



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3RZO
Title : RNA Polymerase II Initiation Complex with a 4-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-12
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

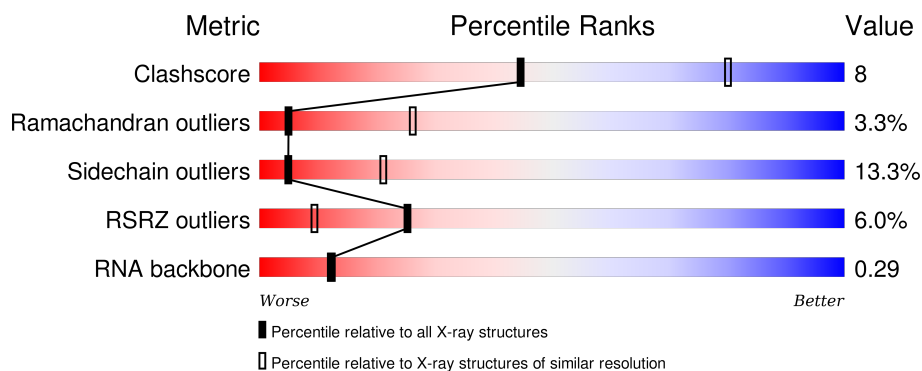
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>8%</div> <div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>4%</div> <div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div>
4	E	215	<div> <div>6%</div> <div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>
5	F	155	<div> <div>43%</div> <div>10%</div> <div>•</div> <div>45%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	146	<div><div></div><div>5%</div><div>61%</div><div>28%</div><div>9%</div></div>
7	I	122	<div><div></div><div>2%</div><div>77%</div><div>19%</div><div></div></div>
8	J	70	<div><div></div><div>56%</div><div>29%</div><div>9%</div><div>7%</div></div>
9	K	120	<div><div></div><div>76%</div><div>14%</div><div>5%</div><div>5%</div></div>
10	L	70	<div><div></div><div>4%</div><div>29%</div><div>26%</div><div>10%</div><div></div><div>34%</div></div>
11	R	4	<div><div></div><div>50%</div><div>100%</div></div>
12	T	29	<div><div></div><div>10%</div><div>7%</div><div>21%</div><div>72%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28547 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	4	Total	C	N	O	P	0	0	0
			88	40	20	25	3			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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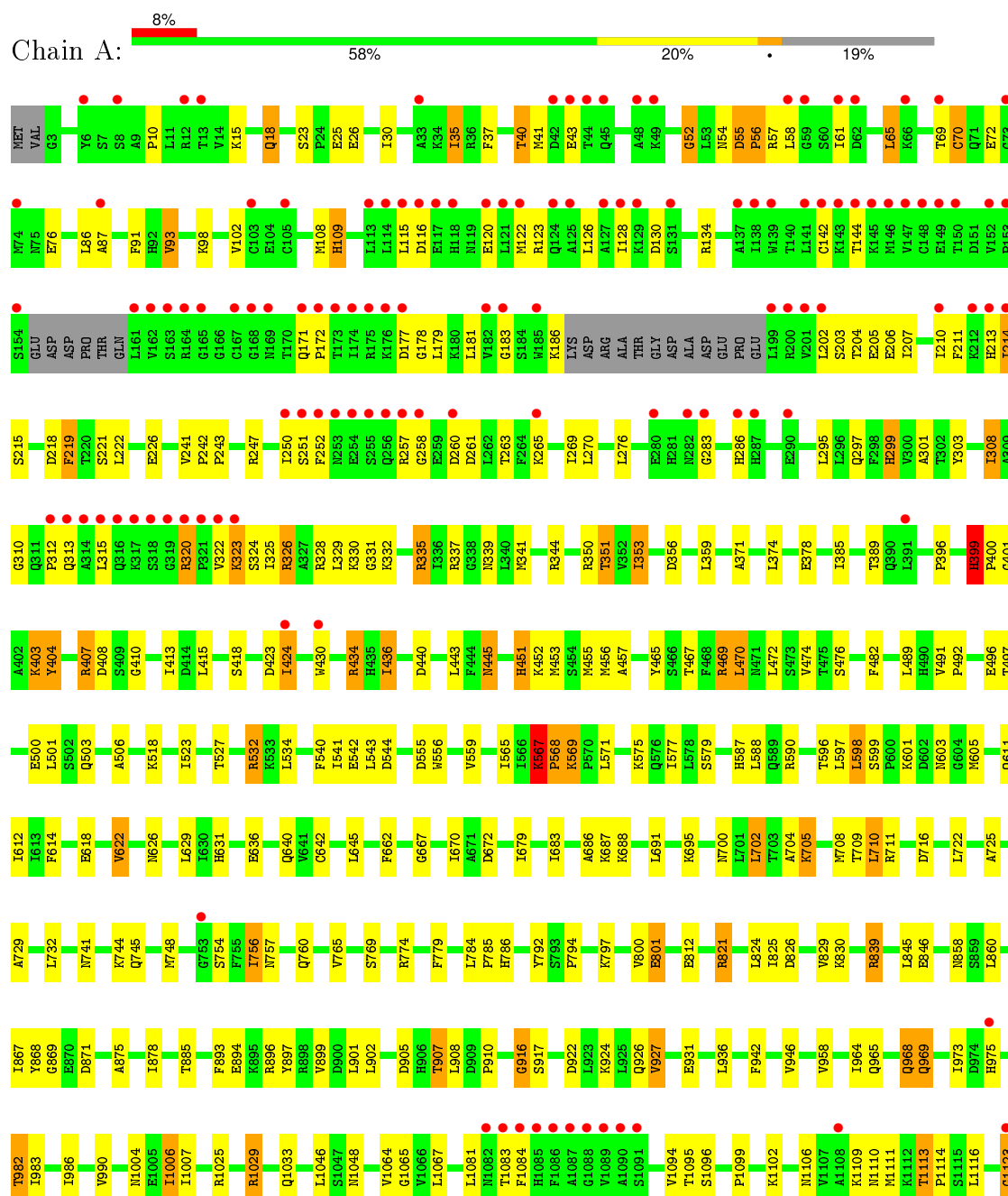
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

