



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 PM UTC

PDB ID : 6JMT / pdb_00006jmt
Title : Crystal structure of GIT/PIX complex
Authors : Zhu, J.; Lin, L.; Xia, Y.; Zhang, R.; Zhang, M.
Deposited on : 2019-03-13
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

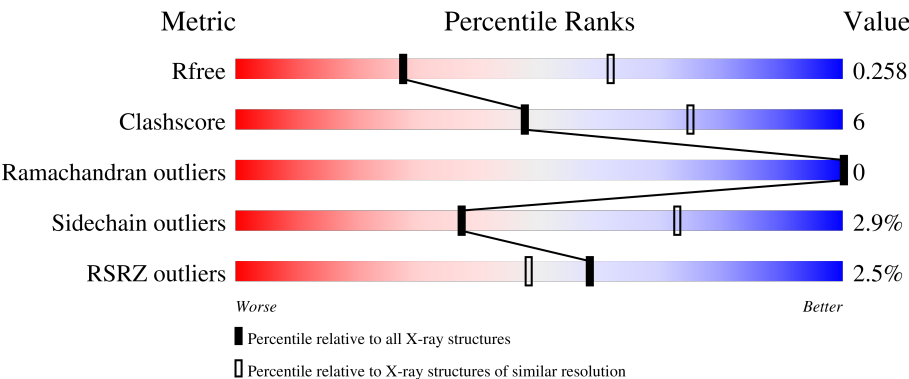
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	364	%81%14%• 5%
1	B	364	%79%15%• •
1	C	364	5%79%13%• 7%
1	D	364	2%82%13%• •
1	E	364	4%81%13%• 6%

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Mol	Chain	Length	Quality of chain
1	F	364	% 79%16%5%
2	I	21	67%10%24%
2	J	21	62%14%24%
2	K	21	67%10%24%
2	L	21	71%5%24%
2	M	21	76%24%
2	N	21	62%14%24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16305 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 ARF GTPase-activating protein GIT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2619	1640	479	489	11			
1	D	350	Total	C	N	O	S	0	0	0
			2634	1645	486	491	12			
1	B	349	Total	C	N	O	S	0	0	0
			2650	1655	487	496	12			
1	C	339	Total	C	N	O	S	0	0	0
			2485	1558	460	458	9			
1	E	343	Total	C	N	O	S	0	0	0
			2544	1596	465	472	11			
1	F	346	Total	C	N	O	S	0	0	0
			2625	1639	482	492	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q80XR8
A	-2	PRO	-	expression tag	UNP Q80XR8
A	-1	GLY	-	expression tag	UNP Q80XR8
A	0	SER	-	expression tag	UNP Q80XR8
A	255	ALA	SER	engineered mutation	UNP Q80XR8
A	256	ALA	SER	engineered mutation	UNP Q80XR8
D	-3	GLY	-	expression tag	UNP Q80XR8
D	-2	PRO	-	expression tag	UNP Q80XR8
D	-1	GLY	-	expression tag	UNP Q80XR8
D	0	SER	-	expression tag	UNP Q80XR8
D	255	ALA	SER	engineered mutation	UNP Q80XR8
D	256	ALA	SER	engineered mutation	UNP Q80XR8
B	-3	GLY	-	expression tag	UNP Q80XR8
B	-2	PRO	-	expression tag	UNP Q80XR8
B	-1	GLY	-	expression tag	UNP Q80XR8
B	0	SER	-	expression tag	UNP Q80XR8
B	255	ALA	SER	engineered mutation	UNP Q80XR8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	256	ALA	SER	engineered mutation	UNP Q80XR8
C	-3	GLY	-	expression tag	UNP Q80XR8
C	-2	PRO	-	expression tag	UNP Q80XR8
C	-1	GLY	-	expression tag	UNP Q80XR8
C	0	SER	-	expression tag	UNP Q80XR8
C	255	ALA	SER	engineered mutation	UNP Q80XR8
C	256	ALA	SER	engineered mutation	UNP Q80XR8
E	-3	GLY	-	expression tag	UNP Q80XR8
E	-2	PRO	-	expression tag	UNP Q80XR8
E	-1	GLY	-	expression tag	UNP Q80XR8
E	0	SER	-	expression tag	UNP Q80XR8
E	255	ALA	SER	engineered mutation	UNP Q80XR8
E	256	ALA	SER	engineered mutation	UNP Q80XR8
F	-3	GLY	-	expression tag	UNP Q80XR8
F	-2	PRO	-	expression tag	UNP Q80XR8
F	-1	GLY	-	expression tag	UNP Q80XR8
F	0	SER	-	expression tag	UNP Q80XR8
F	255	ALA	SER	engineered mutation	UNP Q80XR8
F	256	ALA	SER	engineered mutation	UNP Q80XR8

