



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:12 AM UTC

PDB ID : 3RSE / pdb_00003rse
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

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

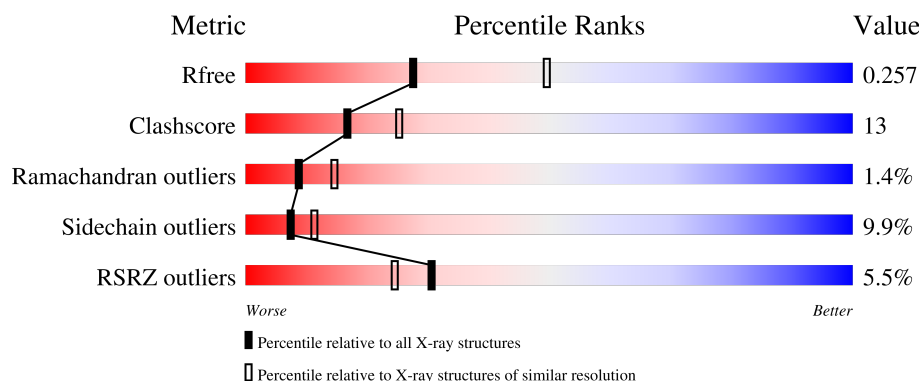
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	418	5% 68% 21% 5% • 5%
2	B	394	6% 31% 15% • 50%
3	C	372	4% 66% 25% • • 5%
4	D	300	2% 72% 18% • 7%
5	E	178	10% 56% 32% 9% •

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Mol	Chain	Length	Quality of chain
6	F	168	% 76% 19% . ..
7	G	151	6% 64% 19% 5% 10%
8	Z	3	67% 33%

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.

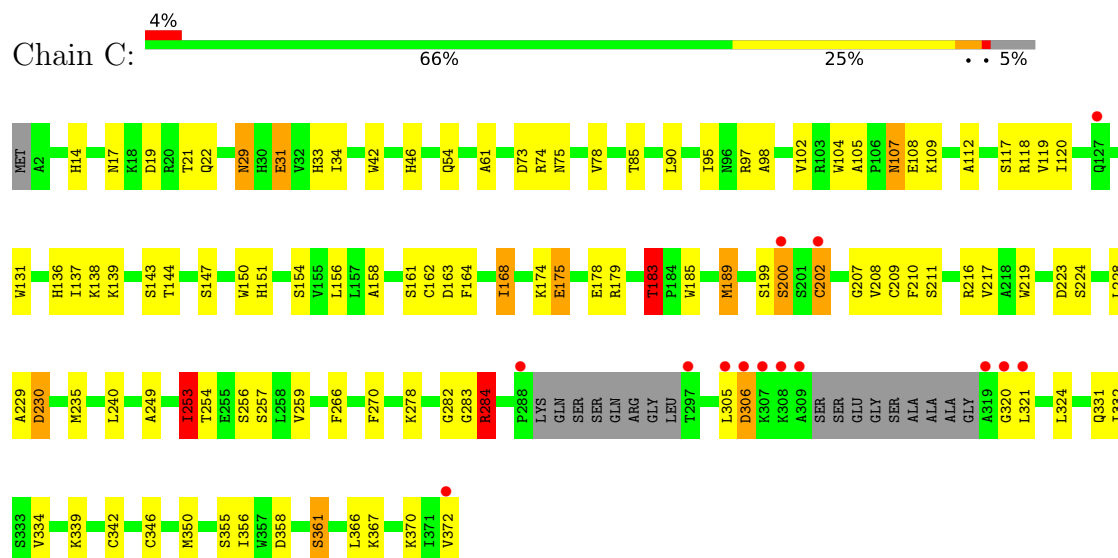
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Z	3	Total	C	N	O	0	0	0
			33	21	4	8			

- Molecule 9 is water.

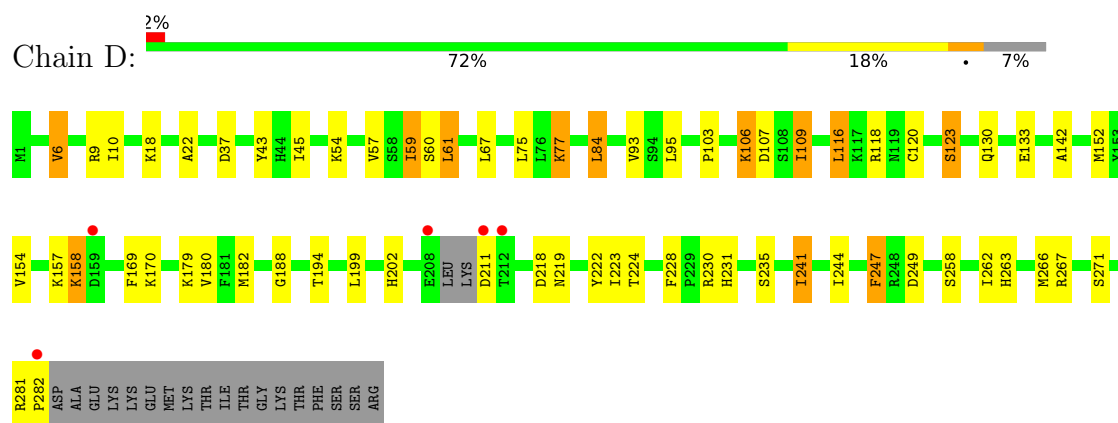
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	51	Total	O	0	0
			51	51		
9	B	13	Total	O	0	0
			13	13		
9	C	52	Total	O	0	0
			52	52		
9	D	47	Total	O	0	0
			47	47		
9	E	1	Total	O	0	0
			1	1		
9	F	35	Total	O	0	0
			35	35		
9	G	9	Total	O	0	0
			9	9		

