 1: MAJOR CAPSID PROTEIN

Chain D: 52% 42% 5%



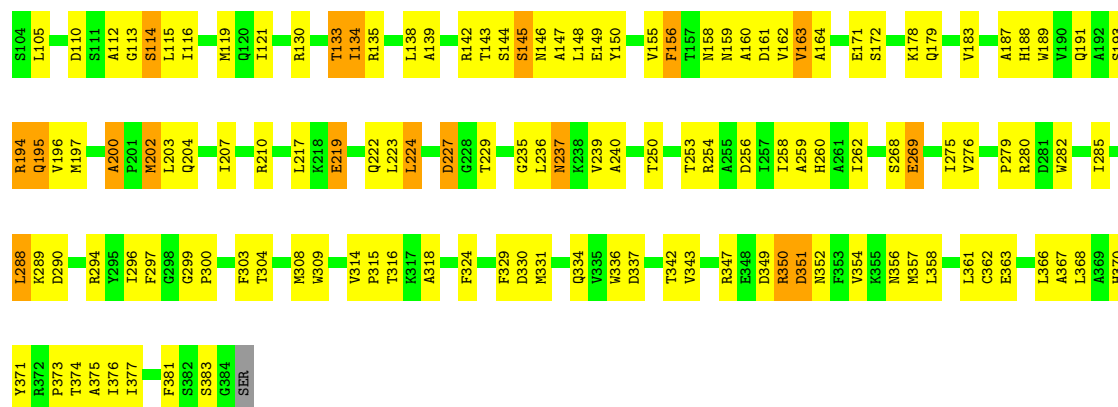
• Molecule 1: MAJOR CAPSID PROTEIN

Chain E: 52% 40% 6%



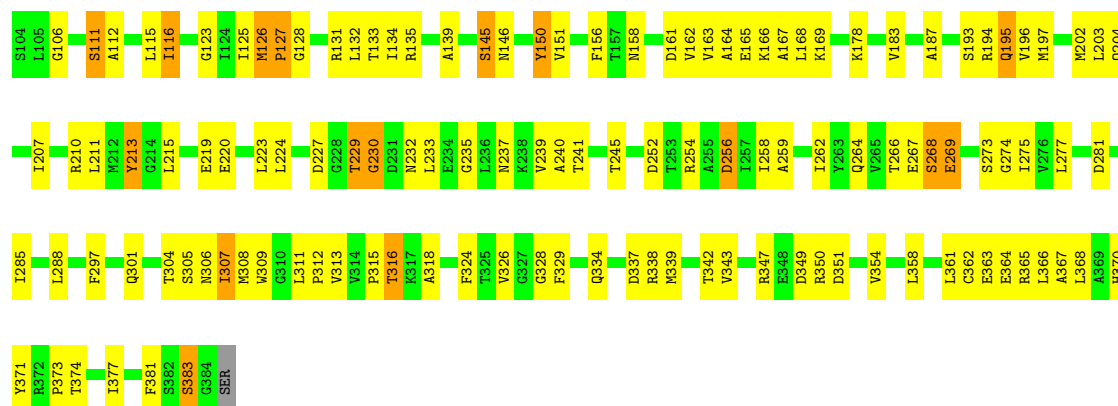
• Molecule 1: MAJOR CAPSID PROTEIN

Chain F: 54% 40% 6%



• Molecule 1: MAJOR CAPSID PROTEIN

Chain G: 55% 39% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	579.70Å 626.65Å 787.20Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	190.13 – 3.45	Depositor
% Data completeness (in resolution range)	65.2 (190.13-3.45)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.373 , 0.374	Depositor
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.326	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-l	Xtriage
Total number of atoms	15070	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: CL, SO4

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	0.57	0/2189	1.03	13/2971 (0.4%)
1	B	0.59	1/2189 (0.0%)	1.03	9/2971 (0.3%)
1	C	0.61	1/2189 (0.0%)	1.04	9/2971 (0.3%)
1	D	0.63	0/2189	1.01	8/2971 (0.3%)
1	E	0.61	1/2189 (0.0%)	1.08	15/2971 (0.5%)
1	F	0.58	1/2189 (0.0%)	1.06	11/2971 (0.4%)
1	G	0.59	1/2189 (0.0%)	1.04	11/2971 (0.4%)
All	All	0.60	5/15323 (0.0%)	1.04	76/20797 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	383	SER	C-N	-5.14	1.26	1.33
1	C	383	SER	C-N	-5.13	1.26	1.33
1	E	383	SER	C-N	-5.12	1.26	1.33
1	B	383	SER	C-N	-5.03	1.26	1.33
1	F	383	SER	C-N	-5.03	1.26	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	GLY	CA-C-N	10.84	133.39	119.84
1	E	299	GLY	C-N-CA	10.84	133.39	119.84
1	B	299	GLY	CA-C-N	6.93	128.50	119.84
1	B	299	GLY	C-N-CA	6.93	128.50	119.84
1	A	106	GLY	N-CA-C	6.91	122.03	112.57
1	C	299	GLY	CA-C-N	6.80	128.34	119.84
1	C	299	GLY	C-N-CA	6.80	128.34	119.84
1	C	200	ALA	CA-C-N	6.72	128.24	119.84
1	C	200	ALA	C-N-CA	6.72	128.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ALA	N-CA-C	6.66	118.54	111.28
1	G	268	SER	N-CA-C	-6.58	105.54	113.97
1	F	200	ALA	CA-C-N	6.50	126.00	119.24
1	F	200	ALA	C-N-CA	6.50	126.00	119.24
1	F	299	GLY	CA-C-N	6.45	127.91	119.84
1	F	299	GLY	C-N-CA	6.45	127.91	119.84
1	F	145	SER	N-CA-C	6.40	118.90	109.24
1	D	299	GLY	CA-C-N	6.38	127.81	119.84
1	D	299	GLY	C-N-CA	6.38	127.81	119.84
1	G	338	ARG	N-CA-C	-6.25	106.19	113.88
1	F	237	ASN	N-CA-C	6.20	118.84	111.71
1	B	116	ILE	N-CA-C	5.97	116.47	107.75
1	G	145	SER	N-CA-C	5.92	118.41	109.41
1	E	116	ILE	N-CA-C	5.89	116.59	107.99
1	E	109	ALA	N-CA-C	5.85	118.16	111.02
1	C	121	ILE	CA-C-N	5.80	127.09	119.84
1	C	121	ILE	C-N-CA	5.80	127.09	119.84
1	E	123	GLY	N-CA-C	5.70	119.86	112.68
1	G	329	PHE	N-CA-C	5.66	117.90	111.11
1	A	125	ILE	N-CA-C	5.64	115.38	107.37
1	G	241	THR	N-CA-C	-5.63	100.49	109.96
1	B	200	ALA	CA-C-N	5.63	126.88	119.84
1	B	200	ALA	C-N-CA	5.63	126.88	119.84
1	B	240	ALA	N-CA-C	5.60	117.51	110.24
1	D	116	ILE	N-CA-C	5.57	116.12	107.99
1	A	155	VAL	N-CA-C	5.56	115.60	107.37
1	A	298	GLY	N-CA-C	5.53	126.28	113.18
1	A	200	ALA	CA-C-N	5.49	126.70	119.84
1	A	200	ALA	C-N-CA	5.49	126.70	119.84
1	G	235	GLY	N-CA-C	5.49	121.68	112.85
1	E	356	ASN	N-CA-C	-5.48	104.17	111.02
1	C	237	ASN	N-CA-C	5.46	118.74	111.75
1	E	298	GLY	N-CA-C	5.43	126.05	113.18
1	F	138	LEU	N-CA-C	5.42	117.87	110.55
1	B	352	ASN	N-CA-C	5.36	122.20	110.80
1	E	237	ASN	N-CA-C	5.35	119.29	112.34
1	A	237	ASN	N-CA-C	5.33	118.88	112.38
1	D	200	ALA	CA-C-N	5.32	126.49	119.84
1	D	200	ALA	C-N-CA	5.32	126.49	119.84
1	C	268	SER	N-CA-C	-5.28	105.98	112.90
1	F	219	GLU	N-CA-C	-5.26	105.44	111.07
1	G	126	MET	CA-C-N	5.21	126.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	126	MET	C-N-CA	5.21	126.35	119.84
1	D	237	ASN	N-CA-C	5.19	118.71	112.38
1	B	155	VAL	N-CA-C	5.18	115.31	107.75
1	C	151	VAL	N-CA-C	5.15	115.54	108.12
1	E	268	SER	N-CA-C	-5.14	106.41	113.30
1	A	296	ILE	CB-CA-C	-5.12	105.22	112.14
1	B	268	SER	N-CA-C	-5.11	107.05	113.28
1	A	338	ARG	N-CA-C	-5.10	104.70	112.04
1	E	200	ALA	CA-C-N	5.10	126.21	119.84
1	E	200	ALA	C-N-CA	5.10	126.21	119.84
1	G	316	THR	N-CA-C	5.10	117.21	108.90
1	F	163	VAL	N-CA-C	5.09	115.24	108.11
1	A	299	GLY	CA-C-N	-5.09	114.88	121.04
1	A	299	GLY	C-N-CA	-5.09	114.88	121.04
1	G	116	ILE	N-CA-C	5.09	115.64	108.36
1	F	240	ALA	N-CA-C	5.09	116.85	110.24
1	D	377	ILE	N-CA-C	5.09	115.44	108.12
1	E	228	GLY	N-CA-C	-5.08	108.64	114.69
1	E	253	THR	N-CA-C	-5.07	103.70	110.55
1	E	297	PHE	N-CA-C	-5.06	106.19	112.93
1	D	235	GLY	N-CA-C	5.03	119.76	112.82
1	G	213	TYR	N-CA-C	-5.03	105.49	110.97
1	A	295	TYR	N-CA-C	5.01	116.96	109.59
1	E	145	SER	N-CA-C	5.00	116.90	109.69
1	F	227	ASP	N-CA-C	5.00	117.39	111.33

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	2152	0	2119	122	0
1	B	2152	0	2119	131	0
1	C	2152	0	2119	133	0
1	D	2152	0	2119	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2152	0	2119	132	0
1	F	2152	0	2119	119	0
1	G	2152	0	2119	104	0
2	A	5	0	0	0	0
3	G	1	0	0	0	0
All	All	15070	0	14833	800	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 27.