- Molecule 2 is a protein called beta PIX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	16	Total	C	N	O	S	0	0	0
			121	77	17	26	1			
2	J	16	Total	C	N	O	S	0	0	0
			121	77	17	26	1			
2	K	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	L	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	M	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	N	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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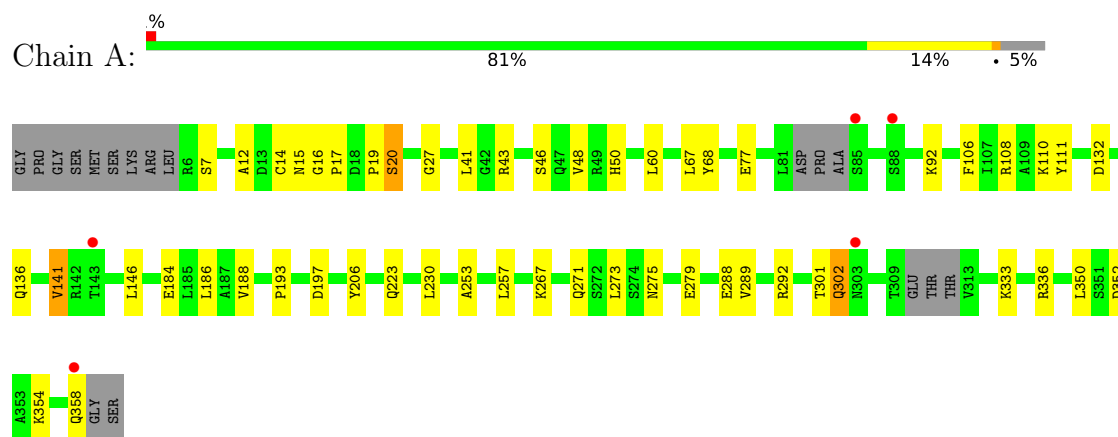
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

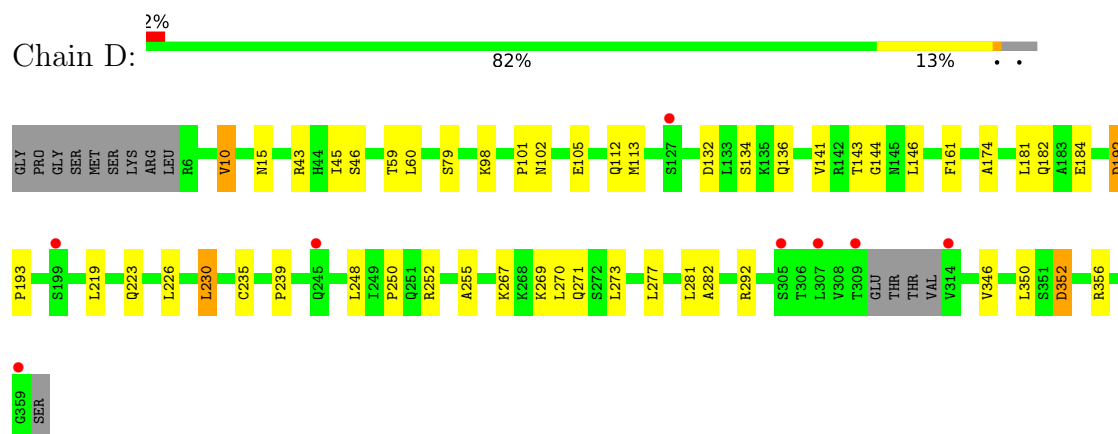
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

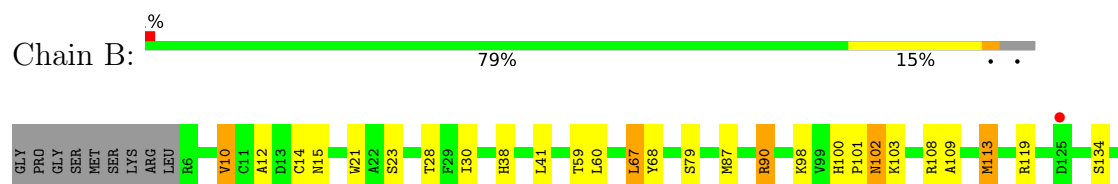
- Molecule 1: ARF GTPase-activating protein GIT2



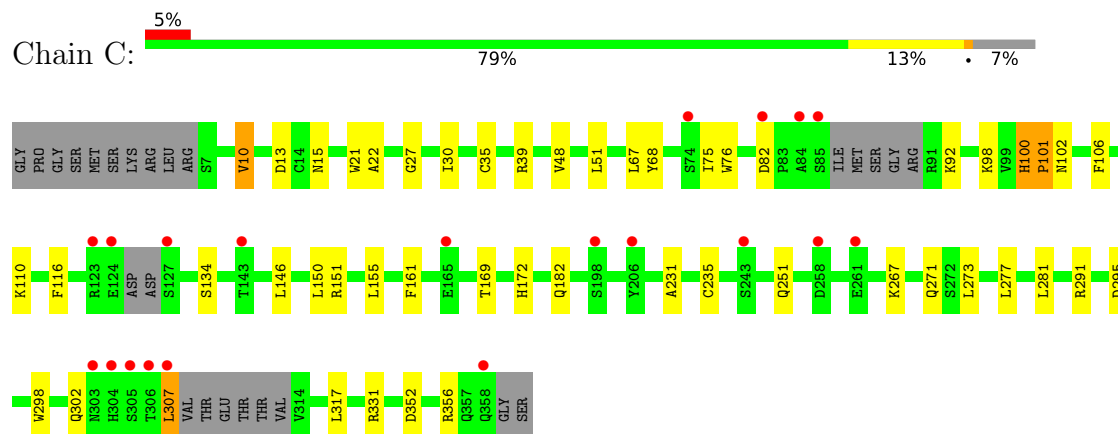
- Molecule 1: ARF GTPase-activating protein GIT2



