



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

PDB ID : 3RSE  
Title : Structural and biochemical characterization of two binding sites for nucleation promoting factor WASp-VCA on Arp2/3 complex  
Authors : Pollard, T.D.; Jurgenson, C.T.; Ti, S.; Nolen, B.J.  
Deposited on : 2011-05-02  
Resolution : 2.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

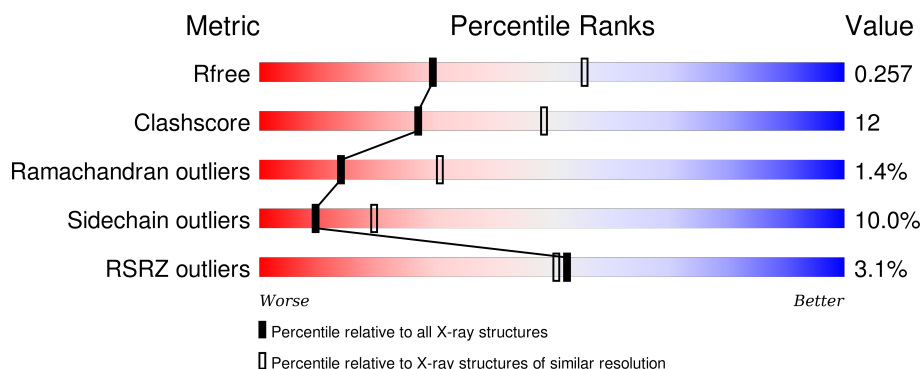
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>2%</div> <div>72% 17% 5%</div> </div>
2	B	394	<div> <div>5%</div> <div>32% 14% 50%</div> </div>
3	C	372	<div> <div>3%</div> <div>70% 20% 5% 5%</div> </div>
4	D	300	<div> <div>%</div> <div>71% 19% 7%</div> </div>
5	E	178	<div> <div>7%</div> <div>58% 30% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	168	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>79%15%5%</div><div></div></div></div>
7	G	151	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>64%21%5%10%</div><div></div></div></div>
8	Z	3	<div><div><div>33%</div><div><div></div><div></div><div></div></div><div>67%33%</div><div></div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13807 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3166	2033	531	588	14			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1566	1005	268	289	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	354	Total	C	N	O	S	0	0	0
			2759	1748	487	505	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	280	Total	C	N	O	S	0	0	0
			2262	1437	392	425	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1411	906	235	261	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	136	Total	C	N	O	S	0	0	0
			1031	647	179	202	3			

- Molecule 8 is a protein called CA fragment of Bos taurus N-WASP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Z	3	Total	C	N	O	0	0	0
			33	21	4	8			

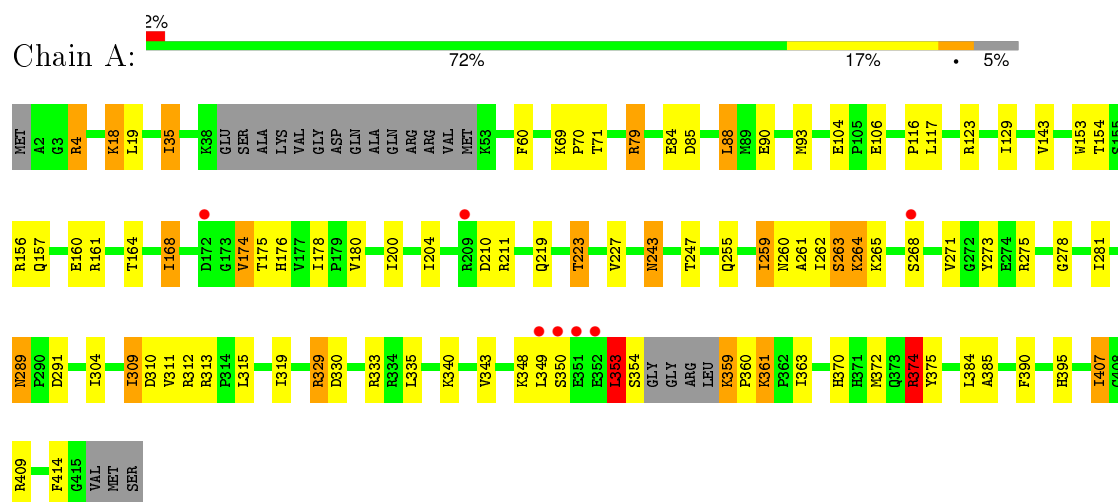
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	51	Total	O	0	0
			51	51		
9	B	13	Total	O	0	0
			13	13		
9	C	52	Total	O	0	0
			52	52		
9	D	47	Total	O	0	0
			47	47		
9	E	1	Total	O	0	0
			1	1		
9	F	35	Total	O	0	0
			35	35		
9	G	9	Total	O	0	0
			9	9		

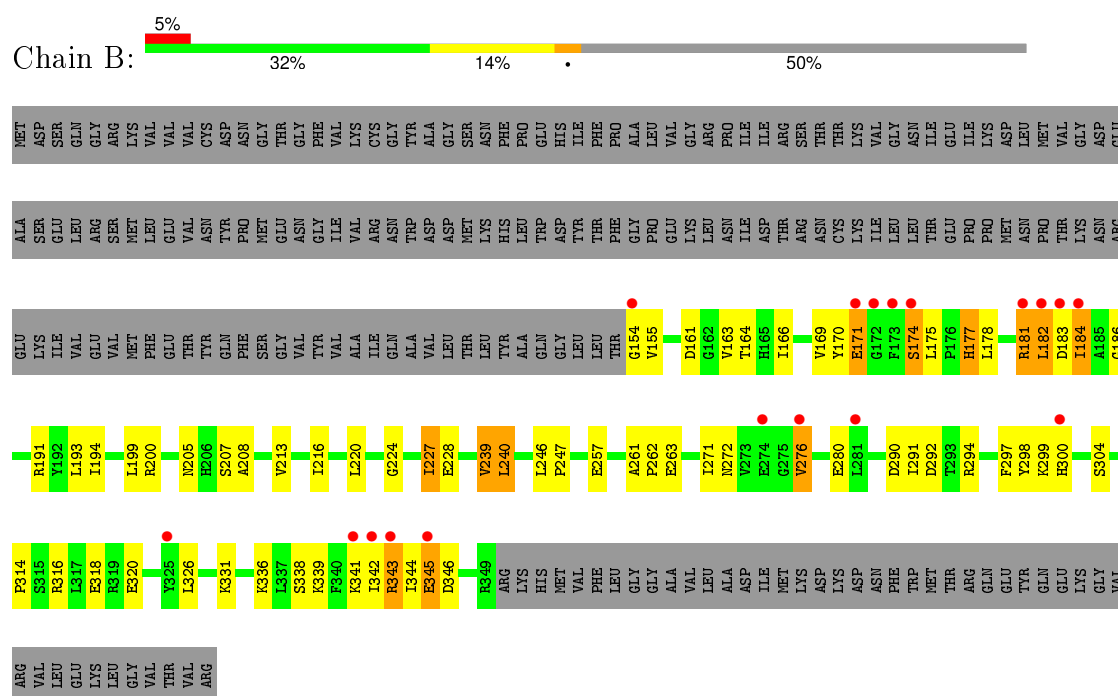
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