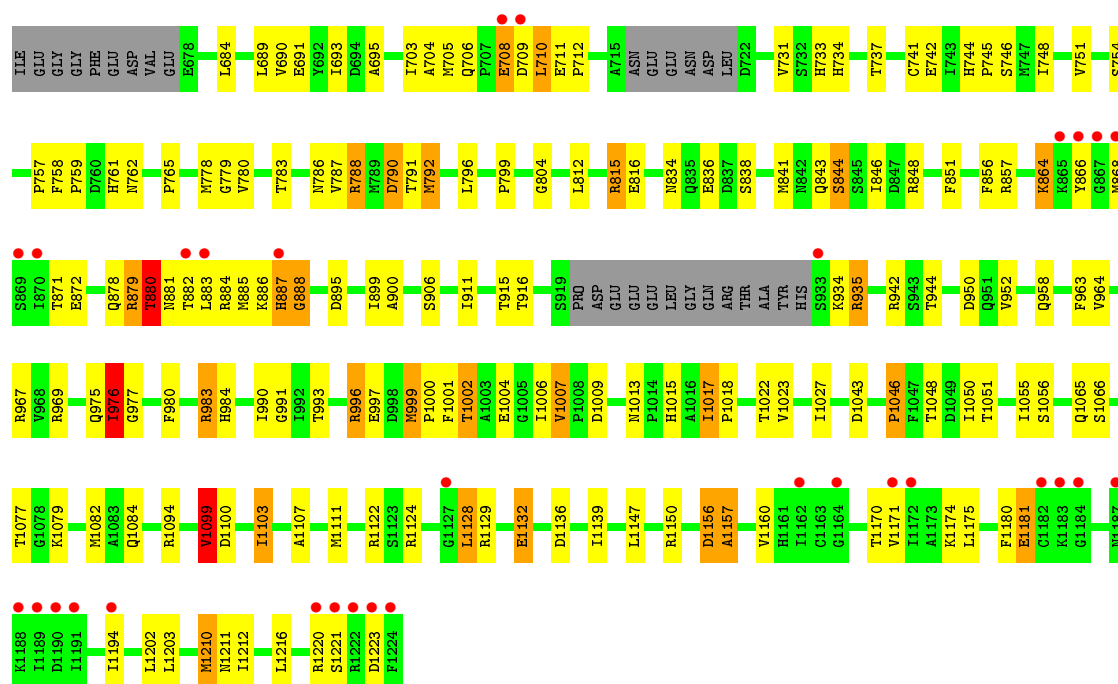
3 Residue-property plots

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

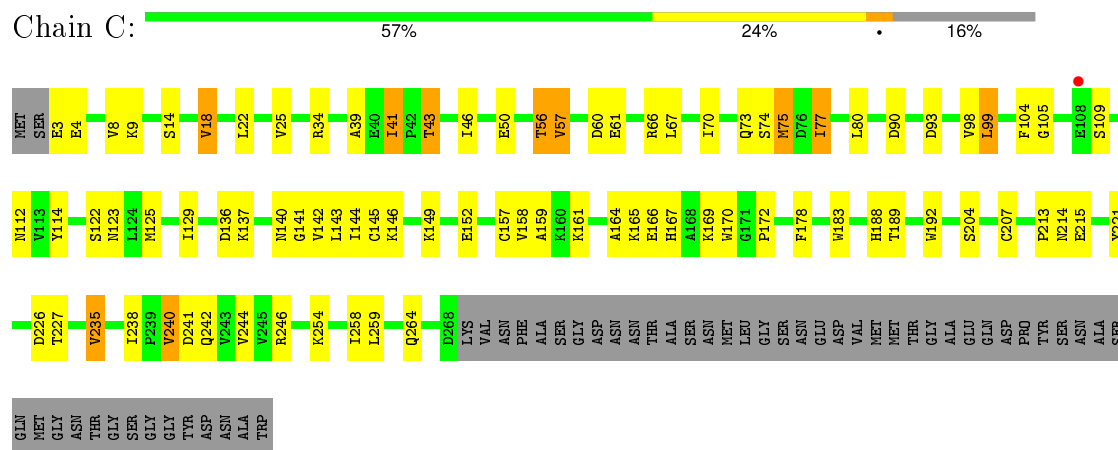
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



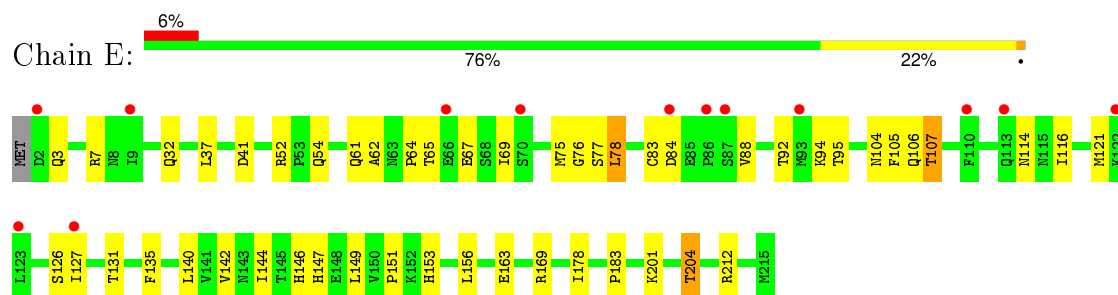




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



MET SER ASP TYR GLU ALA PHE ASN ASP GLY ASN GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU LYS LYS ASP THR THR GLY ASN GLY PRO ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS E71 K72 K76 R79 T82 E89 R90 I93 F108 Y109 D110 L111 L118 K123 K129 PHE PHE LYS ASP R134 R135 R136 S142 T146 W146 D154 L155

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 5% 61% 28% 9%

MET S2 R3 Q11 V12 S13 E14 V15 K22 V23 C24 R25 I26 Q35 F47 S61 S62 L63 ASN LEU GLU ASP THR PRO PRQ ALA ASN ASP SER SER SER ALA T76 R77 S78 Q83 Q84 Q85 D86 R87 S88 L89 A90 D91 D92 Y93 D94 Y95 Y96 N97 T100 S108 K109 D110

L111 T112 A113 G120 L121 L122 E126 R130 M131 L132 L135 K136 Q137 E138 M139 A140 R145 R146

- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 77% 19% 2%

MET T2 N12 L26 E27 E28 V35 E36 E37 P41 Q60 D61 L63 F69 R70 C75 F76 K77 C78 N83 V84 Q87 Q90 D94 D95 S96 M97 L104 T111 K115 R118 T119 Q120 PHE SER

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 56% 29% 9% 7%

M1 I2 V3 R6 C7 C10 G11 K12 V13 V14 W18 E19 L22 Q26 E27 D28 D31 R43 R48 M49 I50 L51 T52 K59 F60 L61 R62 Y63 R64 P65 LEU GLU LYS ARG ASP

- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 76% 14% 5% 5%

M1 R6 F7 F10 L11 E14 G15 E16 A17 K18 L19 K20 I21 K26 V31 V32 I33 L51 V63 E64 H65 P66 F67 R74 L101 E108 W109 W110 L111 L114 ALA ASP ASP ALA PHE

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 4% 29% 26% 10% 34%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 K28 A32 F33 C34 S35 S36 K37 L38 S39 R42 T43 D44 A45 V46 R47 D50 C51 G52 H53 F54 I55 L56 K58 A59 T61 A62 R63 L64

V65 Q66 F67 R70

- Molecule 11: RNA (5'-R(*GP*AP*GP*G)-3')