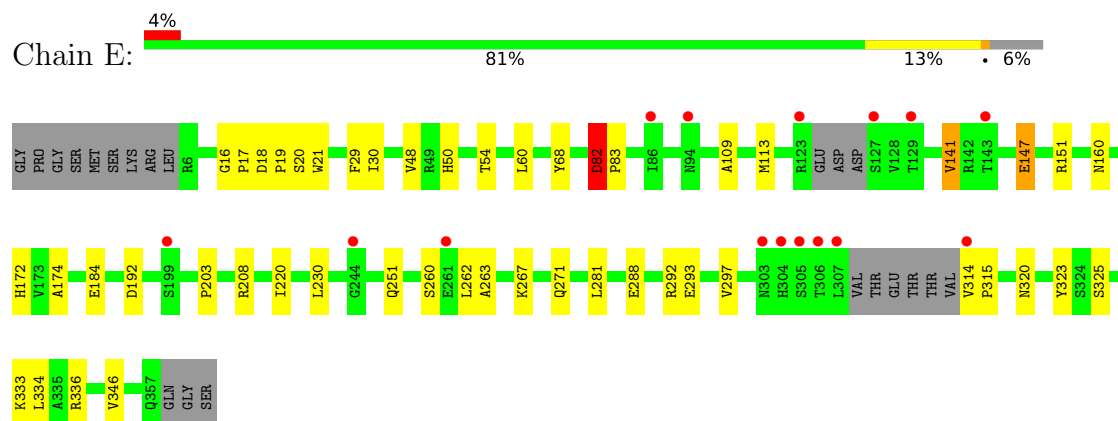
- Molecule 1: ARF GTPase-activating protein GIT2



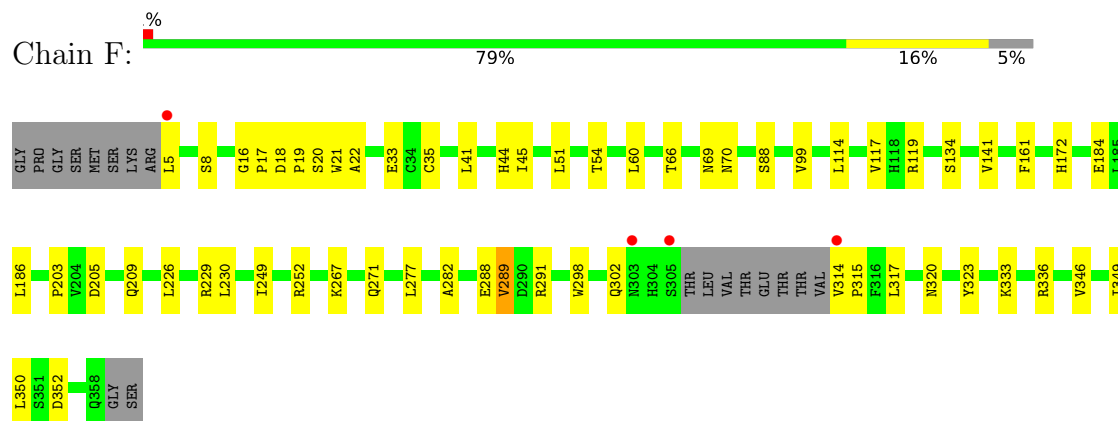
- Molecule 1: ARF GTPase-activating protein GIT2



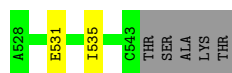
- Molecule 1: ARF GTPase-activating protein GIT2



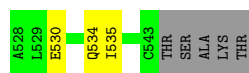
- Molecule 1: ARF GTPase-activating protein GIT2



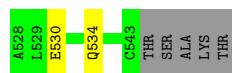
- Molecule 2: beta PIX



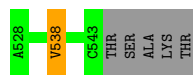
- Molecule 2: beta PIX



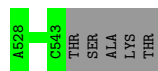
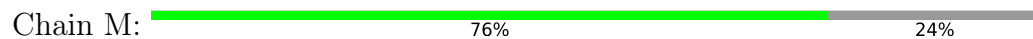
- Molecule 2: beta PIX