All (800) 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:B:316:THR:HG22	1:B:318:ALA:H	1.11	1.09
1:D:316:THR:HG22	1:D:318:ALA:H	1.13	1.09
1:E:316:THR:HG22	1:E:318:ALA:H	1.13	1.09
1:C:316:THR:HG22	1:C:318:ALA:H	1.17	1.06
1:G:316:THR:HG22	1:G:318:ALA:H	1.21	1.05
1:A:316:THR:HG22	1:A:318:ALA:H	1.21	1.02
1:B:258:ILE:HG21	1:B:308:MET:HE3	1.42	1.02
1:E:116:ILE:HG21	1:F:146:ASN:HB2	1.38	1.01
1:C:258:ILE:HG21	1:C:308:MET:HE3	1.44	0.99
1:F:316:THR:HG22	1:F:318:ALA:H	1.27	0.97
1:D:197:MET:HE1	1:D:204:GLN:HB2	1.46	0.96
1:A:258:ILE:HG21	1:A:308:MET:HE3	1.50	0.94
1:G:133:THR:HG22	1:G:135:ARG:H	1.34	0.91
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.54	0.89
1:B:197:MET:HE1	1:B:204:GLN:HB2	1.55	0.88
1:D:194:ARG:NH2	1:D:347:ARG:HH22	1.72	0.88
1:E:295:TYR:HB2	1:E:299:GLY:H	1.39	0.87
1:D:202:MET:HE3	1:D:202:MET:H	1.39	0.87
1:F:200:ALA:HB1	1:F:202:MET:HE1	1.56	0.86
1:D:188:HIS:HB3	1:E:160:ALA:HA	1.58	0.85
1:F:258:ILE:HB	1:F:308:MET:HE1	1.57	0.85
1:E:316:THR:HG22	1:E:318:ALA:N	1.90	0.85
1:E:339:MET:HE1	1:E:363:GLU:HG3	1.59	0.84
1:A:339:MET:HE1	1:A:363:GLU:HG3	1.59	0.83
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.58	0.83
1:F:193:SER:OG	1:F:196:VAL:HG23	1.78	0.83
1:G:197:MET:HE1	1:G:204:GLN:HB2	1.61	0.83
1:G:339:MET:HE1	1:G:363:GLU:HG3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:HIS:HB3	1:C:160:ALA:HA	1.60	0.82
1:D:316:THR:HG22	1:D:318:ALA:N	1.95	0.81
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.62	0.81
1:G:254:ARG:HB3	1:G:381:PHE:CE2	2.16	0.80
1:E:207:ILE:O	1:E:211:LEU:HD13	1.80	0.80
1:F:297:PHE:HB3	1:F:304:THR:HG21	1.66	0.78
1:F:112:ALA:C	1:F:114:SER:H	1.91	0.78
1:A:285:ILE:O	1:A:288:LEU:HB2	1.84	0.77
1:A:160:ALA:HA	1:F:188:HIS:HB3	1.65	0.77
1:G:229:THR:CG2	1:G:232:ASN:HD22	1.98	0.77
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.65	0.77
1:D:285:ILE:O	1:D:288:LEU:HB2	1.84	0.77
1:C:316:THR:HG22	1:C:318:ALA:N	1.99	0.77
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.20	0.76
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.67	0.76
1:E:258:ILE:HD13	1:E:308:MET:HE1	1.66	0.76
1:G:254:ARG:HB3	1:G:381:PHE:HE2	1.50	0.76
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.67	0.75
1:G:150:TYR:H	1:G:150:TYR:HD2	1.34	0.75
1:G:193:SER:HB3	1:G:196:VAL:HG23	1.69	0.74
1:B:215:LEU:HD21	1:B:364:GLU:HB2	1.70	0.74
1:D:119:MET:HE2	1:E:148:LEU:HD22	1.70	0.74
1:D:258:ILE:O	1:D:262:ILE:HG13	1.88	0.74
1:D:339:MET:HE1	1:D:363:GLU:HG3	1.70	0.74
1:F:202:MET:HE2	1:F:203:LEU:N	2.03	0.73
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.69	0.73
1:D:116:ILE:HG21	1:E:146:ASN:CB	2.18	0.73
1:A:316:THR:HG22	1:A:318:ALA:N	2.02	0.73
1:A:297:PHE:HB3	1:A:304:THR:HG21	1.71	0.72
1:F:258:ILE:O	1:F:262:ILE:HG13	1.89	0.72
1:G:197:MET:HE1	1:G:204:GLN:CB	2.20	0.72
1:A:342:THR:HG22	1:A:343:VAL:N	2.04	0.72
1:B:116:ILE:HG21	1:C:146:ASN:HD22	1.55	0.71
1:G:339:MET:CE	1:G:363:GLU:HG3	2.20	0.71
1:C:361:LEU:HD12	1:C:362:CYS:H	1.55	0.71
1:G:195:GLN:H	1:G:195:GLN:HE21	1.39	0.71
1:G:258:ILE:HB	1:G:308:MET:HE1	1.70	0.71
1:E:295:TYR:CD1	1:E:300:PRO:HD3	2.26	0.70
1:G:264:GLN:HB3	1:G:377:ILE:HD13	1.73	0.70
1:F:361:LEU:HD12	1:F:362:CYS:H	1.55	0.70
1:G:229:THR:HG23	1:G:230:GLY:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.74	0.70
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.72	0.70
1:D:297:PHE:HB3	1:D:304:THR:HG21	1.72	0.70
1:B:133:THR:O	1:B:135:ARG:N	2.25	0.70
1:B:303:PHE:HE1	1:C:309:TRP:HB3	1.57	0.69
1:C:244:ASP:OD1	1:C:246:SER:HB3	1.92	0.69
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.74	0.69
1:C:224:LEU:HD13	1:C:237:ASN:ND2	2.07	0.69
1:D:183:VAL:HG23	1:D:366:LEU:O	1.93	0.69
1:A:258:ILE:HD12	1:A:258:ILE:H	1.57	0.68
1:B:239:VAL:HG12	1:B:373:PRO:HB3	1.75	0.68
1:A:258:ILE:O	1:A:262:ILE:HG13	1.94	0.68
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.75	0.68
1:C:258:ILE:O	1:C:262:ILE:HG13	1.94	0.68
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.28	0.68
1:G:229:THR:HG23	1:G:230:GLY:H	1.59	0.68
1:C:254:ARG:HB3	1:C:381:PHE:CE2	2.29	0.68
1:C:285:ILE:O	1:C:288:LEU:HB2	1.94	0.67
1:E:210:ARG:NH2	1:F:156:PHE:HD2	1.93	0.67
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.30	0.67
1:B:316:THR:HG22	1:B:318:ALA:N	1.97	0.67
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.77	0.67
1:A:133:THR:O	1:A:135:ARG:N	2.28	0.66
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.29	0.66
1:C:119:MET:HE2	1:D:148:LEU:HD22	1.76	0.66
1:B:254:ARG:HB3	1:B:381:PHE:CE2	2.31	0.66
1:C:334:GLN:NE2	1:C:371:TYR:OH	2.28	0.66
1:B:297:PHE:HB3	1:B:304:THR:HG21	1.78	0.65
1:A:258:ILE:HD12	1:A:258:ILE:N	2.10	0.65
1:E:361:LEU:HD12	1:E:362:CYS:H	1.62	0.65
1:C:197:MET:HE1	1:C:204:GLN:CB	2.26	0.65
1:B:202:MET:HE3	1:B:202:MET:H	1.62	0.65
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.32	0.65
1:E:295:TYR:HB2	1:E:299:GLY:N	2.10	0.65
1:F:112:ALA:O	1:F:114:SER:N	2.29	0.65
1:D:342:THR:HG22	1:D:343:VAL:N	2.12	0.64
1:G:361:LEU:HD12	1:G:362:CYS:H	1.62	0.64
1:D:219:GLU:HG3	1:D:366:LEU:HD11	1.80	0.64
1:F:202:MET:HE2	1:F:203:LEU:H	1.63	0.64
1:C:193:SER:OG	1:C:196:VAL:HG23	1.97	0.64
1:B:254:ARG:HB3	1:B:381:PHE:HE2	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ILE:O	1:D:211:LEU:HD23	1.98	0.63
1:B:288:LEU:O	1:B:296:ILE:HG12	1.99	0.63
1:G:223:LEU:HD22	1:G:368:LEU:HD22	1.80	0.63
1:E:258:ILE:HG21	1:E:308:MET:CE	2.29	0.63
1:F:258:ILE:HB	1:F:308:MET:CE	2.27	0.63
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.34	0.62
1:D:229:THR:HG23	1:D:232:ASN:HD22	1.64	0.62
1:D:229:THR:HG23	1:D:230:GLY:N	2.13	0.62
1:C:371:TYR:N	1:C:371:TYR:HD1	1.98	0.62
1:F:105:LEU:HD12	1:F:105:LEU:O	2.00	0.62
1:G:259:ALA:HB2	1:G:309:TRP:NE1	2.15	0.62
1:A:187:ALA:HB2	1:A:363:GLU:CB	2.29	0.62
1:C:258:ILE:HG21	1:C:308:MET:CE	2.25	0.62
1:E:119:MET:HB3	1:F:148:LEU:HD22	1.81	0.62
1:B:116:ILE:CG2	1:C:146:ASN:HD22	2.13	0.62
1:C:361:LEU:HD12	1:C:362:CYS:N	2.15	0.62
1:D:361:LEU:HD12	1:D:362:CYS:H	1.65	0.62
1:G:131:ARG:HG3	1:G:132:LEU:O	2.00	0.62
1:D:349:ASP:O	1:D:350:ARG:C	2.42	0.62
1:D:334:GLN:NE2	1:D:371:TYR:OH	2.33	0.61
1:A:107:SER:HB2	1:C:165:GLU:OE2	2.01	0.61
1:E:258:ILE:O	1:E:262:ILE:HG13	2.00	0.61
1:B:361:LEU:HD12	1:B:362:CYS:H	1.64	0.61
1:F:334:GLN:NE2	1:F:371:TYR:OH	2.34	0.61
1:A:119:MET:HE2	1:B:148:LEU:CD2	2.30	0.61
1:G:197:MET:HE1	1:G:204:GLN:CG	2.29	0.61
1:A:135:ARG:NH1	1:A:219:GLU:OE2	2.33	0.61
1:C:124:ILE:N	1:C:124:ILE:HD12	2.15	0.61
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.35	0.61
1:C:342:THR:HG22	1:C:343:VAL:N	2.16	0.61
1:D:256:ASP:O	1:D:259:ALA:HB3	2.01	0.61
1:E:134:ILE:CD1	1:E:224:LEU:HB2	2.30	0.61
1:F:156:PHE:C	1:F:156:PHE:HD1	2.08	0.61
1:G:233:LEU:HD11	1:G:366:LEU:CD1	2.31	0.61
1:F:258:ILE:HD12	1:F:308:MET:HE1	1.83	0.60
1:F:290:ASP:OD2	1:F:294:ARG:HB2	2.01	0.60
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.65	0.60
1:F:115:LEU:HD23	1:G:151:VAL:HG21	1.83	0.60
1:B:197:MET:HE1	1:B:204:GLN:CB	2.29	0.60
1:C:297:PHE:HB3	1:C:304:THR:HG21	1.82	0.60
1:C:289:LYS:HZ1	1:D:253:THR:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ASP:O	1:C:350:ARG:C	2.44	0.60
1:F:156:PHE:C	1:F:156:PHE:CD1	2.77	0.60
1:D:194:ARG:CZ	1:D:347:ARG:NH2	2.65	0.60
1:C:371:TYR:N	1:C:371:TYR:CD1	2.68	0.60
