



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:53 PM GMT

PDB ID : 2Y0S  
Title : Crystal structure of Sulfolobus shibatae RNA polymerase in P21 space group  
Authors : Wojtas, M.; Peralta, B.; Ondiviela, M.; Mogni, M.; Bell, S.D.; Abrescia, N.G.A.  
Deposited on : 2010-12-07  
Resolution : 3.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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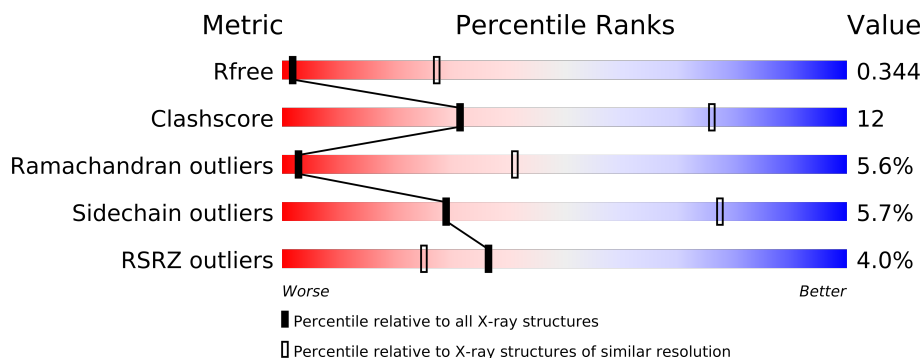
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.80 Å.

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











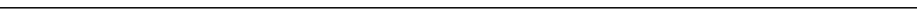



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	880	
1	W	880	
2	B	1131	
2	R	1131	
3	C	395	
3	Y	395	
4	D	265	
4	S	265	
5	E	180	
5	T	180	
6	F	113	
6	U	113	
7	G	132	
7	V	132	

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Mol	Chain	Length	Quality of chain
8	H	84	
8	Z	84	
9	I	95	
9	K	95	
10	J	104	
10	Q	104	
11	L	92	
11	M	92	
12	N	66	
12	O	66	
13	P	48	
13	X	48	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
14	ZN	B	2124	-	X
14	ZN	B	2125	-	X
14	ZN	R	2124	-	X
14	ZN	R	2125	-	X
15	MG	W	1882	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52472 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	831	Total	C	N	O	S	0	0	0
			6620	4211	1170	1212	27			
1	W	831	Total	C	N	O	S	0	0	0
			6620	4211	1170	1212	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1085	Total	C	N	O	S	0	0	0
			8615	5461	1526	1599	29			
2	R	1085	Total	C	N	O	S	0	0	0
			8615	5461	1526	1599	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT A”.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	368	Total	C	N	O	S	0	0	0
			2845	1803	486	548	8			
3	Y	368	Total	C	N	O	S	0	0	0
			2845	1803	486	548	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	262	Total	C	N	O	S	0	0	0
			2081	1338	336	394	13			
4	S	262	Total	C	N	O	S	0	0	0
			2081	1338	336	394	13			

- Molecule 5 is a protein called RNA POLYMERASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	164	Total	C	N	O	S	0	0	0
			1297	833	219	240	5			
5	T	164	Total	C	N	O	S	0	0	0
			1297	833	219	240	5			

- Molecule 6 is a protein called RNA POLYMERASE SUBUNIT 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			
6	U	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			

- Molecule 7 is a protein called RNA POLYMERASE SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	110	Total	C	N	O	S	0	0	0
			878	558	147	169	4			
7	V	110	Total	C	N	O	S	0	0	0
			878	558	147	169	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O	0	0	0
			609	396	108	105			
8	Z	74	Total	C	N	O	0	0	0
			609	396	108	105			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	82	Total	C	N	O	S	0	0	0
			653	419	117	116	1			
9	K	82	Total	C	N	O	S	0	0	0
			653	419	117	116	1			

- Molecule 10 is a protein called RNA POLYMERASE SUBUNIT 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			332	210	54	67	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Q	39	Total	C	N	O	S	0	0	0
			332	210	54	67	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	40	ASN	ASP	CONFLICT	UNP B8YB65
Q	40	ASN	ASP	CONFLICT	UNP B8YB65

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			
11	M	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			
12	O	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 13 is a protein called RNA POLYMERASE SUBUNIT 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	45	Total	C	N	O	S	0	0	0
			369	245	63	56	5			
13	X	45	Total	C	N	O	S	0	0	0
			369	245	63	56	5			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	P	1	Total	Zn	0	0
			1	1		
14	B	3	Total	Zn	0	0
			3	3		
14	W	2	Total	Zn	0	0
			2	2		

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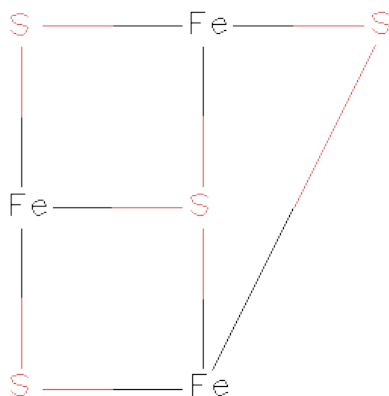
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total 2	Zn 2	0	0
14	N	1	Total 1	Zn 1	0	0
14	X	1	Total 1	Zn 1	0	0
14	O	1	Total 1	Zn 1	0	0
14	R	3	Total 3	Zn 3	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	W	1	Total 1	Mg 1	0	0
15	A	1	Total 1	Mg 1	0	0