- Molecule 2: beta PIX



- Molecule 2: beta PIX



- Molecule 2: beta PIX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.96Å 322.68Å 44.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 2.80 44.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (44.05-2.80) 95.0 (44.05-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.194 , 0.254 0.200 , 0.258	Depositor DCC
R_{free} test set	2988 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16305	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.31% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.63	3/2676 (0.1%)	0.88	3/3642 (0.1%)
1	B	0.69	0/2709	0.90	6/3685 (0.2%)
1	C	0.63	1/2539 (0.0%)	0.92	5/3466 (0.1%)
1	D	0.64	0/2693	0.88	2/3666 (0.1%)
1	E	0.59	3/2601 (0.1%)	0.91	7/3548 (0.2%)
1	F	0.64	4/2684 (0.1%)	0.91	7/3652 (0.2%)
2	I	0.45	0/121	0.80	0/164
2	J	0.48	0/121	0.84	0/164
2	K	0.58	0/125	0.79	0/168
2	L	0.57	0/125	0.81	1/168 (0.6%)
2	M	0.66	0/125	0.79	0/168
2	N	0.59	0/125	0.78	0/168
All	All	0.64	11/16644 (0.1%)	0.90	31/22659 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	ASP	C-N	6.00	1.40	1.33
1	F	16	GLY	C-N	5.84	1.40	1.33
1	A	16	GLY	C-N	5.75	1.40	1.33
1	F	18	ASP	C-N	5.61	1.40	1.33
1	E	16	GLY	C-N	5.48	1.40	1.33
1	C	101	PRO	N-CD	5.43	1.55	1.47
1	F	17	PRO	N-CD	5.25	1.55	1.47
1	A	17	PRO	N-CD	5.24	1.55	1.47
1	A	20	SER	C-O	-5.23	1.17	1.24
1	F	19	PRO	N-CD	5.10	1.54	1.47
1	E	17	PRO	N-CD	5.00	1.54	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	ASP	CA-C-N	9.91	130.96	119.47
1	E	82	ASP	C-N-CA	9.91	130.96	119.47
1	B	102	ASN	N-CA-C	8.02	119.65	111.07
1	C	100	HIS	C-N-CD	7.95	138.08	120.60
1	A	16	GLY	CA-C-N	-7.15	113.30	120.31
1	A	16	GLY	C-N-CA	-7.15	113.30	120.31
1	F	16	GLY	CA-C-N	-6.87	113.58	120.31
1	F	16	GLY	C-N-CA	-6.87	113.58	120.31
1	E	16	GLY	CA-C-N	-6.25	113.51	120.14
1	E	16	GLY	C-N-CA	-6.25	113.51	120.14
1	F	18	ASP	CA-C-N	-6.16	114.30	120.21
1	F	18	ASP	C-N-CA	-6.16	114.30	120.21
1	E	18	ASP	CA-C-N	-6.09	114.00	120.03
1	E	18	ASP	C-N-CA	-6.09	114.00	120.03
1	B	140	SER	N-CA-C	5.95	117.76	111.28
1	F	249	ILE	N-CA-C	5.74	113.23	107.55
1	C	98	LYS	N-CA-C	-5.74	102.54	110.35
1	D	192	ASP	CA-C-N	5.51	125.60	119.87
1	D	192	ASP	C-N-CA	5.51	125.60	119.87
1	B	192	ASP	CA-C-N	5.49	125.16	119.56
1	B	192	ASP	C-N-CA	5.49	125.16	119.56
2	L	538	VAL	N-CA-C	-5.46	105.39	110.53
1	C	82	ASP	CA-C-N	5.45	125.11	119.56
1	C	82	ASP	C-N-CA	5.45	125.11	119.56
1	C	102	ASN	N-CA-C	5.34	116.78	111.07
1	B	320	ASN	CA-C-N	5.15	124.95	119.28
1	B	320	ASN	C-N-CA	5.15	124.95	119.28
1	A	19	PRO	N-CA-C	5.15	119.56	111.38
1	F	317	LEU	CA-C-N	5.15	125.14	119.89
1	F	317	LEU	C-N-CA	5.15	125.14	119.89
1	E	82	ASP	CB-CA-C	5.04	115.69	108.68

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	2619	0	2447	30	0
1	B	2650	0	2501	35	0
1	C	2485	0	2271	30	0
1	D	2634	0	2460	31	0
1	E	2544	0	2342	24	0
1	F	2625	0	2468	27	0
2	I	121	0	113	2	0
2	J	121	0	113	2	0
2	K	125	0	124	1	0
2	L	125	0	124	1	0
2	M	125	0	124	0	0
2	N	125	0	124	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	16305	0	15211	176	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 6.

