



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 PM UTC

PDB ID : 4C3J / pdb_00004c3j
Title : Structure of 14-subunit RNA polymerase I at 3.35 Å resolution, crystal form C2-90
Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on : 2013-08-24
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

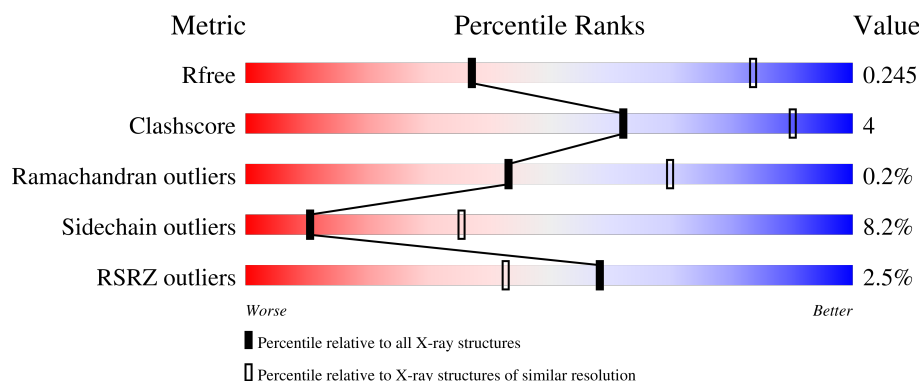
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	155	56%8%35%
7	G	326	6% 66%13%21%
8	H	146	77%15%8%
9	I	125	10% 75%23%..
10	J	70	% 77%13%9%. .
11	K	142	58%13%..27%
12	L	70	56%7%.36%
13	M	415	3% 20%5%75%
14	N	233	6% 52%7%.40%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 34552 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 DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1523	Total	C	N	O	S	0	0	0
			12019	7577	2086	2292	64			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

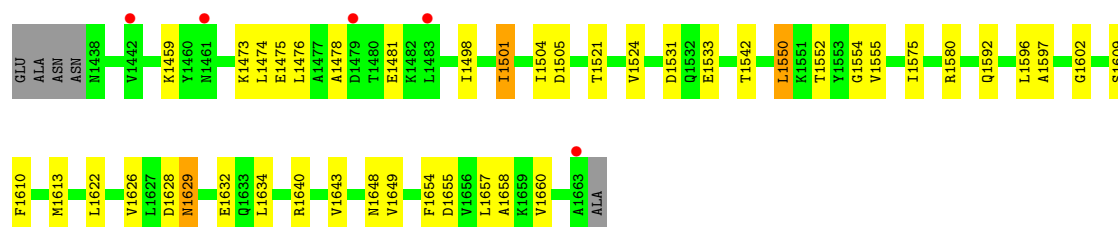
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O	0	0	0
			831	528	137	166			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

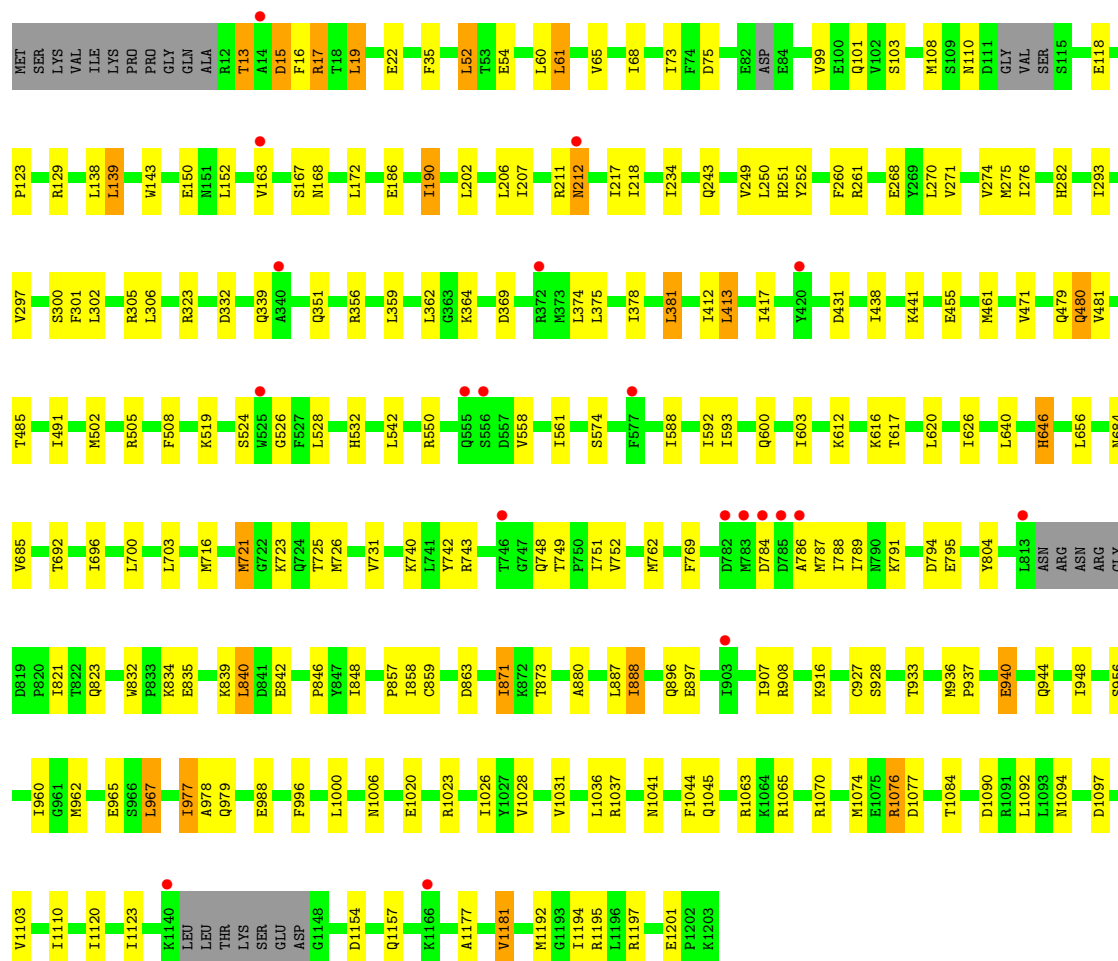
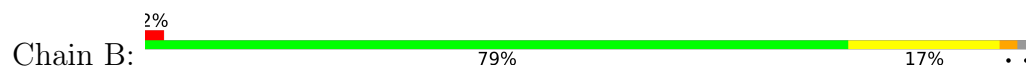
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