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



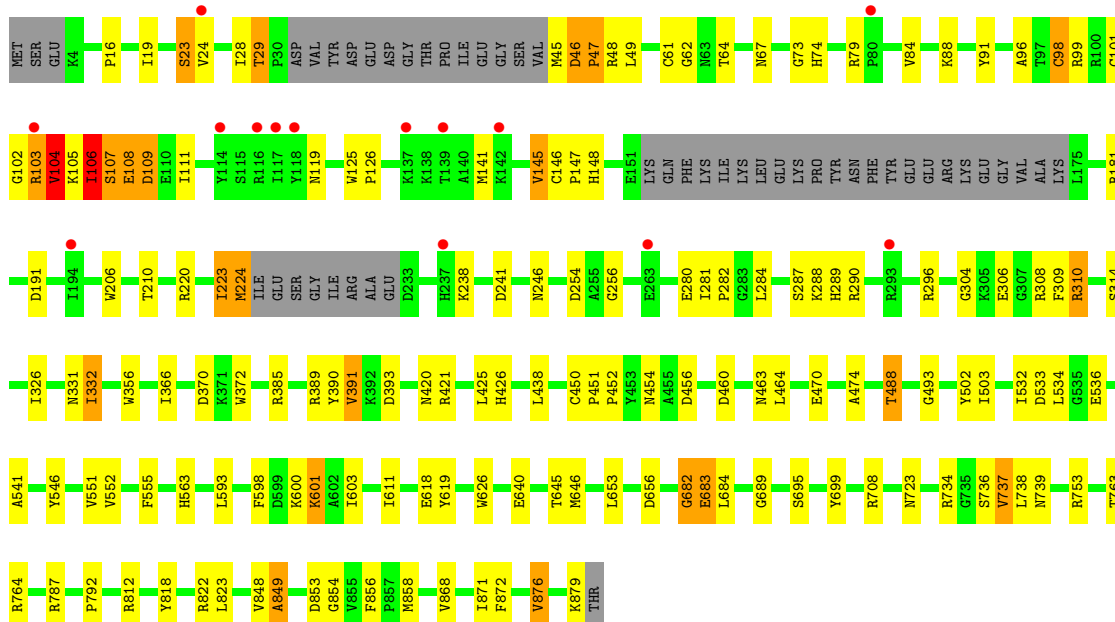
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total 7	Fe 3	S 4	0	0
16	S	1	Total 7	Fe 3	S 4	0	0

### 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.

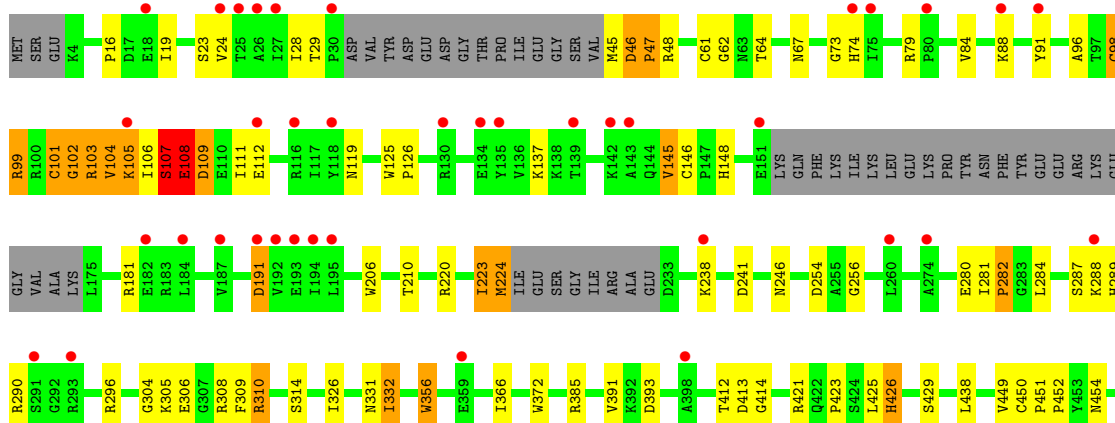
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain A: 

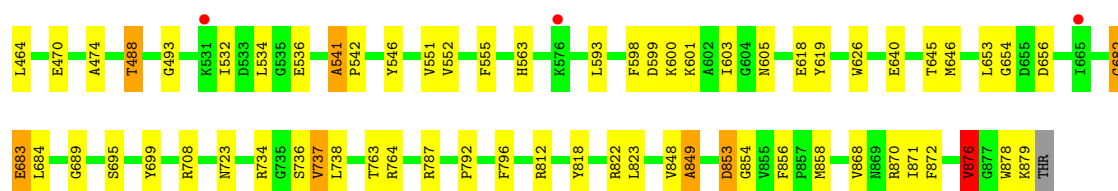


#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain W: 