MET
THR
ARG
GLN
GLU
TVR
GLN
GLY
LVS
VAL
ARG
VAL
LEU
GLU
LVS
LEU
GLY
VAL
THR
VAL
ARG

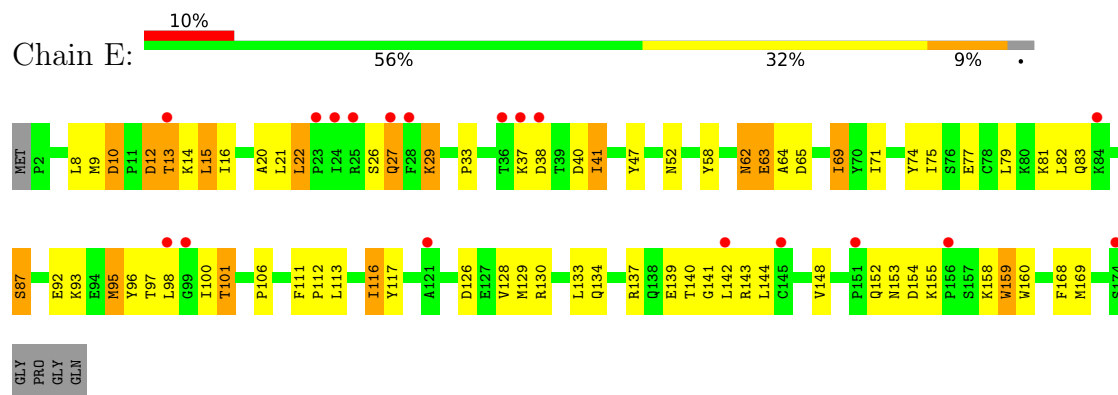
• Molecule 3: Actin-related protein 2/3 complex subunit 1B



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

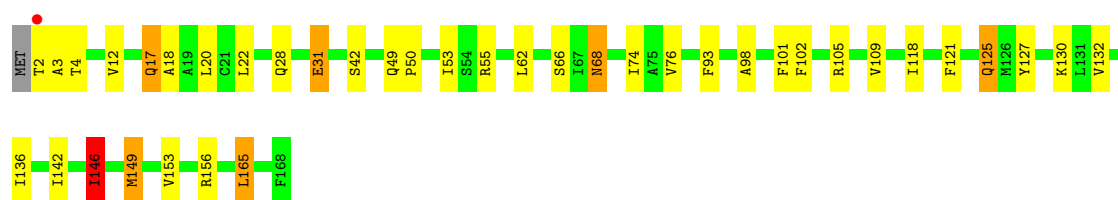


• Molecule 5: Actin-related protein 2/3 complex subunit 3



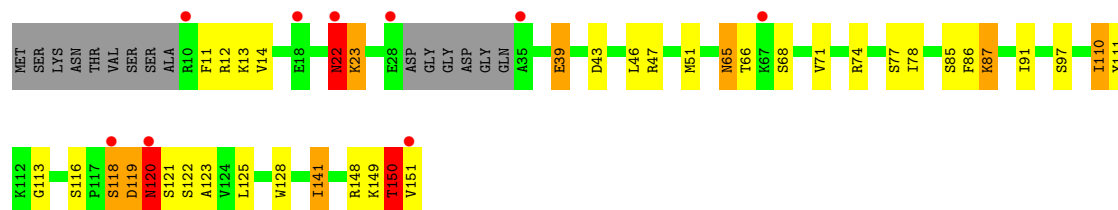
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:  %



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

Chain G:  %



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

Chain Z:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.44Å 129.34Å 204.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.65) 99.4 (50.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.259 0.213 , 0.257	Depositor DCC
R_{free} test set	4355 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13807	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 i