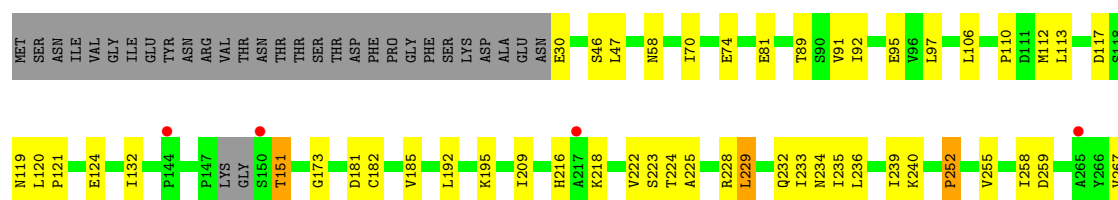
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Zn	0	0
			2	2		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	J	1	Total	Zn	0	0
			1	1		
15	L	1	Total	Zn	0	0
			1	1		



• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135



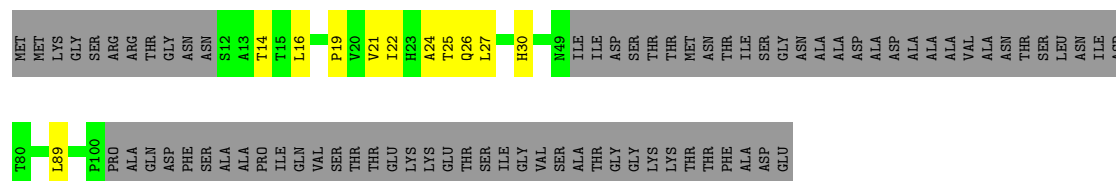
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1





• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D: 35% 8% 57%



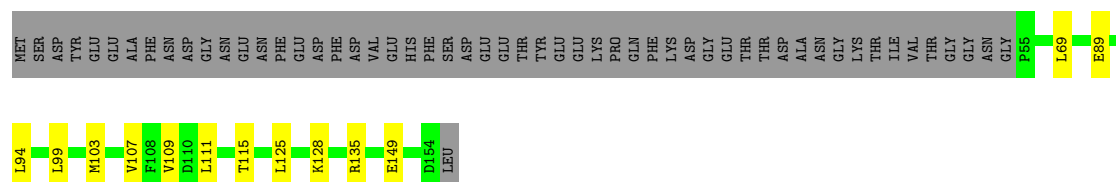
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E: 87% 12%



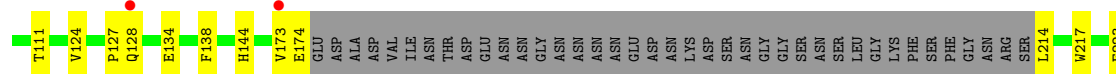
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F: 56% 8% 35%



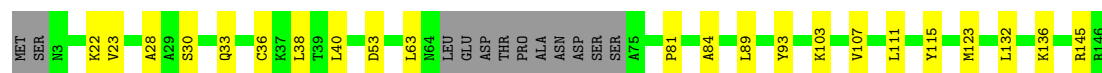
• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain G: 6% 66% 13% 21%

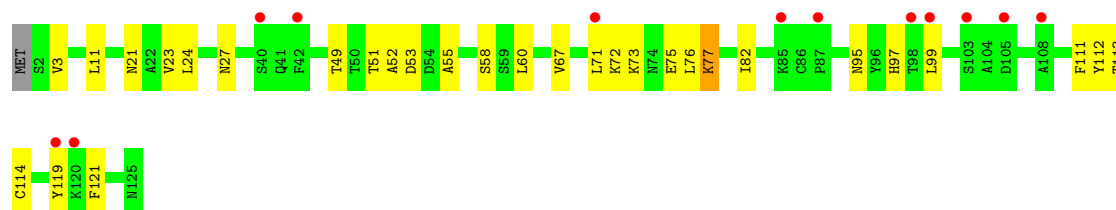
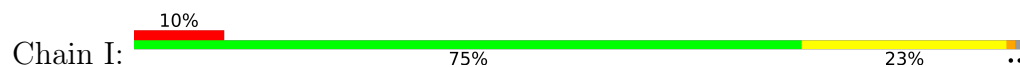


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

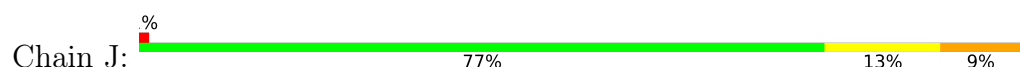
Chain H: 77% 15% 8%



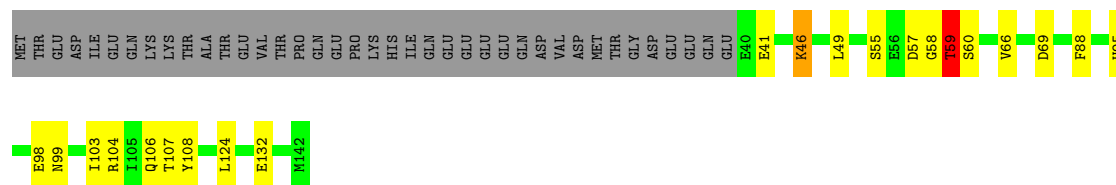
• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



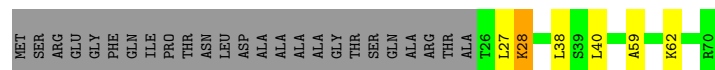
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