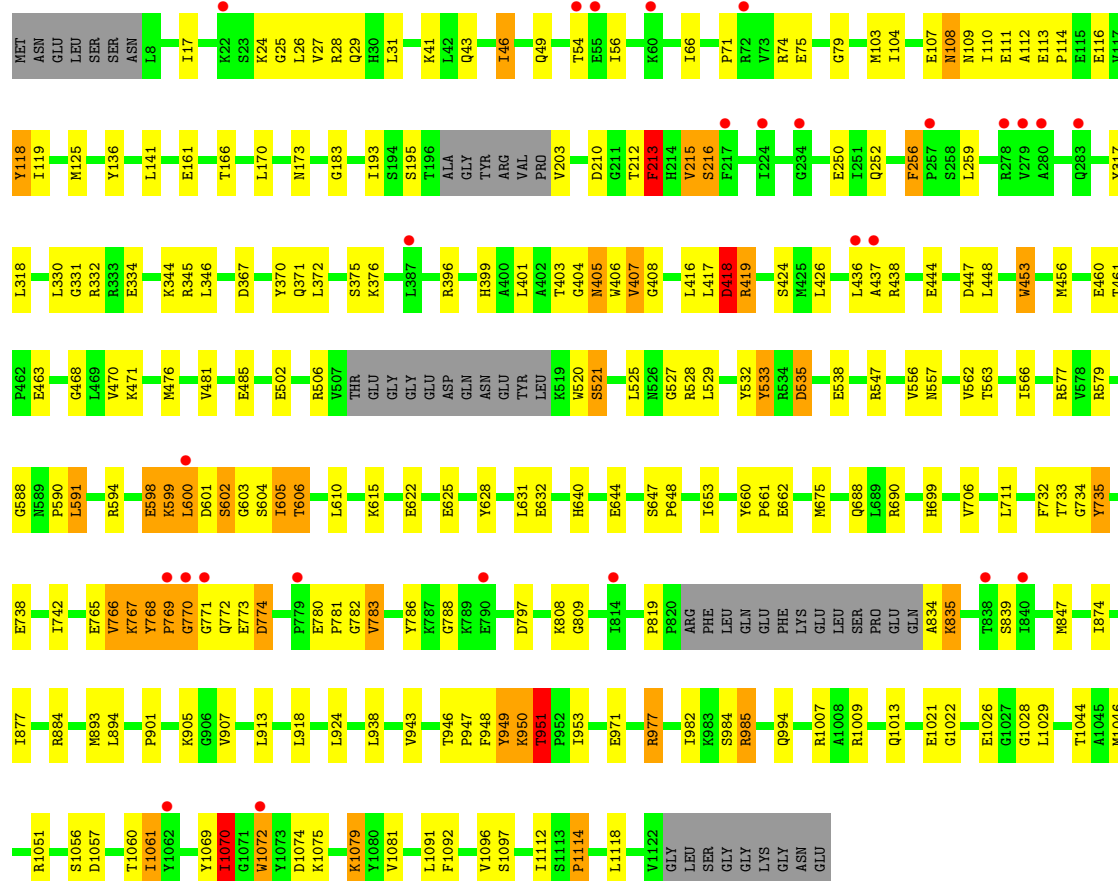






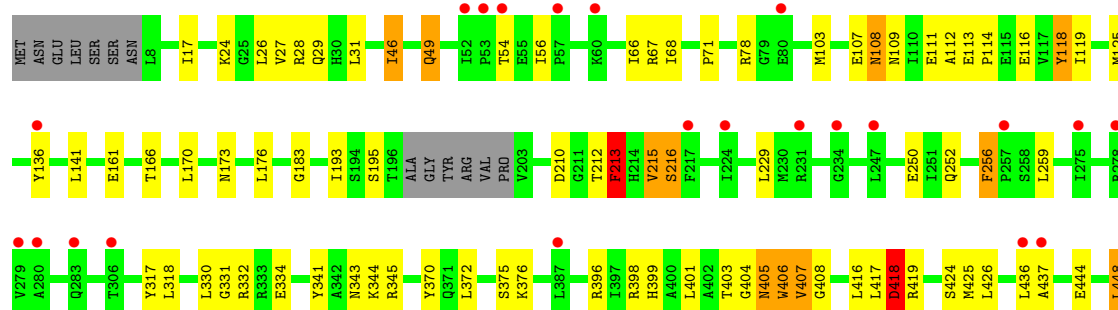
### • Molecule 2: DNA-DIRECTED RNA POLYMERASE

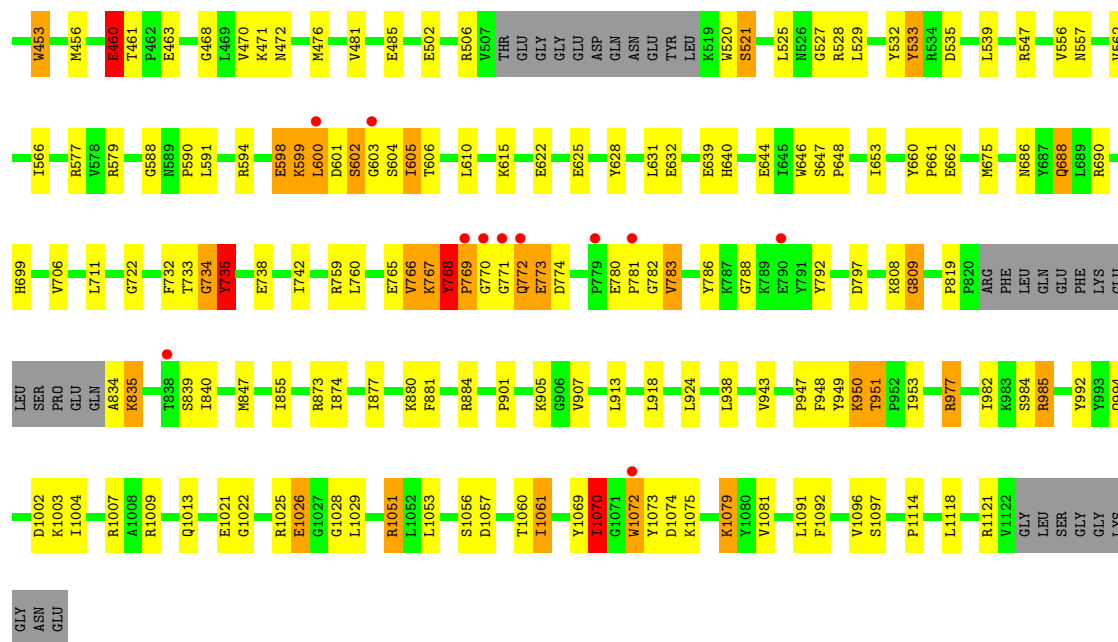
Chain B:



### • Molecule 2: DNA-DIRECTED RNA POLYMERASE

Chain R:





• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT A”

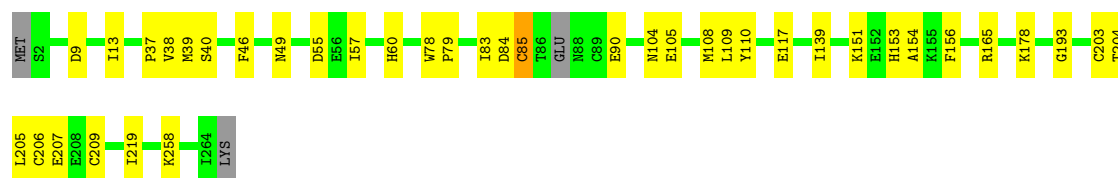
Chain C:

• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT A”

Chain Y:

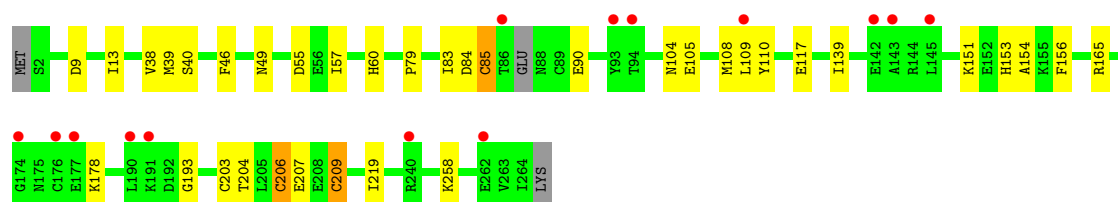
• Molecule 4: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