1:C:288:LEU:O	1:C:296:ILE:HG12	2.01	0.60
1:C:133:THR:O	1:C:134:ILE:C	2.45	0.59
1:E:116:ILE:CG2	1:F:146:ASN:HB2	2.24	0.59
1:G:223:LEU:CD2	1:G:368:LEU:HD22	2.32	0.59
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.37	0.59
1:C:254:ARG:HB3	1:C:381:PHE:HE2	1.66	0.59
1:E:156:PHE:C	1:E:156:PHE:CD2	2.79	0.59
1:C:135:ARG:NH2	1:C:219:GLU:OE2	2.36	0.59
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.36	0.59
1:G:183:VAL:HA	1:G:367:ALA:HB2	1.84	0.59
1:B:349:ASP:OD1	1:B:350:ARG:HG2	2.03	0.59
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.31	0.59
1:G:366:LEU:C	1:G:366:LEU:HD12	2.27	0.59
1:G:227:ASP:OD1	1:G:229:THR:HB	2.02	0.59
1:A:259:ALA:HB2	1:A:309:TRP:NE1	2.18	0.59
1:C:156:PHE:HD1	1:C:156:PHE:C	2.11	0.59
1:A:258:ILE:H	1:A:258:ILE:CD1	2.16	0.59
1:B:349:ASP:O	1:B:350:ARG:HG3	2.03	0.58
1:E:112:ALA:HB1	1:E:115:LEU:HD12	1.84	0.58
1:E:264:GLN:HB3	1:E:377:ILE:CD1	2.33	0.58
1:E:354:VAL:HG12	1:E:354:VAL:O	2.04	0.58
1:G:194:ARG:CZ	1:G:347:ARG:NH2	2.66	0.58
1:G:307:ILE:HA	1:G:311:LEU:O	2.03	0.58
1:C:156:PHE:C	1:C:156:PHE:CD1	2.81	0.58
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.86	0.58
1:D:258:ILE:HG21	1:D:308:MET:CE	2.33	0.58
1:B:197:MET:CE	1:B:204:GLN:HB2	2.32	0.58
1:C:119:MET:HE2	1:D:148:LEU:CD2	2.33	0.58
1:C:354:VAL:HG12	1:C:354:VAL:O	2.04	0.58
1:D:259:ALA:HB2	1:D:309:TRP:NE1	2.18	0.58
1:F:239:VAL:HG12	1:F:373:PRO:HB3	1.86	0.58
1:G:239:VAL:HG12	1:G:373:PRO:HB3	1.86	0.58
1:G:193:SER:HB3	1:G:196:VAL:CG2	2.33	0.58
1:G:354:VAL:HG12	1:G:354:VAL:O	2.03	0.58
1:G:112:ALA:HB1	1:G:115:LEU:HD12	1.85	0.58
1:F:227:ASP:CG	1:F:229:THR:HG22	2.29	0.58
1:G:252:ASP:HB2	1:G:256:ASP:CG	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:O	1:A:354:VAL:HG12	2.03	0.58
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.39	0.58
1:A:342:THR:HG22	1:A:343:VAL:H	1.66	0.57
1:G:339:MET:HB3	1:G:365:ARG:HG2	1.84	0.57
1:D:258:ILE:HD13	1:D:308:MET:HE1	1.86	0.57
1:B:135:ARG:NH1	1:B:219:GLU:OE2	2.38	0.57
1:B:285:ILE:O	1:B:288:LEU:HB2	2.04	0.57
1:A:148:LEU:HD22	1:F:119:MET:HE2	1.86	0.57
1:F:259:ALA:HB2	1:F:309:TRP:NE1	2.19	0.57
1:G:229:THR:HG22	1:G:232:ASN:HD22	1.69	0.57
1:E:187:ALA:HB2	1:E:363:GLU:CB	2.35	0.57
1:E:223:LEU:O	1:E:236:LEU:HD22	2.05	0.57
1:B:292:GLU:OE2	1:B:292:GLU:HA	2.05	0.57
1:B:334:GLN:NE2	1:B:371:TYR:OH	2.38	0.57
1:E:197:MET:HE1	1:E:204:GLN:HA	1.86	0.57
1:F:194:ARG:NH2	1:F:347:ARG:HH21	2.03	0.57
1:A:254:ARG:HB3	1:A:381:PHE:HE2	1.69	0.56
1:A:334:GLN:NE2	1:A:371:TYR:OH	2.38	0.56
1:F:147:ALA:HA	1:F:183:VAL:HG23	1.87	0.56
1:B:303:PHE:CE1	1:C:309:TRP:HB3	2.38	0.56
1:F:223:LEU:HD23	1:F:368:LEU:HD22	1.88	0.56
1:F:254:ARG:HB3	1:F:381:PHE:CE2	2.40	0.56
1:A:258:ILE:HG21	1:A:308:MET:CE	2.30	0.56
1:B:256:ASP:O	1:B:259:ALA:HB3	2.05	0.56
1:C:259:ALA:HB2	1:C:309:TRP:NE1	2.19	0.56
1:B:342:THR:HG22	1:B:343:VAL:N	2.19	0.56
1:C:156:PHE:CE1	1:C:158:ASN:HB2	2.41	0.56
1:C:244:ASP:HB2	1:C:264:GLN:HE22	1.71	0.56
1:A:168:LEU:HD22	1:A:169:LYS:O	2.05	0.56
1:A:295:TYR:HB2	1:A:299:GLY:H	1.70	0.56
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.20	0.56
1:A:288:LEU:O	1:A:296:ILE:HG12	2.05	0.56
1:B:163:VAL:HG12	1:B:164:ALA:O	2.04	0.56
1:B:289:LYS:HZ1	1:C:253:THR:HG23	1.71	0.56
1:D:183:VAL:HB	1:D:367:ALA:HB2	1.87	0.56
1:G:168:LEU:HD12	1:G:169:LYS:N	2.20	0.56
1:B:134:ILE:HD13	1:B:224:LEU:HB2	1.87	0.56
1:D:227:ASP:OD1	1:D:229:THR:HB	2.05	0.56
1:B:354:VAL:HG12	1:B:354:VAL:O	2.06	0.56
1:D:342:THR:HG22	1:D:343:VAL:H	1.70	0.56
1:E:227:ASP:OD1	1:E:229:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ASP:C	1:F:350:ARG:HG3	2.31	0.56
1:G:361:LEU:HD12	1:G:362:CYS:N	2.20	0.56
1:D:194:ARG:CZ	1:D:347:ARG:HH22	2.19	0.56
1:E:224:LEU:HG	1:E:237:ASN:ND2	2.21	0.56
1:C:150:TYR:CE1	1:C:179:GLN:HB2	2.40	0.55
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.50	0.55
1:A:126:MET:HE3	1:A:210:ARG:HD2	1.88	0.55
1:F:105:LEU:HD12	1:F:105:LEU:C	2.31	0.55
1:F:133:THR:O	1:F:134:ILE:C	2.49	0.55
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.72	0.55
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.19	0.55
1:F:361:LEU:HD12	1:F:362:CYS:N	2.22	0.55
1:G:316:THR:HG22	1:G:318:ALA:N	2.06	0.55
1:A:256:ASP:O	1:A:259:ALA:HB3	2.06	0.55
1:G:165:GLU:O	1:G:166:LYS:HB2	2.06	0.55
1:G:258:ILE:HG21	1:G:275:ILE:HD13	1.89	0.55
1:A:324:PHE:HB3	1:A:381:PHE:HE1	1.71	0.55
1:E:342:THR:HG22	1:E:343:VAL:N	2.22	0.55
1:A:156:PHE:C	1:A:156:PHE:CD1	2.84	0.55
1:A:197:MET:HE1	1:A:204:GLN:CB	2.37	0.55
1:C:256:ASP:O	1:C:259:ALA:HB3	2.06	0.55
1:F:276:VAL:HA	1:F:314:VAL:HG23	1.89	0.55
1:G:139:ALA:HB3	1:G:334:GLN:HB3	1.88	0.55
1:B:224:LEU:HD13	1:B:237:ASN:ND2	2.21	0.55
1:B:258:ILE:HG21	1:B:308:MET:CE	2.28	0.55
1:B:258:ILE:HG21	1:B:275:ILE:HD13	1.89	0.55
1:A:193:SER:HB3	1:A:196:VAL:CG2	2.36	0.55
1:C:299:GLY:O	1:C:301:GLN:N	2.39	0.55
1:E:119:MET:HE2	1:F:148:LEU:HD22	1.89	0.55
1:E:259:ALA:HB2	1:E:309:TRP:NE1	2.22	0.55
1:F:143:THR:OG1	1:F:144:SER:N	2.40	0.55
1:A:200:ALA:HB1	1:A:202:MET:HE1	1.89	0.55
1:A:134:ILE:HD13	1:A:224:LEU:HB2	1.89	0.54
1:A:239:VAL:HG21	1:A:370:HIS:CG	2.41	0.54
1:D:292:GLU:OE1	1:D:292:GLU:HA	2.06	0.54
1:G:227:ASP:HB3	1:G:229:THR:HG22	1.88	0.54
1:A:223:LEU:HD23	1:A:368:LEU:HD22	1.90	0.54
1:C:244:ASP:CG	1:C:246:SER:HB3	2.32	0.54
1:G:127:PRO:HB2	1:G:210:ARG:HH12	1.72	0.54
1:C:224:LEU:HD13	1:C:237:ASN:HD21	1.72	0.54
1:D:135:ARG:NH1	1:D:219:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ILE:O	1:F:377:ILE:HD13	2.07	0.54
1:C:187:ALA:HB2	1:C:363:GLU:CB	2.38	0.54
1:F:235:GLY:O	1:F:236:LEU:C	2.48	0.54
1:F:324:PHE:HD2	1:F:381:PHE:CE1	2.26	0.54
1:G:161:ASP:CG	1:G:162:VAL:H	2.15	0.54
1:G:264:GLN:HB3	1:G:377:ILE:CD1	2.38	0.54
1:A:119:MET:HE2	1:B:148:LEU:HD22	1.89	0.54
1:D:188:HIS:ND1	1:E:160:ALA:HB2	2.23	0.54
1:D:229:THR:HG23	1:D:230:GLY:H	1.71	0.54
1:D:329:PHE:O	1:D:331:MET:N	2.40	0.54
1:B:263:TYR:O	1:B:266:THR:N	2.40	0.54
1:F:183:VAL:HG13	1:F:366:LEU:O	2.08	0.54
1:E:163:VAL:HG12	1:E:164:ALA:O	2.07	0.54
1:E:334:GLN:NE2	1:E:371:TYR:OH	2.40	0.54
1:F:135:ARG:NH1	1:F:219:GLU:OE2	2.41	0.54
1:F:258:ILE:CB	1:F:308:MET:HE1	2.33	0.54
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.23	0.54
1:A:226:GLY:HA3	1:A:235:GLY:H	1.72	0.54
1:F:189:TRP:HZ3	1:F:191:GLN:HG2	1.73	0.53
1:E:299:GLY:O	1:E:301:GLN:N	2.41	0.53
1:A:155:VAL:H	1:A:175:THR:HB	1.74	0.53
1:A:339:MET:CE	1:A:363:GLU:HG3	2.35	0.53
1:D:146:ASN:C	1:D:183:VAL:HG12	2.33	0.53
1:D:229:THR:CG2	1:D:232:ASN:ND2	2.71	0.53
1:B:258:ILE:O	1:B:262:ILE:HG13	2.07	0.53
1:E:189:TRP:CZ2	1:F:171:GLU:HB2	2.43	0.53
1:G:305:SER:OG	1:G:306:ASN:N	2.41	0.53
1:D:155:VAL:H	1:D:175:THR:HB	1.74	0.53
1:A:342:THR:CG2	1:A:343:VAL:N	2.71	0.53
1:D:156:PHE:C	1:D:156:PHE:CD2	2.83	0.53
1:D:187:ALA:HB2	1:D:363:GLU:HA	1.91	0.53
1:A:156:PHE:C	1:A:156:PHE:HD1	2.17	0.53
1:B:143:THR:OG1	1:B:144:SER:N	2.42	0.53
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.23	0.53
1:D:119:MET:HE2	1:E:148:LEU:CD2	2.38	0.53
1:D:133:THR:O	1:D:134:ILE:C	2.51	0.53
1:F:145:SER:O	1:F:183:VAL:HG21	2.08	0.53
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.43	0.53
1:A:226:GLY:HA3	1:A:235:GLY:N	2.24	0.53
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.23	0.53
1:D:290:ASP:OD2	1:D:294:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.23	0.53