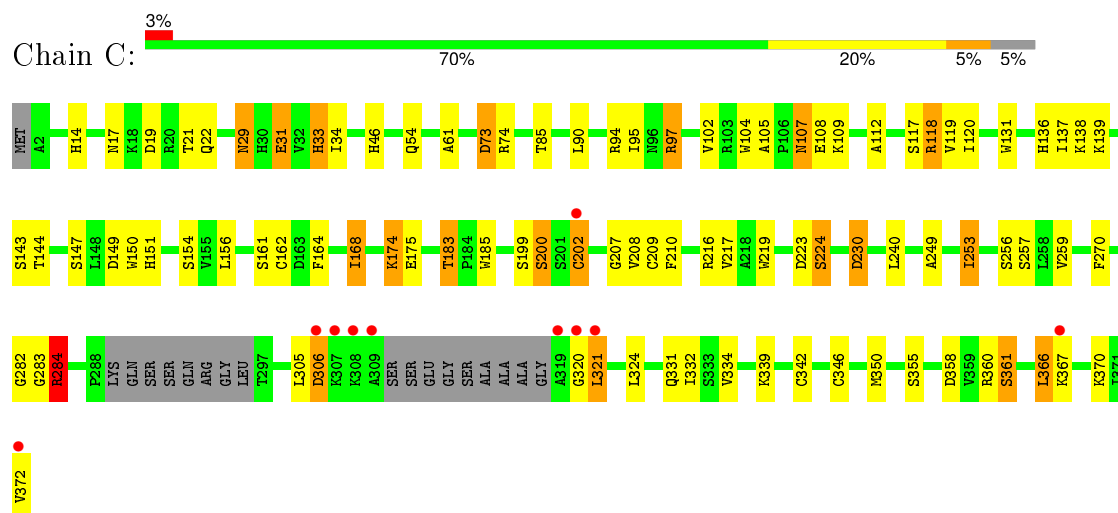
#### • Molecule 1: Actin-related protein 3



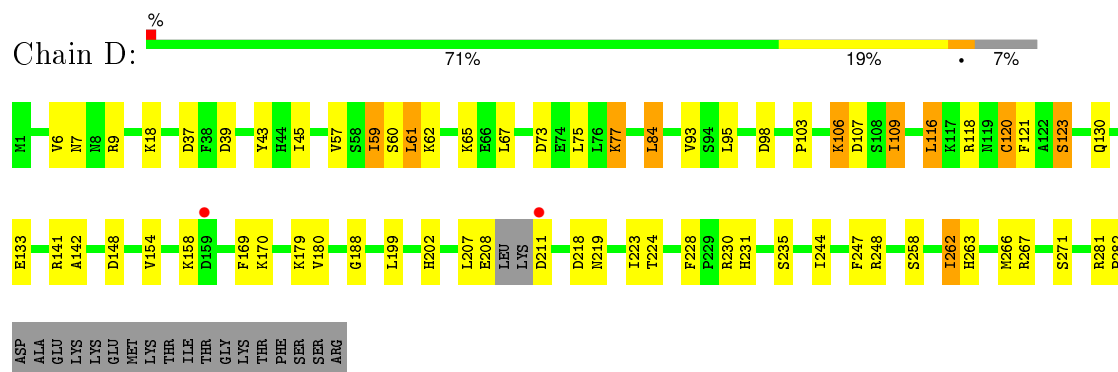
#### • Molecule 2: Actin-related protein 2



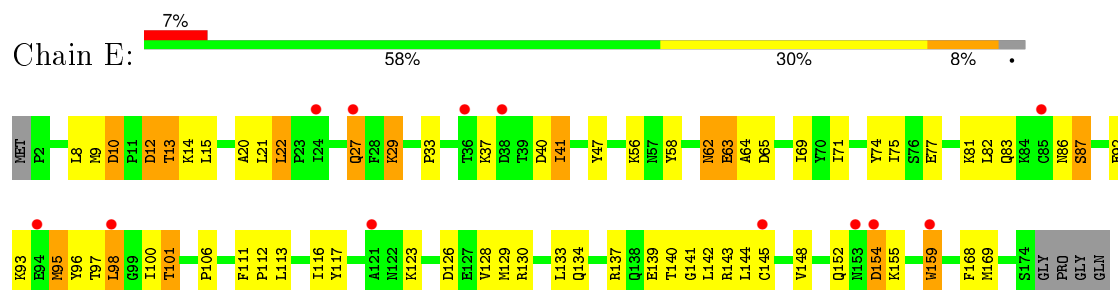
- Molecule 3: Actin-related protein 2/3 complex subunit 1B



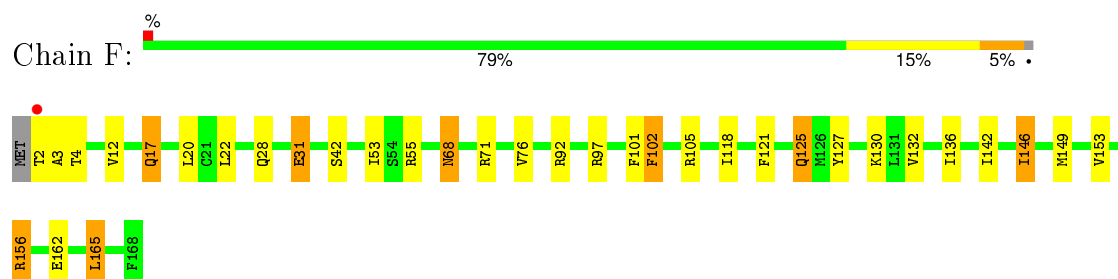
- Molecule 4: Actin-related protein 2/3 complex subunit 2