Chain R: 50% 100%



● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.04Å 221.15Å 192.88Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	40.01 – 3.00 40.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.01-3.00) 99.3 (40.01-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.236 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 132696 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28547	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.48	0/11241	0.76	2/15199 (0.0%)
2	B	0.52	0/9033	0.79	4/12181 (0.0%)
3	C	0.47	0/2133	0.80	0/2891
4	E	0.45	0/1788	0.71	0/2406
5	F	0.46	0/700	0.70	0/945
6	H	0.47	0/1086	0.82	1/1470 (0.1%)
7	I	0.48	0/989	0.79	0/1331
8	J	0.55	0/541	0.86	0/727
9	K	0.45	0/937	0.70	0/1265
10	L	0.54	0/365	0.93	1/485 (0.2%)
11	R	0.88	0/99	1.45	0/154
12	T	1.25	0/176	2.19	12/268 (4.5%)
All	All	0.50	0/29088	0.80	20/39322 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.75	114.12	108.00
2	B	647	GLY	C-N-CA	8.32	142.50	121.70
12	T	22	DT	P-O3'-C3'	7.60	128.82	119.70
12	T	16	DC	C2-N1-C1'	6.96	126.45	118.80
12	T	20	DC	O4'-C1'-N1	6.96	112.87	108.00
12	T	19	DT	O4'-C1'-N1	6.89	112.83	108.00
2	B	648	HIS	N-CA-CB	6.82	122.87	110.60
12	T	16	DC	N1-C2-O2	6.67	122.90	118.90
12	T	23	DC	O4'-C1'-N1	6.36	112.45	108.00
12	T	16	DC	P-O3'-C3'	5.68	126.52	119.70
1	A	451	HIS	CB-CA-C	-5.60	99.19	110.40
12	T	16	DC	C6-N1-C1'	-5.57	114.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	N1-C1'-C2'	5.38	122.82	112.60
6	H	2	SER	C-N-CA	5.37	135.13	121.70
2	B	140	ILE	C-N-CA	5.25	134.81	121.70
10	L	50	ASP	C-N-CA	5.18	134.65	121.70
12	T	17	DG	O4'-C4'-C3'	-5.16	102.44	104.50
1	A	399	HIS	N-CA-CB	5.12	119.82	110.60
2	B	476	ARG	C-N-CA	5.07	134.36	121.70
12	T	17	DG	C1'-O4'-C4'	-5.03	105.07	110.10

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	11043	0	11133	182	0
2	B	8861	0	8884	190	0
3	C	2095	0	2051	51	0
4	E	1752	0	1776	18	0
5	F	688	0	707	9	0
6	H	1068	0	1040	12	0
7	I	971	0	927	7	0
8	J	532	0	542	20	0
9	K	919	0	929	16	0
10	L	363	0	386	13	0
11	R	88	0	46	0	0
12	T	159	0	91	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28547	0	28512	452	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 8.