1:C:183:VAL:HG13	1:C:366:LEU:O	2.09	0.52
1:C:188:HIS:HB3	1:D:160:ALA:CA	2.36	0.52
1:C:200:ALA:HB1	1:C:202:MET:HE1	1.89	0.52
1:F:256:ASP:O	1:F:259:ALA:HB3	2.08	0.52
1:G:258:ILE:CB	1:G:308:MET:HE1	2.36	0.52
1:E:106:GLY:O	1:E:111:SER:HB3	2.09	0.52
1:E:361:LEU:HD12	1:E:362:CYS:N	2.23	0.52
1:G:133:THR:C	1:G:135:ARG:N	2.65	0.52
1:G:215:LEU:HD21	1:G:364:GLU:HB3	1.90	0.52
1:G:163:VAL:HG12	1:G:164:ALA:O	2.09	0.52
1:G:324:PHE:HB3	1:G:381:PHE:HE1	1.73	0.52
1:C:133:THR:O	1:C:136:ASP:N	2.43	0.52
1:D:112:ALA:HB1	1:D:115:LEU:HD12	1.90	0.52
1:D:119:MET:HB3	1:E:148:LEU:CD2	2.39	0.52
1:E:254:ARG:HB3	1:E:381:PHE:CE2	2.45	0.52
1:A:187:ALA:CB	1:A:363:GLU:HB3	2.39	0.52
1:A:361:LEU:HD12	1:A:362:CYS:H	1.73	0.52
1:C:263:TYR:O	1:C:266:THR:N	2.40	0.52
1:D:361:LEU:HD12	1:D:362:CYS:N	2.25	0.52
1:C:297:PHE:HB3	1:C:304:THR:CG2	2.39	0.52
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.90	0.52
1:E:193:SER:HA	1:E:357:MET:SD	2.50	0.52
1:D:354:VAL:HG12	1:D:354:VAL:O	2.09	0.52
1:B:119:MET:HB3	1:C:148:LEU:CD2	2.40	0.52
1:D:135:ARG:NH2	1:D:337:ASP:OD1	2.42	0.52
1:D:207:ILE:O	1:D:211:LEU:CD2	2.57	0.52
1:A:119:MET:HB3	1:B:148:LEU:CD2	2.40	0.52
1:B:119:MET:HE2	1:C:148:LEU:HD22	1.92	0.51
1:C:239:VAL:HG12	1:C:373:PRO:HB3	1.92	0.51
1:E:295:TYR:HD1	1:E:300:PRO:HD3	1.72	0.51
1:E:339:MET:CE	1:E:363:GLU:HG3	2.36	0.51
1:F:161:ASP:CG	1:F:162:VAL:H	2.18	0.51
1:A:260:HIS:O	1:A:263:TYR:HB3	2.10	0.51
1:D:289:LYS:NZ	1:E:253:THR:HG23	2.25	0.51
1:G:194:ARG:CZ	1:G:347:ARG:HH21	2.23	0.51
1:C:268:SER:O	1:C:269:GLU:HB2	2.09	0.51
1:B:371:TYR:CD1	1:B:371:TYR:N	2.77	0.51
1:D:263:TYR:O	1:D:266:THR:N	2.39	0.51
1:E:149:GLU:CD	1:E:178:LYS:HE2	2.36	0.51
1:E:290:ASP:OD2	1:E:294:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:HB1	1:A:115:LEU:HD12	1.92	0.51
1:A:125:ILE:O	1:A:125:ILE:HG22	2.09	0.51
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.26	0.51
1:E:134:ILE:HD12	1:E:224:LEU:HB2	1.93	0.51
1:F:373:PRO:C	1:F:375:ALA:H	2.19	0.51
1:G:150:TYR:CD2	1:G:150:TYR:N	2.79	0.51
1:C:303:PHE:HE1	1:D:309:TRP:HB3	1.76	0.51
1:E:139:ALA:O	1:E:334:GLN:HG3	2.11	0.51
1:E:159:ASN:O	1:E:160:ALA:C	2.54	0.51
1:E:235:GLY:O	1:E:236:LEU:C	2.54	0.51
1:F:187:ALA:HB2	1:F:363:GLU:CB	2.41	0.51
1:G:313:VAL:O	1:G:315:PRO:HD3	2.11	0.51
1:A:187:ALA:HB2	1:A:363:GLU:HB3	1.92	0.51
1:A:297:PHE:HB3	1:A:304:THR:CG2	2.39	0.51
1:C:258:ILE:N	1:C:258:ILE:HD12	2.25	0.51
1:D:253:THR:HB	1:D:288:LEU:HD11	1.92	0.51
1:A:272:ALA:HB3	1:A:311:LEU:HD11	1.93	0.51
1:B:187:ALA:HB2	1:B:363:GLU:HA	1.92	0.51
1:G:258:ILE:HD12	1:G:308:MET:HE1	1.93	0.50
1:G:339:MET:HE1	1:G:363:GLU:CG	2.38	0.50
1:E:190:VAL:HG22	1:F:172:SER:O	2.11	0.50
1:F:135:ARG:NH2	1:F:337:ASP:OD1	2.44	0.50
1:B:295:TYR:HD1	1:B:300:PRO:HD3	1.76	0.50
1:D:219:GLU:HG3	1:D:366:LEU:CD1	2.41	0.50
1:E:227:ASP:CG	1:E:229:THR:HB	2.36	0.50
1:E:236:LEU:HD13	1:E:370:HIS:HE1	1.76	0.50
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.41	0.50
1:B:235:GLY:O	1:B:236:LEU:C	2.53	0.50
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.77	0.50
1:E:285:ILE:O	1:E:288:LEU:HB2	2.12	0.50
1:C:303:PHE:CE1	1:D:309:TRP:HB3	2.46	0.50
1:E:258:ILE:HG21	1:E:308:MET:HE3	1.92	0.50
1:F:159:ASN:O	1:F:160:ALA:C	2.54	0.50
1:F:163:VAL:HG12	1:F:164:ALA:O	2.11	0.50
1:C:275:ILE:HG23	1:C:326:VAL:HG22	1.92	0.50
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.45	0.50
1:D:260:HIS:O	1:D:263:TYR:HB3	2.12	0.50
1:E:324:PHE:HD2	1:E:381:PHE:CE1	2.29	0.50
1:F:297:PHE:HB3	1:F:304:THR:CG2	2.40	0.50
1:A:197:MET:HE1	1:A:204:GLN:HB2	1.92	0.50
1:E:258:ILE:HG21	1:E:308:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:LEU:O	1:F:296:ILE:HG12	2.12	0.49
1:G:266:THR:C	1:G:268:SER:H	2.20	0.49
1:A:156:PHE:CE1	1:A:158:ASN:HB2	2.47	0.49
1:A:258:ILE:CG2	1:A:275:ILE:HD13	2.42	0.49
1:B:289:LYS:NZ	1:C:253:THR:HG23	2.26	0.49
1:E:297:PHE:CB	1:E:304:THR:HG21	2.42	0.49
1:G:268:SER:O	1:G:269:GLU:HB2	2.12	0.49
1:C:235:GLY:O	1:C:236:LEU:C	2.55	0.49
1:G:197:MET:HE1	1:G:204:GLN:HG3	1.94	0.49
1:F:297:PHE:CB	1:F:304:THR:HG21	2.40	0.49
1:F:316:THR:HG22	1:F:318:ALA:N	2.11	0.49
1:C:133:THR:O	1:C:135:ARG:N	2.46	0.49
1:G:128:GLY:HA2	1:G:213:TYR:CZ	2.48	0.49
1:C:161:ASP:CG	1:C:162:VAL:H	2.21	0.49
1:A:163:VAL:HG12	1:A:164:ALA:O	2.12	0.49
1:A:263:TYR:O	1:A:266:THR:N	2.35	0.49
1:B:156:PHE:C	1:B:156:PHE:CD2	2.88	0.49
1:C:145:SER:OG	1:C:146:ASN:N	2.45	0.49
1:C:258:ILE:HD11	1:C:381:PHE:CZ	2.48	0.49
1:D:119:MET:HB3	1:E:148:LEU:HD22	1.94	0.49
1:B:297:PHE:HB3	1:B:304:THR:CG2	2.42	0.49
1:D:187:ALA:HB2	1:D:363:GLU:CB	2.42	0.49
1:G:224:LEU:HG	1:G:237:ASN:ND2	2.27	0.49
1:A:107:SER:HB2	1:C:165:GLU:CD	2.38	0.48
1:A:193:SER:CB	1:A:196:VAL:HG23	2.43	0.48
1:B:329:PHE:C	1:B:331:MET:H	2.21	0.48
1:F:149:GLU:CD	1:F:178:LYS:HE2	2.38	0.48
1:B:295:TYR:OH	1:C:256:ASP:OD1	2.31	0.48
1:D:299:GLY:O	1:D:301:GLN:N	2.46	0.48
1:B:219:GLU:HG3	1:B:366:LEU:HD11	1.94	0.48
1:B:253:THR:OG1	1:B:255:ALA:HB3	2.13	0.48
1:D:125:ILE:HD13	1:E:371:TYR:HB3	1.95	0.48
1:A:119:MET:HE2	1:B:148:LEU:HD21	1.95	0.48
1:B:210:ARG:NH2	1:C:156:PHE:HD2	2.11	0.48
1:E:349:ASP:O	1:E:352:ASN:HB2	2.13	0.48
1:F:224:LEU:HD22	1:F:237:ASN:ND2	2.28	0.48
1:F:276:VAL:HG22	1:F:314:VAL:CG2	2.44	0.48
1:G:342:THR:HG22	1:G:343:VAL:N	2.28	0.48
1:C:159:ASN:O	1:C:160:ALA:C	2.55	0.48
1:D:193:SER:OG	1:D:196:VAL:HG23	2.13	0.48
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:LEU:HG	1:E:237:ASN:HD22	1.79	0.48
1:D:297:PHE:CB	1:D:304:THR:HG21	2.41	0.48
1:E:156:PHE:C	1:E:156:PHE:HD2	2.20	0.48
1:F:347:ARG:HG3	1:F:347:ARG:HH11	1.77	0.48
1:B:193:SER:HB3	1:B:196:VAL:HG23	1.96	0.48
1:C:163:VAL:HG12	1:C:164:ALA:O	2.14	0.48
1:C:268:SER:HB2	1:C:374:THR:HB	1.96	0.48
1:D:159:ASN:O	1:D:160:ALA:C	2.56	0.48
1:E:202:MET:SD	1:E:202:MET:N	2.86	0.48
1:F:376:ILE:C	1:F:377:ILE:HD13	2.39	0.48
1:E:145:SER:OG	1:E:146:ASN:N	2.44	0.48
1:F:148:LEU:HD12	1:F:336:TRP:CD1	2.49	0.48
1:A:371:TYR:N	1:A:371:TYR:CD2	2.81	0.47
1:D:235:GLY:O	1:D:236:LEU:C	2.58	0.47
1:D:339:MET:CE	1:D:363:GLU:HG3	2.40	0.47
1:B:119:MET:HE1	1:C:336:TRP:CZ3	2.49	0.47
1:B:369:ALA:HB1	1:B:371:TYR:HE1	1.79	0.47
1:D:223:LEU:HD23	1:D:368:LEU:HD22	1.96	0.47
1:A:258:ILE:CG2	1:A:308:MET:HE3	2.32	0.47
1:B:316:THR:HG22	1:B:317:LYS:N	2.29	0.47
1:D:190:VAL:CG2	1:D:211:LEU:HD11	2.44	0.47
1:D:324:PHE:HB3	1:D:381:PHE:HE1	1.79	0.47
1:C:324:PHE:HD2	1:C:381:PHE:CE1	2.32	0.47
1:G:349:ASP:O	1:G:350:ARG:C	2.56	0.47
1:B:239:VAL:HG21	1:B:370:HIS:CG	2.49	0.47
1:F:187:ALA:HB2	1:F:363:GLU:HB3	1.96	0.47
1:A:282:TRP:HE3	1:A:282:TRP:HA	1.80	0.47
1:B:159:ASN:O	1:B:160:ALA:C	2.56	0.47
1:A:235:GLY:O	1:A:236:LEU:C	2.57	0.47
1:A:258:ILE:N	1:A:258:ILE:CD1	2.76	0.47
1:A:342:THR:CG2	1:A:343:VAL:H	2.27	0.47
1:B:187:ALA:HB2	1:B:363:GLU:CB	2.45	0.47
1:B:203:LEU:O	1:B:207:ILE:HG13	2.14	0.47
1:C:188:HIS:CG	1:D:160:ALA:HB2	2.48	0.47
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.79	0.47
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.45	0.47
1:B:339:MET:HE1	1:B:363:GLU:HG3	1.96	0.47
1:D:163:VAL:HG12	1:D:164:ALA:O	2.15	0.47
1:E:135:ARG:NH1	1:E:219:GLU:OE2	2.48	0.47
1:E:295:TYR:CB	1:E:299:GLY:H	2.18	0.47
1:F:354:VAL:O	1:F:354:VAL:HG12	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASN:C	1:D:183:VAL:CG1	2.87	0.47
1:D:268:SER:O	1:D:269:GLU:HB2	2.15	0.47