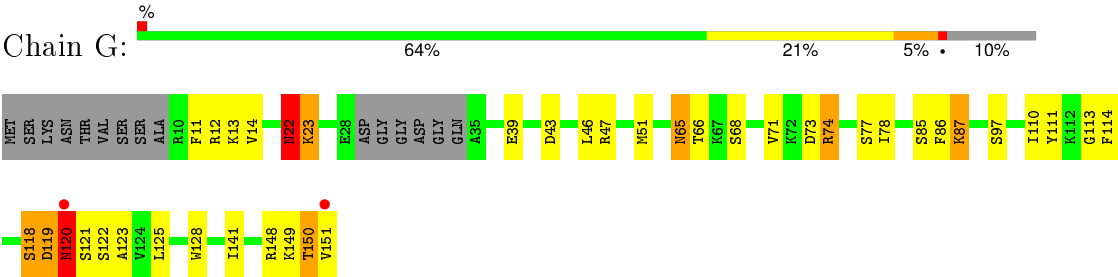
- Molecule 5: Actin-related protein 2/3 complex subunit 3



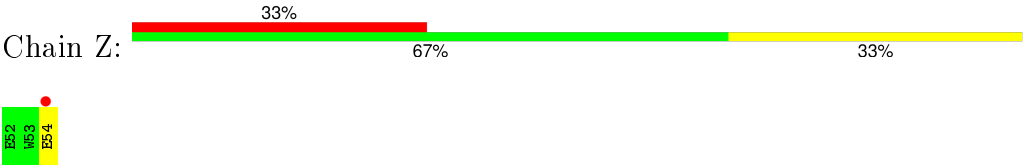
- Molecule 6: Actin-related protein 2/3 complex subunit 4



● Molecule 7: Actin-related protein 2/3 complex subunit 5



● Molecule 8: CA fragment of Bos taurus N-WASP





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.44Å 129.34Å 204.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 49.64 – 2.64	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.65) 99.1 (49.64-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.65Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.213 , 0.259 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	4317 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 86740 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	1/3247 (0.0%)	0.91	2/4406 (0.0%)
2	B	0.90	1/1596 (0.1%)	0.89	0/2157
3	C	1.04	2/2828 (0.1%)	1.03	12/3833 (0.3%)
4	D	1.04	3/2310 (0.1%)	0.96	4/3118 (0.1%)
5	E	0.84	0/1445	0.87	1/1949 (0.1%)
6	F	1.14	2/1393 (0.1%)	1.06	7/1868 (0.4%)
7	G	0.91	1/1043 (0.1%)	0.88	0/1403
8	Z	1.44	0/34	0.93	0/44
All	All	1.00	10/13896 (0.1%)	0.95	26/18778 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	CYS	CB-SG	7.64	1.95	1.82
4	D	120	CYS	CB-SG	-6.96	1.70	1.82
4	D	208	GLU	CG-CD	6.25	1.61	1.51
4	D	39	ASP	CB-CG	5.97	1.64	1.51
6	F	102	PHE	CE1-CZ	5.90	1.48	1.37
1	A	374	ARG	CG-CD	5.68	1.66	1.51
7	G	114	PHE	CE2-CZ	5.36	1.47	1.37
3	C	224	SER	CB-OG	-5.18	1.35	1.42
6	F	162	GLU	CG-CD	5.18	1.59	1.51
2	B	239	VAL	CB-CG1	-5.03	1.42	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	284	ARG	NE-CZ-NH1	7.73	124.17	120.30
5	E	98	LEU	CA-CB-CG	7.61	132.81	115.30
3	C	321	LEU	CA-CB-CG	7.54	132.65	115.30
1	A	168	ILE	CG1-CB-CG2	-6.77	96.50	111.40
4	D	73	ASP	CB-CG-OD1	6.77	124.39	118.30
3	C	97	ARG	NE-CZ-NH2	-6.59	117.00	120.30
6	F	92	ARG	NE-CZ-NH1	6.51	123.55	120.30
3	C	73	ASP	CB-CG-OD1	6.44	124.09	118.30
3	C	94	ARG	NE-CZ-NH1	6.35	123.47	120.30
4	D	207	LEU	CA-CB-CG	5.97	129.02	115.30
6	F	146	ILE	CG1-CB-CG2	-5.89	98.44	111.40
6	F	71	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	C	230	ASP	CB-CG-OD2	-5.68	113.19	118.30
6	F	156	ARG	NE-CZ-NH1	-5.65	117.47	120.30
3	C	118	ARG	NE-CZ-NH2	-5.64	117.48	120.30
4	D	98	ASP	CB-CG-OD2	-5.64	113.22	118.30
4	D	262	ILE	CG1-CB-CG2	-5.63	99.02	111.40
6	F	17	GLN	CB-CA-C	5.57	121.54	110.40
3	C	149	ASP	CB-CG-OD1	-5.34	113.50	118.30
3	C	366	LEU	CA-CB-CG	5.31	127.51	115.30
3	C	284	ARG	NE-CZ-NH2	-5.28	117.66	120.30
6	F	71	ARG	NE-CZ-NH1	5.19	122.89	120.30
6	F	97	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	93	MET	CG-SD-CE	-5.17	91.93	100.20
3	C	200	SER	N-CA-C	-5.14	97.13	111.00
3	C	230	ASP	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	282	GLY	Peptide