Chain D: 



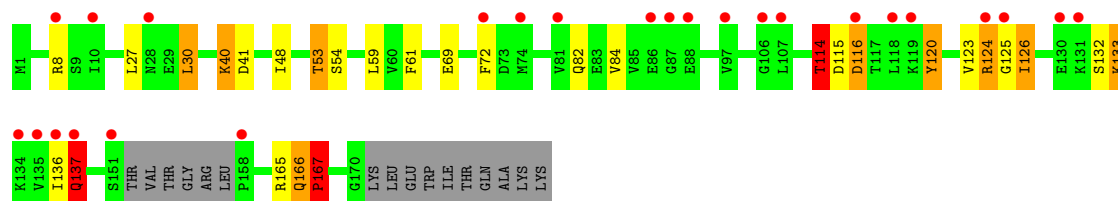
- Molecule 4: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

Chain S: 



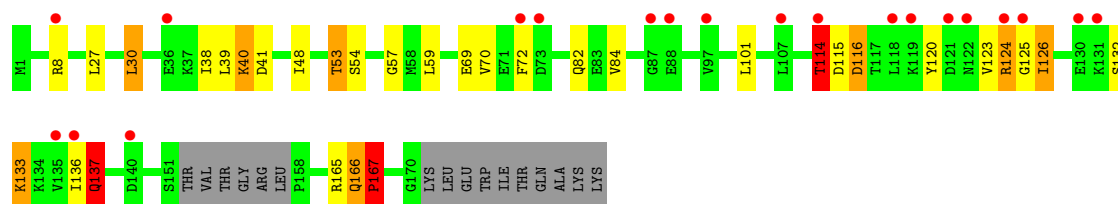
- Molecule 5: RNA POLYMERASE SUBUNIT 4

Chain E: 



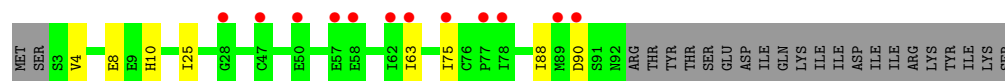
- Molecule 5: RNA POLYMERASE SUBUNIT 4

Chain T: 



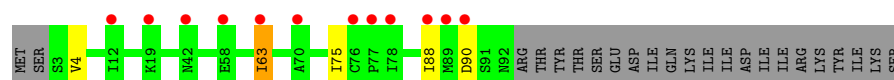
- Molecule 6: RNA POLYMERASE SUBUNIT 7

Chain F:



- Molecule 6: RNA POLYMERASE SUBUNIT 7

Chain U: 



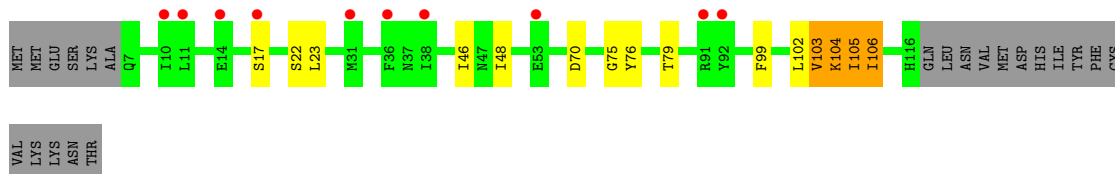
- Molecule 7: RNA POLYMERASE SUBUNIT 8

Chain G:



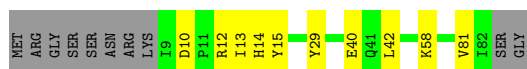
- Molecule 7: RNA POLYMERASE SUBUNIT 8

Chain V:



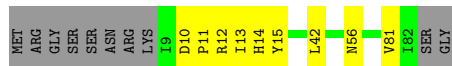
- Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H

Chain H:



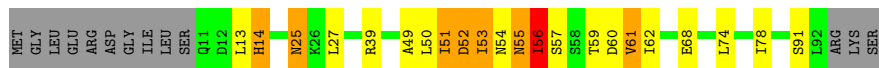
- Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H

Chain Z:



- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

Chain I:



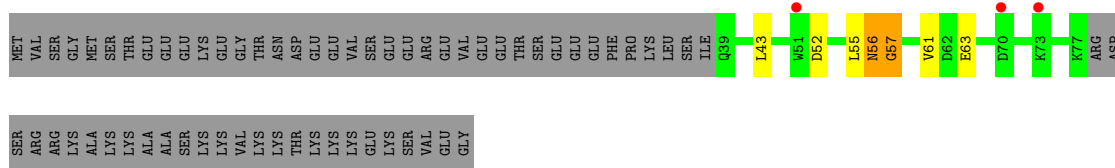
- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

Chain K:



- Molecule 10: RNA POLYMERASE SUBUNIT 13

Chain J:



- Molecule 10: RNA POLYMERASE SUBUNIT 13

Chain Q:

- Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain L:

- Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain M:

- Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

Chain N:

- Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

Chain O:

- Molecule 13: RNA POLYMERASE SUBUNIT 12

Chain P:

- Molecule 13: RNA POLYMERASE SUBUNIT 12

Chain X:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.33Å 195.91Å 212.45Å 90.00° 105.73° 90.00°	Depositor
Resolution (Å)	29.86 – 3.80 47.12 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.86-3.80) 98.6 (47.12-3.79)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.300 , 0.354 0.287 , 0.344	Depositor DCC
$R_{free}$ test set	4995 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.6	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.3	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 99994 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	52472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6829e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, F3S, MG