All (452) 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:A:756:ILE:CD1	1:A:756:ILE:CG1	1.77	1.56
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.90	1.06
1:A:869:GLY:O	4:E:204:THR:HG21	1.63	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.89	0.88
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.88
6:H:2:SER:HB2	6:H:3:ASN:HB2	1.56	0.88
8:J:48:ARG:O	8:J:52:THR:HG22	1.76	0.84
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.22	0.83
3:C:56:THR:HG21	3:C:145:CYS:SG	2.20	0.82
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.61	0.82
1:A:901:LEU:HA	1:A:907:THR:HG23	1.60	0.82
1:A:741:ASN:HD22	1:A:744:LYS:H	1.29	0.81
5:F:110:ASP:O	5:F:123:LYS:HE2	1.81	0.80
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.63	0.79
1:A:754:SER:H	1:A:757:ASN:HD22	1.30	0.77
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.66	0.76
2:B:276:ILE:HG13	2:B:334:ILE:HG23	1.68	0.76
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.69	0.74
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.74
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.72	0.72
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.54	0.72
3:C:167:HIS:HD2	3:C:169:LYS:H	1.36	0.71
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.74	0.69
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.58	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.38	0.69
1:A:756:ILE:H	1:A:756:ILE:HD13	1.58	0.69
4:E:77:SER:HB3	4:E:105:PHE:HA	1.74	0.68
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.58	0.68
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.76	0.67
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.77	0.67
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.67
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.43	0.66
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.66
1:A:1364:ASN:HD21	1:A:1366:ARG:HD2	1.61	0.65
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.62	0.65
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.79	0.64
2:B:848:ARG:HH22	2:B:996:ARG:NH1	1.95	0.64
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:HA	2:B:838:SER:HB2	1.78	0.64
2:B:516:ASN:HD22	2:B:516:ASN:H	1.46	0.64
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.80	0.63
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.12	0.63
1:A:946:VAL:HG13	4:E:201:LYS:HB3	1.81	0.63
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.79	0.63
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.80	0.63
2:B:54:PHE:HA	2:B:58:THR:HB	1.80	0.63
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.81	0.63
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.81	0.63
2:B:864:LYS:HB3	2:B:872:GLU:H	1.61	0.62
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.64	0.62
1:A:469:ARG:NH2	2:B:991:GLY:O	2.32	0.62
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.14	0.62
1:A:567:LYS:HB3	6:H:96:VAL:H	1.63	0.62
3:C:165:LYS:O	9:K:6:ARG:NH1	2.33	0.62
1:A:705:LYS:HE3	1:A:705:LYS:H	1.65	0.62
2:B:260:GLY:O	2:B:267:ARG:HD3	1.99	0.62
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.64	0.61
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.82	0.61
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.81	0.61
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.81	0.61
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.81	0.61
3:C:73:GLN:HE21	3:C:75:MET:H	1.49	0.61
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.54	0.60
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.31	0.60
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.67	0.60
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.84	0.60
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.84	0.60
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.83	0.60
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.84	0.59
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.83	0.59
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.84	0.59
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.48	0.59
1:A:404:TYR:HA	1:A:413:ILE:O	2.03	0.59
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.84	0.59
2:B:345:LYS:HA	2:B:347:LYS:H	1.67	0.59
2:B:887:HIS:HA	2:B:888:GLY:O	2.03	0.58
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.84	0.58
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.51	0.58
8:J:48:ARG:O	8:J:52:THR:CG2	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.39	0.58
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.03	0.58
3:C:41:ILE:HD12	3:C:246:ARG:HB2	1.86	0.58
9:K:65:HIS:CD2	9:K:67:PHE:H	2.22	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.58
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.86	0.57
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.85	0.57
2:B:887:HIS:HA	2:B:888:GLY:C	2.24	0.57
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.86	0.57
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.40	0.57
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.85	0.57
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.87	0.57
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.86	0.57
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.57
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.86	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.87	0.56
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.87	0.56
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.88	0.56
2:B:843:GLN:HB2	2:B:993:THR:HB	1.86	0.56
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.89	0.56
1:A:924:LYS:O	1:A:927:VAL:HG12	2.06	0.56
2:B:975:GLN:HG2	2:B:976:ILE:H	1.69	0.56
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.88	0.55
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.88	0.55
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.05	0.55
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.35	0.55
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.89	0.55
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.31	0.54
2:B:705:MET:H	2:B:710:LEU:HG	1.73	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.40	0.54
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.43	0.54
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.88	0.54
1:A:313:GLN:HG2	1:A:322:VAL:HG22	1.88	0.54
2:B:357:GLN:HG2	2:B:368:GLU:HA	1.89	0.54
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.43	0.54
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.54	0.54
1:A:741:ASN:ND2	1:A:744:LYS:H	2.00	0.54
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.54
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.72	0.54
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.43	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.54
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.54
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.90	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.89	0.53
2:B:915:THR:HG21	2:B:934:LYS:HD2	1.89	0.53
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.88	0.53
2:B:213:ILE:HG12	2:B:481:GLN:HG3	1.90	0.53
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.90	0.53
8:J:6:ARG:HG2	8:J:11:GLY:O	2.09	0.53
2:B:222:ILE:HD13	2:B:403:LYS:HG3	1.90	0.53
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.44	0.53
2:B:983:ARG:HB2	2:B:983:ARG:HH11	1.74	0.52
2:B:999:MET:HA	2:B:999:MET:CE	2.39	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.90	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.52
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.74	0.52
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.39	0.52
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.52
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.44	0.52
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.92	0.52
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.90	0.52
9:K:65:HIS:HD2	9:K:67:PHE:H	1.56	0.52
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.92	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.09	0.51
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.91	0.51
2:B:516:ASN:ND2	2:B:516:ASN:H	2.08	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HG12	1.93	0.51
1:A:1096:SER:O	1:A:1099:PRO:HD2	2.11	0.51
2:B:58:THR:O	2:B:62:ILE:HG12	2.10	0.51
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.92	0.51
8:J:12:LYS:HD2	8:J:43:ARG:HH12	1.76	0.51
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50
3:C:46:ILE:HA	3:C:159:ALA:HA	1.93	0.50
2:B:976:ILE:HG23	2:B:977:GLY:H	1.75	0.50
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:VAL:HG13	6:H:78:SER:HA	1.93	0.50
5:F:111:LEU:H	5:F:111:LEU:HD12	1.77	0.50
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.75	0.50
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.92	0.50
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.50
1:A:756:ILE:CD1	1:A:756:ILE:H	2.23	0.50
2:B:705:MET:N	2:B:710:LEU:HG	2.27	0.50
2:B:804:GLY:O	2:B:983:ARG:NH2	2.45	0.50
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.94	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.93	0.50
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.93	0.50
1:A:826:ASP:HA	1:A:829:VAL:HB	1.94	0.50
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.77	0.49
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.94	0.49
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.47	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.93	0.49
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.93	0.49
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.92	0.49
10:L:27:LEU:HB3	10:L:37:LYS:HG2	1.94	0.49
4:E:65:THR:HG22	4:E:67:GLU:H	1.77	0.49
2:B:466:TRP:HB3	2:B:475:SER:HB3	1.93	0.49
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.93	0.49
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.12	0.49
2:B:476:ARG:O	2:B:478:GLY:N	2.45	0.49
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.49
2:B:256:VAL:HG12	2:B:385:LEU:HD22	1.93	0.49
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.25	0.49
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.44	0.49
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.95	0.49
1:A:626:ASN:O	1:A:631:HIS:CD2	2.66	0.49
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.49
1:A:371:ALA:HA	1:A:436:ILE:HG22	1.95	0.49
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.37	0.49
1:A:128:ILE:HG23	1:A:134:ARG:HG3	1.94	0.48
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.43	0.48
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.13	0.48
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.94	0.48
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.78	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.96	0.48
1:A:744:LYS:O	1:A:748:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:CD2	3:C:169:LYS:H	2.24	0.48
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.48
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.48
2:B:640:VAL:HG13	2:B:649:LYS:HB3	1.95	0.48
2:B:708:GLU:O	2:B:710:LEU:N	2.46	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.95	0.48
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.48	0.48
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.96	0.47
2:B:637:LEU:HD12	2:B:693:ILE:HG13	1.95	0.47
2:B:492:LEU:O	2:B:496:ARG:HG3	2.14	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.14	0.47
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.96	0.47
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.47
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.97	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.47
2:B:880:THR:C	2:B:882:THR:H	2.17	0.47
1:A:55:ASP:O	1:A:57:ARG:N	2.47	0.47
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.97	0.47
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.96	0.47
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.96	0.47
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.97	0.47
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.79	0.47
1:A:323:LYS:HG3	1:A:328:ARG:HG3	1.96	0.47
2:B:705:MET:CE	2:B:742:GLU:HG2	2.45	0.47
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.44	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.47
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.97	0.47