## 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	3166	0	3108	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1566	0	1596	52	0
3	C	2759	0	2716	57	0
4	D	2262	0	2223	54	0
5	E	1411	0	1413	52	0
6	F	1371	0	1410	32	0
7	G	1031	0	1041	26	0
8	Z	33	0	21	1	0
9	A	51	0	0	3	0
9	B	13	0	0	2	0
9	C	52	0	0	0	0
9	D	47	0	0	3	0
9	E	1	0	0	0	0
9	F	35	0	0	2	0
9	G	9	0	0	0	0
All	All	13807	0	13528	326	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 (326) 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)
3:C:183:THR:HG22	3:C:185:TRP:H	1.11	1.05
5:E:29:LYS:H	5:E:29:LYS:HD2	1.23	1.02
4:D:77:LYS:NZ	9:D:316:HOH:O	2.01	0.92
4:D:109:ILE:HD13	4:D:109:ILE:H	1.35	0.92
1:A:313:ARG:HD3	1:A:361:LYS:NZ	1.84	0.91
2:B:184:ILE:HD13	2:B:271:ILE:HD11	1.48	0.91
3:C:119:VAL:HG23	3:C:137:ILE:O	1.71	0.90
3:C:183:THR:HG22	3:C:185:TRP:N	1.86	0.89
2:B:200:ARG:HD3	9:B:405:HOH:O	1.73	0.89
1:A:71:THR:HG22	9:A:430:HOH:O	1.72	0.88
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.56	0.88
2:B:205:ASN:HD22	2:B:208:ALA:H	1.21	0.86
3:C:183:THR:CG2	3:C:185:TRP:H	1.90	0.85
3:C:107:ASN:ND2	3:C:109:LYS:H	1.74	0.85
1:A:374:ARG:CG	1:A:374:ARG:HH11	1.90	0.84
1:A:313:ARG:HD3	1:A:361:LYS:HZ2	1.39	0.83
1:A:359:LYS:N	1:A:360:PRO:HD3	1.95	0.82
2:B:184:ILE:CD1	2:B:271:ILE:HD11	2.09	0.81
5:E:10:ASP:HB2	5:E:13:THR:OG1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:ILE:HD13	3:C:46:HIS:HB2	1.62	0.80
4:D:228:PHE:H	4:D:231:HIS:HD2	1.29	0.80
6:F:4:THR:HG23	6:F:55:ARG:HE	1.45	0.80
3:C:256:SER:HB2	3:C:372:VAL:HG13	1.64	0.78
3:C:14:HIS:H	3:C:331:GLN:HE22	1.31	0.78
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.50	0.77
1:A:374:ARG:HH11	1:A:374:ARG:HG2	1.49	0.77
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.19	0.76
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.50	0.76
4:D:45:ILE:CD1	4:D:57:VAL:HG22	2.17	0.75
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.68	0.75
1:A:4:ARG:HH11	1:A:4:ARG:CG	1.99	0.75
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.67	0.74
4:D:281:ARG:HH21	6:F:125:GLN:HE22	1.36	0.74
3:C:107:ASN:HD22	3:C:107:ASN:C	1.91	0.73
2:B:290:ASP:O	2:B:292:ASP:N	2.22	0.73
4:D:211:ASP:HB3	9:D:310:HOH:O	1.89	0.72
5:E:27:GLN:HA	5:E:27:GLN:HE21	1.56	0.71
1:A:85:ASP:OD2	1:A:88:LEU:HD22	1.88	0.71
4:D:59:ILE:HD12	4:D:61:LEU:HD11	1.72	0.70
1:A:204:ILE:HD11	1:A:278:GLY:HA3	1.74	0.70
4:D:263:HIS:HD2	4:D:266:MET:CE	2.03	0.70
6:F:121:PHE:O	6:F:125:GLN:HG2	1.92	0.70
3:C:253:ILE:HD12	3:C:259:VAL:HG23	1.75	0.69
3:C:95:ILE:HD12	3:C:97:ARG:O	1.92	0.69
4:D:281:ARG:HH21	6:F:125:GLN:NE2	1.90	0.69
5:E:22:LEU:HD23	5:E:41:ILE:HD13	1.75	0.69
4:D:228:PHE:H	4:D:231:HIS:CD2	2.11	0.68
2:B:299:LYS:HE2	2:B:300:HIS:HE1	1.58	0.68
2:B:154:GLY:HA2	2:B:297:PHE:HD2	1.57	0.68
3:C:17:ASN:ND2	3:C:22:GLN:HB2	2.07	0.68
1:A:262:ILE:O	1:A:263:SER:HB3	1.94	0.68
1:A:289:ASN:HD22	1:A:291:ASP:H	1.42	0.68
6:F:76:VAL:HG13	6:F:142:ILE:CD1	2.23	0.67
1:A:200:ILE:O	1:A:204:ILE:HG12	1.94	0.67
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.77	0.67
5:E:144:LEU:O	5:E:148:VAL:HG23	1.95	0.67
3:C:199:SER:O	3:C:200:SER:C	2.34	0.67
3:C:107:ASN:HD22	3:C:109:LYS:H	1.42	0.66
5:E:29:LYS:HD2	5:E:29:LYS:N	2.05	0.66
4:D:281:ARG:NH2	6:F:125:GLN:NE2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ILE:CD1	2:B:271:ILE:CD1	2.72	0.66
2:B:163:VAL:HG22	2:B:164:THR:H	1.61	0.66
1:A:129:ILE:HD11	4:D:267:ARG:NH2	2.11	0.66
4:D:281:ARG:NH2	6:F:125:GLN:HE22	1.94	0.65
1:A:313:ARG:CD	1:A:361:LYS:NZ	2.59	0.65
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.24	0.65
5:E:27:GLN:HA	5:E:27:GLN:NE2	2.11	0.65
4:D:59:ILE:HD12	4:D:61:LEU:CD1	2.26	0.65
5:E:8:LEU:HD12	5:E:41:ILE:HD12	1.78	0.64
3:C:31:GLU:OE1	3:C:33:HIS:HE1	1.81	0.64
5:E:29:LYS:CD	5:E:29:LYS:H	1.89	0.64
5:E:74:TYR:OH	5:E:98:LEU:HD13	1.98	0.64
7:G:22:ASN:HD22	7:G:22:ASN:N	1.96	0.64
2:B:345:GLU:OE2	2:B:346:ASP:N	2.31	0.63
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.80	0.63
2:B:227:ILE:HD12	2:B:227:ILE:H	1.64	0.63
2:B:343:ARG:NE	2:B:343:ARG:H	1.97	0.63
3:C:253:ILE:HB	3:C:342:CYS:HB3	1.81	0.63
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.33	0.62
4:D:130:GLN:OE1	4:D:130:GLN:HA	1.99	0.62
6:F:76:VAL:HG13	6:F:142:ILE:HD11	1.81	0.62
5:E:74:TYR:O	5:E:77:GLU:N	2.33	0.62
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.80	0.62
3:C:253:ILE:CD1	3:C:257:SER:HB3	2.30	0.62
1:A:304:ILE:HD12	1:A:315:LEU:HB3	1.81	0.62
4:D:180:VAL:HG11	6:F:153:VAL:HG12	1.81	0.61
2:B:314:PRO:O	2:B:318:GLU:HG3	1.99	0.61
1:A:219:GLN:O	1:A:223:THR:OG1	2.18	0.61
4:D:103:PRO:HG2	4:D:109:ILE:CD1	2.31	0.61
3:C:107:ASN:HD22	3:C:108:GLU:N	1.97	0.61
7:G:120:ASN:O	7:G:123:ALA:N	2.24	0.61
4:D:59:ILE:CD1	4:D:61:LEU:HG	2.32	0.60
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.31	0.60
2:B:299:LYS:HE2	2:B:300:HIS:CE1	2.36	0.60
5:E:62:ASN:HD22	5:E:62:ASN:C	2.05	0.60
5:E:20:ALA:HB3	5:E:22:LEU:HD22	1.83	0.60
6:F:146:ILE:HA	6:F:149:MET:CE	2.32	0.60
3:C:208:VAL:HG12	3:C:219:TRP:HB3	1.84	0.60
3:C:119:VAL:CG2	3:C:137:ILE:O	2.45	0.60
5:E:14:LYS:O	5:E:21:LEU:N	2.24	0.59
5:E:71:ILE:O	5:E:75:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:HB2	1:A:265:LYS:O	2.03	0.58
1:A:343:VAL:HG11	1:A:363:ILE:HB	1.84	0.58
1:A:374:ARG:CB	1:A:374:ARG:HH11	2.17	0.58
1:A:289:ASN:ND2	1:A:291:ASP:H	2.01	0.58
4:D:103:PRO:HG2	4:D:109:ILE:HD11	1.85	0.58
2:B:154:GLY:HA2	2:B:297:PHE:CD2	2.37	0.57
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.86	0.57