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	0.54	3/6762 (0.0%)	0.81	7/9151 (0.1%)
1	W	0.44	2/6762 (0.0%)	0.62	4/9151 (0.0%)
2	B	0.50	0/8778	0.81	1/11873 (0.0%)
2	R	0.42	0/8778	0.60	0/11873
3	C	0.50	1/2869 (0.0%)	0.80	0/3862
3	Y	0.41	0/2869	0.61	0/3862
4	D	0.39	0/2116	0.64	0/2859
4	S	0.32	0/2116	0.48	0/2859
5	E	0.40	0/1316	0.71	0/1775
5	T	0.36	1/1316 (0.1%)	0.53	0/1775
6	F	0.28	0/709	0.62	0/961
6	U	0.25	0/709	0.41	0/961
7	G	0.40	0/890	0.67	0/1194
7	V	0.33	0/890	0.51	0/1194
8	H	0.53	0/623	0.77	0/845
8	Z	0.42	0/623	0.58	0/845
9	I	1.29	3/662 (0.5%)	0.90	5/896 (0.6%)
9	K	1.33	4/662 (0.6%)	1.01	5/896 (0.6%)
10	J	0.36	0/336	0.51	0/450
10	Q	0.43	0/336	0.71	0/450
11	L	0.40	0/717	0.68	0/968
11	M	0.31	0/717	0.52	0/968
12	N	0.43	0/524	0.68	0/706
12	O	0.35	0/524	0.52	0/706
13	P	0.49	0/378	0.80	0/507
13	X	0.44	0/378	0.66	0/507
All	All	0.49	14/53360 (0.0%)	0.69	22/72094 (0.0%)