1:E:211:LEU:HD12	1:E:211:LEU:N	2.29	0.47
1:B:349:ASP:C	1:B:350:ARG:CG	2.88	0.47
1:D:139:ALA:O	1:D:334:GLN:HG3	2.14	0.47
1:E:210:ARG:HH21	1:F:156:PHE:HD2	1.63	0.47
1:G:347:ARG:HB3	1:G:347:ARG:CZ	2.45	0.47
1:D:282:TRP:HE3	1:D:282:TRP:HA	1.81	0.46
1:G:135:ARG:NH2	1:G:337:ASP:OD1	2.47	0.46
1:B:150:TYR:CE1	1:B:179:GLN:HB2	2.51	0.46
1:B:286:ALA:C	1:B:288:LEU:H	2.23	0.46
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.31	0.46
1:D:188:HIS:NE2	1:D:211:LEU:HD12	2.30	0.46
1:E:236:LEU:HD12	1:E:376:ILE:HD13	1.97	0.46
1:A:282:TRP:HA	1:A:282:TRP:CE3	2.50	0.46
1:D:222:GLN:O	1:D:223:LEU:C	2.59	0.46
1:D:371:TYR:N	1:D:371:TYR:CD2	2.83	0.46
1:E:146:ASN:C	1:E:183:VAL:HG23	2.40	0.46
1:E:290:ASP:OD1	1:E:290:ASP:C	2.58	0.46
1:G:134:ILE:CD1	1:G:224:LEU:HB2	2.44	0.46
1:A:280:ARG:CZ	1:B:247:LEU:HD21	2.46	0.46
1:E:146:ASN:O	1:E:183:VAL:HG23	2.16	0.46
1:G:139:ALA:O	1:G:334:GLN:HB2	2.16	0.46
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.80	0.46
1:C:189:TRP:HB3	1:C:361:LEU:HD13	1.98	0.46
1:D:335:VAL:HG22	1:D:368:LEU:HD13	1.97	0.46
1:E:155:VAL:H	1:E:175:THR:HB	1.79	0.46
1:E:339:MET:HE1	1:E:363:GLU:CG	2.39	0.46
1:B:258:ILE:HD12	1:B:258:ILE:N	2.31	0.46
1:D:148:LEU:HD11	1:D:336:TRP:CG	2.49	0.46
1:E:297:PHE:HB3	1:E:304:THR:HG21	1.98	0.46
1:A:150:TYR:HB3	1:F:121:ILE:HD12	1.98	0.46
1:D:119:MET:HE1	1:E:336:TRP:CZ3	2.51	0.46
1:E:119:MET:HE2	1:F:148:LEU:CD2	2.44	0.46
1:F:156:PHE:CE1	1:F:158:ASN:HB2	2.50	0.46
1:F:282:TRP:HA	1:F:282:TRP:CE3	2.51	0.46
1:C:168:LEU:HD22	1:C:169:LYS:O	2.16	0.46
1:E:258:ILE:CD1	1:E:308:MET:HE1	2.42	0.46
1:E:263:TYR:O	1:E:266:THR:N	2.46	0.46
1:G:197:MET:CE	1:G:204:GLN:HB2	2.39	0.46
1:B:183:VAL:HG13	1:B:366:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TRP:HD1	1:E:169:LYS:HB3	1.81	0.46
1:D:286:ALA:C	1:D:288:LEU:H	2.23	0.46
1:F:373:PRO:C	1:F:375:ALA:N	2.72	0.46
1:E:116:ILE:HG21	1:F:146:ASN:CB	2.28	0.46
1:F:142:ARG:NH1	1:F:142:ARG:HB3	2.31	0.46
1:B:361:LEU:HD12	1:B:362:CYS:N	2.30	0.45
1:D:126:MET:HE2	1:D:206:TYR:CE1	2.51	0.45
1:D:146:ASN:O	1:D:147:ALA:HB2	2.16	0.45
1:F:329:PHE:O	1:F:331:MET:N	2.49	0.45
1:A:146:ASN:CG	1:F:116:ILE:HG21	2.42	0.45
1:C:292:GLU:OE2	1:C:292:GLU:HA	2.15	0.45
1:D:156:PHE:CE2	1:D:158:ASN:HB2	2.51	0.45
1:B:260:HIS:O	1:B:263:TYR:HB3	2.16	0.45
1:C:125:ILE:HD13	1:D:371:TYR:HB3	1.98	0.45
1:D:197:MET:HE1	1:D:204:GLN:CB	2.32	0.45
1:D:280:ARG:CZ	1:E:247:LEU:HD21	2.46	0.45
1:G:133:THR:O	1:G:134:ILE:C	2.57	0.45
1:A:148:LEU:CD1	1:A:336:TRP:CG	2.99	0.45
1:A:188:HIS:CG	1:B:160:ALA:HB2	2.52	0.45
1:B:329:PHE:O	1:B:331:MET:N	2.49	0.45
1:B:349:ASP:O	1:B:350:ARG:C	2.58	0.45
1:A:126:MET:HE3	1:A:210:ARG:CD	2.46	0.45
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.98	0.45
1:E:215:LEU:HD21	1:E:364:GLU:HB3	1.99	0.45
1:E:336:TRP:HB2	1:E:367:ALA:HB3	1.98	0.45
1:A:376:ILE:C	1:A:377:ILE:HD13	2.41	0.45
1:C:121:ILE:HA	1:C:122:PRO:HD3	1.80	0.45
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.82	0.45
1:D:189:TRP:CZ2	1:E:171:GLU:HB2	2.51	0.45
1:D:282:TRP:HA	1:D:282:TRP:CE3	2.51	0.45
1:E:156:PHE:CE2	1:E:158:ASN:HB2	2.51	0.45
1:A:295:TYR:HB2	1:A:299:GLY:N	2.32	0.45
1:D:193:SER:HA	1:D:357:MET:SD	2.57	0.45
1:D:229:THR:CG2	1:D:230:GLY:H	2.28	0.45
1:F:314:VAL:HG23	1:F:314:VAL:O	2.17	0.45
1:F:336:TRP:HB2	1:F:367:ALA:HB3	1.98	0.45
1:G:187:ALA:HB2	1:G:363:GLU:CB	2.46	0.45
1:A:188:HIS:CE1	1:B:160:ALA:HB2	2.52	0.45
1:B:132:LEU:HD22	1:B:220:GLU:HG3	1.99	0.45
1:A:135:ARG:NH2	1:A:337:ASP:OD1	2.46	0.45
1:D:163:VAL:HG21	1:D:169:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:GLN:O	1:E:368:LEU:HD12	2.17	0.45
1:F:196:VAL:HG12	1:F:203:LEU:HD22	1.98	0.45
1:B:148:LEU:HD11	1:B:336:TRP:CG	2.51	0.45
1:B:279:PRO:HD3	1:B:316:THR:O	2.15	0.45
1:C:148:LEU:HD12	1:C:336:TRP:CD1	2.52	0.45
1:D:143:THR:OG1	1:D:144:SER:N	2.49	0.45
1:D:202:MET:H	1:D:202:MET:CE	2.22	0.45
1:A:249:ALA:O	1:A:250:THR:C	2.60	0.44
1:D:288:LEU:O	1:D:296:ILE:HG12	2.18	0.44
1:F:145:SER:OG	1:F:146:ASN:N	2.50	0.44
1:A:258:ILE:HD11	1:A:381:PHE:CZ	2.52	0.44
1:A:339:MET:HE1	1:A:363:GLU:CG	2.38	0.44
1:B:189:TRP:HB3	1:B:361:LEU:HD13	2.00	0.44
1:C:135:ARG:HH21	1:C:219:GLU:CD	2.24	0.44
1:E:134:ILE:HD13	1:E:224:LEU:HB2	1.97	0.44
1:F:139:ALA:O	1:F:334:GLN:HG3	2.17	0.44
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.84	0.44
1:D:239:VAL:HG21	1:D:370:HIS:CG	2.52	0.44
1:A:361:LEU:HD12	1:A:362:CYS:N	2.32	0.44
1:B:299:GLY:O	1:B:301:GLN:N	2.50	0.44
1:E:324:PHE:CZ	1:E:379:GLY:HA3	2.52	0.44
1:E:350:ARG:O	1:E:352:ASN:N	2.49	0.44
1:A:300:PRO:HG2	1:B:296:ILE:HG22	2.00	0.44
1:F:347:ARG:HD2	1:F:358:LEU:HD11	2.00	0.44
1:C:189:TRP:CZ2	1:D:171:GLU:HB2	2.53	0.44
1:D:133:THR:O	1:D:135:ARG:N	2.51	0.44
1:D:146:ASN:HA	1:D:183:VAL:CG1	2.48	0.44
1:E:134:ILE:HD13	1:E:224:LEU:HD13	1.99	0.44
1:E:168:LEU:HD22	1:E:169:LYS:O	2.17	0.44
1:A:146:ASN:O	1:A:147:ALA:HB2	2.18	0.44
1:B:201:PRO:HD2	1:B:202:MET:HE1	1.99	0.44
1:F:195:GLN:O	1:F:196:VAL:C	2.61	0.44
1:C:345:VAL:HG13	1:C:360:ILE:HG12	1.98	0.44
1:E:373:PRO:C	1:E:375:ALA:H	2.25	0.44
1:F:282:TRP:HA	1:F:282:TRP:HE3	1.81	0.44
1:C:286:ALA:C	1:C:288:LEU:H	2.26	0.44
1:B:195:GLN:O	1:B:196:VAL:C	2.61	0.43
1:E:239:VAL:HG21	1:E:370:HIS:CG	2.53	0.43
1:G:123:GLY:H	1:G:202:MET:CE	2.29	0.43
1:C:290:ASP:OD1	1:C:290:ASP:C	2.61	0.43
1:D:146:ASN:HA	1:D:183:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:OD1	1:D:343:VAL:HG11	2.19	0.43
1:G:135:ARG:NH1	1:G:219:GLU:CD	2.76	0.43
1:D:229:THR:HG23	1:D:232:ASN:ND2	2.31	0.43
1:E:134:ILE:HD11	1:E:224:LEU:HD22	2.00	0.43
1:F:114:SER:HB3	1:G:178:LYS:HB2	2.00	0.43
1:G:233:LEU:HD11	1:G:366:LEU:HD11	1.99	0.43
1:B:119:MET:HE2	1:C:148:LEU:CD2	2.48	0.43
1:B:283:HIS:NE2	1:C:260:HIS:HA	2.34	0.43
1:C:197:MET:CE	1:C:204:GLN:HB2	2.38	0.43
1:F:197:MET:HE1	1:F:204:GLN:HA	1.99	0.43
1:A:254:ARG:HB3	1:A:381:PHE:CE2	2.50	0.43
1:D:156:PHE:C	1:D:156:PHE:HD2	2.23	0.43
1:D:369:ALA:HB1	1:D:371:TYR:HE2	1.83	0.43
1:E:288:LEU:O	1:E:296:ILE:HG12	2.19	0.43
1:F:350:ARG:HB2	1:F:351:ASP:H	1.52	0.43
1:G:275:ILE:HG12	1:G:326:VAL:HG22	2.01	0.43
1:G:366:LEU:CD1	1:G:366:LEU:C	2.91	0.43
1:B:134:ILE:HD11	1:B:224:LEU:HG	2.00	0.43
1:B:224:LEU:HD22	1:B:237:ASN:ND2	2.33	0.43
1:B:280:ARG:CZ	1:C:247:LEU:HD21	2.48	0.43
1:B:314:VAL:HA	1:B:315:PRO:HD3	1.74	0.43
1:C:155:VAL:H	1:C:175:THR:HB	1.82	0.43
1:C:208:ASN:OD1	1:C:343:VAL:HG11	2.19	0.43
1:G:133:THR:HG22	1:G:134:ILE:N	2.32	0.43
1:A:253:THR:HG23	1:F:289:LYS:NZ	2.34	0.43
1:A:352:ASN:O	1:A:353:PHE:C	2.61	0.43
1:B:295:TYR:HE1	1:B:300:PRO:HG3	1.84	0.43
1:D:249:ALA:O	1:D:250:THR:C	2.62	0.43
1:E:135:ARG:NH1	1:E:219:GLU:CD	2.77	0.43
1:F:276:VAL:HG22	1:F:314:VAL:HG21	2.00	0.43
1:B:371:TYR:N	1:B:371:TYR:HD1	2.17	0.43
1:D:186:ILE:HA	1:E:161:ASP:O	2.18	0.43
1:E:289:LYS:NZ	1:F:253:THR:HG23	2.34	0.43
1:E:373:PRO:C	1:E:375:ALA:N	2.77	0.43
1:G:196:VAL:HG12	1:G:203:LEU:CD2	2.48	0.43
1:G:274:GLY:HA2	1:G:312:PRO:HD2	2.00	0.43
1:A:119:MET:HB3	1:B:148:LEU:HD22	2.01	0.43
1:A:253:THR:O	1:A:254:ARG:C	2.62	0.43
1:B:134:ILE:CD1	1:B:224:LEU:HG	2.49	0.43
1:B:155:VAL:H	1:B:175:THR:HB	1.82	0.43
1:C:139:ALA:O	1:C:334:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:CD1	1:C:336:TRP:CG	3.02	0.43
1:G:277:LEU:HD13	1:G:285:ILE:HD12	2.01	0.43
1:B:289:LYS:C	1:B:296:ILE:HD11	2.44	0.43