3:C:168:ILE:HD11	3:C:217:VAL:HG11	1.84	0.57
3:C:144:THR:H	6:F:28:GLN:NE2	2.02	0.57
5:E:87:SER:HA	5:E:154:ASP:HA	1.85	0.57
7:G:151:VAL:O	7:G:151:VAL:HG23	2.04	0.57
1:A:84:GLU:HG2	9:A:433:HOH:O	2.04	0.57
6:F:12:VAL:HA	6:F:53:ILE:HD13	1.86	0.57
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.87	0.57
4:D:59:ILE:HD13	4:D:60:SER:N	2.20	0.57
2:B:343:ARG:N	2:B:343:ARG:NE	2.53	0.57
2:B:177:HIS:O	2:B:178:LEU:HB2	2.05	0.57
1:A:384:LEU:HB3	1:A:414:PHE:CZ	2.40	0.56
4:D:84:LEU:HD21	4:D:93:VAL:HG13	1.87	0.56
4:D:118:ARG:HD3	4:D:118:ARG:C	2.26	0.56
6:F:2:THR:HG23	6:F:3:ALA:H	1.70	0.56
1:A:370:HIS:HD2	1:A:372:MET:H	1.52	0.55
3:C:283:GLY:O	3:C:284:ARG:HB2	2.07	0.55
4:D:169:PHE:O	4:D:219:ASN:ND2	2.34	0.54
7:G:111:TYR:OH	7:G:141:ILE:HD12	2.07	0.54
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.90	0.54
1:A:262:ILE:O	1:A:263:SER:CB	2.55	0.54
4:D:75:LEU:O	4:D:75:LEU:HD23	2.07	0.54
4:D:263:HIS:CD2	4:D:266:MET:HE2	2.37	0.53
5:E:40:ASP:OD1	5:E:143:ARG:NH1	2.37	0.53
4:D:67:LEU:HD13	4:D:120:CYS:O	2.08	0.53
4:D:103:PRO:O	4:D:106:LYS:HE3	2.08	0.53
3:C:29:ASN:ND2	3:C:31:GLU:H	2.07	0.53
4:D:258:SER:O	4:D:262:ILE:HD13	2.08	0.53
1:A:271:VAL:HG12	1:A:275:ARG:HG3	1.89	0.53
7:G:113:GLY:HA3	7:G:125:LEU:HD11	1.88	0.53
7:G:43:ASP:O	7:G:47:ARG:HG3	2.09	0.53
3:C:143:SER:OG	3:C:162:CYS:HB2	2.09	0.53
1:A:219:GLN:HE22	1:A:261:ALA:H	1.56	0.53
7:G:119:ASP:OD1	7:G:120:ASN:N	2.41	0.53
1:A:123:ARG:NH1	1:A:409:ARG:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ILE:HD13	3:C:257:SER:HB3	1.90	0.52
1:A:313:ARG:CD	1:A:361:LYS:HZ1	2.23	0.52
1:A:374:ARG:CB	1:A:374:ARG:NH1	2.72	0.52
4:D:142:ALA:HB3	4:D:154:VAL:HB	1.92	0.52
1:A:104:GLU:OE1	1:A:106:GLU:HG3	2.09	0.52
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.62	0.52
7:G:65:ASN:ND2	7:G:65:ASN:N	2.57	0.52
4:D:202:HIS:HE1	4:D:218:ASP:O	1.93	0.52
6:F:2:THR:HG23	6:F:3:ALA:N	2.25	0.52
3:C:358:ASP:HB3	3:C:361:SER:OG	2.11	0.51
3:C:107:ASN:ND2	3:C:109:LYS:N	2.53	0.51
2:B:166:ILE:HD12	2:B:166:ILE:N	2.25	0.51
4:D:109:ILE:N	4:D:109:ILE:HD13	2.16	0.51
1:A:153:TRP:CD2	1:A:161:ARG:HG3	2.46	0.51
3:C:14:HIS:H	3:C:331:GLN:NE2	2.05	0.51
3:C:102:VAL:HA	3:C:112:ALA:O	2.10	0.51
5:E:65:ASP:O	5:E:69:ILE:HG12	2.11	0.51
5:E:98:LEU:HA	5:E:101:THR:CG2	2.40	0.51
2:B:343:ARG:HE	2:B:343:ARG:H	1.58	0.51
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.26	0.50
3:C:107:ASN:C	3:C:107:ASN:ND2	2.61	0.50
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.12	0.50
2:B:290:ASP:C	2:B:292:ASP:H	2.15	0.50
2:B:169:VAL:HG22	2:B:174:SER:HB3	1.92	0.50
2:B:166:ILE:CD1	2:B:166:ILE:N	2.75	0.50
1:A:260:ASN:O	1:A:264:LYS:HA	2.12	0.49
3:C:19:ASP:HB3	3:C:21:THR:HG23	1.94	0.49
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.47	0.49
5:E:10:ASP:CB	5:E:13:THR:OG1	2.56	0.49
2:B:227:ILE:H	2:B:227:ILE:CD1	2.22	0.49
6:F:146:ILE:HA	6:F:149:MET:HE2	1.95	0.49
7:G:110:ILE:HD12	7:G:128:TRP:HB3	1.94	0.49
4:D:109:ILE:H	4:D:109:ILE:CD1	2.17	0.49
3:C:253:ILE:HD11	3:C:257:SER:HB3	1.93	0.49
6:F:146:ILE:HA	6:F:149:MET:HE3	1.94	0.49
2:B:213:VAL:HA	2:B:216:ILE:HD12	1.95	0.49
5:E:133:LEU:HB3	5:E:137:ARG:HH12	1.77	0.49
3:C:117:SER:O	3:C:118:ARG:HB2	2.13	0.49
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.49
1:A:359:LYS:N	1:A:360:PRO:CD	2.72	0.49
6:F:127:TYR:HB2	6:F:130:LYS:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:SER:HB3	9:D:341:HOH:O	2.13	0.49
3:C:306:ASP:N	3:C:306:ASP:OD1	2.46	0.48
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.41	0.48
1:A:164:THR:HA	1:A:180:VAL:O	2.13	0.48
5:E:168:PHE:CE2	5:E:169:MET:CE	2.95	0.48
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.95	0.48
4:D:199:LEU:HB2	4:D:224:THR:HB	1.94	0.48
4:D:45:ILE:HD13	4:D:57:VAL:HA	1.94	0.48
3:C:210:PHE:O	3:C:339:LYS:HE2	2.14	0.48
2:B:299:LYS:HD2	2:B:341:LYS:NZ	2.27	0.48
5:E:152:GLN:O	5:E:155:LYS:HD2	2.14	0.48
5:E:69:ILE:HB	5:E:117:TYR:OH	2.14	0.47
1:A:223:THR:O	1:A:227:VAL:HG23	2.14	0.47
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.49	0.47
5:E:40:ASP:OD2	5:E:143:ARG:NH2	2.33	0.47
3:C:174:LYS:HG2	3:C:175:GLU:N	2.29	0.47
1:A:348:LYS:C	1:A:350:SER:H	2.18	0.47
2:B:257:GLU:CD	2:B:257:GLU:H	2.18	0.47
1:A:129:ILE:HD11	4:D:267:ARG:HH21	1.79	0.47
5:E:95:MET:HE2	5:E:98:LEU:HD12	1.97	0.47
2:B:299:LYS:HA	2:B:343:ARG:NE	2.29	0.47
1:A:90:GLU:OE2	1:A:129:ILE:HD12	2.15	0.47
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.62	0.47
1:A:174:VAL:HG23	1:A:175:THR:N	2.29	0.47
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.49	0.47
5:E:100:ILE:HA	5:E:134:GLN:HE21	1.80	0.46
2:B:299:LYS:O	2:B:300:HIS:ND1	2.48	0.46
2:B:193:LEU:HD23	2:B:213:VAL:HG12	1.97	0.46
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.97	0.46
1:A:168:ILE:HD13	1:A:319:ILE:CG2	2.46	0.46
3:C:223:ASP:O	3:C:224:SER:HB2	2.16	0.46
1:A:4:ARG:NH1	1:A:4:ARG:CG	2.65	0.46
4:D:45:ILE:HD12	4:D:57:VAL:HG22	1.96	0.46
5:E:69:ILE:HD12	5:E:169:MET:HE2	1.97	0.46
1:A:176:HIS:HB2	1:A:178:ILE:HD11	1.98	0.46
6:F:68:ASN:HA	6:F:68:ASN:HD22	1.36	0.45
7:G:65:ASN:HD22	7:G:65:ASN:H	1.64	0.45
7:G:68:SER:CB	7:G:71:VAL:HG12	2.45	0.45
5:E:40:ASP:CG	5:E:143:ARG:HH12	2.19	0.45
5:E:96:TYR:O	5:E:100:ILE:HG12	2.16	0.45
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:TYR:O	5:E:75:ILE:C	2.53	0.45
7:G:119:ASP:C	7:G:121:SER:H	2.20	0.45
1:A:168:ILE:CD1	1:A:319:ILE:HG23	2.47	0.45
6:F:121:PHE:O	6:F:125:GLN:CG	2.62	0.45
5:E:140:THR:O	5:E:142:LEU:N	2.50	0.45
5:E:27:GLN:CA	5:E:27:GLN:HE21	2.25	0.45