All (176) 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:E:147:GLU:OE2	1:E:151:ARG:NH1	2.15	0.80
1:A:275:ASN:O	1:A:279:GLU:HG3	1.82	0.79
1:A:197:ASP:OD2	1:A:206:TYR:OH	2.01	0.78
1:F:60:LEU:HA	1:F:184:GLU:HG2	1.71	0.71
1:E:333:LYS:HA	1:E:336:ARG:HD3	1.74	0.70
1:C:317:LEU:HD12	1:C:331:ARG:HB3	1.73	0.69
1:D:60:LEU:HA	1:D:184:GLU:HG2	1.75	0.69
1:E:60:LEU:HA	1:E:184:GLU:HG2	1.73	0.69
1:A:60:LEU:HA	1:A:184:GLU:HG2	1.76	0.66
1:C:277:LEU:HD21	2:I:531:GLU:HB3	1.78	0.65
1:C:231:ALA:O	1:C:235:CYS:HB2	1.96	0.64
1:A:14:CYS:O	1:A:15:ASN:HB2	1.96	0.64
2:K:530:GLU:OE2	2:K:534:GLN:NE2	2.30	0.64
1:A:67:LEU:HD13	1:A:146:LEU:HB3	1.80	0.64
1:D:352:ASP:OD2	1:D:356:ARG:NH1	2.30	0.64
1:D:10:VAL:HG13	1:D:15:ASN:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:PRO:O	1:D:105:GLU:HG3	1.99	0.63
1:A:267:LYS:O	1:A:271:GLN:HG3	1.99	0.63
1:F:66:THR:O	1:F:70:ASN:ND2	2.33	0.61
1:D:45:ILE:HD13	1:D:112:GLN:HG3	1.83	0.60
1:B:59:THR:HG23	1:B:184:GLU:OE2	2.02	0.60
1:C:39:ARG:NH2	1:C:295:ASP:OD1	2.32	0.60
1:C:10:VAL:HG13	1:C:15:ASN:HA	1.84	0.59
1:D:273:LEU:HD11	2:N:538:VAL:HG21	1.85	0.59
1:A:302:GLN:HE21	1:A:302:GLN:N	2.01	0.58
1:C:281:LEU:HD13	2:I:535:ILE:HG23	1.85	0.58
1:C:13:ASP:OD1	1:C:110:LYS:NZ	2.33	0.57
1:B:10:VAL:HG13	1:B:15:ASN:HA	1.86	0.57
1:D:239:PRO:HG3	1:D:248:LEU:HB2	1.85	0.57
1:A:273:LEU:HD11	2:L:538:VAL:HG21	1.87	0.56
1:F:134:SER:HB3	1:F:161:PHE:CD2	2.39	0.56
1:C:267:LYS:O	1:C:271:GLN:HG3	2.06	0.56
1:F:5:LEU:HA	1:F:69:ASN:ND2	2.20	0.56
1:A:193:PRO:HB2	1:A:223:GLN:HG3	1.88	0.55
1:B:23:SER:HB3	1:B:28:THR:HG22	1.89	0.55
1:B:60:LEU:HA	1:B:184:GLU:HG2	1.89	0.55
1:A:50:HIS:CD2	1:A:301:THR:HG21	2.43	0.54
1:B:109:ALA:HA	1:B:113:MET:HB2	1.89	0.54
1:B:179:GLN:HB3	1:B:182:GLN:HG3	1.89	0.54
1:F:267:LYS:O	1:F:271:GLN:HG3	2.08	0.54
1:A:77:GLU:HG3	1:A:110:LYS:HE3	1.89	0.54
1:F:141:VAL:HG11	1:F:186:LEU:HD11	1.90	0.53
1:D:267:LYS:O	1:D:271:GLN:HG3	2.09	0.53
1:C:92:LYS:HG3	1:C:106:PHE:CE2	2.44	0.53
1:A:230:LEU:HD22	1:A:289:VAL:HG21	1.90	0.53
1:C:271:GLN:HG2	1:C:352:ASP:OD2	2.09	0.53
1:C:273:LEU:O	1:C:356:ARG:NH2	2.42	0.52
1:B:144:GLY:O	1:B:182:GLN:NE2	2.43	0.52
1:D:143:THR:HG22	1:D:144:GLY:N	2.24	0.52
1:A:302:GLN:NE2	1:A:302:GLN:CA	2.73	0.52
1:C:298:TRP:HE1	1:C:307:LEU:HD11	1.75	0.51
1:E:160:ASN:HD21	1:E:192:ASP:HB2	1.74	0.51
1:D:230:LEU:HD13	1:D:346:VAL:HG13	1.92	0.51
1:C:21:TRP:CG	1:C:35:CYS:HG	2.29	0.51
1:E:267:LYS:O	1:E:271:GLN:HG3	2.11	0.51
1:B:98:LYS:O	1:B:102:ASN:HB2	2.11	0.51
1:F:333:LYS:O	1:F:336:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:HG3	1:A:106:PHE:CZ	2.46	0.50
1:E:260:SER:HB2	1:E:263:ALA:H	1.77	0.49
1:D:45:ILE:CD1	1:D:112:GLN:HG3	2.41	0.49
1:B:59:THR:HG21	1:B:218:ARG:HG2	1.94	0.49
1:D:235:CYS:SG	1:D:250:PRO:HB3	2.53	0.49
1:D:143:THR:HG22	1:D:144:GLY:H	1.78	0.49
1:D:193:PRO:HB2	1:D:223:GLN:HG3	1.95	0.48
1:A:43:ARG:HA	1:A:46:SER:O	2.14	0.48
1:C:67:LEU:HD13	1:C:146:LEU:HB3	1.96	0.48
1:E:230:LEU:HB3	1:E:346:VAL:HG13	1.94	0.48
1:B:23:SER:HB3	1:B:28:THR:CG2	2.43	0.48
1:D:134:SER:HB3	1:D:161:PHE:CG	2.48	0.47
2:J:530:GLU:O	2:J:534:GLN:HG3	2.14	0.47
1:C:76:TRP:O	1:C:116:PHE:HB2	2.14	0.47
1:B:14:CYS:CB	1:B:103:LYS:HE2	2.45	0.47
1:A:141:VAL:HG21	1:A:186:LEU:HD11	1.96	0.47
1:C:169:THR:O	1:C:172:HIS:HB2	2.15	0.47
1:B:176:LYS:HE2	1:B:206:TYR:CE1	2.49	0.47
1:B:321:PRO:HB2	1:F:88:SER:HB3	1.97	0.47
1:F:33:GLU:HB3	1:F:99:VAL:HG22	1.95	0.47
1:F:298:TRP:O	1:F:302:GLN:HG2	2.14	0.47
1:E:288:GLU:OE1	1:E:292:ARG:NH1	2.47	0.47
1:C:22:ALA:HB2	1:C:51:LEU:HD21	1.96	0.46
1:A:288:GLU:HG3	1:A:292:ARG:HD2	1.98	0.46
1:B:38:HIS:HA	1:B:41:LEU:HD12	1.98	0.46
1:D:146:LEU:HD11	1:D:181:LEU:HB3	1.98	0.46
1:D:98:LYS:O	1:D:102:ASN:HB2	2.16	0.46
1:C:291:ARG:HD3	1:C:317:LEU:HD23	1.97	0.46
1:A:184:GLU:O	1:A:188:VAL:HG23	2.16	0.46
1:A:302:GLN:N	1:A:302:GLN:NE2	2.64	0.45
1:C:317:LEU:HD13	1:C:331:ARG:NH2	2.31	0.45
1:B:248:LEU:O	1:B:250:PRO:HD3	2.17	0.45
1:A:132:ASP:O	1:A:136:GLN:HG3	2.17	0.45
1:F:22:ALA:HB2	1:F:51:LEU:HD21	1.98	0.45
1:A:12:ALA:O	1:A:110:LYS:NZ	2.50	0.45
1:A:41:LEU:HD21	1:A:108:ARG:HG2	1.99	0.45
1:C:67:LEU:HD21	1:C:150:LEU:HD22	1.99	0.45
1:E:208:ARG:HH21	1:E:220:ILE:HD11	1.81	0.45
1:E:60:LEU:HA	1:E:184:GLU:CG	2.46	0.45
1:B:41:LEU:HD21	1:B:108:ARG:HG2	1.99	0.45
1:F:41:LEU:HD13	1:F:45:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:TRP:O	1:C:302:GLN:HG2	2.17	0.44
1:C:27:GLY:O	1:C:68:TYR:HB2	2.18	0.44
1:F:277:LEU:HD23	1:F:277:LEU:HA	1.81	0.44
1:E:320:ASN:HB3	1:E:323:TYR:CD2	2.53	0.44