5.1 Standard geometry i

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	1.19	6/3247 (0.2%)	1.24	17/4406 (0.4%)
2	B	1.07	1/1596 (0.1%)	1.14	0/2157
3	C	1.26	5/2828 (0.2%)	1.31	18/3833 (0.5%)
4	D	1.26	6/2310 (0.3%)	1.21	4/3118 (0.1%)
5	E	0.98	0/1445	1.20	6/1949 (0.3%)
6	F	1.37	4/1393 (0.3%)	1.30	4/1868 (0.2%)
7	G	1.10	0/1043	1.21	6/1403 (0.4%)
8	Z	1.05	0/34	1.08	0/44
All	All	1.20	22/13896 (0.2%)	1.24	55/18778 (0.3%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	LEU	CA-CB	7.49	1.63	1.54
3	C	202	CYS	CA-C	6.57	1.60	1.52
1	A	309	ILE	CA-CB	6.27	1.61	1.54
6	F	74	ILE	C-O	6.19	1.30	1.24
4	D	22	ALA	CA-CB	-6.05	1.43	1.53
4	D	6	VAL	C-O	-5.90	1.16	1.24
4	D	241	ILE	CA-CB	5.74	1.61	1.54
3	C	158	ALA	CA-CB	-5.72	1.45	1.53
4	D	249	ASP	N-CA	-5.69	1.39	1.46
6	F	98	ALA	CA-CB	-5.55	1.44	1.53
3	C	211	SER	N-CA	5.52	1.53	1.45
1	A	262	ILE	CA-CB	5.50	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	222	TYR	CA-C	-5.49	1.46	1.52
1	A	87	ASP	C-O	-5.41	1.17	1.24
6	F	50	PRO	C-O	-5.38	1.17	1.23
6	F	18	ALA	CA-CB	-5.29	1.45	1.53
2	B	189	ILE	C-O	-5.25	1.18	1.24
4	D	152	MET	CA-C	5.18	1.58	1.52
1	A	125	TYR	C-O	5.15	1.30	1.24
3	C	78	VAL	CA-CB	-5.14	1.48	1.54
1	A	28	GLN	N-CA	-5.10	1.39	1.46
3	C	42	TRP	C-O	-5.10	1.17	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	200	SER	N-CA-C	-9.30	97.13	110.24
1	A	67	ILE	N-CA-C	8.38	118.40	110.53
1	A	289	ASN	CA-C-N	-8.37	111.00	120.04
1	A	289	ASN	C-N-CA	-8.37	111.00	120.04
5	E	26	SER	N-CA-C	7.93	121.53	109.23
1	A	373	GLN	N-CA-C	7.58	120.20	111.11
3	C	183	THR	CA-C-N	-7.28	112.30	119.87
3	C	183	THR	C-N-CA	-7.28	112.30	119.87
4	D	6	VAL	CB-CA-C	-6.99	102.87	112.24
4	D	6	VAL	N-CA-C	6.88	118.50	111.00
6	F	109	VAL	N-CA-C	-6.84	100.70	109.80
6	F	17	GLN	CB-CA-C	6.79	121.54	110.88
6	F	146	ILE	N-CA-C	-6.74	103.74	110.62
5	E	153	ASN	N-CA-C	6.43	119.83	109.79
7	G	141	ILE	CB-CA-C	-6.15	103.74	112.22
6	F	149	MET	N-CA-C	-6.11	104.70	111.36
7	G	116	SER	CA-C-N	-6.07	113.53	119.78
7	G	116	SER	C-N-CA	-6.07	113.53	119.78
5	E	69	ILE	CB-CA-C	-6.01	104.28	111.97
1	A	143	VAL	N-CA-CB	5.91	116.97	110.53
3	C	75	ASN	N-CA-C	5.82	118.41	110.55
3	C	230	ASP	N-CA-CB	5.78	119.65	110.57
7	G	150	THR	N-CA-C	5.78	118.64	110.14
4	D	194	THR	N-CA-C	5.71	119.50	112.54
1	A	155	SER	CA-C-N	5.69	127.90	120.28
1	A	155	SER	C-N-CA	5.69	127.90	120.28
3	C	253	ILE	CB-CA-C	5.68	117.94	110.84
1	A	166	THR	CA-C-N	-5.67	115.74	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	THR	C-N-CA	-5.67	115.74	123.12
1	A	84	GLU	N-CA-C	-5.58	107.02	113.88
3	C	278	LYS	N-CA-C	5.57	117.86	109.23
3	C	189	MET	CA-C-N	-5.56	114.05	119.78
3	C	189	MET	C-N-CA	-5.56	114.05	119.78
3	C	163	ASP	N-CA-C	-5.52	106.86	113.21
3	C	202	CYS	N-CA-C	5.48	117.46	108.52
5	E	38	ASP	N-CA-C	5.43	119.60	112.92
3	C	284	ARG	N-CA-C	-5.41	99.28	110.80
5	E	15	LEU	N-CA-C	5.37	118.48	107.69
3	C	266	PHE	CA-C-N	5.36	125.26	119.85
3	C	266	PHE	C-N-CA	5.36	125.26	119.85
1	A	368	ILE	CB-CA-C	-5.35	104.49	110.96
1	A	374	ARG	CB-CG-CD	5.29	123.48	111.30
3	C	230	ASP	N-CA-C	5.29	117.59	109.07
3	C	98	ALA	N-CA-C	5.26	118.10	110.42
1	A	35	ILE	CA-CB-CG1	5.22	119.27	110.40
1	A	189	CYS	N-CA-C	5.21	119.73	113.17
4	D	247	PHE	N-CA-C	5.17	117.32	111.11
7	G	110	ILE	CB-CA-C	-5.15	105.29	112.04
1	A	143	VAL	N-CA-C	5.12	115.65	108.89
7	G	39	GLU	N-CA-C	5.12	116.86	111.28
3	C	229	ALA	CA-C-N	-5.07	116.00	123.00
3	C	229	ALA	C-N-CA	-5.07	116.00	123.00
5	E	52	ASN	N-CA-C	5.07	118.23	111.75
1	A	141	ILE	CB-CA-C	-5.02	103.64	110.96
1	A	239	VAL	N-CA-CB	5.00	116.41	110.55

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	70	0
2	B	1566	0	1596	57	0
3	C	2759	0	2716	66	0
4	D	2262	0	2223	57	0
5	E	1411	0	1413	53	0
6	F	1371	0	1410	33	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	3	0
9	G	9	0	0	0	0
All	All	13807	0	13528	348	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 13.