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

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
5	E	0	1
5	T	0	1
9	I	0	1
9	K	0	1
All	All	0	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	56	ILE	C-N	-22.63	0.82	1.34
9	K	55	ASN	C-N	21.74	1.84	1.34
9	K	56	ILE	C-N	-21.68	0.84	1.34
9	I	55	ASN	C-N	20.09	1.80	1.34
1	A	104	VAL	CB-CG2	-9.48	1.32	1.52
1	W	101	CYS	CB-SG	8.03	1.95	1.82
3	C	80	GLU	CG-CD	7.09	1.62	1.51
1	A	104	VAL	CB-CG1	-7.06	1.38	1.52
1	A	146	CYS	CB-SG	-5.68	1.72	1.81
5	T	57	GLY	C-N	-5.39	1.21	1.34
1	W	104	VAL	CB-CG1	-5.15	1.42	1.52
9	I	25	ASN	C-N	5.13	1.45	1.34
9	K	25	ASN	C-N	5.10	1.45	1.34
9	K	70	LYS	N-CA	-5.08	1.36	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	55	ASN	O-C-N	9.91	138.56	122.70
9	K	55	ASN	CA-C-N	-9.88	95.47	117.20
9	I	55	ASN	CA-C-N	-9.78	95.68	117.20
9	I	56	ILE	O-C-N	-9.40	107.66	122.70
9	K	55	ASN	O-C-N	9.26	137.52	122.70
1	W	98	CYS	CA-CB-SG	8.54	129.38	114.00
9	K	56	ILE	O-C-N	-8.41	109.24	122.70
1	A	102	GLY	N-CA-C	-7.68	93.91	113.10
9	I	56	ILE	C-N-CA	6.55	138.07	121.70
9	K	56	ILE	C-N-CA	6.40	137.70	121.70
1	A	456	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	98	CYS	CA-CB-SG	6.29	125.32	114.00
1	W	105	LYS	CD-CE-NZ	-5.97	97.96	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	102	GLY	N-CA-C	-5.81	98.58	113.10
2	B	774	ASP	CB-CG-OD2	5.73	123.46	118.30
9	I	56	ILE	CA-C-N	5.61	129.53	117.20
1	A	106	ILE	CG1-CB-CG2	5.60	123.73	111.40
1	A	104	VAL	CG1-CB-CG2	5.53	119.74	110.90
1	W	104	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	A	533	ASP	N-CA-CB	5.20	119.96	110.60
9	K	91	SER	N-CA-C	5.08	124.70	111.00
1	A	460	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	VAL	Mainchain
5	E	167	PRO	Peptide
9	I	56	ILE	Mainchain
9	K	56	ILE	Mainchain
5	T	167	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6620	0	0	85	0
1	W	6620	0	0	86	0
2	B	8615	0	0	115	0
2	R	8615	0	0	107	0
3	C	2845	0	0	48	0
3	Y	2845	0	0	49	0
4	D	2081	0	0	19	0
4	S	2081	0	0	19	0
5	E	1297	0	0	20	0
5	T	1297	0	0	24	0
6	F	701	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	701	0	0	2	0
7	G	878	0	0	6	0
7	V	878	0	0	7	0
8	H	609	0	0	5	0
8	Z	609	0	0	2	0
9	I	653	0	0	21	0
9	K	653	0	0	20	0
10	J	332	0	0	3	0
10	Q	332	0	0	5	0
11	L	707	0	0	2	0
11	M	707	0	0	2	0
12	N	514	0	0	2	0
12	O	514	0	0	4	0
13	P	369	0	0	6	0
13	X	369	0	0	8	0
14	A	2	0	0	0	0
14	B	3	0	0	0	0
14	N	1	0	0	0	0
14	O	1	0	0	0	0
14	P	1	0	0	0	0
14	R	3	0	0	0	0
14	W	2	0	0	0	0
14	X	1	0	0	0	0
15	A	1	0	0	0	0
15	W	1	0	0	0	0
16	D	7	0	0	3	0
16	S	7	0	0	5	0
All	All	52472	0	0	606	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (606) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:55:ASN:C	9:I:56:ILE:N	1.80	1.32
9:K:55:ASN:C	9:K:56:ILE:N	1.84	1.30
9:I:56:ILE:O	9:I:57:SER:N	1.67	1.24
9:K:56:ILE:O	9:K:57:SER:N	1.71	1.19
9:I:56:ILE:C	9:I:57:SER:CA	2.13	1.17
9:K:56:ILE:C	9:K:57:SER:CA	2.14	1.15
9:K:56:ILE:CA	9:K:57:SER:N	2.14	1.10
9:I:56:ILE:CA	9:I:57:SER:N	2.14	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:HIS:CE1	3:C:80:GLU:OE2	2.13	1.01
1:A:426:HIS:ND1	3:C:80:GLU:OE2	1.98	0.97
1:W:426:HIS:CE1	3:Y:80:GLU:OE2	2.18	0.97
1:W:98:CYS:O	1:W:146:CYS:SG	2.25	0.95
9:K:56:ILE:C	9:K:57:SER:N	0.84	0.89
1:W:426:HIS:ND1	3:Y:80:GLU:OE2	2.06	0.88
9:I:56:ILE:C	9:I:57:SER:N	0.82	0.87
1:A:104:VAL:CG1	1:A:104:VAL:O	2.21	0.85
1:A:103:ARG:NE	1:A:191:ASP:OD1	2.14	0.81
1:W:104:VAL:CG1	1:W:137:LYS:CB	2.58	0.81
2:B:767:LYS:CB	2:B:768:TYR:CD1	2.65	0.78
2:R:767:LYS:CB	2:R:768:TYR:CD1	2.67	0.78
9:I:55:ASN:CA	9:I:56:ILE:N	2.47	0.76
3:Y:168:GLN:CG	3:Y:204:ASN:OD1	2.34	0.75
9:K:55:ASN:CA	9:K:56:ILE:N	2.49	0.75
1:W:103:ARG:CB	1:W:191:ASP:OD1	2.34	0.74
2:B:767:LYS:CB	2:B:768:TYR:CA	2.66	0.74
2:B:768:TYR:CB	2:B:769:PRO:CD	2.66	0.73
3:C:168:GLN:CG	3:C:204:ASN:OD1	2.36	0.73
1:A:241:ASP:OD2	1:A:289:HIS:CE1	2.43	0.72
1:A:426:HIS:NE2	3:C:80:GLU:OE1	2.23	0.72
1:A:618:GLU:O	1:A:619:TYR:CG	2.43	0.72
13:X:5:ARG:O	13:X:6:CYS:SG	2.48	0.72
1:W:107:SER:O	1:W:109:ASP:N	2.23	0.71
9:K:50:LEU:O	9:K:51:ILE:O	2.08	0.71
1:W:241:ASP:OD2	1:W:289:HIS:CE1	2.44	0.71
1:A:107:SER:O	1:A:109:ASP:N	2.23	0.70