1:D:141:VAL:HG13	1:D:182:GLN:HB3	1.98	0.44
1:B:249:ILE:HD12	1:B:351:SER:HA	1.99	0.44
1:E:29:PHE:HB2	1:E:68:TYR:CE2	2.53	0.44
1:D:141:VAL:CG1	1:D:174:ALA:HB2	2.48	0.44
1:B:100:HIS:HA	1:B:101:PRO:HA	1.82	0.44
1:C:30:ILE:HD12	1:C:35:CYS:HA	2.00	0.44
1:F:172:HIS:NE2	1:F:203:PRO:HD3	2.33	0.44
1:F:205:ASP:O	1:F:209:GLN:HG3	2.18	0.44
1:A:336:ARG:HG2	1:A:336:ARG:HH11	1.81	0.44
1:B:137:LEU:O	1:B:141:VAL:HG13	2.18	0.44
1:B:87:MET:HE2	1:B:87:MET:HB3	1.91	0.44
1:C:298:TRP:NE1	1:C:307:LEU:HD11	2.33	0.44
1:A:333:LYS:O	1:A:336:ARG:HG3	2.18	0.43
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.84	0.43
1:A:27:GLY:O	1:A:68:TYR:HB2	2.18	0.43
1:E:281:LEU:HD13	2:J:535:ILE:HG23	2.00	0.43
1:A:354:LYS:O	1:A:358:GLN:HG3	2.17	0.43
1:D:43:ARG:HA	1:D:46:SER:O	2.18	0.43
1:D:134:SER:HB3	1:D:161:PHE:CD2	2.53	0.43
1:A:110:LYS:HD3	1:A:111:TYR:CE2	2.53	0.43
1:B:230:LEU:HD22	1:B:289:VAL:HG21	1.99	0.43
1:F:134:SER:HB3	1:F:161:PHE:CG	2.54	0.43
1:F:288:GLU:OE1	1:F:291:ARG:NH1	2.51	0.43
1:D:281:LEU:HD13	2:N:535:ILE:HG23	2.00	0.43
1:A:253:ALA:HB1	1:B:250:PRO:HB3	2.01	0.43
1:B:79:SER:OG	1:B:90:ARG:NH1	2.52	0.42
1:B:134:SER:HB3	1:B:161:PHE:CG	2.54	0.42
1:D:226:LEU:HD21	1:D:282:ALA:HB1	2.02	0.42
1:D:277:LEU:HD23	1:D:277:LEU:HA	1.83	0.42
1:E:172:HIS:NE2	1:E:203:PRO:HD3	2.34	0.42
1:C:134:SER:HB3	1:C:161:PHE:CG	2.54	0.42
1:C:151:ARG:O	1:C:155:LEU:HG	2.20	0.42
1:E:160:ASN:HD21	1:E:192:ASP:CB	2.31	0.42
1:F:230:LEU:HB3	1:F:346:VAL:HG13	2.02	0.42
1:D:252:ARG:NH1	1:D:255:ALA:HA	2.35	0.42
1:B:333:LYS:O	1:B:336:ARG:HG2	2.20	0.42
1:F:320:ASN:HB3	1:F:323:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.81	0.42
1:A:230:LEU:HB2	1:A:350:LEU:HD21	2.02	0.42
1:F:21:TRP:CG	1:F:35:CYS:HG	2.37	0.42
1:F:350:LEU:HD23	1:F:350:LEU:HA	1.83	0.42
1:E:82:ASP:HA	1:E:83:PRO:HD3	1.83	0.42
1:A:12:ALA:HB2	1:A:68:TYR:CE1	2.55	0.41
1:B:12:ALA:HB2	1:B:68:TYR:CE1	2.55	0.41
1:D:132:ASP:O	1:D:136:GLN:HG3	2.19	0.41
1:C:134:SER:HB3	1:C:161:PHE:CD2	2.55	0.41
1:E:293:GLU:O	1:E:297:VAL:HG23	2.20	0.41
1:D:277:LEU:HD22	2:N:535:ILE:HD11	2.03	0.41
1:B:322:GLU:OE1	1:F:88:SER:OG	2.35	0.41
1:F:314:VAL:N	1:F:315:PRO:HD3	2.36	0.41
1:D:113:MET:HE2	1:D:113:MET:HB3	1.80	0.41
1:B:21:TRP:HB2	1:B:30:ILE:HG13	2.03	0.41
1:E:21:TRP:CE2	1:E:50:HIS:HD2	2.39	0.41
1:C:100:HIS:HA	1:C:101:PRO:HA	1.66	0.41
1:E:109:ALA:HA	1:E:113:MET:HE3	2.03	0.41
1:E:141:VAL:HG13	1:E:174:ALA:HB2	2.03	0.41
1:C:298:TRP:CE2	1:C:302:GLN:HG3	2.56	0.41
1:F:226:LEU:HD21	1:F:282:ALA:HB1	2.02	0.41
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.89	0.40
1:C:75:ILE:HD11	1:C:151:ARG:HB2	2.02	0.40
1:E:262:LEU:HD23	1:E:262:LEU:HA	1.95	0.40
1:E:334:LEU:HD23	1:E:334:LEU:HA	1.97	0.40
1:B:14:CYS:O	1:B:15:ASN:HB2	2.22	0.40
1:B:67:LEU:HD21	1:B:150:LEU:HD22	2.03	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.78	0.40
1:E:19:PRO:HB2	1:E:30:ILE:O	2.22	0.40
1:E:314:VAL:HA	1:E:315:PRO:HD3	1.83	0.40
1:F:44:HIS:CE1	1:F:320:ASN:HA	2.56	0.40
1:B:149:CYS:SG	1:B:185:LEU:HD23	2.62	0.40
1:B:235:CYS:SG	1:B:250:PRO:HG3	2.62	0.40
1:F:229:ARG:HH21	1:F:289:VAL:HG12	1.85	0.40
1:D:192:ASP:HA	1:D:193:PRO:HD3	1.80	0.40
1:B:87:MET:HG3	1:B:90:ARG:HG3	2.03	0.40
1:F:114:LEU:O	1:F:117:VAL:HG22	2.22	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	341/364 (94%)	337 (99%)	4 (1%)	0	100	100
1	B	345/364 (95%)	335 (97%)	10 (3%)	0	100	100
1	C	331/364 (91%)	320 (97%)	11 (3%)	0	100	100
1	D	346/364 (95%)	340 (98%)	6 (2%)	0	100	100
1	E	337/364 (93%)	330 (98%)	7 (2%)	0	100	100
1	F	342/364 (94%)	336 (98%)	6 (2%)	0	100	100
2	I	14/21 (67%)	14 (100%)	0	0	100	100
2	J	14/21 (67%)	14 (100%)	0	0	100	100
2	K	14/21 (67%)	14 (100%)	0	0	100	100
2	L	14/21 (67%)	14 (100%)	0	0	100	100
2	M	14/21 (67%)	14 (100%)	0	0	100	100
2	N	14/21 (67%)	14 (100%)	0	0	100	100
All	All	2126/2310 (92%)	2082 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	262/311 (84%)	255 (97%)	7 (3%)	39	74
1	B	270/311 (87%)	260 (96%)	10 (4%)	30	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	235/311 (76%)	230 (98%)	5 (2%)	47	79
1	D	263/311 (85%)	255 (97%)	8 (3%)	36	72
1	E	247/311 (79%)	239 (97%)	8 (3%)	34	70
1	F	267/311 (86%)	259 (97%)	8 (3%)	36	72
2	I	12/17 (71%)	12 (100%)	0	100	100
2	J	12/17 (71%)	12 (100%)	0	100	100
2	K	13/17 (76%)	13 (100%)	0	100	100
2	L	13/17 (76%)	13 (100%)	0	100	100
2	M	13/17 (76%)	13 (100%)	0	100	100
2	N	13/17 (76%)	12 (92%)	1 (8%)	12	36
All	All	1620/1968 (82%)	1573 (97%)	47 (3%)	37	73