All (348) 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
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.07	0.89
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: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
1:A:313:ARG:HD3	1:A:361:LYS:HZ2	1.45	0.79
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
3:C:107:ASN:C	3:C:107:ASN:HD22	1.91	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: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
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
1:A:85:ASP:OD2	1:A:88:LEU:HD22	1.88	0.71
5:E:27:GLN:HE21	5:E:27:GLN:HA	1.56	0.71
3:C:199:SER:O	3:C:200:SER:C	2.34	0.71
4:D:263:HIS:HD2	4:D:266:MET:CE	2.03	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
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
1:A:10:VAL:HG11	1:A:93:MET:HE1	1.75	0.68
2:B:154:GLY:HA2	2:B:297:PHE:HD2	1.57	0.68
2:B:299:LYS:HE2	2:B:300:HIS:HE1	1.58	0.68
3:C:17:ASN:ND2	3:C:22:GLN:HB2	2.07	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
5:E:95:MET:HE2	5:E:98:LEU:HD12	1.77	0.66
3:C:107:ASN:HD22	3:C:109:LYS:H	1.42	0.66
1:A:262:ILE:O	1:A:263:SER:HB3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:163:VAL:HG22	2:B:164:THR:H	1.61	0.66
2:B:184:ILE:CD1	2:B:271:ILE:CD1	2.72	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:62:ASN:C	5:E:62:ASN:HD22	2.05	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:H	5:E:29:LYS:CD	1.89	0.64
5:E:74:TYR:OH	5:E:98:LEU:HD13	1.98	0.64
7:G:22:ASN:N	7:G:22:ASN:HD22	1.96	0.64
2:B:345:GLU:OE2	2:B:346:ASP:N	2.31	0.63
2:B:227:ILE:HD12	2:B:227:ILE:H	1.64	0.63
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.80	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
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.64	0.62
4:D:130:GLN:OE1	4:D:130:GLN:HA	1.99	0.62
5:E:27:GLN:HA	5:E:27:GLN:NE2	2.11	0.62
6:F:76:VAL:HG13	6:F:142:ILE:HD11	1.81	0.62
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.80	0.62
5:E:74:TYR:O	5:E:77:GLU:N	2.33	0.62
1:A:304:ILE:HD12	1:A:315:LEU:HB3	1.81	0.62
3:C:253:ILE:CD1	3:C:257:SER:HB3	2.30	0.62
4:D:180:VAL:HG11	6:F:153:VAL:HG12	1.81	0.61
1:A:219:GLN:O	1:A:223:THR:OG1	2.18	0.61
2:B:314:PRO:O	2:B:318:GLU:HG3	1.99	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:118:ARG:HD3	4:D:118:ARG:C	2.26	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
6:F:146:ILE:HA	6:F:149:MET:HE2	1.83	0.60
5:E:20:ALA:HB3	5:E:22:LEU:HD22	1.83	0.60
3:C:208:VAL:HG12	3:C:219:TRP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:146:ILE:HA	6:F:149:MET:CE	2.32	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
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:HH11	1:A:374:ARG:CB	2.17	0.58
1:A:289:ASN:ND2	1:A:291:ASP:H	2.01	0.58
1:A:313:ARG:CD	1:A:361:LYS:HZ1	2.17	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
3:C:168:ILE:HD11	3:C:217:VAL:HG11	1.84	0.57
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.86	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:HG23	7:G:151:VAL:O	2.04	0.57
1:A:84:GLU:HG2	9:A:433:HOH:O	2.04	0.57
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.87	0.57
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.40	0.57
6:F:12:VAL:HA	6:F:53:ILE:HD13	1.86	0.57
2:B:343:ARG:NE	2:B:343:ARG:N	2.53	0.57
4:D:59:ILE:HD13	4:D:60:SER:N	2.20	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
3:C:107:ASN:ND2	3:C:107:ASN:C	2.61	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
2:B:290:ASP:C	2:B:292:ASP:H	2.15	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:HD23	4:D:75:LEU:O	2.07	0.54
4:D:67:LEU:HD13	4:D:120:CYS:O	2.08	0.53
5:E:40:ASP:OD1	5:E:143:ARG:NH1	2.37	0.53
1:A:271:VAL:HG12	1:A:275:ARG:HG3	1.89	0.53
3:C:29:ASN:ND2	3:C:31:GLU:H	2.07	0.53
4:D:103:PRO:O	4:D:106:LYS:HE3	2.08	0.53
4:D:258:SER:O	4:D:262:ILE:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:113:GLY:HA3	7:G:125:LEU:HD11	1.88	0.53
3:C:143:SER:OG	3:C:162:CYS:HB2	2.09	0.53
7:G:43:ASP:O	7:G:47:ARG:HG3	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
3:C:253:ILE:HD13	3:C:257:SER:HB3	1.90	0.52