1:W:426:HIS:NE2	3:Y:80:GLU:OE1	2.25	0.70
4:S:209:CYS:SG	16:S:1001:F3S:S2	2.89	0.70
1:W:618:GLU:O	1:W:619:TYR:CG	2.44	0.70
1:W:618:GLU:O	1:W:619:TYR:CD2	2.45	0.69
1:W:98:CYS:C	1:W:146:CYS:SG	2.65	0.68
2:B:396:ARG:NH2	2:B:406:TRP:CH2	2.61	0.68
9:I:50:LEU:O	9:I:51:ILE:O	2.11	0.67
2:R:768:TYR:CB	2:R:769:PRO:CD	2.72	0.67
2:R:161:GLU:OE2	2:R:690:ARG:NH2	2.28	0.67
2:R:767:LYS:CB	2:R:768:TYR:CA	2.72	0.67
5:E:165:ARG:C	5:E:167:PRO:CD	2.63	0.67
5:E:114:THR:CB	5:E:115:ASP:CA	2.75	0.65
5:T:114:THR:CB	5:T:115:ASP:CA	2.75	0.65
1:W:103:ARG:NE	1:W:191:ASP:OD1	2.30	0.65
1:W:426:HIS:CG	3:Y:80:GLU:OE2	2.51	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:618:GLU:O	1:A:619:TYR:CD2	2.50	0.64
1:A:682:GLY:O	1:A:684:LEU:N	2.30	0.64
1:A:426:HIS:CG	3:C:80:GLU:OE2	2.50	0.64
13:P:5:ARG:O	13:P:6:CYS:SG	2.56	0.64
13:P:5:ARG:O	13:P:6:CYS:CB	2.45	0.64
1:A:108:GLU:O	1:A:111:ILE:N	2.30	0.64
9:I:56:ILE:O	9:I:57:SER:CA	2.33	0.64
4:S:203:CYS:SG	16:S:1001:F3S:S1	2.96	0.64
2:B:161:GLU:OE2	2:B:690:ARG:NH2	2.31	0.64
2:R:396:ARG:NH2	2:R:406:TRP:CH2	2.66	0.64
3:C:216:ILE:O	3:C:217:ALA:CB	2.45	0.64
1:A:309:PHE:O	1:A:310:ARG:CG	2.45	0.64
4:S:206:CYS:SG	16:S:1001:F3S:FE4	1.89	0.63
4:D:203:CYS:SG	16:D:1001:F3S:FE3	1.89	0.63
9:K:51:ILE:O	9:K:52:ASP:CB	2.45	0.63
3:Y:216:ILE:O	3:Y:217:ALA:CB	2.46	0.63
2:R:406:TRP:CG	2:R:407:VAL:N	2.66	0.63
2:B:406:TRP:O	2:B:408:GLY:N	2.31	0.63
2:B:1007:ARG:NH1	2:B:1028:GLY:O	2.32	0.63
1:W:104:VAL:CG1	1:W:137:LYS:CA	2.76	0.62
2:B:766:VAL:CG1	2:B:774:ASP:OD2	2.47	0.62
13:X:5:ARG:O	13:X:6:CYS:CB	2.48	0.62
1:A:372:TRP:C	1:A:372:TRP:CD1	2.73	0.62
1:W:104:VAL:CG1	1:W:137:LYS:CG	2.78	0.62
5:T:165:ARG:C	5:T:167:PRO:CD	2.68	0.61
3:Y:176:ASP:O	3:Y:177:LYS:CB	2.48	0.61
9:K:56:ILE:O	9:K:57:SER:CA	2.38	0.61
1:A:854:GLY:O	3:C:64:ILE:CG2	2.48	0.61
2:R:1007:ARG:NH1	2:R:1028:GLY:C	2.54	0.61
9:I:51:ILE:O	9:I:52:ASP:CB	2.49	0.60
2:B:1007:ARG:NH1	2:B:1028:GLY:C	2.55	0.60
1:A:848:VAL:O	1:A:849:ALA:CB	2.50	0.60
1:W:682:GLY:O	1:W:684:LEU:N	2.34	0.60
2:B:601:ASP:O	2:B:602:SER:CB	2.50	0.60
2:R:601:ASP:O	2:R:602:SER:CB	2.50	0.60
2:R:418:ASP:OD1	2:R:424:SER:OG	2.19	0.60
5:T:166:GLN:N	5:T:167:PRO:CD	2.65	0.59
1:A:426:HIS:CD2	3:C:80:GLU:CD	2.75	0.59
2:R:520:TRP:O	2:R:521:SER:CB	2.51	0.59
2:R:418:ASP:OD1	2:R:418:ASP:O	2.21	0.59
3:C:176:ASP:O	3:C:177:LYS:CB	2.50	0.59
1:W:108:GLU:O	1:W:111:ILE:N	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:166:GLN:N	5:E:167:PRO:CD	2.65	0.59
2:B:834:ALA:O	2:B:835:LYS:CB	2.51	0.59
1:W:426:HIS:CD2	3:Y:80:GLU:OE1	2.56	0.59
2:B:406:TRP:CG	2:B:407:VAL:N	2.71	0.59
1:W:426:HIS:CD2	3:Y:80:GLU:CD	2.75	0.59
2:B:557:ASN:OD1	2:B:577:ARG:NH1	2.35	0.58
2:R:1072:TRP:CZ3	1:W:67:ASN:OD1	2.56	0.58
2:B:520:TRP:O	2:B:521:SER:CB	2.50	0.58
2:B:418:ASP:OD1	2:B:418:ASP:O	2.22	0.58
2:R:834:ALA:O	2:R:835:LYS:CB	2.51	0.58
5:T:115:ASP:O	5:T:116:ASP:CB	2.50	0.58
5:T:132:SER:O	5:T:133:LYS:CB	2.51	0.58
2:R:1007:ARG:NH1	2:R:1028:GLY:O	2.36	0.58
2:R:766:VAL:CG1	2:R:774:ASP:OD2	2.52	0.58
3:C:328:GLN:OE1	3:C:331:ARG:NH1	2.37	0.58
3:C:231:ILE:CG2	3:C:232:LYS:N	2.66	0.57
1:W:309:PHE:O	1:W:310:ARG:CB	2.52	0.57
1:W:848:VAL:O	1:W:849:ALA:CB	2.51	0.57
1:W:534:LEU:CB	1:W:546:TYR:CE2	2.88	0.57
2:B:418:ASP:OD1	2:B:424:SER:OG	2.22	0.57
1:A:600:LYS:O	1:A:601:LYS:CB	2.53	0.57
2:R:765:GLU:O	2:R:766:VAL:O	2.22	0.57
2:R:774:ASP:OD1	2:R:819:PRO:CD	2.52	0.57
9:K:39:ARG:NE	9:K:68:GLU:OE2	2.38	0.57
3:Y:231:ILE:CG2	3:Y:232:LYS:N	2.68	0.56
4:D:60:HIS:CD2	4:D:60:HIS:C	2.78	0.56
3:Y:323:THR:O	3:Y:325:VAL:N	2.39	0.56
9:I:39:ARG:NE	9:I:68:GLU:OE2	2.38	0.56
1:A:534:LEU:CB	1:A:546:TYR:CE1	2.89	0.56
5:E:115:ASP:O	5:E:116:ASP:CB	2.53	0.56
2:B:1057:ASP:OD1	2:B:1057:ASP:N	2.39	0.56
1:A:281:ILE:N	1:A:282:PRO:CD	2.68	0.56
2:B:774:ASP:OD1	2:B:819:PRO:CD	2.54	0.56
1:A:385:ARG:NH1	2:B:1009:ARG:NH2	2.54	0.56
9:I:54:ASN:ND2	1:W:356:TRP:CE3	2.73	0.56
2:B:765:GLU:O	2:B:766:VAL:O	2.24	0.55
4:S:209:CYS:SG	16:S:1001:F3S:S3	3.04	0.55
1:W:853:ASP:CB	3:Y:311:ARG:NH1	2.70	0.55
1:A:736:SER:O	1:A:738:LEU:N	2.40	0.55
5:E:132:SER:O	5:E:133:LYS:CB	2.54	0.55
2:R:107:GLU:O	2:R:108:ASN:CB	2.54	0.55