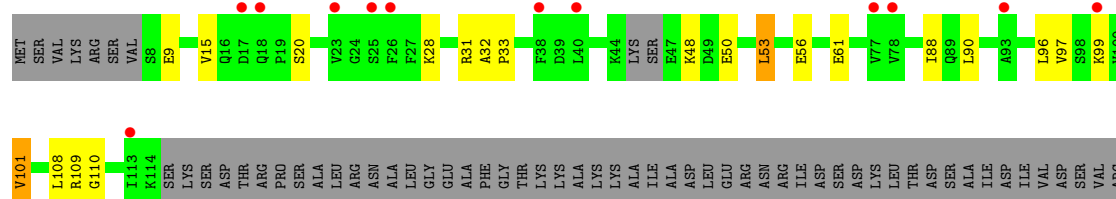
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	401.02Å 139.84Å 140.94Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	49.05 – 3.35 49.05 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.05-3.35) 99.5 (49.05-3.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.213 , 0.220 0.237 , 0.245	Depositor DCC
R_{free} test set	5612 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34552	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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	0.74	0/12233	1.29	22/16523 (0.1%)
2	B	0.74	0/9527	1.24	10/12879 (0.1%)
3	C	0.75	1/2469 (0.0%)	1.22	8/3347 (0.2%)
4	D	0.74	0/472	1.33	0/639
5	E	0.76	0/1795	1.20	4/2416 (0.2%)
6	F	0.72	0/838	1.23	0/1129
7	G	0.75	0/2094	1.19	3/2843 (0.1%)
8	H	0.75	1/1090 (0.1%)	1.01	0/1476
9	I	0.76	0/954	1.19	0/1285
10	J	0.77	0/578	1.32	0/775
11	K	0.72	0/821	1.28	2/1108 (0.2%)
12	L	0.70	0/361	1.11	2/478 (0.4%)
13	M	0.72	0/846	0.98	0/1136
14	N	0.77	0/1124	1.05	2/1512 (0.1%)
All	All	0.74	2/35202 (0.0%)	1.23	53/47546 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	252	PRO	CA-C	5.40	1.54	1.51
8	H	81	PRO	CA-C	5.10	1.54	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	ILE	N-CA-C	7.82	118.29	111.56
1	A	1218	GLY	CA-C-N	7.14	124.74	120.24
1	A	1218	GLY	C-N-CA	7.14	124.74	120.24
3	C	173	GLY	CA-C-N	6.24	129.49	120.38
3	C	173	GLY	C-N-CA	6.24	129.49	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	121	PRO	CA-C-N	6.15	128.81	120.38
3	C	121	PRO	C-N-CA	6.15	128.81	120.38
7	G	138	PHE	CA-CB-CG	6.08	119.88	113.80
3	C	151	THR	CA-C-N	5.95	129.13	120.51
3	C	151	THR	C-N-CA	5.95	129.13	120.51
2	B	212	ASN	CA-CB-CG	5.92	118.52	112.60
2	B	1006	ASN	CA-C-N	5.88	128.43	120.38
2	B	1006	ASN	C-N-CA	5.88	128.43	120.38
1	A	365	THR	CA-C-N	5.79	128.31	120.38
1	A	365	THR	C-N-CA	5.79	128.31	120.38
3	C	124	GLU	CA-C-N	5.69	127.84	120.44
3	C	124	GLU	C-N-CA	5.69	127.84	120.44
1	A	1225	ILE	CA-C-N	5.68	127.92	120.60
1	A	1225	ILE	C-N-CA	5.68	127.92	120.60
1	A	1629	ASN	CA-C-N	5.60	128.79	120.90
1	A	1629	ASN	C-N-CA	5.60	128.79	120.90
1	A	1035	ASP	CA-CB-CG	5.56	118.16	112.60
11	K	69	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	852	ASP	CA-C-N	5.40	127.78	120.38
1	A	852	ASP	C-N-CA	5.40	127.78	120.38
2	B	1044	PHE	CA-CB-CG	5.40	119.20	113.80
2	B	167	SER	CA-C-N	5.36	127.72	120.38
2	B	167	SER	C-N-CA	5.36	127.72	120.38
2	B	751	ILE	N-CA-C	-5.34	105.51	110.53
1	A	271	ARG	CA-C-N	5.31	127.39	120.28
1	A	271	ARG	C-N-CA	5.31	127.39	120.28
1	A	691	GLN	CA-C-N	5.30	127.33	120.44
1	A	691	GLN	C-N-CA	5.30	127.33	120.44
14	N	163	VAL	CA-C-N	5.23	128.19	120.82
14	N	163	VAL	C-N-CA	5.23	128.19	120.82
1	A	1053	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	75	ASP	CA-CB-CG	5.19	117.79	112.60
2	B	834	LYS	CA-C-N	5.19	131.45	121.54
2	B	834	LYS	C-N-CA	5.19	131.45	121.54
1	A	1136	VAL	N-CA-CB	-5.18	103.77	112.47
7	G	29	ASP	CA-C-N	5.17	131.42	121.54
7	G	29	ASP	C-N-CA	5.17	131.42	121.54
1	A	1524	VAL	CA-C-N	5.11	128.48	121.33
1	A	1524	VAL	C-N-CA	5.11	128.48	121.33
1	A	994	GLU	CA-C-N	5.09	127.06	120.44
1	A	994	GLU	C-N-CA	5.09	127.06	120.44
5	E	17	ARG	CA-C-N	5.03	127.02	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	17	ARG	C-N-CA	5.03	127.02	120.28
12	L	28	LYS	CA-C-N	5.03	129.73	121.58
12	L	28	LYS	C-N-CA	5.03	129.73	121.58
5	E	161	LYS	CA-C-N	5.02	127.25	120.38
5	E	161	LYS	C-N-CA	5.02	127.25	120.38
11	K	59	THR	N-CA-C	5.01	116.74	111.28

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	12019	0	12051	123	0
2	B	9322	0	9187	97	0
3	C	2418	0	2401	22	0
4	D	466	0	466	4	0
5	E	1759	0	1788	10	0
6	F	823	0	841	7	0
7	G	2052	0	2016	14	0
8	H	1072	0	1042	6	0
9	I	942	0	933	13	0
10	J	569	0	585	13	0
11	K	810	0	801	13	0
12	L	359	0	381	1	0
13	M	831	0	820	12	0
14	N	1103	0	1106	6	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	34552	0	34418	280	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 4.