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	20	SER
1	A	48	VAL
1	A	141	VAL
1	A	257	LEU
1	A	302	GLN
1	A	352	ASP
1	D	10	VAL
1	D	59	THR
1	D	79	SER
1	D	230	LEU
1	D	269	LYS
1	D	270	LEU
1	D	292	ARG
1	D	352	ASP
1	B	10	VAL
1	B	67	LEU
1	B	90	ARG
1	B	113	MET
1	B	119	ARG
1	B	230	LEU
1	B	259	LEU
1	B	292	ARG

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Mol	Chain	Res	Type
1	B	306	THR
1	B	352	ASP
1	C	10	VAL
1	C	48	VAL
1	C	182	GLN
1	C	251	GLN
1	C	307	LEU
1	E	20	SER
1	E	48	VAL
1	E	54	THR
1	E	82	ASP
1	E	141	VAL
1	E	147	GLU
1	E	251	GLN
1	E	325	SER
1	F	8	SER
1	F	20	SER
1	F	54	THR
1	F	119	ARG
1	F	252	ARG
1	F	289	VAL
1	F	349	ILE
1	F	352	ASP
2	N	543	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	245	GLN
1	A	271	GLN
1	A	304	HIS
1	D	78	HIS
1	D	118	HIS
1	D	138	HIS
1	D	340	HIS
1	B	44	HIS
1	B	62	GLN
1	B	112	GLN
1	B	212	HIS
1	B	251	GLN
1	B	304	HIS