1:A:104:GLU:OE1	1:A:106:GLU:HG3	2.09	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
4:D:263:HIS:HA	4:D:266:MET:HE2	1.90	0.52
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.62	0.52
4:D:202:HIS:HE1	4:D:218:ASP:O	1.93	0.52
7:G:65:ASN:N	7:G:65:ASN:ND2	2.57	0.52
1:A:348:LYS:C	1:A:350:SER:H	2.18	0.52
6:F:2:THR:HG23	6:F:3:ALA:N	2.25	0.52
2:B:257:GLU:H	2:B:257:GLU:CD	2.18	0.52
3:C:358:ASP:HB3	3:C:361:SER:OG	2.11	0.51
2:B:166:ILE:HD12	2:B:166:ILE:N	2.25	0.51
3:C:107:ASN:ND2	3:C:109:LYS:N	2.53	0.51
1:A:153:TRP:CD2	1:A:161:ARG:HG3	2.46	0.51
3:C:185:TRP:HE3	3:C:235:MET:HE2	1.75	0.51
4:D:109:ILE:HD13	4:D:109:ILE:N	2.16	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
1:A:313:ARG:HD3	1:A:361:LYS:HZ1	1.73	0.51
2:B:343:ARG:H	2:B:343:ARG:HE	1.58	0.51
3:C:254:THR:HG1	3:C:372:VAL:HG22	1.76	0.50
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.26	0.50
2:B:169:VAL:HG22	2:B:174:SER:HB3	1.92	0.50
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.12	0.50
2:B:166:ILE:N	2:B:166:ILE:CD1	2.75	0.50
5:E:40:ASP:CG	5:E:143:ARG:HH12	2.19	0.50
5:E:74:TYR:O	5:E:75:ILE:C	2.53	0.50
7:G:119:ASP:C	7:G:121:SER:H	2.20	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
2:B:227:ILE:H	2:B:227:ILE:CD1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:ASP:CB	5:E:13:THR:OG1	2.56	0.49
2:B:343:ARG:C	2:B:343:ARG:CZ	2.85	0.49
7:G:110:ILE:HD12	7:G:128:TRP:HB3	1.94	0.49
2:B:213:VAL:HA	2:B:216:ILE:HD12	1.95	0.49
3:C:117:SER:O	3:C:118:ARG:HB2	2.13	0.49
3:C:253:ILE:HD11	3:C:257:SER:HB3	1.93	0.49
4:D:109:ILE:H	4:D:109:ILE:CD1	2.17	0.49
5:E:62:ASN:C	5:E:62:ASN:ND2	2.71	0.49
5:E:133:LEU:HB3	5:E:137:ARG:HH12	1.77	0.49
7:G:120:ASN:C	7:G:120:ASN:HD22	2.21	0.49
1:A:359:LYS:N	1:A:360:PRO:CD	2.72	0.49
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.49
4:D:123:SER:HB3	9:D:341:HOH:O	2.13	0.49
6:F:127:TYR:HB2	6:F:130:LYS:CG	2.43	0.49
3:C:306:ASP:N	3:C:306:ASP:OD1	2.46	0.48
1:A:164:THR:HA	1:A:180:VAL:O	2.13	0.48
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.41	0.48
5:E:16:ILE:HG13	5:E:129:MET:HE3	1.94	0.48
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.95	0.48
4:D:182:MET:HE2	4:D:223:ILE:HG13	1.95	0.48
4:D:75:LEU:HD23	4:D:75:LEU:C	2.39	0.48
4:D:199:LEU:HB2	4:D:224:THR:HB	1.94	0.48
3:C:210:PHE:O	3:C:339:LYS:HE2	2.14	0.48
4:D:45:ILE:HD13	4:D:57:VAL:HA	1.94	0.48
2:B:299:LYS:HD2	2:B:341:LYS:NZ	2.27	0.48
2:B:290:ASP:C	2:B:292:ASP:N	2.72	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
3:C:183:THR:HB	3:C:189:MET:HE1	1.95	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:129:ILE:HD11	4:D:267:ARG:HH21	1.79	0.47
5:E:128:VAL:O	5:E:129:MET:C	2.58	0.47
1:A:90:GLU:OE2	1:A:129:ILE:HD12	2.15	0.47
2:B:299:LYS:HA	2:B:343:ARG:NE	2.29	0.47
1:A:174:VAL:HG23	1:A:175:THR:N	2.29	0.47
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.62	0.47
3:C:350:MET:HE3	9:F:176:HOH:O	2.15	0.47
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ILE:HA	5:E:134:GLN:HE21	1.80	0.46
2:B:193:LEU:HD23	2:B:213:VAL:HG12	1.97	0.46
2:B:299:LYS:O	2:B:300:HIS:ND1	2.48	0.46
7:G:119:ASP:CG	7:G:120:ASN:N	2.72	0.46
2:B:170:TYR:O	2:B:171:GLU:C	2.57	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:162:CYS:C	3:C:164:PHE:H	2.23	0.46
3:C:156:LEU:HD21	3:C:189:MET:HE2	1.98	0.46
3:C:223:ASP:O	3:C:224:SER:HB2	2.16	0.46
1:A:4:ARG:CG	1:A:4:ARG:NH1	2.65	0.46
1:A:176:HIS:HB2	1:A:178:ILE:HD11	1.98	0.46
4:D:45:ILE:HD12	4:D:57:VAL:HG22	1.96	0.46
6:F:68:ASN:HD22	6:F:68:ASN:HA	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
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.99	0.45
5:E:96:TYR:O	5:E:100:ILE:HG12	2.16	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
7:G:11:PHE:C	7:G:13:LYS:H	2.24	0.45
1:A:35:ILE:HD11	1:A:60:PHE:CD1	2.51	0.45
5:E:27:GLN:HE21	5:E:27:GLN:CA	2.25	0.45
6:F:22:LEU:HA	9:F:180:HOH:O	2.17	0.45
1:A:395:HIS:HB3	1:A:407:ILE:CD1	2.47	0.45
2:B:318:GLU:HG2	2:B:344:ILE:HD12	1.98	0.45
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.16	0.44
4:D:6:VAL:O	4:D:6:VAL:HG12	2.16	0.44
5:E:9:MET:HB2	5:E:64:ALA:HB2	1.99	0.44
1:A:353:LEU:O	1:A:354:SER:HB3	2.18	0.44