6:F:22:LEU:HA	9:F:180:HOH:O	2.17	0.45
1:A:35:ILE:HD11	1:A:60:PHE:CD1	2.51	0.45
2:B:318:GLU:HG2	2:B:344:ILE:HD12	1.98	0.45
1:A:395:HIS:HB3	1:A:407:ILE:CD1	2.47	0.45
2:B:343:ARG:CZ	2:B:343:ARG:C	2.85	0.44
5:E:9:MET:HB2	5:E:64:ALA:HB2	1.99	0.44
3:C:350:MET:HE1	9:F:250:HOH:O	2.17	0.44
4:D:6:VAL:HG12	4:D:6:VAL:O	2.16	0.44
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.16	0.44
4:D:266:MET:HB2	4:D:266:MET:HE3	1.83	0.44
1:A:353:LEU:O	1:A:354:SER:HB3	2.18	0.44
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.53	0.44
5:E:96:TYR:CZ	5:E:100:ILE:HD11	2.52	0.44
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.52	0.44
7:G:120:ASN:HD22	7:G:120:ASN:C	2.21	0.44
5:E:62:ASN:ND2	5:E:62:ASN:C	2.71	0.44
4:D:179:LYS:HE2	4:D:202:HIS:CD2	2.52	0.44
6:F:127:TYR:HB2	6:F:130:LYS:HG2	1.98	0.44
4:D:18:LYS:HD3	4:D:18:LYS:HA	1.87	0.44
6:F:76:VAL:CG1	6:F:142:ILE:CD1	2.94	0.44
3:C:210:PHE:O	3:C:339:LYS:CE	2.66	0.43
4:D:106:LYS:HA	4:D:109:ILE:HD11	2.00	0.43
6:F:156:ARG:HH11	6:F:156:ARG:HD2	1.66	0.43
2:B:200:ARG:CD	9:B:405:HOH:O	2.50	0.43
4:D:75:LEU:C	4:D:75:LEU:HD23	2.39	0.43
1:A:79:ARG:NH2	9:A:468:HOH:O	2.51	0.43
2:B:290:ASP:C	2:B:292:ASP:N	2.72	0.43
2:B:299:LYS:HG3	2:B:300:HIS:ND1	2.33	0.43
7:G:87:LYS:H	7:G:87:LYS:HE2	1.84	0.43
5:E:137:ARG:HH11	5:E:137:ARG:HG3	1.84	0.43
5:E:139:GLU:OE2	5:E:139:GLU:HA	2.17	0.43
5:E:95:MET:HG2	5:E:141:GLY:O	2.18	0.43
7:G:150:THR:HG23	7:G:151:VAL:OXT	2.18	0.43
8:Z:54:GLU:OE1	8:Z:54:GLU:HA	2.18	0.43
1:A:204:ILE:HD11	1:A:278:GLY:CA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ARG:N	2:B:343:ARG:HE	2.16	0.43
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.99	0.43
3:C:346:CYS:HA	3:C:355:SER:O	2.18	0.43
1:A:35:ILE:HD11	1:A:60:PHE:HB2	2.00	0.43
2:B:276:VAL:HB	2:B:280:GLU:HB3	2.01	0.43
4:D:244:ILE:HD12	4:D:244:ILE:HG23	1.68	0.43
1:A:329:ARG:O	1:A:330:ASP:HB2	2.19	0.43
1:A:260:ASN:HB3	1:A:265:LYS:H	1.83	0.42
7:G:119:ASP:OD1	7:G:120:ASN:ND2	2.52	0.42
6:F:20:LEU:HD21	6:F:118:ILE:HG21	2.01	0.42
1:A:35:ILE:CD1	1:A:60:PHE:HB2	2.49	0.42
2:B:263:GLU:OE2	2:B:316:ARG:NH1	2.45	0.42
7:G:119:ASP:CG	7:G:120:ASN:N	2.72	0.42
4:D:282:PRO:HB3	6:F:127:TYR:OH	2.19	0.42
2:B:170:TYR:O	2:B:171:GLU:C	2.57	0.42
5:E:128:VAL:O	5:E:129:MET:C	2.58	0.42
1:A:313:ARG:HD3	1:A:361:LYS:CE	2.49	0.42
6:F:118:ILE:N	6:F:118:ILE:HD12	2.35	0.42
3:C:73:ASP:O	3:C:74:ARG:HB2	2.18	0.42
2:B:320:GLU:HG3	7:G:11:PHE:HE1	1.84	0.42
1:A:370:HIS:HD2	1:A:372:MET:N	2.17	0.42
7:G:148:ARG:HA	7:G:148:ARG:HD2	1.82	0.42
5:E:106:PRO:HD3	5:E:111:PHE:CE1	2.55	0.42
2:B:343:ARG:O	2:B:343:ARG:HD2	2.20	0.42
3:C:162:CYS:C	3:C:164:PHE:H	2.23	0.41
2:B:339:LYS:HE2	2:B:339:LYS:HB3	1.88	0.41
3:C:147:SER:OG	3:C:207:GLY:HA2	2.20	0.41
2:B:193:LEU:HD23	2:B:213:VAL:CG1	2.49	0.41
4:D:62:LYS:NZ	4:D:148:ASP:OD2	2.47	0.41
2:B:224:GLY:O	2:B:316:ARG:HD3	2.20	0.41
1:A:69:LYS:HA	1:A:70:PRO:HD2	1.90	0.41
5:E:112:PRO:O	5:E:113:LEU:HB2	2.20	0.41
7:G:46:LEU:HD23	7:G:46:LEU:HA	1.79	0.41
3:C:105:ALA:HB2	3:C:150:TRP:CE2	2.55	0.41
3:C:209:CYS:SG	3:C:339:LYS:HE3	2.60	0.41
4:D:84:LEU:HD23	4:D:95:LEU:HD23	2.01	0.41
1:A:289:ASN:HD22	1:A:291:ASP:N	2.13	0.41
1:A:219:GLN:NE2	1:A:261:ALA:H	2.18	0.41
5:E:62:ASN:HD21	5:E:64:ALA:HB3	1.86	0.41
3:C:144:THR:O	3:C:161:SER:HB2	2.21	0.41
1:A:385:ALA:HA	1:A:390:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	2.19	0.41
1:A:116:PRO:O	1:A:117:LEU:CB	2.69	0.41
6:F:31:GLU:O	6:F:31:GLU:HG3	2.20	0.41
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.51	0.41
7:G:74:ARG:O	7:G:78:ILE:HG12	2.20	0.41
1:A:309:ILE:O	1:A:312:ARG:HG3	2.21	0.41
3:C:283:GLY:O	3:C:284:ARG:CB	2.69	0.40
7:G:125:LEU:HA	7:G:125:LEU:HD23	1.88	0.40
3:C:74:ARG:HH11	3:C:74:ARG:HD3	1.73	0.40
1:A:18:LYS:HD3	1:A:375:TYR:CD2	2.57	0.40
3:C:240:LEU:HD23	3:C:270:PHE:CD2	2.56	0.40
3:C:144:THR:H	6:F:28:GLN:HE21	1.69	0.40
6:F:132:VAL:O	6:F:136:ILE:HD12	2.22	0.40
4:D:9:ARG:HD3	4:D:9:ARG:HH11	1.74	0.40
6:F:101:PHE:O	6:F:102:PHE:HB2	2.21	0.40
4:D:59:ILE:HG22	4:D:93:VAL:HB	2.02	0.40
3:C:61:ALA:HB2	3:C:104:TRP:CG	2.57	0.40
7:G:11:PHE:C	7:G:13:LYS:H	2.24	0.40
6:F:105:ARG:HD3	6:F:105:ARG:HH11	1.74	0.40
2:B:181:ARG:NE	2:B:181:ARG:H	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/418 (93%)	360 (92%)	23 (6%)	7 (2%)	11	23
2	B	194/394 (49%)	173 (89%)	17 (9%)	4 (2%)	9	20
3	C	348/372 (94%)	322 (92%)	24 (7%)	2 (1%)	30	54
4	D	276/300 (92%)	267 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	171/178 (96%)	142 (83%)	23 (14%)	6 (4%)	4	9
6	F	165/168 (98%)	158 (96%)	7 (4%)	0	100	100
7	G	132/151 (87%)	119 (90%)	9 (7%)	4 (3%)	5	11
8	Z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	1677/1984 (84%)	1541 (92%)	113 (7%)	23 (1%)	14	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	263	SER
1	A	264	LYS
1	A	349	LEU
2	B	291	ILE
2	B	338	SER
5	E	12	ASP
2	B	171	GLU
5	E	33	PRO
7	G	120	ASN
1	A	273	TYR
2	B	331	LYS
3	C	284	ARG
5	E	87	SER
5	E	159	TRP
7	G	23	LYS
7	G	118	SER
5	E	82	LEU
5	E	97	THR
1	A	353	LEU
7	G	22	ASN
3	C	320	GLY
1	A	259	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/363 (95%)	313 (91%)	31 (9%)	12	24
2	B	171/345 (50%)	146 (85%)	25 (15%)	4	8
3	C	301/313 (96%)	274 (91%)	27 (9%)	12	24
4	D	246/264 (93%)	226 (92%)	20 (8%)	15	30
5	E	156/159 (98%)	136 (87%)	20 (13%)	5	11
6	F	154/155 (99%)	148 (96%)	6 (4%)	39	67
7	G	110/123 (89%)	91 (83%)	19 (17%)	2	5
8	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	1485/1725 (86%)	1337 (90%)	148 (10%)	9	19