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Mol	Chain	Res	Type
1	B	340	HIS
1	C	136	GLN
1	C	163	HIS
1	C	213	HIS
1	C	251	GLN
1	C	276	HIS
1	C	340	HIS
1	E	47	GLN
1	E	100	HIS
1	E	160	ASN
1	E	179	GLN
1	E	213	HIS
1	F	118	HIS
1	F	209	GLN
1	F	251	GLN
1	F	271	GLN
2	L	534	GLN

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 [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	347/364 (95%)	-0.14	5 (1%) 73 64	21, 41, 80, 100	0
1	B	349/364 (95%)	-0.38	3 (0%) 81 74	17, 35, 63, 93	0
1	C	339/364 (93%)	0.25	20 (5%) 28 21	29, 56, 92, 113	0
1	D	350/364 (96%)	-0.22	8 (2%) 61 51	21, 38, 74, 113	0
1	E	343/364 (94%)	0.16	15 (4%) 39 31	27, 52, 86, 118	0
1	F	346/364 (95%)	-0.27	4 (1%) 76 68	21, 37, 62, 110	0
2	I	16/21 (76%)	-0.11	0 100 100	43, 49, 65, 67	0
2	J	16/21 (76%)	-0.33	0 100 100	33, 40, 62, 62	0
2	K	16/21 (76%)	-0.41	0 100 100	26, 35, 54, 60	0
2	L	16/21 (76%)	-0.38	0 100 100	31, 40, 51, 54	0
2	M	16/21 (76%)	-0.65	0 100 100	20, 30, 41, 42	0
2	N	16/21 (76%)	-0.31	0 100 100	28, 34, 48, 51	0
All	All	2170/2310 (93%)	-0.12	55 (2%) 58 48	17, 42, 82, 118	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	303	ASN	5.5
1	F	305	SER	5.0
1	A	303	ASN	4.9
1	B	125	ASP	4.2
1	C	165	GLU	4.0
1	C	358	GLN	3.5
1	E	305	SER	3.5
1	E	199	SER	3.4
1	C	307	LEU	3.3
1	E	127	SER	3.3
1	E	303	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	358	GLN	3.3
1	C	85	SER	3.3
1	F	5	LEU	3.2
1	D	309	THR	3.2
1	C	206	TYR	3.0
1	E	123	ARG	2.9
1	C	303	ASN	2.9
1	E	304	HIS	2.8
1	E	306	THR	2.8
1	C	82	ASP	2.8
1	C	74	SER	2.7
1	C	127	SER	2.7
1	B	303	ASN	2.7
1	E	307	LEU	2.7
1	A	143	THR	2.7
1	E	261	GLU	2.6
1	A	85	SER	2.6
1	D	305	SER	2.6
1	C	305	SER	2.6
1	C	258	ASP	2.5
1	E	314	VAL	2.4
1	E	94	ASN	2.4
1	C	304	HIS	2.4
1	D	127	SER	2.4
1	D	307	LEU	2.3
1	B	305	SER	2.3
1	D	245	GLN	2.2
1	C	198	SER	2.2
1	C	84	ALA	2.2
1	E	129	THR	2.2
1	C	243	SER	2.2
1	D	359	GLY	2.2
1	C	124	GLU	2.2
1	E	143	THR	2.2
1	C	306	THR	2.1
1	D	199	SER	2.1
1	C	123	ARG	2.1
1	C	261	GLU	2.1
1	A	88	SER	2.0
1	E	244	GLY	2.0
1	C	143	THR	2.0
1	E	86	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	314	VAL	2.0
1	F	314	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	401	1/1	0.99	0.03	53,53,53,53	0
3	ZN	D	401	1/1	1.00	0.01	41,41,41,41	0
3	ZN	B	401	1/1	1.00	0.01	28,28,28,28	0
3	ZN	A	401	1/1	1.00	0.03	39,39,39,39	0
3	ZN	E	401	1/1	1.00	0.01	51,51,51,51	0
3	ZN	F	401	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.