2:B:165:HIS:C	2:B:166:ILE:HD12	2.42	0.44
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.52	0.44
5:E:96:TYR:CZ	5:E:100:ILE:HD11	2.52	0.44
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.53	0.44
4:D:179:LYS:HE2	4:D:202:HIS:CD2	2.52	0.44
4:D:18:LYS:HD3	4:D:18:LYS:HA	1.87	0.44
6:F:127:TYR:HB2	6:F:130:LYS:HG2	1.98	0.44
3:C:199:SER:C	3:C:200:SER:O	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:79:ARG:NH2	9:A:468:HOH:O	2.51	0.43
2:B:299:LYS:HG3	2:B:300:HIS:ND1	2.33	0.43
5:E:137:ARG:HG3	5:E:137:ARG:HH11	1.84	0.43
5:E:139:GLU:OE2	5:E:139:GLU:HA	2.17	0.43
7:G:87:LYS:HE2	7:G:87:LYS:H	1.84	0.43
3:C:228:LEU:C	3:C:228:LEU:HD23	2.44	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
4:D:263:HIS:HD2	4:D:266:MET:HE1	1.83	0.43
8:Z:54:GLU:HA	8:Z:54:GLU:OE1	2.18	0.43
1:A:204:ILE:HD11	1:A:278:GLY:CA	2.47	0.43
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.99	0.43
2:B:343:ARG:N	2:B:343:ARG:HE	2.16	0.43
3:C:346:CYS:HA	3:C:355:SER:O	2.18	0.43
4:D:157:LYS:O	4:D:158:LYS:C	2.62	0.43
1:A:35:ILE:HD11	1:A:60:PHE:HB2	2.00	0.43
1:A:329:ARG:O	1:A:330:ASP:HB2	2.19	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:260:ASN:HB3	1:A:265:LYS:H	1.83	0.42
6:F:20:LEU:HD21	6:F:118:ILE:HG21	2.01	0.42
7:G:119:ASP:OD1	7:G:120:ASN:ND2	2.52	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
4:D:282:PRO:HB3	6:F:127:TYR:OH	2.19	0.42
1:A:313:ARG:HD3	1:A:361:LYS:CE	2.49	0.42
2:B:320:GLU:HG3	7:G:11:PHE:HE1	1.84	0.42
2:B:330:LEU:O	2:B:331:LYS:C	2.63	0.42
3:C:73:ASP:O	3:C:74:ARG:HB2	2.18	0.42
6:F:118:ILE:N	6:F:118:ILE:HD12	2.35	0.42
1:A:370:HIS:HD2	1:A:372:MET:N	2.17	0.42
3:C:29:ASN:C	3:C:29:ASN:HD22	2.28	0.42
5:E:106:PRO:HD3	5:E:111:PHE:CE1	2.55	0.42
7:G:148:ARG:HD2	7:G:148:ARG:HA	1.82	0.42
2:B:343:ARG:HD2	2:B:343:ARG:O	2.20	0.42
3:C:178:GLU:O	3:C:179:ARG:C	2.63	0.42
2:B:339:LYS:HE2	2:B:339:LYS:HB3	1.88	0.41
2:B:345:GLU:CD	2:B:345:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:310:TYR:O	2:B:311:PRO:C	2.62	0.41
1:A:69:LYS:HA	1:A:70:PRO:HD2	1.90	0.41
2:B:224:GLY:O	2:B:316:ARG:HD3	2.20	0.41
1:A:111:LEU:HD23	1:A:111:LEU:C	2.45	0.41
5:E:112:PRO:O	5:E:113:LEU:HB2	2.20	0.41
5:E:158:LYS:C	5:E:160:TRP:H	2.28	0.41
1:A:193:ILE:C	1:A:195:ILE:H	2.28	0.41
3:C:105:ALA:HB2	3:C:150:TRP:CE2	2.55	0.41
7:G:46:LEU:HD23	7:G:46:LEU:HA	1.79	0.41
3:C:209:CYS:SG	3:C:339:LYS:HE3	2.60	0.41
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	2.19	0.41
1:A:219:GLN:NE2	1:A:261:ALA:H	2.18	0.41
1:A:289:ASN:HD22	1:A:291:ASP:N	2.13	0.41
1:A:385:ALA:HA	1:A:390:PHE:CG	2.56	0.41
3:C:144:THR:O	3:C:161:SER:HB2	2.21	0.41
4:D:84:LEU:HD23	4:D:95:LEU:HD23	2.01	0.41
5:E:62:ASN:HD21	5:E:64:ALA:HB3	1.86	0.41
1:A:116:PRO:O	1:A:117:LEU:CB	2.69	0.41
1:A:309:ILE:O	1:A:312:ARG:HG3	2.21	0.41
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.51	0.41
3:C:350:MET:HE1	9:F:250:HOH:O	2.20	0.41
6:F:31:GLU:O	6:F:31:GLU:HG3	2.20	0.41
7:G:74:ARG:O	7:G:78:ILE:HG12	2.20	0.41
5:E:100:ILE:O	5:E:101:THR:C	2.63	0.41
6:F:66:SER:C	6:F:68:ASN:H	2.28	0.41
1:A:18:LYS:HD3	1:A:375:TYR:CD2	2.57	0.40
2:B:307:SER:O	2:B:307:SER:OG	2.36	0.40
3:C:74:ARG:HH11	3:C:74:ARG:HD3	1.73	0.40
3:C:240:LEU:HD23	3:C:270:PHE:CD2	2.56	0.40
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:144:THR:H	6:F:28:GLN:HE21	1.69	0.40
4:D:9:ARG:HH11	4:D:9:ARG:HD3	1.74	0.40
6:F:101:PHE:O	6:F:102:PHE:HB2	2.21	0.40
6:F:132:VAL:O	6:F:136:ILE:HD12	2.22	0.40
3:C:61:ALA:HB2	3:C:104:TRP:CG	2.57	0.40
4:D:59:ILE:HG22	4:D:93:VAL:HB	2.02	0.40
2:B:181:ARG:NE	2:B:181:ARG:H	2.19	0.40
4:D:263:HIS:CD2	4:D:266:MET:HE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:ARG:HH11	6:F:105:ARG:HD3	1.74	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%)	6	11
2	B	194/394 (49%)	173 (89%)	17 (9%)	4 (2%)	5	9
3	C	348/372 (94%)	322 (92%)	24 (7%)	2 (1%)	21	34
4	D	276/300 (92%)	267 (97%)	9 (3%)	0	100	100
5	E	171/178 (96%)	142 (83%)	23 (14%)	6 (4%)	3	4
6	F	165/168 (98%)	158 (96%)	7 (4%)	0	100	100
7	G	132/151 (87%)	119 (90%)	9 (7%)	4 (3%)	3	5
8	Z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	1677/1984 (84%)	1541 (92%)	113 (7%)	23 (1%)	9	14