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.97	0.47
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.97	0.47
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.97	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.12	0.47
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.14	0.47
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.96	0.47
1:A:324:SER:O	1:A:326:ARG:N	2.40	0.47
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.15	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47
3:C:98:VAL:H	3:C:122:SER:HB2	1.80	0.47
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.96	0.46
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.97	0.46
1:A:702:LEU:O	1:A:710:LEU:HD11	2.14	0.46
2:B:370:PHE:O	2:B:372:SER:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LEU:O	2:B:428:ILE:HG12	2.15	0.46
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.51	0.46
2:B:601:ARG:HG2	2:B:615:MET:HE3	1.97	0.46
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.96	0.46
2:B:487:THR:HG22	2:B:490:SER:HB3	1.98	0.46
3:C:166:GLU:HG2	9:K:6:ARG:HB2	1.97	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD21	1.98	0.46
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.97	0.46
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.97	0.46
1:A:467:THR:HG23	2:B:976:ILE:HG23	1.97	0.46
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HD12	1.96	0.46
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.46	0.46
1:A:704:ALA:H	1:A:710:LEU:HD22	1.81	0.46
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.97	0.46
1:A:907:THR:HG22	1:A:908:LEU:H	1.81	0.45
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.97	0.45
1:A:23:SER:HB3	1:A:26:GLU:HB2	1.99	0.45
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.98	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.45
2:B:783:THR:HG23	8:J:59:LYS:HB3	1.97	0.45
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.99	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.51	0.45
1:A:1102:LYS:HE2	1:A:1106:ASN:HD21	1.81	0.45
2:B:654:ARG:H	2:B:657:HIS:HD2	1.63	0.45
5:F:93:ILE:HD13	5:F:134:ILE:HD11	1.98	0.45
1:A:942:PHE:O	1:A:946:VAL:HG23	2.17	0.45
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.99	0.45
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.98	0.45
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.98	0.45
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.50	0.45
2:B:1103:ILE:O	2:B:1122:ARG:HD2	2.16	0.45
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.99	0.45
6:H:135:LEU:C	6:H:137:GLN:H	2.20	0.45
5:F:72:LYS:HE2	5:F:142:SER:HB3	1.98	0.45
3:C:8:VAL:HG12	9:K:108:GLU:HG3	1.97	0.45
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.81	0.45
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	1.99	0.45
3:C:146:LYS:HB3	8:J:61:LEU:HD11	1.98	0.45
1:A:55:ASP:H	1:A:56:PRO:HD2	1.82	0.45
1:A:982:THR:HG22	1:A:983:ILE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.80	0.45
1:A:700:ASN:HD22	7:I:115:LYS:HB2	1.82	0.45
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.52	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.35	0.45
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.99	0.45
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.50	0.45
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.99	0.44
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.82	0.44
4:E:64:PRO:HD3	4:E:76:GLY:CA	2.48	0.44
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.47	0.44
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.17	0.44
2:B:778:MET:HB3	2:B:796:LEU:HD13	1.99	0.44
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.98	0.44
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.47	0.44
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.00	0.44
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.99	0.44
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.44
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.33	0.44
2:B:302:CYS:HA	2:B:310:MET:HE3	1.99	0.44
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.83	0.44
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.44
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.44
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.83	0.44
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.83	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.99	0.44
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.83	0.44
2:B:976:ILE:O	2:B:990:ILE:HB	2.17	0.44
2:B:815:ARG:HG2	2:B:816:GLU:OE1	2.17	0.44
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.99	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.17	0.44
2:B:169:ARG:HH22	2:B:958:GLN:HE22	1.64	0.44
2:B:515:HIS:HD2	2:B:517:THR:H	1.65	0.44
1:A:702:LEU:HD12	1:A:710:LEU:HD13	2.00	0.44
1:A:341:MET:HB3	2:B:1132:GLU:HB3	2.00	0.44
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.53	0.44
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.99	0.44
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.15	0.44
1:A:729:ALA:O	1:A:732:LEU:HB2	2.17	0.44
5:F:108:PHE:HB3	5:F:129:LYS:HD2	1.99	0.44
1:A:579:SER:HB3	1:A:611:GLN:HA	1.99	0.43
2:B:51:PHE:O	2:B:55:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.51	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.18	0.43
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.00	0.43
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.43
1:A:687:LYS:HD2	1:A:794:PRO:HG2	2.00	0.43
3:C:41:ILE:HG12	3:C:172:PRO:HG3	2.01	0.43
2:B:123:THR:HA	2:B:204:ILE:O	2.18	0.43
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.53	0.43
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.01	0.43
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.99	0.43
5:F:76:LYS:HG2	5:F:79:ARG:HH12	1.82	0.43
7:I:75:CYS:O	7:I:78:CYS:O	2.35	0.43
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.66	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.99	0.43
2:B:227:LYS:HG3	2:B:395:GLN:HB2	2.00	0.43
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.54	0.43
1:A:709:THR:HG22	1:A:711:ARG:H	1.83	0.43
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.43
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.15	0.43
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.19	0.43
10:L:28:LYS:HB2	10:L:39:SER:HB2	2.01	0.43
1:A:134:ARG:HH11	1:A:221:SER:HA	1.83	0.43
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.71	0.43
3:C:56:THR:HG22	3:C:57:VAL:H	1.83	0.42
10:L:27:LEU:HD13	10:L:59:ALA:HB1	2.01	0.42
1:A:686:ALA:HB2	1:A:725:ALA:HB2	2.01	0.42
1:A:786:HIS:HE1	2:B:742:GLU:OE1	2.02	0.42
1:A:181:LEU:HB2	1:A:202:LEU:HB2	2.01	0.42
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.01	0.42
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.55	0.42
2:B:1210:MET:HB3	2:B:1212:ILE:HD12	2.00	0.42
1:A:98:LYS:O	1:A:102:VAL:HG23	2.19	0.42
3:C:60:ASP:HB3	10:L:67:PHE:CZ	2.53	0.42
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	2.01	0.42
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.72	0.42
4:E:151:PRO:HD2	4:E:153:HIS:HE1	1.84	0.42
1:A:792:TYR:HA	1:A:797:LYS:HD2	2.00	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.49	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.54	0.42
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:ASN:HB2	1:A:1351:GLU:OE2	2.20	0.42
1:A:120:GLU:HA	1:A:123:ARG:HH11	1.84	0.42
3:C:14:SER:HA	9:K:114:LEU:HD22	2.01	0.42
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.01	0.42
1:A:134:ARG:HD2	1:A:221:SER:O	2.20	0.42
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.42
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.35	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HG3	2.02	0.42
1:A:1284:MET:HA	1:A:1306:LEU:HD23	2.02	0.42
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.55	0.42
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.55	0.42
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.20	0.42
3:C:183:TRP:HB3	3:C:213:PRO:HD3	2.01	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.38	0.42
2:B:241:ARG:HG2	2:B:253:THR:HG22	2.01	0.42
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	2.01	0.42
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.02	0.42
2:B:844:SER:HB2	2:B:996:ARG:H	1.85	0.41
2:B:880:THR:HB	2:B:934:LYS:HE2	2.01	0.41
10:L:34:CYS:SG	10:L:36:SER:HB2	2.60	0.41
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.02	0.41
1:A:109:HIS:H	1:A:210:ILE:HD12	1.85	0.41
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.56	0.41
2:B:487:THR:HG22	2:B:490:SER:H	1.85	0.41
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.02	0.41
3:C:50:GLU:HG2	10:L:66:GLN:HG3	2.01	0.41
6:H:113:ALA:HB2	6:H:126:GLU:HG3	2.01	0.41
2:B:114:PRO:HB3	2:B:174:LEU:HD21	2.01	0.41
1:A:577:ILE:H	1:A:577:ILE:HG13	1.76	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:451:HIS:HB3	1:A:453:MET:H	1.85	0.41
10:L:46:VAL:HG12	10:L:47:ARG:H	1.85	0.41
3:C:43:THR:HG22	3:C:170:TRP:HD1	1.85	0.41
2:B:383:ASN:O	2:B:387:LEU:HB2	2.21	0.41
9:K:26:LYS:H	9:K:26:LYS:HG2	1.48	0.41
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.21	0.41
1:A:403:LYS:HA	1:A:415:LEU:HB2	2.02	0.41
2:B:520:GLY:HA2	2:B:748:ILE:HA	2.03	0.41
10:L:47:ARG:HA	10:L:53:HIS:O	2.20	0.41
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.50	0.41
2:B:552:MET:HA	2:B:555:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:116:ILE:HG22	4:E:121:MET:HG2	2.03	0.41
4:E:64:PRO:HG2	4:E:69:ILE:HD11	2.01	0.41
1:A:251:SER:HB3	1:A:258:GLY:HA3	2.01	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.41
1:A:172:PRO:HB2	1:A:183:GLY:HA3	2.02	0.41
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.61	0.41
2:B:345:LYS:N	2:B:346:GLU:HB3	2.36	0.41
2:B:757:PRO:HG3	2:B:983:ARG:NH1	2.36	0.41
2:B:555:ILE:H	2:B:555:ILE:HG13	1.71	0.41
3:C:98:VAL:HG22	3:C:158:VAL:HG22	2.03	0.41
2:B:950:ASP:HB3	2:B:967:ARG:HG2	2.03	0.41
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.89	0.41
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.86	0.41
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.02	0.41
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.45	0.41
2:B:209:GLU:HB3	2:B:483:LEU:HD23	2.02	0.41
2:B:400:HIS:CD2	2:B:517:THR:HG21	2.55	0.41
2:B:515:HIS:H	2:B:518:HIS:CD2	2.39	0.41
9:K:108:GLU:HA	9:K:111:LEU:HD12	2.02	0.41
2:B:879:ARG:HD3	2:B:879:ARG:HA	1.93	0.41
1:A:353:ILE:HB	1:A:470:LEU:HD21	2.02	0.41
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.41
4:E:107:THR:HA	4:E:131:THR:O	2.20	0.41
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.02	0.41
2:B:706:GLN:H	2:B:710:LEU:HG	1.86	0.41
2:B:175:ARG:NH2	2:B:181:LEU:O	2.54	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.03	0.41
7:I:60:GLN:HE21	7:I:60:GLN:HA	1.85	0.41
9:K:21:ILE:HG13	9:K:33:ILE:HG12	2.03	0.41
3:C:74:SER:O	3:C:77:ILE:HB	2.21	0.40
1:A:540:PHE:HB3	1:A:571:LEU:HG	2.03	0.40
1:A:91:PHE:H	1:A:297:GLN:HE22	1.69	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.95	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.21	0.40
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.03	0.40
1:A:601:LYS:HE3	1:A:603:ASN:HD21	1.86	0.40
2:B:950:ASP:OD2	2:B:967:ARG:NH1	2.54	0.40
1:A:965:GLN:HE21	1:A:965:GLN:HB2	1.71	0.40
1:A:964:ILE:HG22	1:A:968:GLN:OE1	2.21	0.40
1:A:587:HIS:HE1	1:A:969:GLN:HE21	1.70	0.40
2:B:952:VAL:HB	10:L:58:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.03	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.40
1:A:1153:TYR:HD2	7:I:41:PRO:HG2	1.86	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.74	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	1395/1733 (80%)	1239 (89%)	110 (8%)	46 (3%)	5	26
2	B	1096/1224 (90%)	962 (88%)	91 (8%)	43 (4%)	4	21
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	13	50
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	21	64
5	F	83/155 (54%)	77 (93%)	5 (6%)	1 (1%)	16	56
6	H	129/146 (88%)	101 (78%)	21 (16%)	7 (5%)	2	14
7	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	11	46
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	3	17
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	21	64
10	L	44/70 (63%)	31 (70%)	7 (16%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3115 (89%)	285 (8%)	115 (3%)	5	26