All (280) 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)
11:K:59:THR:HG22	11:K:107:THR:OG1	1.46	1.13
11:K:60:SER:OG	11:K:106:GLN:HG2	1.63	0.97
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.58	0.84
1:A:1382:VAL:HA	2:B:1070:ARG:NH1	1.94	0.81
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.68	0.75
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.73
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.72
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.53	0.72
1:A:432:ASN:HD21	1:A:444:GLN:H	1.37	0.72
1:A:712:ILE:H	11:K:106:GLN:HE22	1.39	0.70
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.74	0.69
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.77	0.67
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.78	0.66
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.77	0.65
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.61	0.64
5:E:147:HIS:HD2	5:E:149:LEU:H	1.46	0.63
2:B:749:THR:O	10:J:52:THR:HG23	1.99	0.62
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.81	0.62
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.82	0.62
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.64	0.62
1:A:713:VAL:H	1:A:738:ASN:HD21	1.49	0.61
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.82	0.60
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.83	0.60
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.83	0.60
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.84	0.59
1:A:332:GLN:HE22	1:A:350:VAL:H	1.50	0.59
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.83	0.59
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.84	0.59
2:B:190:ILE:HD13	2:B:190:ILE:H	1.68	0.59
2:B:211:ARG:HH22	2:B:243:GLN:HE22	1.51	0.58
11:K:59:THR:HG22	11:K:107:THR:HG1	1.63	0.58
1:A:701:ARG:H	1:A:706:HIS:HD2	1.50	0.58
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.58
1:A:943:ILE:HG12	2:B:960:ILE:HD11	1.85	0.58
1:A:130:ILE:HB	5:E:215:MET:HE2	1.85	0.57
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.87	0.57
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.86	0.56
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.86	0.56
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.87	0.56
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HG23	2:B:461:MET:HE1	1.87	0.56
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.87	0.55
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.87	0.55
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.88	0.55
2:B:300:SER:HB3	9:I:49:THR:HG22	1.89	0.55
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.88	0.55
1:A:970:LYS:HE2	2:B:685:VAL:HG21	1.89	0.55
1:A:1017:GLY:O	1:A:1384:TYR:HB3	2.05	0.55
2:B:791:LYS:O	2:B:795:GLU:HG2	2.07	0.55
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.88	0.55
10:J:48:ARG:O	10:J:52:THR:HB	2.06	0.55
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.87	0.54
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.89	0.54
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.89	0.54
3:C:92:ILE:HG12	10:J:2:ILE:HD11	1.89	0.54
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.90	0.54
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.55	0.54
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.88	0.54
1:A:701:ARG:H	1:A:706:HIS:CD2	2.26	0.53
2:B:282:HIS:HD2	13:M:99:LYS:HD2	1.73	0.53
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.53
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.53
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.89	0.53
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.91	0.53
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.90	0.53
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.91	0.53
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.90	0.53
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.90	0.53
1:A:1055:ILE:HD13	1:A:1063:MET:HE1	1.90	0.53
2:B:52:LEU:HG	2:B:61:LEU:HD13	1.90	0.53
2:B:787:MET:HE3	2:B:927:CYS:HA	1.91	0.53
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.91	0.52
7:G:134:GLU:HB3	7:G:228:LYS:HE2	1.90	0.52
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.09	0.52
1:A:891:ILE:HG23	9:I:71:LEU:HG	1.89	0.52
1:A:1613:MET:HE3	1:A:1622:LEU:HB2	1.90	0.52
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.91	0.52
1:A:1239:THR:HB	1:A:1542:THR:HB	1.91	0.52
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.91	0.52
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.92	0.52
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.92	0.52
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.92	0.51
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.91	0.51
2:B:646:HIS:CD2	2:B:646:HIS:H	2.29	0.51
3:C:333:ILE:HG22	11:K:49:LEU:HB2	1.92	0.51
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.75	0.51
11:K:104:ARG:HD2	11:K:106:GLN:HG3	1.92	0.51
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.92	0.51
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.92	0.51
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.92	0.51
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.93	0.50
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.92	0.50
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.92	0.50
1:A:1265:GLU:HA	9:I:58:SER:HB3	1.94	0.50
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.93	0.50
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.94	0.50
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.91	0.50