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

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Mol	Chain	Res	Type
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%)	308 (90%)	36 (10%)	6	10
2	B	171/345 (50%)	147 (86%)	24 (14%)	3	5
3	C	301/313 (96%)	276 (92%)	25 (8%)	10	18
4	D	246/264 (93%)	228 (93%)	18 (7%)	13	22
5	E	156/159 (98%)	139 (89%)	17 (11%)	6	9
6	F	154/155 (99%)	145 (94%)	9 (6%)	18	31
7	G	110/123 (89%)	92 (84%)	18 (16%)	2	3
8	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	1485/1725 (86%)	1338 (90%)	147 (10%)	7	11

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG

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Mol	Chain	Res	Type
1	A	18	LYS
1	A	19	LEU
1	A	35	ILE
1	A	79	ARG
1	A	88	LEU
1	A	96	VAL
1	A	129	ILE
1	A	135	ASN
1	A	143	VAL
1	A	154	THR
1	A	156	ARG
1	A	157	GLN
1	A	174	VAL
1	A	191	LYS
1	A	210	ASP
1	A	223	THR
1	A	243	ASN
1	A	255	GLN
1	A	259	ILE
1	A	265	LYS
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	333	ARG
1	A	335	LEU
1	A	340	LYS
1	A	348	LYS
1	A	353	LEU
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	179	THR
2	B	181	ARG
2	B	182	LEU
2	B	183	ASP

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Mol	Chain	Res	Type
2	B	184	ILE
2	B	191	ARG
2	B	199	LEU
2	B	200	ARG
2	B	207	SER
2	B	220	LEU
2	B	227	ILE
2	B	232	LYS
2	B	240	LEU
2	B	276	VAL
2	B	294	ARG
2	B	298	TYR
2	B	326	LEU
2	B	327	GLU
2	B	342	ILE
2	B	343	ARG
2	B	345	GLU
3	C	29	ASN
3	C	31	GLU
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	175	GLU
3	C	183	THR
3	C	202	CYS
3	C	253	ILE
3	C	305	LEU
3	C	306	ASP
3	C	321	LEU
3	C	324	LEU
3	C	334	VAL
3	C	356	ILE
3	C	361	SER
3	C	366	LEU
3	C	367	LYS
3	C	370	LYS