1:C:342:THR:CG2	1:C:343:VAL:N	2.82	0.43
1:D:129:LEU:HD12	1:D:129:LEU:HA	1.77	0.43
1:D:368:LEU:HD12	1:D:368:LEU:HA	1.80	0.43
1:E:148:LEU:HD11	1:E:336:TRP:CG	2.54	0.43
1:G:211:LEU:HD23	1:G:211:LEU:HA	1.88	0.43
1:A:183:VAL:HG13	1:A:366:LEU:O	2.19	0.42
1:G:134:ILE:HB	1:G:220:GLU:HG3	2.00	0.42
1:A:183:VAL:HG22	1:A:367:ALA:HB2	2.01	0.42
1:B:210:ARG:HD2	1:B:210:ARG:HA	1.89	0.42
1:B:329:PHE:C	1:B:331:MET:N	2.77	0.42
1:C:207:ILE:O	1:C:211:LEU:HG	2.18	0.42
1:C:224:LEU:CD1	1:C:237:ASN:HD21	2.31	0.42
1:D:253:THR:OG1	1:D:255:ALA:HB3	2.18	0.42
1:C:329:PHE:O	1:C:331:MET:N	2.52	0.42
1:F:148:LEU:HD11	1:F:336:TRP:CD2	2.54	0.42
1:F:222:GLN:O	1:F:223:LEU:C	2.62	0.42
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.42
1:C:352:ASN:O	1:C:353:PHE:C	2.63	0.42
1:D:373:PRO:C	1:D:375:ALA:N	2.77	0.42
1:E:266:THR:C	1:E:268:SER:H	2.28	0.42
1:E:275:ILE:HD13	1:E:308:MET:CE	2.50	0.42
1:G:334:GLN:HG2	1:G:371:TYR:OH	2.19	0.42
1:A:294:ARG:H	1:A:294:ARG:HG2	1.42	0.42
1:D:297:PHE:HB3	1:D:304:THR:CG2	2.46	0.42
1:E:121:ILE:HG13	1:F:150:TYR:HB3	2.02	0.42
1:A:168:LEU:C	1:A:168:LEU:CD2	2.92	0.42
1:A:222:GLN:O	1:A:223:LEU:C	2.62	0.42
1:C:268:SER:O	1:C:269:GLU:CB	2.67	0.42
1:D:258:ILE:HG21	1:D:308:MET:HE3	2.00	0.42
1:D:258:ILE:HD13	1:D:308:MET:CE	2.48	0.42
1:E:256:ASP:O	1:E:259:ALA:HB3	2.19	0.42
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.34	0.42
1:E:297:PHE:CD1	1:E:297:PHE:N	2.87	0.42
1:F:203:LEU:HG	1:F:207:ILE:HD11	2.01	0.42
1:G:165:GLU:C	1:G:167:ALA:H	2.27	0.42
1:A:283:HIS:NE2	1:B:260:HIS:HA	2.34	0.42
1:B:224:LEU:HD13	1:B:237:ASN:HD22	1.85	0.42
1:C:258:ILE:HG21	1:C:275:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:THR:CG2	1:D:343:VAL:N	2.80	0.42
1:E:203:LEU:HG	1:E:207:ILE:HD11	2.02	0.42
1:E:349:ASP:C	1:E:350:ARG:HG3	2.44	0.42
1:E:371:TYR:N	1:E:371:TYR:CD2	2.87	0.42
1:B:146:ASN:O	1:B:147:ALA:HB2	2.19	0.42
1:C:143:THR:OG1	1:C:144:SER:N	2.52	0.42
1:C:148:LEU:HD11	1:C:336:TRP:CG	2.54	0.42
1:F:342:THR:HG22	1:F:343:VAL:N	2.35	0.42
1:A:245:THR:O	1:A:245:THR:HG22	2.19	0.42
1:D:148:LEU:HD11	1:D:336:TRP:CD2	2.54	0.42
1:D:249:ALA:N	1:D:252:ASP:OD2	2.46	0.42
1:F:268:SER:O	1:F:269:GLU:HB2	2.18	0.42
1:B:222:GLN:O	1:B:223:LEU:C	2.61	0.42
1:B:342:THR:CG2	1:B:343:VAL:N	2.83	0.42
1:D:145:SER:OG	1:D:146:ASN:N	2.52	0.42
1:F:258:ILE:HG21	1:F:275:ILE:HD13	2.00	0.42
1:A:145:SER:OG	1:A:146:ASN:N	2.51	0.41
1:A:373:PRO:C	1:A:375:ALA:N	2.77	0.41
1:C:148:LEU:HD11	1:C:336:TRP:CD2	2.55	0.41
1:C:254:ARG:O	1:C:258:ILE:HD13	2.19	0.41
1:C:258:ILE:H	1:C:258:ILE:CD1	2.33	0.41
1:E:254:ARG:HB3	1:E:381:PHE:HE2	1.83	0.41
1:F:112:ALA:C	1:F:114:SER:N	2.62	0.41
1:F:133:THR:O	1:F:135:ARG:N	2.52	0.41
1:F:324:PHE:CD1	1:F:324:PHE:C	2.97	0.41
1:G:106:GLY:O	1:G:111:SER:HB3	2.20	0.41
1:A:159:ASN:O	1:A:160:ALA:C	2.61	0.41
1:B:335:VAL:HG22	1:B:368:LEU:HD13	2.02	0.41
1:B:349:ASP:C	1:B:350:ARG:HG3	2.45	0.41
1:F:290:ASP:OD1	1:F:290:ASP:C	2.63	0.41
1:F:349:ASP:CG	1:F:350:ARG:HG3	2.45	0.41
1:B:272:ALA:HB3	1:B:311:LEU:HD11	2.02	0.41
1:C:202:MET:HE2	1:C:203:LEU:N	2.35	0.41
1:C:243:TYR:HA	1:C:264:GLN:OE1	2.20	0.41
1:C:342:THR:HG22	1:C:343:VAL:H	1.83	0.41
1:D:189:TRP:CD1	1:E:169:LYS:HB3	2.55	0.41
1:D:373:PRO:C	1:D:375:ALA:H	2.26	0.41
1:G:156:PHE:CZ	1:G:158:ASN:HB2	2.54	0.41
1:B:188:HIS:CE1	1:C:160:ALA:HB2	2.55	0.41
1:B:280:ARG:NH1	1:C:247:LEU:HD23	2.34	0.41
1:B:350:ARG:HB2	1:B:351:ASP:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:PHE:CE1	1:D:379:GLY:HA3	2.56	0.41
1:G:229:THR:CG2	1:G:230:GLY:H	2.20	0.41
1:G:254:ARG:HB3	1:G:381:PHE:CD2	2.55	0.41
1:C:195:GLN:O	1:C:196:VAL:C	2.63	0.41
1:D:135:ARG:NH1	1:D:219:GLU:CD	2.79	0.41
1:D:227:ASP:CG	1:D:229:THR:HG22	2.45	0.41
1:E:351:ASP:CG	1:E:351:ASP:O	2.63	0.41
1:G:281:ASP:O	1:G:285:ILE:HG13	2.20	0.41
1:G:350:ARG:HB2	1:G:351:ASP:H	1.61	0.41
1:A:290:ASP:C	1:A:290:ASP:OD1	2.63	0.41
1:C:119:MET:HB3	1:D:148:LEU:CD2	2.50	0.41
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.41
1:A:112:ALA:O	1:A:113:GLY:C	2.64	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.82	0.41
1:A:329:PHE:C	1:A:331:MET:H	2.29	0.41
1:A:373:PRO:C	1:A:375:ALA:H	2.28	0.41
1:C:295:TYR:HD1	1:C:300:PRO:HD3	1.86	0.41
1:D:130:ARG:CZ	1:D:217:LEU:HD21	2.51	0.41
1:G:128:GLY:HA2	1:G:213:TYR:CE1	2.56	0.41
1:A:324:PHE:CE1	1:A:379:GLY:HA3	2.54	0.41
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.83	0.41
1:B:376:ILE:C	1:B:377:ILE:HG13	2.46	0.41
1:A:120:GLN:O	1:A:122:PRO:HD3	2.19	0.41
1:B:148:LEU:HD11	1:B:336:TRP:CD2	2.56	0.41
1:C:187:ALA:HB2	1:C:363:GLU:HB3	2.02	0.41
1:C:187:ALA:HB2	1:C:363:GLU:HA	2.02	0.41
1:C:224:LEU:HD12	1:C:225:ASN:ND2	2.36	0.41
1:C:265:VAL:HG23	1:C:377:ILE:HD12	2.03	0.41
1:E:222:GLN:O	1:E:223:LEU:C	2.63	0.41
1:E:222:GLN:HB3	1:E:233:LEU:HB2	2.03	0.41
1:E:229:THR:HG22	1:E:232:ASN:HD22	1.86	0.41
1:F:285:ILE:O	1:F:288:LEU:HB2	2.21	0.41
1:G:239:VAL:HG21	1:G:370:HIS:CD2	2.56	0.41
1:G:349:ASP:C	1:G:350:ARG:CG	2.94	0.41
1:A:206:TYR:CZ	1:A:210:ARG:HD3	2.56	0.41
1:B:147:ALA:O	1:B:148:LEU:HD23	2.21	0.41
1:B:227:ASP:OD1	1:B:227:ASP:C	2.64	0.41
1:C:124:ILE:N	1:C:124:ILE:CD1	2.84	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.83	0.41
1:D:224:LEU:HG	1:D:237:ASN:ND2	2.36	0.41
1:F:303:PHE:HD2	1:F:303:PHE:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:LEU:HD11	1:G:207:ILE:HD11	2.03	0.41
1:G:227:ASP:C	1:G:229:THR:H	2.29	0.41
1:D:255:ALA:HA	1:D:258:ILE:HD12	2.02	0.40
1:E:324:PHE:CD1	1:E:324:PHE:C	2.99	0.40
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.85	0.40
1:A:314:VAL:HA	1:A:315:PRO:HD3	1.78	0.40
1:B:268:SER:HB2	1:B:374:THR:CG2	2.51	0.40
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.85	0.40
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.03	0.40
1:E:147:ALA:O	1:E:148:LEU:HD23	2.21	0.40
1:E:282:TRP:CE3	1:E:282:TRP:HA	2.56	0.40
1:F:210:ARG:HD2	1:F:210:ARG:HA	1.82	0.40
1:G:126:MET:HA	1:G:127:PRO:HD3	1.85	0.40
1:G:194:ARG:NH1	1:G:347:ARG:NH2	2.69	0.40
1:G:258:ILE:O	1:G:262:ILE:HG13	2.21	0.40
1:B:126:MET:HA	1:B:127:PRO:HD3	1.84	0.40
1:D:196:VAL:HG12	1:D:203:LEU:CD2	2.52	0.40
1:A:269:GLU:HG2	1:F:130:ARG:HA	2.03	0.40
1:A:278:ASN:O	1:A:279:PRO:C	2.64	0.40
1:B:145:SER:OG	1:B:146:ASN:N	2.55	0.40
1:B:223:LEU:HD23	1:B:368:LEU:HD22	2.04	0.40
1:B:259:ALA:HB2	1:B:309:TRP:NE1	2.36	0.40
1:C:324:PHE:CD1	1:C:324:PHE:C	2.99	0.40
1:F:356:ASN:OD1	1:G:363:GLU:OE2	2.40	0.40
1:G:273:SER:H	1:G:328:GLY:HA2	1.86	0.40
1:G:306:ASN:HB3	1:G:313:VAL:HB	2.03	0.40
1:B:148:LEU:CD1	1:B:336:TRP:CG	3.05	0.40
1:B:282:TRP:CE3	1:B:282:TRP:HA	2.56	0.40
1:C:314:VAL:HA	1:C:315:PRO:HD3	1.78	0.40
1:C:371:TYR:HD1	1:C:371:TYR:H	1.64	0.40
1:E:211:LEU:N	1:E:211:LEU:CD1	2.85	0.40
1:E:282:TRP:HA	1:E:282:TRP:HE3	1.86	0.40
1:F:347:ARG:HG3	1:F:347:ARG:NH1	2.35	0.40
1:G:145:SER:OG	1:G:146:ASN:N	2.54	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	279/282 (99%)	237 (85%)	36 (13%)	6 (2%)	5	30
1	B	279/282 (99%)	229 (82%)	43 (15%)	7 (2%)	4	28
1	C	279/282 (99%)	236 (85%)	34 (12%)	9 (3%)	3	24
1	D	279/282 (99%)	232 (83%)	39 (14%)	8 (3%)	3	26
1	E	279/282 (99%)	240 (86%)	32 (12%)	7 (2%)	4	28
1	F	279/282 (99%)	231 (83%)	40 (14%)	8 (3%)	3	26
1	G	279/282 (99%)	232 (83%)	38 (14%)	9 (3%)	3	24
All	All	1953/1974 (99%)	1637 (84%)	262 (13%)	54 (3%)	4	26