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO

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Mol	Chain	Res	Type
1	A	109	HIS
1	A	260	ASP
1	A	286	HIS
1	A	399	HIS
1	A	418	SER
1	A	424	ILE
1	A	569	LYS
1	A	597	LEU
2	B	67	SER
2	B	137	TYR
2	B	139	ALA
2	B	364	ILE
2	B	367	LEU
2	B	477	ALA
2	B	648	HIS
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	880	THR
2	B	883	LEU
2	B	976	ILE
2	B	1046	PRO
2	B	1156	ASP
3	C	227	THR
6	H	90	ALA
6	H	109	LYS
6	H	131	ASN
7	I	118	ARG
8	J	2	ILE
8	J	6	ARG
1	A	250	ILE
1	A	283	GLY
1	A	312	PRO
1	A	325	ILE
1	A	556	TRP
1	A	846	GLU
1	A	1083	THR
1	A	1123	GLY
1	A	1221	LYS
1	A	1437	GLY
2	B	138	GLU

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Mol	Chain	Res	Type
2	B	371	GLU
2	B	483	LEU
2	B	531	GLN
2	B	695	ALA
2	B	712	PRO
2	B	881	ASN
2	B	888	GLY
2	B	1124	ARG
2	B	1157	ALA
2	B	1180	PHE
2	B	1181	GLU
3	C	141	GLY
4	E	126	SER
10	L	51	CYS
10	L	64	LEU
1	A	332	LYS
1	A	410	GLY
1	A	662	PHE
1	A	975	HIS
2	B	65	GLU
2	B	737	THR
2	B	887	HIS
2	B	1171	VAL
2	B	1223	ASP
3	C	90	ASP
6	H	140	ALA
7	I	77	LYS
10	L	39	SER
10	L	56	LEU
1	A	35	ILE
1	A	52	GLY
1	A	65	LEU
1	A	214	ILE
1	A	257	ARG
1	A	308	ILE
1	A	310	GLY
1	A	404	TYR
2	B	526	GLU
2	B	644	GLU
2	B	1221	SER
5	F	154	ASP
6	H	84	ALA

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Mol	Chain	Res	Type
8	J	26	GLN
9	K	18	LYS
10	L	46	VAL
10	L	55	ILE
1	A	213	HIS
1	A	299	HIS
1	A	400	PRO
1	A	567	LYS
1	A	958	VAL
2	B	646	LEU
2	B	647	GLY
2	B	792	MET
3	C	142	VAL
6	H	108	SER
1	A	331	GLY
1	A	385	ILE
1	A	543	LEU
1	A	599	SER
4	E	3	GLN
6	H	61	SER
1	A	568	PRO
2	B	592	ASN
2	B	1017	ILE
2	B	711	GLU
2	B	1099	VAL
1	A	178	GLY
1	A	916	GLY
1	A	1384	VAL

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	1225/1520 (81%)	1066 (87%)	159 (13%)	5	22
2	B	967/1061 (91%)	842 (87%)	125 (13%)	5	23
3	C	234/274 (85%)	205 (88%)	29 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	196/197 (100%)	170 (87%)	26 (13%)	5	21
5	F	75/137 (55%)	71 (95%)	4 (5%)	28	67
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	9
7	I	113/116 (97%)	98 (87%)	15 (13%)	5	21
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	11
9	K	99/102 (97%)	86 (87%)	13 (13%)	5	22
10	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
All	All	3126/3657 (86%)	2710 (87%)	416 (13%)	5	21

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	18	GLN
1	A	25	GLU
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	69	THR
1	A	70	CYS
1	A	86	LEU
1	A	93	VAL
1	A	108	MET
1	A	116	ASP
1	A	122	MET
1	A	126	LEU
1	A	130	ASP
1	A	144	THR
1	A	171	GLN
1	A	177	ASP
1	A	179	LEU
1	A	186	LYS
1	A	204	THR
1	A	205	GLU
1	A	219	PHE
1	A	222	LEU
1	A	252	PHE

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Mol	Chain	Res	Type
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	295	LEU
1	A	303	TYR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	389	THR
1	A	403	LYS
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	452	LYS
1	A	456	MET
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	476	SER
1	A	489	LEU
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	541	ILE
1	A	542	GLU

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Mol	Chain	Res	Type
1	A	544	ASP
1	A	555	ASP
1	A	567	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS
1	A	708	MET
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	801	GLU
1	A	821	ARG
1	A	830	LYS
1	A	839	ARG
1	A	867	ILE
1	A	878	ILE
1	A	894	GLU
1	A	896	ARG
1	A	905	ASP
1	A	907	THR
1	A	917	SER
1	A	922	ASP
1	A	927	VAL
1	A	931	GLU
1	A	968	GLN
1	A	969	GLN
1	A	973	ILE
1	A	982	THR

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Mol	Chain	Res	Type
1	A	1006	ILE
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1046	LEU
1	A	1048	ASN
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1095	THR
1	A	1109	LYS
1	A	1110	ASN
1	A	1113	THR
1	A	1129	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1229	SER
1	A	1230	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1264	GLU
1	A	1274	ARG
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1350	LYS
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL

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Mol	Chain	Res	Type
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	121	ASN
2	B	134	LYS
2	B	135	ARG
2	B	140	ILE
2	B	175	ARG
2	B	199	MET
2	B	217	ARG
2	B	218	SER
2	B	221	ASN
2	B	223	VAL
2	B	225	VAL
2	B	233	PRO
2	B	234	ILE
2	B	240	ILE
2	B	249	ARG
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	285	ILE
2	B	299	GLU
2	B	312	GLU
2	B	323	VAL
2	B	325	GLN
2	B	327	ARG

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Mol	Chain	Res	Type
2	B	355	ILE
2	B	357	GLN
2	B	363	HIS
2	B	365	THR
2	B	371	GLU
2	B	376	PHE
2	B	393	LYS
2	B	394	ASP
2	B	413	LEU
2	B	416	LEU
2	B	437	GLU
2	B	451	LYS
2	B	458	LYS
2	B	461	LEU
2	B	471	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	516	ASN
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	576	ASP
2	B	578	THR
2	B	579	ARG
2	B	591	ARG
2	B	604	ARG
2	B	614	SER
2	B	616	ILE
2	B	624	LEU
2	B	629	ASP
2	B	653	VAL
2	B	660	LYS
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	733	HIS
2	B	762	ASN
2	B	780	VAL

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Mol	Chain	Res	Type
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	791	THR
2	B	799	PRO
2	B	815	ARG
2	B	844	SER
2	B	864	LYS
2	B	866	TYR
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	885	MET
2	B	886	LYS
2	B	895	ASP
2	B	906	SER
2	B	935	ARG
2	B	944	THR
2	B	963	PHE
2	B	964	VAL
2	B	976	ILE
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1065	GLN
2	B	1077	THR
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1132	GLU
2	B	1147	LEU
2	B	1150	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1194	ILE

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1210	MET
2	B	1211	ASN
2	B	1216	LEU
3	C	3	GLU
3	C	4	GLU
3	C	9	LYS
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	41	ILE
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	75	MET
3	C	77	ILE
3	C	80	LEU
3	C	93	ASP
3	C	99	LEU
3	C	109	SER
3	C	136	ASP
3	C	137	LYS
3	C	204	SER
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	264	GLN
4	E	7	ARG
4	E	32	GLN
4	E	37	LEU
4	E	41	ASP
4	E	52	ARG
4	E	54	GLN
4	E	61	GLN
4	E	75	MET
4	E	78	LEU

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Mol	Chain	Res	Type
4	E	83	CYS
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	104	ASN
4	E	106	GLN
4	E	107	THR
4	E	114	ASN
4	E	127	ILE
4	E	144	ILE
4	E	146	HIS
4	E	149	LEU
4	E	156	LEU
4	E	169	ARG
4	E	178	ILE
4	E	204	THR
5	F	76	LYS
5	F	82	THR
5	F	93	ILE
5	F	118	LEU
6	H	11	GLN
6	H	13	SER
6	H	14	GLU
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	35	GLN
6	H	63	LEU
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	91	ASP
6	H	92	ASP
6	H	100	THR
6	H	109	LYS
6	H	110	ASP
6	H	111	LEU
6	H	130	ARG
6	H	132	LEU

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Mol	Chain	Res	Type
6	H	136	LYS
6	H	139	ASN
7	I	28	GLU
7	I	35	VAL
7	I	60	GLN
7	I	61	ASP
7	I	70	ARG
7	I	77	LYS
7	I	83	ASN
7	I	87	GLN
7	I	90	GLN
7	I	94	ASP
7	I	96	SER
7	I	97	MET
7	I	104	LEU
7	I	111	THR
7	I	119	THR
8	J	1	MET
8	J	3	VAL
8	J	10	CYS
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	28	ASP
8	J	31	ASP
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
9	K	11	LEU
9	K	14	GLU
9	K	16	GLU
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	26	LYS
9	K	31	VAL
9	K	33	ILE
9	K	51	LEU
9	K	63	VAL
9	K	74	ARG
9	K	114	LEU
10	L	27	LEU

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Mol	Chain	Res	Type
10	L	38	LEU
10	L	42	ARG
10	L	43	THR
10	L	44	ASP
10	L	47	ARG
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	64	LEU
10	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	83	HIS
1	A	225	ASN
1	A	256	GLN
1	A	297	GLN
1	A	339	ASN
1	A	445	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	603	ASN
1	A	631	HIS
1	A	700	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	969	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1110	ASN
1	A	1140	HIS