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.50
7:G:50:ALA:H	7:G:64:GLN:HE22	1.58	0.50
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.94	0.50
9:I:97:HIS:HB3	9:I:111:PHE:HB2	1.94	0.50
1:A:940:VAL:HG13	1:A:944:MET:HE3	1.92	0.50
1:A:1382:VAL:HA	2:B:1070:ARG:HH11	1.74	0.50
7:G:18:LYS:HA	7:G:21:LYS:HD2	1.94	0.49
13:M:109:ARG:HG3	13:M:110:GLY:H	1.76	0.49
1:A:518:GLU:HG3	6:F:115:THR:HG21	1.94	0.49
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.93	0.49
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.95	0.49
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.94	0.49
3:C:216:HIS:HD2	3:C:218:LYS:H	1.61	0.49
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.94	0.49
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.94	0.49
10:J:68:LYS:HD3	10:J:69:ARG:HD2	1.94	0.49
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.95	0.49
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.95	0.49
1:A:1348:VAL:HG11	2:B:270:LEU:HD12	1.94	0.48
11:K:55:SER:HB2	11:K:60:SER:HB2	1.95	0.48
1:A:986:PHE:HB2	2:B:960:ILE:HD12	1.95	0.48
2:B:908:ARG:HD2	3:C:95:GLU:HG2	1.94	0.48
2:B:656:LEU:HB3	14:N:148:ILE:HG12	1.95	0.48
7:G:14:ALA:HA	7:G:17:ILE:HD12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.48
1:A:952:LEU:HD23	1:A:1004:GLU:HG3	1.95	0.48
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.48
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.96	0.48
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.96	0.47
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.95	0.47
9:I:52:ALA:HB3	9:I:55:ALA:HB2	1.96	0.47
2:B:129:ARG:HA	2:B:888:ILE:HG21	1.96	0.47
2:B:740:LYS:HA	2:B:804:TYR:O	2.14	0.47
1:A:836:THR:HG23	1:A:839:GLY:H	1.80	0.47
1:A:727:THR:H	1:A:730:GLN:HE21	1.63	0.47
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.97	0.47
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.45	0.47
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.97	0.47
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.97	0.47
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.47
1:A:898:SER:HB2	9:I:77:LYS:HB2	1.95	0.47
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.97	0.47
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.96	0.47
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.97	0.47
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.14	0.47
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.97	0.46
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.46
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.45	0.46
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.50	0.46
7:G:47:VAL:HG21	7:G:61:VAL:HG13	1.98	0.46
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.81	0.46
5:E:56:LYS:HE2	5:E:84:ASP:H	1.81	0.46
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.80	0.46
1:A:986:PHE:CB	2:B:960:ILE:HD12	2.45	0.46
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.98	0.46
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.97	0.46
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.98	0.46
2:B:480:GLN:HE21	2:B:508:PHE:H	1.63	0.46
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.98	0.46
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.98	0.46
9:I:114:CYS:HB3	9:I:119:TYR:H	1.81	0.46
2:B:748:GLN:HB3	10:J:52:THR:CG2	2.45	0.46
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.97	0.46
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.97	0.45
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.97	0.45
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.97	0.45
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.52	0.45
2:B:721:MET:O	2:B:725:THR:HG23	2.16	0.45
1:A:438:ILE:HD12	2:B:1192:MET:HA	1.99	0.45
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.98	0.45
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.98	0.45
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.99	0.45
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.98	0.45
1:A:1032:VAL:HG21	1:A:1179:ILE:HG12	1.99	0.45
11:K:59:THR:CG2	11:K:108:TYR:O	2.65	0.45
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.99	0.45
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.98	0.45
1:A:1014:SER:HA	1:A:1223:ARG:HH22	1.82	0.45
9:I:72:LYS:HB2	9:I:75:GLU:HB2	1.98	0.45
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.82	0.44
1:A:657:TYR:HA	1:A:667:ARG:HG3	1.99	0.44
2:B:940:GLU:OE2	3:C:228:ARG:HB2	2.17	0.44
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.98	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	2.00	0.44
1:A:1384:TYR:HE2	2:B:1077:ASP:OD2	2.00	0.44
2:B:65:VAL:HA	2:B:68:ILE:HG12	1.98	0.44
3:C:195:LYS:HB3	10:J:61:LEU:HD11	1.99	0.44
2:B:480:GLN:CD	2:B:480:GLN:H	2.26	0.44
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.99	0.44
5:E:141:VAL:HG12	5:E:142:VAL:HG23	1.99	0.44
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.99	0.44
7:G:30:GLU:HG2	7:G:32:ASN:HB2	1.99	0.44
1:A:671:GLN:HE22	2:B:784:ASP:HB2	1.83	0.44
2:B:13:THR:HG21	2:B:977:ILE:HB	2.00	0.44
1:A:128:GLY:H	1:A:207:SER:HB3	1.82	0.44
6:F:107:VAL:HG12	6:F:109:VAL:H	1.83	0.44
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.00	0.44
1:A:124:LEU:HD21	1:A:189:VAL:HA	1.98	0.43
1:A:862:THR:HA	9:I:67:VAL:HG12	1.99	0.43
2:B:788:ILE:HB	2:B:948:ILE:HB	2.00	0.43
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.00	0.43
1:A:1626:VAL:HG21	2:B:1194:ILE:HG12	1.99	0.43
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	2.00	0.43