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	PRO
1	B	352	ASN
1	C	134	ILE
1	C	300	PRO
1	D	229	THR
1	E	300	PRO
1	F	352	ASN
1	G	127	PRO
1	G	229	THR
1	G	297	PHE
1	A	226	GLY
1	C	269	GLU
1	D	134	ILE
1	D	230	GLY
1	D	300	PRO
1	D	330	ASP
1	D	350	ARG
1	E	230	GLY

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Mol	Chain	Res	Type
1	E	298	GLY
1	E	350	ARG
1	F	113	GLY
1	F	134	ILE
1	F	300	PRO
1	F	330	ASP
1	G	301	GLN
1	A	227	ASP
1	B	230	GLY
1	B	330	ASP
1	C	330	ASP
1	D	269	GLU
1	E	236	LEU
1	F	269	GLU
1	G	230	GLY
1	G	240	ALA
1	G	267	GLU
1	G	269	GLU
1	A	240	ALA
1	B	134	ILE
1	B	329	PHE
1	C	226	GLY
1	C	227	ASP
1	C	350	ARG
1	E	330	ASP
1	F	351	ASP
1	B	315	PRO
1	A	315	PRO
1	E	315	PRO
1	G	304	THR
1	A	230	GLY
1	D	226	GLY
1	A	134	ILE
1	C	315	PRO
1	C	196	VAL
1	F	315	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%)	212 (92%)	18 (8%)	11	37
1	B	230/231 (100%)	217 (94%)	13 (6%)	18	46
1	C	230/231 (100%)	213 (93%)	17 (7%)	13	39
1	D	230/231 (100%)	221 (96%)	9 (4%)	28	56
1	E	230/231 (100%)	209 (91%)	21 (9%)	9	32
1	F	230/231 (100%)	213 (93%)	17 (7%)	13	39
1	G	230/231 (100%)	218 (95%)	12 (5%)	21	49
All	All	1610/1617 (100%)	1503 (93%)	107 (7%)	15	43