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	LYS
1	A	19	LEU
1	A	35	ILE
1	A	79	ARG
1	A	88	LEU
1	A	143	VAL
1	A	154	THR
1	A	156	ARG
1	A	157	GLN
1	A	174	VAL
1	A	210	ASP
1	A	223	THR
1	A	243	ASN
1	A	255	GLN
1	A	259	ILE
1	A	268	SER
1	A	281	ILE
1	A	289	ASN
1	A	309	ILE
1	A	310	ASP
1	A	311	VAL
1	A	329	ARG
1	A	333	ARG
1	A	335	LEU
1	A	340	LYS
1	A	353	LEU

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Mol	Chain	Res	Type
1	A	359	LYS
1	A	361	LYS
1	A	374	ARG
1	A	407	ILE
2	B	155	VAL
2	B	174	SER
2	B	175	LEU
2	B	177	HIS
2	B	181	ARG
2	B	182	LEU
2	B	183	ASP
2	B	184	ILE
2	B	191	ARG
2	B	199	LEU
2	B	207	SER
2	B	220	LEU
2	B	227	ILE
2	B	228	GLU
2	B	240	LEU
2	B	272	ASN
2	B	276	VAL
2	B	294	ARG
2	B	298	TYR
2	B	304	SER
2	B	326	LEU
2	B	336	LYS
2	B	342	ILE
2	B	343	ARG
2	B	345	GLU
3	C	29	ASN
3	C	31	GLU
3	C	33	HIS
3	C	54	GLN
3	C	85	THR
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	138	LYS
3	C	139	LYS
3	C	154	SER
3	C	168	ILE
3	C	174	LYS