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.18	0.43
2:B:61:LEU:HD21	2:B:413:LEU:HD13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:HB2	2:B:716:MET:HE1	2.00	0.43
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.01	0.43
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.00	0.43
6:F:94:LEU:HD21	6:F:125:LEU:HD22	2.00	0.43
3:C:229:LEU:HD21	3:C:295:ARG:HA	2.01	0.43
3:C:229:LEU:HD23	3:C:293:ARG:HB3	2.00	0.43
10:J:32:GLU:H	10:J:32:GLU:HG2	1.52	0.43
11:K:57:ASP:HA	11:K:58:GLY:HA2	1.82	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.18	0.43
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.01	0.43
1:A:1261:VAL:HG11	1:A:1308:VAL:HG21	2.00	0.43
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.00	0.43
2:B:526:GLY:HA2	2:B:696:ILE:HA	2.01	0.43
13:M:9:GLU:HA	14:N:71:PRO:HA	2.01	0.42
1:A:387:SER:HA	1:A:390:LEU:HD12	2.01	0.42
1:A:490:ILE:HG22	1:A:606:ARG:HD3	2.01	0.42
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.01	0.42
1:A:456:VAL:HG21	2:B:1192:MET:HG3	2.01	0.42
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.01	0.42
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.42
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.01	0.42
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.02	0.42
2:B:561:ILE:HG12	2:B:620:LEU:HD12	2.00	0.42
1:A:385:LEU:HD13	1:A:437:PHE:HA	2.01	0.42
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.01	0.42
1:A:646:GLU:HB3	2:B:1084:THR:OG1	2.20	0.42
2:B:15:ASP:HA	2:B:978:ALA:HB3	2.01	0.42
2:B:19:LEU:HD11	10:J:26:GLN:HG2	2.01	0.42
2:B:251:HIS:HE1	2:B:261:ARG:HD2	1.85	0.42
11:K:59:THR:HG21	11:K:108:TYR:O	2.20	0.42
12:L:28:LYS:HB2	12:L:59:ALA:HB3	2.02	0.42
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.02	0.42
2:B:139:LEU:HD22	2:B:417:ILE:HD13	2.02	0.41
2:B:703:LEU:HD11	2:B:762:MET:HE3	2.02	0.41
3:C:233:ILE:HB	3:C:267:VAL:HG11	2.01	0.41
2:B:207:ILE:HB	2:B:505:ARG:HA	2.02	0.41
13:M:20:SER:HB3	14:N:36:LYS:HB2	2.01	0.41
2:B:840:LEU:HA	2:B:846:PRO:HA	2.03	0.41
1:A:805:VAL:O	1:A:809:VAL:HG23	2.20	0.41
1:A:827:THR:HG21	2:B:1026:ILE:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:ALA:HB2	2:B:907:ILE:HG13	2.01	0.41
2:B:260:PHE:HB3	2:B:271:VAL:HG23	2.03	0.41
7:G:264:ARG:H	7:G:267:ALA:HB3	1.85	0.41
9:I:95:ASN:HB2	9:I:113:THR:HB	2.02	0.41
13:M:32:ALA:HB1	13:M:33:PRO:HD2	2.03	0.41
5:E:6:GLU:HA	5:E:9:ILE:HD12	2.03	0.41
8:H:93:TYR:HA	8:H:145:ARG:HG3	2.03	0.41
1:A:502:ALA:HA	1:A:581:ILE:HG22	2.02	0.41
1:A:855:ARG:HH21	1:A:867:ASP:HB3	1.84	0.41
1:A:1384:TYR:CE2	2:B:1074:MET:HG2	2.56	0.41
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.02	0.41
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
2:B:211:ARG:HH22	2:B:243:GLN:NE2	2.18	0.41
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.03	0.41
9:I:112:TYR:HB2	9:I:121:PHE:HB3	2.03	0.41
1:A:1344:ILE:HG12	2:B:275:MET:HE1	2.03	0.41
2:B:967:LEU:HD13	2:B:996:PHE:HB2	2.03	0.41
2:B:1076:ARG:HG3	2:B:1092:LEU:HD11	2.03	0.41
3:C:223:SER:HB2	3:C:303:GLU:HB2	2.03	0.41
3:C:252:PRO:HD2	3:C:255:VAL:HG21	2.03	0.41
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
1:A:233:CYS:HB3	1:A:236:CYS:O	2.21	0.40
2:B:17:ARG:H	2:B:17:ARG:HG2	1.64	0.40
8:H:40:LEU:HB2	8:H:123:MET:HG3	2.02	0.40
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.03	0.40
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	2.03	0.40
2:B:962:MET:HE3	2:B:1031:VAL:HG11	2.04	0.40
9:I:11:LEU:HD22	13:M:31:ARG:HG3	2.03	0.40
8:H:28:ALA:HB3	8:H:38:LEU:HB3	2.03	0.40
1:A:49:LEU:HD12	1:A:368:ARG:HH21	1.85	0.40
1:A:990:ILE:HD12	1:A:995:TYR:HA	2.04	0.40
4:D:26:GLN:HB2	7:G:42:PRO:HG2	2.02	0.40
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.04	0.40
1:A:1121:ASP:HA	5:E:207:ARG:HH22	1.85	0.40
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.02	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	1503/1664 (90%)	1422 (95%)	79 (5%)	2 (0%)	48	76
2	B	1166/1203 (97%)	1094 (94%)	68 (6%)	4 (0%)	36	63
3	C	300/335 (90%)	283 (94%)	17 (6%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	95 (97%)	3 (3%)	0	100	100
7	G	251/326 (77%)	232 (92%)	17 (7%)	2 (1%)	16	44
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	16	44
9	I	120/125 (96%)	108 (90%)	12 (10%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	95 (94%)	5 (5%)	1 (1%)	12	38
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	M	101/415 (24%)	94 (93%)	7 (7%)	0	100	100
14	N	131/233 (56%)	122 (93%)	9 (7%)	0	100	100
All	All	4279/5236 (82%)	4020 (94%)	249 (6%)	10 (0%)	43	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1389	GLU
1	A	237	GLY
2	B	532	HIS
2	B	1154	ASP
11	K	46	LYS
2	B	339	GLN
2	B	359	LEU
8	H	84	ALA
7	G	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	127	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1343/1465 (92%)	1251 (93%)	92 (7%)	14	40
2	B	1024/1053 (97%)	922 (90%)	102 (10%)	7	26
3	C	269/296 (91%)	241 (90%)	28 (10%)	7	24
4	D	56/116 (48%)	50 (89%)	6 (11%)	6	23
5	E	197/197 (100%)	188 (95%)	9 (5%)	24	50
6	F	90/137 (66%)	86 (96%)	4 (4%)	25	51
7	G	234/291 (80%)	216 (92%)	18 (8%)	12	37
8	H	116/128 (91%)	108 (93%)	8 (7%)	14	40
9	I	109/110 (99%)	97 (89%)	12 (11%)	6	22
10	J	64/65 (98%)	56 (88%)	8 (12%)	4	17
11	K	93/130 (72%)	87 (94%)	6 (6%)	15	42
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	26
13	M	94/371 (25%)	87 (93%)	7 (7%)	13	38
14	N	128/220 (58%)	114 (89%)	14 (11%)	6	22
All	All	3857/4636 (83%)	3539 (92%)	318 (8%)	10	35