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

Mol	Chain	Res	Type
1	A	107	SER
1	A	108	ASP
1	A	114	SER
1	A	124	ILE
1	A	133	THR
1	A	142	ARG
1	A	156	PHE
1	A	157	THR
1	A	168	LEU
1	A	202	MET
1	A	217	LEU
1	A	220	GLU
1	A	224	LEU
1	A	250	THR
1	A	288	LEU
1	A	292	GLU
1	A	301	GLN
1	A	374	THR
1	B	133	THR
1	B	151	VAL
1	B	157	THR
1	B	169	LYS
1	B	191	GLN
1	B	194	ARG
1	B	220	GLU
1	B	224	LEU

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Mol	Chain	Res	Type
1	B	250	THR
1	B	268	SER
1	B	279	PRO
1	B	288	LEU
1	B	374	THR
1	C	114	SER
1	C	124	ILE
1	C	133	THR
1	C	156	PHE
1	C	168	LEU
1	C	195	GLN
1	C	202	MET
1	C	215	LEU
1	C	224	LEU
1	C	234	GLU
1	C	250	THR
1	C	256	ASP
1	C	280	ARG
1	C	288	LEU
1	C	345	VAL
1	C	371	TYR
1	C	374	THR
1	D	114	SER
1	D	133	THR
1	D	151	VAL
1	D	180	THR
1	D	183	VAL
1	D	210	ARG
1	D	217	LEU
1	D	250	THR
1	D	288	LEU
1	E	111	SER
1	E	126	MET
1	E	133	THR
1	E	151	VAL
1	E	156	PHE
1	E	168	LEU
1	E	169	LYS
1	E	202	MET
1	E	205	SER
1	E	215	LEU
1	E	217	LEU

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Mol	Chain	Res	Type
1	E	229	THR
1	E	236	LEU
1	E	239	VAL
1	E	250	THR
1	E	279	PRO
1	E	288	LEU
1	E	297	PHE
1	E	300	PRO
1	E	358	LEU
1	E	374	THR
1	F	110	ASP
1	F	114	SER
1	F	133	THR
1	F	155	VAL
1	F	156	PHE
1	F	194	ARG
1	F	195	GLN
1	F	202	MET
1	F	217	LEU
1	F	224	LEU
1	F	250	THR
1	F	279	PRO
1	F	280	ARG
1	F	288	LEU
1	F	350	ARG
1	F	357	MET
1	F	374	THR
1	G	111	SER
1	G	116	ILE
1	G	125	ILE
1	G	150	TYR
1	G	195	GLN
1	G	245	THR
1	G	256	ASP
1	G	288	LEU
1	G	307	ILE
1	G	358	LEU
1	G	374	THR
1	G	383	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	182	ASN
1	A	204	GLN
1	A	225	ASN
1	A	237	ASN
1	A	334	GLN
1	B	158	ASN
1	B	191	GLN
1	B	237	ASN
1	B	334	GLN
1	C	140	GLN
1	C	146	ASN
1	C	182	ASN
1	C	204	GLN
1	C	225	ASN
1	C	237	ASN
1	C	291	ASN
1	C	334	GLN
1	D	120	GLN
1	D	232	ASN
1	D	291	ASN
1	D	334	GLN
1	E	191	GLN
1	E	208	ASN
1	E	232	ASN
1	E	237	ASN
1	E	334	GLN
1	F	158	ASN
1	F	182	ASN
1	F	204	GLN
1	F	232	ASN
1	F	237	ASN
1	F	334	GLN
1	G	140	GLN
1	G	195	GLN
1	G	232	ASN
1	G	334	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1384	-	4,4,4	1.87	2 (50%)	6,6,6	0.18	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1384	SO4	O2-S	2.38	1.59	1.44
2	A	1384	SO4	O1-S	2.38	1.59	1.44

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.