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Mol	Chain	Res	Type
3	C	183	THR
3	C	202	CYS
3	C	253	ILE
3	C	284	ARG
3	C	305	LEU
3	C	306	ASP
3	C	321	LEU
3	C	324	LEU
3	C	334	VAL
3	C	360	ARG
3	C	361	SER
3	C	366	LEU
3	C	367	LYS
3	C	370	LYS
4	D	7	ASN
4	D	59	ILE
4	D	61	LEU
4	D	65	LYS
4	D	77	LYS
4	D	84	LEU
4	D	106	LYS
4	D	107	ASP
4	D	109	ILE
4	D	116	LEU
4	D	121	PHE
4	D	123	SER
4	D	133	GLU
4	D	141	ARG
4	D	158	LYS
4	D	170	LYS
4	D	230	ARG
4	D	235	SER
4	D	248	ARG
4	D	271	SER
5	E	10	ASP
5	E	13	THR
5	E	22	LEU
5	E	27	GLN
5	E	29	LYS
5	E	37	LYS
5	E	41	ILE
5	E	56	LYS

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Mol	Chain	Res	Type
5	E	62	ASN
5	E	63	GLU
5	E	81	LYS
5	E	83	GLN
5	E	86	ASN
5	E	92	GLU
5	E	93	LYS
5	E	95	MET
5	E	101	THR
5	E	123	LYS
5	E	145	CYS
5	E	154	ASP
6	F	17	GLN
6	F	31	GLU
6	F	42	SER
6	F	68	ASN
6	F	125	GLN
6	F	165	LEU
7	G	12	ARG
7	G	14	VAL
7	G	22	ASN
7	G	23	LYS
7	G	39	GLU
7	G	65	ASN
7	G	66	THR
7	G	73	ASP
7	G	74	ARG
7	G	77	SER
7	G	85	SER
7	G	87	LYS
7	G	97	SER
7	G	118	SER
7	G	119	ASP
7	G	120	ASN
7	G	122	SER
7	G	149	LYS
7	G	150	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	144	GLN
1	A	219	GLN
1	A	255	GLN
1	A	289	ASN
1	A	305	GLN
1	A	318	ASN
1	A	370	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	28	ASN
3	C	29	ASN
3	C	33	HIS
3	C	54	GLN
3	C	65	ASN
3	C	107	ASN
3	C	129	ASN
3	C	136	HIS
3	C	303	GLN
3	C	331	GLN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	E	27	GLN
5	E	62	ASN
5	E	102	ASN
5	E	138	GLN
5	E	167	GLN
6	F	28	GLN
6	F	68	ASN
6	F	125	GLN
7	G	65	ASN
7	G	96	GLN
7	G	120	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	396/418 (94%)	-0.01	7 (1%) 71 70	25, 48, 95, 106	0
2	B	196/394 (49%)	0.44	18 (9%) 11 9	30, 60, 104, 110	0
3	C	354/372 (95%)	-0.15	10 (2%) 56 55	26, 42, 81, 116	0
4	D	280/300 (93%)	-0.19	2 (0%) 89 89	25, 42, 66, 89	0
5	E	173/178 (97%)	0.49	12 (6%) 20 17	47, 70, 100, 112	0
6	F	167/168 (99%)	-0.15	1 (0%) 90 91	26, 36, 52, 78	0
7	G	136/151 (90%)	0.00	2 (1%) 76 75	30, 59, 82, 87	0
8	Z	3/3 (100%)	1.20	1 (33%) 0 0	73, 73, 83, 84	0
All	All	1705/1984 (85%)	0.03	53 (3%) 52 51	25, 48, 94, 116	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173	PHE	7.1
3	C	306	ASP	4.1
2	B	183	ASP	4.0
5	E	94	GLU	3.9
2	B	276	VAL	3.9
4	D	211	ASP	3.9
2	B	182	LEU	3.7
5	E	38	ASP	3.6
3	C	307	LYS	3.5
2	B	181	ARG	3.4
3	C	308	LYS	3.2
2	B	172	GLY	3.1
5	E	36	THR	3.1
2	B	174	SER	3.0
7	G	120	ASN	3.0
1	A	349	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	343	ARG	3.0
5	E	85	CYS	3.0
2	B	281	LEU	2.9
1	A	268	SER	2.9
5	E	153	ASN	2.9
5	E	24	ILE	2.8
3	C	319	ALA	2.8
1	A	350	SER	2.8
2	B	341	LYS	2.8
4	D	159	ASP	2.7
2	B	184	ILE	2.7
7	G	151	VAL	2.7
2	B	154	GLY	2.7
2	B	300	HIS	2.6
1	A	351	GLU	2.6
5	E	159	TRP	2.6
2	B	171	GLU	2.6
6	F	2	THR	2.6
1	A	209	ARG	2.5
5	E	98	LEU	2.4
3	C	320	GLY	2.4
2	B	325	TYR	2.4
8	Z	54	GLU	2.4
2	B	345	GLU	2.4
3	C	321	LEU	2.3
3	C	367	LYS	2.3
3	C	309	ALA	2.3
5	E	154	ASP	2.3
3	C	372	VAL	2.3
5	E	121	ALA	2.2
2	B	342	ILE	2.1
1	A	172	ASP	2.1
5	E	145	CYS	2.1
1	A	352	GLU	2.1
5	E	27	GLN	2.1
3	C	202	CYS	2.1
2	B	274	GLU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.