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	49	LEU
1	A	59	ARG
1	A	94	LEU
1	A	103	LEU
1	A	113	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	227	LEU
1	A	250	LYS
1	A	270	ILE
1	A	322	ASN
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	373	LEU
1	A	398	ASP
1	A	399	LEU
1	A	403	LEU
1	A	413	LEU
1	A	423	LEU
1	A	484	ILE
1	A	518	GLU
1	A	536	ILE
1	A	539	GLU
1	A	562	LEU
1	A	572	THR
1	A	586	VAL
1	A	587	VAL
1	A	632	GLU
1	A	684	ASP
1	A	715	LEU
1	A	727	THR
1	A	743	ASP
1	A	747	ILE
1	A	821	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR
1	A	862	THR
1	A	878	ARG
1	A	880	GLN
1	A	952	LEU
1	A	957	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	960	MET
1	A	1004	GLU
1	A	1059	LYS
1	A	1065	GLN
1	A	1086	ILE
1	A	1136	VAL
1	A	1164	LYS
1	A	1169	LEU
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1190	SER
1	A	1193	VAL
1	A	1205	PHE
1	A	1217	LEU
1	A	1227	MET
1	A	1240	LEU
1	A	1242	ILE
1	A	1252	ASP
1	A	1263	LEU
1	A	1273	THR
1	A	1313	LEU
1	A	1343	ASP
1	A	1365	LEU
1	A	1380	GLN
1	A	1388	ASP
1	A	1389	GLU
1	A	1392	ILE
1	A	1396	ARG
1	A	1474	LEU
1	A	1475	GLU
1	A	1481	GLU
1	A	1501	ILE
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1550	LEU
1	A	1552	THR
1	A	1592	GLN
1	A	1609	SER
1	A	1628	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1629	ASN
1	A	1649	VAL
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	60	LEU
2	B	61	LEU
2	B	73	ILE
2	B	101	GLN
2	B	108	MET
2	B	139	LEU
2	B	150	GLU
2	B	163	VAL
2	B	168	ASN
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	212	ASN
2	B	217	ILE
2	B	218	ILE
2	B	234	ILE
2	B	250	LEU
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	297	VAL
2	B	306	LEU
2	B	332	ASP
2	B	356	ARG
2	B	364	LYS
2	B	374	LEU
2	B	381	LEU
2	B	413	LEU
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	455	GLU
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	491	ILE
2	B	502	MET
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	588	ILE
2	B	592	ILE
2	B	593	ILE
2	B	616	LYS
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	723	LYS
2	B	743	ARG
2	B	752	VAL
2	B	789	ILE
2	B	794	ASP
2	B	821	ILE
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	858	ILE
2	B	859	CYS
2	B	871	ILE
2	B	873	THR
2	B	887	LEU
2	B	888	ILE
2	B	896	GLN
2	B	897	GLU
2	B	933	THR
2	B	940	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	944	GLN
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE
2	B	988	GLU
2	B	1000	LEU
2	B	1020	GLU
2	B	1028	VAL
2	B	1037	ARG
2	B	1041	ASN
2	B	1065	ARG
2	B	1076	ARG
2	B	1103	VAL
2	B	1110	ILE
2	B	1120	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	119	ASN
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	185	VAL
3	C	209	ILE
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	239	ILE
3	C	240	LYS
3	C	258	ILE
3	C	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU
3	C	311	GLU
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL
4	D	25	THR
4	D	27	LEU
4	D	89	LEU
5	E	84	ASP
5	E	106	GLN
5	E	122	LYS
5	E	127	ILE
5	E	154	ILE
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
5	E	204	THR
6	F	69	LEU
6	F	99	LEU
6	F	103	MET
6	F	111	LEU
7	G	22	LYS
7	G	32	ASN
7	G	54	LEU
7	G	75	ASN
7	G	85	GLU
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	111	THR
7	G	128	GLN
7	G	144	HIS
7	G	174	GLU
7	G	214	LEU
7	G	217	TRP
7	G	223	GLU
7	G	248	THR
7	G	250	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	316	GLU
8	H	22	LYS
8	H	23	VAL
8	H	33	GLN
8	H	53	ASP
8	H	63	LEU
8	H	89	LEU
8	H	132	LEU
8	H	136	LYS
9	I	3	VAL
9	I	23	VAL
9	I	24	LEU
9	I	27	ASN
9	I	51	THR
9	I	53	ASP
9	I	60	LEU
9	I	73	LYS
9	I	76	LEU
9	I	77	LYS
9	I	82	ILE
9	I	99	LEU
10	J	2	ILE
10	J	14	VAL
10	J	22	LEU
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	41	GLU
11	K	59	THR
11	K	99	ASN
11	K	103	ILE
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	40	LEU
12	L	62	LYS
13	M	48	LYS
13	M	50	GLU
13	M	53	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	56	GLU
13	M	88	ILE
13	M	101	VAL
13	M	108	LEU
14	N	25	ILE
14	N	36	LYS
14	N	49	LYS
14	N	67	LEU
14	N	74	PHE
14	N	78	THR
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	164	GLU
14	N	166	LEU
14	N	168	LEU
14	N	178	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	260	GLN
1	A	263	ASN
1	A	332	GLN
1	A	431	GLN
1	A	432	ASN
1	A	538	ASN
1	A	580	HIS
1	A	590	ASN
1	A	592	GLN
1	A	610	ASN
1	A	636	HIS
1	A	639	GLN
1	A	642	ASN
1	A	671	GLN
1	A	693	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	748	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	753	ASN
1	A	785	GLN
1	A	798	HIS
1	A	819	ASN
1	A	901	ASN
1	A	926	GLN
1	A	949	GLN
1	A	1026	GLN
1	A	1113	HIS
1	A	1171	GLN
1	A	1293	HIS
1	A	1299	ASN
1	A	1319	ASN
1	A	1320	GLN
1	A	1323	HIS
1	A	1373	GLN
1	A	1380	GLN
1	A	1440	ASN
1	A	1599	ASN
1	A	1647	ASN
2	B	80	ASN
2	B	87	ASN
2	B	128	GLN
2	B	146	ASN
2	B	151	ASN
2	B	166	GLN
2	B	182	GLN
2	B	212	ASN
2	B	213	HIS
2	B	243	GLN
2	B	251	HIS
2	B	282	HIS
2	B	344	GLN
2	B	351	GLN
2	B	361	HIS
2	B	400	GLN
2	B	479	GLN
2	B	480	GLN
2	B	547	HIS
2	B	636	GLN
2	B	646	HIS
2	B	683	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	735	HIS
2	B	755	ASN
2	B	767	ASN
2	B	875	HIS
2	B	912	GLN
2	B	975	HIS
2	B	999	GLN
2	B	1041	ASN
2	B	1089	GLN
2	B	1094	ASN
2	B	1199	ASN
3	C	58	ASN
3	C	232	GLN
3	C	248	GLN
4	D	30	HIS
5	E	5	ASN
5	E	147	HIS
5	E	179	GLN
6	F	100	GLN
7	G	26	ASN
7	G	64	GLN
7	G	65	HIS
7	G	128	GLN
7	G	140	GLN
7	G	150	HIS
7	G	160	ASN
7	G	170	HIS
7	G	216	HIS
7	G	261	ASN
7	G	275	ASN
8	H	11	GLN
8	H	33	GLN
8	H	35	GLN
8	H	64	ASN
9	I	91	ASN
9	I	100	GLN
10	J	64	ASN
11	K	64	GLN
11	K	106	GLN
13	M	16	GLN
13	M	71	GLN
14	N	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	132	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 7 ligands modelled in this entry, 7 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	79:GLY	C	80:ALA	N	4.36