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Mol	Chain	Res	Type
1	A	1211	GLN
1	A	1258	HIS
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	215	GLN
2	B	363	HIS
2	B	395	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	957	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1074	ASN
2	B	1084	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	54	GLN
4	E	147	HIS
6	H	11	GLN
7	I	60	GLN
9	K	65	HIS
9	K	89	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	1405/1733 (81%)	0.28	130 (9%) 11 4	63, 111, 202, 234	0
2	B	1114/1224 (91%)	0.07	54 (4%) 34 14	62, 96, 166, 219	0
3	C	266/318 (83%)	-0.09	1 (0%) 93 80	67, 94, 132, 186	0
4	E	214/215 (99%)	0.21	13 (6%) 25 9	81, 139, 193, 210	0
5	F	85/155 (54%)	0.09	0 100 100	81, 115, 159, 172	0
6	H	133/146 (91%)	0.36	7 (5%) 30 12	109, 151, 177, 187	0
7	I	119/122 (97%)	0.01	2 (1%) 73 45	78, 114, 150, 167	0
8	J	65/70 (92%)	-0.08	0 100 100	65, 83, 114, 130	0
9	K	114/120 (95%)	-0.11	0 100 100	66, 102, 126, 149	0
10	L	46/70 (65%)	0.11	3 (6%) 22 8	82, 119, 152, 176	0
11	R	4/4 (100%)	2.15	2 (50%) 0 0	210, 216, 218, 219	0
12	T	8/29 (27%)	2.22	3 (37%) 0 0	200, 204, 210, 211	0
All	All	3573/4206 (84%)	0.16	215 (6%) 25 9	62, 106, 192, 234	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	9.3
1	A	1087	ALA	9.1
1	A	182	VAL	8.7
1	A	1090	ALA	6.6
2	B	647	GLY	6.5
1	A	250	ILE	6.5
1	A	1082	ASN	6.5
6	H	86	ASP	6.4
1	A	116	ASP	6.4
1	A	199	LEU	6.2
6	H	85	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	171	GLN	5.9
1	A	113	LEU	5.9
1	A	147	VAL	5.8
1	A	161	LEU	5.7
4	E	93	MET	5.7
2	B	865	LYS	5.7
2	B	1224	PHE	5.6
1	A	45	GLN	5.6
1	A	49	LYS	5.5
1	A	115	LEU	5.5
1	A	258	GLY	5.4
1	A	114	LEU	5.4
2	B	883	LEU	5.3
1	A	69	THR	5.3
1	A	201	VAL	5.2
12	T	19	DT	5.2
1	A	253	ASN	5.2
1	A	183	GLY	5.0
1	A	168	GLY	5.0
1	A	313	GLN	4.9
1	A	177	ASP	4.9
1	A	1123	GLY	4.9
1	A	174	ILE	4.9
1	A	141	LEU	4.8
2	B	867	GLY	4.8
1	A	148	CYS	4.7
1	A	1086	PHE	4.7
1	A	139	TRP	4.7
1	A	44	THR	4.7
1	A	314	ALA	4.7
1	A	149	GLU	4.7
1	A	146	MET	4.6
2	B	474	SER	4.5
1	A	144	THR	4.5
1	A	1085	HIS	4.5
1	A	137	ALA	4.5
1	A	1091	SER	4.4
2	B	136	THR	4.4
1	A	280	GLU	4.4
2	B	1222	ARG	4.4
1	A	173	THR	4.4
1	A	318	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	SER	4.3
1	A	152	VAL	4.2
1	A	127	ALA	4.1
1	A	1088	GLY	4.1
10	L	50	ASP	4.1
2	B	1184	GLY	4.0
1	A	131	SER	4.0
1	A	1083	THR	4.0
1	A	122	MET	3.9
1	A	316	GLN	3.9
2	B	471	LYS	3.9
2	B	469	GLN	3.9
4	E	110	PHE	3.9
1	A	251	SER	3.9
1	A	172	PRO	3.8
2	B	866	TYR	3.8
2	B	477	ALA	3.8
2	B	869	SER	3.8
11	R	7	G	3.8
1	A	202	LEU	3.7
1	A	214	ILE	3.7
1	A	200	ARG	3.6
12	T	22	DT	3.6
1	A	319	GLY	3.6
1	A	169	ASN	3.6
1	A	62	ASP	3.6
2	B	1221	SER	3.5
1	A	12	ARG	3.5
2	B	645	SER	3.5
4	E	122	LYS	3.5
2	B	870	ILE	3.5
2	B	1171	VAL	3.4
4	E	84	ASP	3.4
2	B	1223	ASP	3.4
1	A	66	LYS	3.4
1	A	256	GLN	3.4
1	A	1173	HIS	3.4
1	A	163	SER	3.3
6	H	109	LYS	3.3
2	B	429	PHE	3.2
1	A	105	CYS	3.2
1	A	175	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	ASP	3.2
6	H	84	ALA	3.2
1	A	254	GLU	3.1
1	A	287	HIS	3.1
2	B	1183	LYS	3.1
1	A	58	LEU	3.1
1	A	128	ILE	3.1
4	E	86	PRO	3.1
1	A	176	LYS	3.0
1	A	321	PRO	3.0
1	A	213	HIS	3.0
2	B	709	ASP	3.0
1	A	315	LEU	3.0
1	A	317	LYS	3.0
10	L	45	ALA	3.0
2	B	933	SER	3.0
1	A	145	LYS	3.0
2	B	135	ARG	2.9
6	H	83	GLN	2.9
1	A	118	HIS	2.9
2	B	1164	GLY	2.9
1	A	286	HIS	2.9
2	B	1188	LYS	2.8
1	A	257	ARG	2.8
1	A	283	GLY	2.8
1	A	164	ARG	2.8
1	A	1089	VAL	2.8
2	B	1187	ASN	2.8
1	A	185	TRP	2.8
1	A	753	GLY	2.8
2	B	1172	ILE	2.8
1	A	117	GLU	2.7
1	A	323	LYS	2.7
2	B	662	MET	2.7
2	B	1190	ASP	2.7
1	A	1108	ALA	2.7
6	H	88	SER	2.7
1	A	312	PRO	2.7
4	E	2	ASP	2.7
2	B	1194	ILE	2.6
2	B	472	ALA	2.6
1	A	162	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	2.6
1	A	87	ALA	2.6
2	B	882	THR	2.6
1	A	120	GLU	2.6
4	E	123	LEU	2.5
2	B	470	LYS	2.5
1	A	167	CYS	2.5
6	H	132	LEU	2.5
1	A	74	MET	2.5
1	A	260	ASP	2.5
2	B	468	GLU	2.5
2	B	887	HIS	2.5
1	A	975	HIS	2.5
1	A	150	THR	2.5
2	B	868	MET	2.5
1	A	125	ALA	2.5
2	B	246	LYS	2.5
11	R	8	A	2.4
2	B	657	HIS	2.4
1	A	430	TRP	2.4
2	B	134	LYS	2.4
1	A	153	PRO	2.4
1	A	282	ASN	2.4
1	A	165	GLY	2.4
2	B	1189	ILE	2.4
1	A	391	LEU	2.4
1	A	290	GLU	2.3
4	E	9	ILE	2.3
1	A	124	GLN	2.3
1	A	252	PHE	2.3
1	A	33	ALA	2.3
1	A	320	ARG	2.3
2	B	167	ILE	2.3
1	A	1124	HIS	2.3
1	A	142	CYS	2.2
2	B	708	GLU	2.2
12	T	23	DC	2.2
2	B	355	ILE	2.2
1	A	103	CYS	2.2
1	A	1391	ARG	2.2
1	A	212	LYS	2.2
1	A	13	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	113	GLN	2.2
1	A	129	LYS	2.2
3	C	108	GLU	2.2
1	A	424	ILE	2.2
4	E	70	SER	2.2
4	E	66	GLU	2.2
1	A	138	ILE	2.2
2	B	1191	ILE	2.2
1	A	1084	PHE	2.2
2	B	1220	ARG	2.2
1	A	210	ILE	2.2
1	A	322	VAL	2.2
2	B	1127	GLY	2.2
2	B	1182	CYS	2.1
1	A	154	SER	2.1
1	A	143	LYS	2.1
1	A	6	TYR	2.1
1	A	59	GLY	2.1
1	A	8	SER	2.1
4	E	127	ILE	2.1
4	E	87	SER	2.1
7	I	104	LEU	2.1
2	B	138	GLU	2.1
1	A	73	GLY	2.1
2	B	430	ARG	2.1
10	L	27	LEU	2.1
1	A	43	GLU	2.1
1	A	48	ALA	2.1
2	B	475	SER	2.1
1	A	1236	LEU	2.1
2	B	432	MET	2.1
7	I	2	THR	2.0
1	A	265	LYS	2.0
1	A	61	ILE	2.0
2	B	1162	ILE	2.0
2	B	263	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
13	ZN	L	105	1/1	0.94	0.11	-0.70	111,111,111,111	0
13	ZN	A	1734	1/1	0.22	0.26	-0.97	300,300,300,300	0
13	ZN	J	101	1/1	0.93	0.15	-1.25	88,88,88,88	0
13	ZN	B	1307	1/1	0.79	0.07	-1.95	206,206,206,206	0
13	ZN	A	1735	1/1	0.74	0.05	-2.14	177,177,177,177	0
13	ZN	I	204	1/1	0.95	0.05	-2.45	90,90,90,90	0
13	ZN	I	203	1/1	0.94	0.04	-2.68	113,113,113,113	0
13	ZN	C	319	1/1	0.92	0.05	-3.21	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.