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Mol	Chain	Res	Type
4	D	10	ILE
4	D	54	LYS
4	D	59	ILE
4	D	61	LEU
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	123	SER
4	D	133	GLU
4	D	158	LYS
4	D	170	LYS
4	D	230	ARG
4	D	235	SER
4	D	241	ILE
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	62	ASN
5	E	63	GLU
5	E	79	LEU
5	E	81	LYS
5	E	83	GLN
5	E	92	GLU
5	E	93	LYS
5	E	95	MET
5	E	101	THR
5	E	116	ILE
6	F	17	GLN
6	F	31	GLU
6	F	42	SER
6	F	49	GLN
6	F	62	LEU
6	F	68	ASN
6	F	125	GLN

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Mol	Chain	Res	Type
6	F	146	ILE
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	77	SER
7	G	85	SER
7	G	87	LYS
7	G	91	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	144	GLN
1	A	219	GLN
1	A	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	366	GLN
1	A	370	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
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	75	ASN

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Mol	Chain	Res	Type
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	197	GLN
4	D	202	HIS
4	D	231	HIS
5	E	27	GLN
5	E	62	ASN
5	E	90	GLN
5	E	102	ASN
5	E	138	GLN
5	E	167	GLN
6	F	24	ASN
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	396/418 (94%)	0.09	20 (5%) 33 26	25, 48, 95, 106	0
2	B	196/394 (49%)	0.56	25 (12%) 7 6	30, 60, 104, 110	0
3	C	354/372 (95%)	-0.09	14 (3%) 42 34	26, 42, 81, 116	0
4	D	280/300 (93%)	-0.25	5 (1%) 67 63	25, 42, 66, 89	0
5	E	173/178 (97%)	0.96	18 (10%) 11 9	47, 70, 100, 112	0
6	F	167/168 (99%)	-0.40	1 (0%) 85 83	26, 36, 52, 78	0
7	G	136/151 (90%)	0.32	9 (6%) 24 18	30, 59, 82, 87	0
8	Z	3/3 (100%)	2.10	2 (66%) 0 0	73, 73, 83, 84	0
All	All	1705/1984 (85%)	0.11	94 (5%) 30 24	25, 48, 94, 116	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	28	GLU	6.7
7	G	10	ARG	5.5
1	A	259	ILE	5.4
3	C	309	ALA	5.3
3	C	321	LEU	4.9
2	B	173	PHE	4.5
2	B	349	ARG	4.4
7	G	35	ALA	4.2
3	C	202	CYS	4.2
1	A	262	ILE	4.2
2	B	345	GLU	4.1
1	A	353	LEU	4.1
1	A	172	ASP	4.0
2	B	291	ILE	3.8
4	D	159	ASP	3.7
3	C	305	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	211	ASP	3.6
3	C	308	LYS	3.6
2	B	183	ASP	3.6
3	C	319	ALA	3.6
3	C	200	SER	3.5
7	G	151	VAL	3.4
3	C	320	GLY	3.3
5	E	156	PRO	3.3
1	A	2	ALA	3.3
1	A	264	LYS	3.2
2	B	181	ARG	3.2
3	C	307	LYS	3.2
5	E	37	LYS	3.1
5	E	36	THR	3.1
2	B	343	ARG	3.1
2	B	348	PRO	3.1
1	A	415	GLY	3.1
2	B	341	LYS	3.1
5	E	142	LEU	3.0
7	G	67	LYS	3.0
5	E	24	ILE	3.0
2	B	177	HIS	3.0
3	C	306	ASP	2.9
5	E	151	PRO	2.9
7	G	120	ASN	2.9
1	A	202	TYR	2.9
4	D	212	THR	2.9
1	A	361	LYS	2.9
6	F	2	THR	2.9
1	A	221	LEU	2.8
2	B	346	ASP	2.8
2	B	182	LEU	2.7
5	E	25	ARG	2.7
8	Z	52	GLU	2.7
3	C	297	THR	2.7
2	B	206	HIS	2.7
1	A	354	SER	2.7
3	C	372	VAL	2.7
2	B	342	ILE	2.6
2	B	344	ILE	2.6
2	B	175	LEU	2.6
2	B	329	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	174	SER	2.6
3	C	288	PRO	2.6
1	A	349	LEU	2.6
2	B	178	LEU	2.5
2	B	325	TYR	2.5
8	Z	54	GLU	2.5
1	A	156	ARG	2.4
2	B	172	GLY	2.4
5	E	23	PRO	2.4
5	E	99	GLY	2.4
2	B	334	VAL	2.4
5	E	121	ALA	2.4
5	E	13	THR	2.4
5	E	84	LYS	2.4
1	A	158	VAL	2.3
4	D	208	GLU	2.3
5	E	145	CYS	2.3
1	A	261	ALA	2.3
2	B	336	LYS	2.3
7	G	118	SER	2.3
2	B	300	HIS	2.3
4	D	282	PRO	2.2
1	A	213	VAL	2.2
2	B	170	TYR	2.2
5	E	27	GLN	2.2
1	A	344	ASP	2.2
5	E	38	ASP	2.2
1	A	268	SER	2.2
7	G	18	GLU	2.1
5	E	98	LEU	2.1
7	G	22	ASN	2.1
1	A	192	HIS	2.1
2	B	203	ALA	2.0
3	C	127	GLN	2.0
5	E	28	PHE	2.0
1	A	159	GLY	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 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.