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	1523/1664 (91%)	0.07	27 (1%) 67 51	82, 114, 166, 248	0
2	B	1176/1203 (97%)	0.17	20 (1%) 69 53	80, 119, 170, 238	0
3	C	304/335 (90%)	0.05	4 (1%) 75 61	108, 134, 171, 191	0
4	D	59/137 (43%)	-0.11	0 100 100	114, 157, 188, 193	0
5	E	215/215 (100%)	0.12	2 (0%) 81 69	95, 143, 193, 201	0
6	F	100/155 (64%)	-0.32	0 100 100	88, 115, 156, 167	0
7	G	259/326 (79%)	0.42	18 (6%) 23 18	102, 167, 256, 274	0
8	H	134/146 (91%)	0.21	0 100 100	114, 141, 173, 184	0
9	I	124/125 (99%)	0.60	12 (9%) 13 12	105, 177, 215, 229	0
10	J	69/70 (98%)	0.11	1 (1%) 73 59	105, 124, 150, 176	0
11	K	103/142 (72%)	-0.10	0 100 100	101, 125, 165, 206	0
12	L	45/70 (64%)	0.21	0 100 100	130, 156, 183, 191	0
13	M	105/415 (25%)	0.85	12 (11%) 10 10	161, 209, 254, 264	0
14	N	139/233 (59%)	0.65	14 (10%) 12 12	113, 211, 252, 271	0
All	All	4355/5236 (83%)	0.16	110 (2%) 58 43	80, 126, 209, 274	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ILE	4.1
7	G	95	LEU	4.1
9	I	103	SER	4.0
14	N	107	MET	4.0
13	M	17	ASP	3.9
9	I	99	LEU	3.9
7	G	314	THR	3.9
1	A	1205	PHE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	70	LEU	3.8
1	A	1340	THR	3.7
1	A	1663	ALA	3.7
2	B	1140	LYS	3.6
1	A	269	PHE	3.5
1	A	264	ASN	3.5
9	I	108	ALA	3.5
14	N	111	VAL	3.4
13	M	77	VAL	3.4
1	A	1483	LEU	3.3
3	C	150	SER	3.3
9	I	87	PRO	3.2
1	A	328	PHE	3.2
2	B	577	PHE	3.2
7	G	245	VAL	3.2
14	N	125	ALA	3.1
14	N	54	TRP	3.1
14	N	106	ASN	3.1
13	M	25	SER	3.1
13	M	40	LEU	3.0
14	N	56	ILE	3.0
9	I	120	LYS	3.0
1	A	266	VAL	3.0
1	A	1388	ASP	2.9
2	B	746	THR	2.9
14	N	55	LEU	2.9
1	A	97	TYR	2.9
1	A	141	LEU	2.9
14	N	109	LEU	2.9
1	A	1442	VAL	2.8
2	B	556	SER	2.7
13	M	38	PHE	2.7
1	A	128	GLY	2.7
9	I	71	LEU	2.7
14	N	121	ILE	2.6
7	G	237	HIS	2.6
2	B	903	ILE	2.6
2	B	14	ALA	2.6
14	N	108	THR	2.6
9	I	85	LYS	2.6
14	N	30	LYS	2.6
14	N	113	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	23	GLN	2.6
7	G	304	ASN	2.5
1	A	1013	THR	2.5
1	A	628	PHE	2.5
1	A	1342	PRO	2.5
13	M	23	VAL	2.5
1	A	1290	TYR	2.5
7	G	273	VAL	2.5
9	I	105	ASP	2.4
13	M	93	ALA	2.4
13	M	78	VAL	2.4
7	G	128	GLN	2.4
7	G	303	ASP	2.4
3	C	217	ALA	2.4
1	A	355	PHE	2.4
1	A	406	LEU	2.4
3	C	144	PRO	2.4
7	G	173	VAL	2.4
2	B	782	ASP	2.4
2	B	785	ASP	2.3
1	A	251	ILE	2.3
7	G	267	ALA	2.3
2	B	555	GLN	2.3
10	J	69	ARG	2.3
2	B	420	TYR	2.3
9	I	42	PHE	2.3
2	B	783	MET	2.3
14	N	40	LEU	2.3
1	A	1461	ASN	2.3
7	G	315	SER	2.3
1	A	1026	GLN	2.3
7	G	251	SER	2.2
7	G	74	ASN	2.2
7	G	244	SER	2.2
5	E	3	GLN	2.2
13	M	18	GLN	2.2
9	I	98	THR	2.2
2	B	163	VAL	2.2
13	M	113	ILE	2.2
3	C	265	ALA	2.2
2	B	813	LEU	2.1
2	B	786	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	26	PHE	2.1
5	E	2	ASP	2.1
7	G	24	VAL	2.1
9	I	119	TYR	2.1
2	B	372	ARG	2.1
1	A	1479	ASP	2.1
2	B	525	TRP	2.1
1	A	963	GLY	2.1
7	G	271	PRO	2.1
7	G	283	GLU	2.1
13	M	99	LYS	2.0
1	A	1016	SER	2.0
9	I	40	SER	2.0
2	B	784	ASP	2.0
2	B	1166	LYS	2.0
1	A	1374	SER	2.0
2	B	212	ASN	2.0
2	B	340	ALA	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
15	ZN	I	1127	1/1	0.97	0.09	156,156,156,156	0
15	ZN	I	1126	1/1	0.99	0.08	151,151,151,151	0
15	ZN	A	2664	1/1	0.99	0.03	122,122,122,122	0
15	ZN	L	1071	1/1	0.99	0.02	136,136,136,136	0
15	ZN	B	2204	1/1	1.00	0.02	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ZN	J	1070	1/1	1.00	0.06	111,111,111,111	0
15	ZN	A	2665	1/1	1.00	0.02	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.