1:A:792:PRO:CG	2:B:948:PHE:CE1	2.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:323:THR:O	3:C:325:VAL:N	2.40	0.55
2:R:1060:THR:O	2:R:1061:ILE:C	2.45	0.55
4:D:49:ASN:OD1	4:D:139:ILE:CD1	2.55	0.55
2:B:27:VAL:O	2:B:29:GLN:N	2.40	0.55
3:Y:104:LEU:N	3:Y:105:PRO:CD	2.69	0.55
3:C:104:LEU:N	3:C:105:PRO:CD	2.69	0.55
1:W:281:ILE:N	1:W:282:PRO:CD	2.69	0.55
1:W:854:GLY:O	3:Y:64:ILE:CG1	2.55	0.55
1:A:103:ARG:CB	1:A:191:ASP:OD1	2.54	0.55
1:W:309:PHE:O	1:W:310:ARG:CG	2.55	0.55
2:B:1060:THR:O	2:B:1061:ILE:C	2.46	0.55
1:A:426:HIS:CE1	3:C:80:GLU:CD	2.79	0.54
1:W:854:GLY:O	3:Y:64:ILE:CG2	2.54	0.54
1:W:372:TRP:CD1	1:W:372:TRP:C	2.79	0.54
5:E:30:LEU:CD1	5:E:72:PHE:CE2	2.91	0.54
1:A:47:PRO:O	1:A:48:ARG:CB	2.55	0.54
1:A:98:CYS:SG	1:A:145:VAL:O	2.65	0.54
1:A:736:SER:O	1:A:737:VAL:C	2.46	0.54
2:B:603:GLY:C	2:B:605:ILE:N	2.60	0.54
4:S:49:ASN:OD1	4:S:139:ILE:CD1	2.55	0.54
2:R:628:TYR:CE2	2:R:640:HIS:CE1	2.96	0.54
5:T:30:LEU:CD2	5:T:72:PHE:CE2	2.91	0.54
9:I:52:ASP:O	9:I:53:ILE:CB	2.56	0.53
2:R:557:ASN:OD1	2:R:577:ARG:NH1	2.41	0.53
1:W:600:LYS:O	1:W:601:LYS:CB	2.56	0.53
1:W:145:VAL:O	1:W:146:CYS:SG	2.66	0.53
2:R:416:LEU:O	2:R:418:ASP:N	2.42	0.53
1:A:792:PRO:CA	2:B:948:PHE:CE1	2.92	0.53
2:B:416:LEU:O	2:B:418:ASP:N	2.41	0.53
2:B:453:TRP:CZ3	2:B:644:GLU:OE2	2.60	0.53
1:A:450:CYS:N	1:A:451:PRO:CD	2.72	0.53
1:W:125:TRP:N	1:W:126:PRO:CD	2.71	0.53
2:R:604:SER:O	2:R:605:ILE:O	2.27	0.53
2:B:17:ILE:CD1	2:B:476:MET:SD	2.97	0.53
1:W:47:PRO:O	1:W:48:ARG:CB	2.56	0.53
1:A:125:TRP:N	1:A:126:PRO:CD	2.72	0.53
1:A:426:HIS:CD2	3:C:80:GLU:OE1	2.62	0.52
2:R:647:SER:N	2:R:648:PRO:CD	2.72	0.52
1:W:736:SER:O	1:W:737:VAL:C	2.48	0.52
13:X:10:TRP:CB	13:X:31:TYR:CE2	2.93	0.52
3:C:30:GLU:CG	3:C:31:ASP:N	2.73	0.52
2:R:406:TRP:O	2:R:408:GLY:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:451:PRO:N	1:W:452:PRO:CD	2.73	0.52
2:B:647:SER:N	2:B:648:PRO:CD	2.73	0.52
3:C:210:PHE:O	3:C:211:ALA:CB	2.57	0.52
1:A:818:TYR:CD2	1:A:822:ARG:NH1	2.78	0.52
3:C:11:SER:N	3:C:45:ARG:NH2	2.58	0.52
2:B:215:VAL:CG1	2:B:216:SER:N	2.72	0.52
4:D:203:CYS:SG	16:D:1001:F3S:S1	3.07	0.52
13:P:10:TRP:CB	13:P:31:TYR:CE2	2.93	0.52
1:W:736:SER:O	1:W:738:LEU:N	2.43	0.52
2:B:107:GLU:O	2:B:108:ASN:CB	2.57	0.52
3:C:46:ASP:O	3:C:47:GLU:OE1	2.28	0.52
1:W:223:ILE:CG1	1:W:224:MET:N	2.73	0.52
2:B:461:THR:CG2	2:B:468:GLY:N	2.72	0.52
1:A:107:SER:O	1:A:108:GLU:C	2.46	0.52
2:R:453:TRP:CZ3	2:R:644:GLU:OE2	2.63	0.52
1:A:309:PHE:O	1:A:310:ARG:CB	2.58	0.51
5:E:123:VAL:O	5:E:124:ARG:O	2.29	0.51
4:D:104:ASN:O	4:D:105:GLU:C	2.49	0.51
1:A:356:TRP:CE3	9:K:54:ASN:ND2	2.78	0.51
1:A:879:LYS:NZ	3:C:44:THR:O	2.43	0.51
3:Y:30:GLU:CG	3:Y:31:ASP:N	2.73	0.51
4:S:60:HIS:CD2	4:S:60:HIS:C	2.83	0.51
3:C:80:GLU:N	3:C:81:PRO:CD	2.73	0.51
3:Y:11:SER:N	3:Y:45:ARG:NH2	2.58	0.51
2:R:461:THR:CG2	2:R:468:GLY:N	2.74	0.51
3:Y:210:PHE:O	3:Y:211:ALA:CB	2.57	0.51
1:W:421:ARG:CZ	1:W:454:ASN:O	2.59	0.51
2:B:628:TYR:CE2	2:B:640:HIS:CE1	2.98	0.51
2:R:984:SER:O	2:R:985:ARG:CB	2.58	0.51
3:Y:328:GLN:OE1	3:Y:331:ARG:NH1	2.44	0.51
2:R:112:ALA:O	2:R:113:GLU:CG	2.59	0.51
1:W:98:CYS:O	1:W:99:ARG:CB	2.59	0.51
3:Y:46:ASP:O	3:Y:47:GLU:OE1	2.29	0.51
1:A:246:ASN:O	1:A:246:ASN:CG	2.50	0.51
1:W:246:ASN:O	1:W:246:ASN:CG	2.50	0.51
4:D:209:CYS:SG	4:D:219:ILE:CD1	2.99	0.50
2:R:773:GLU:CG	2:R:774:ASP:N	2.74	0.50
1:W:450:CYS:N	1:W:451:PRO:CD	2.74	0.50
7:V:104:LYS:O	7:V:105:ILE:C	2.49	0.50
5:E:132:SER:O	5:E:133:LYS:CG	2.58	0.50
8:H:12:ARG:O	8:H:14:HIS:N	2.44	0.50
2:B:113:GLU:CB	2:B:114:PRO:CD	2.89	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:112:ALA:O	2:B:113:GLU:CG	2.59	0.50
2:R:448:LEU:CD2	1:W:796:PHE:CZ	2.94	0.50
2:B:118:TYR:CD1	2:B:118:TYR:C	2.85	0.50
2:R:109:ASN:CG	2:R:109:ASN:O	2.50	0.50
9:K:52:ASP:O	9:K:53:ILE:CB	2.59	0.50
2:R:1057:ASP:N	2:R:1057:ASP:OD1	2.44	0.50
2:R:17:ILE:CD1	2:R:476:MET:SD	2.99	0.50
3:C:176:ASP:O	3:C:177:LYS:CG	2.59	0.50
1:W:107:SER:O	1:W:108:GLU:C	2.48	0.50
2:R:628:TYR:CE2	2:R:640:HIS:ND1	2.80	0.50
4:D:84:ASP:O	4:D:85:CYS:C	2.49	0.50
1:W:695:SER:O	1:W:699:TYR:CD2	2.65	0.50
1:A:792:PRO:N	2:B:948:PHE:CE1	2.80	0.50
3:C:348:GLU:O	3:C:349:VAL:C	2.50	0.50
2:R:330:LEU:O	2:R:332:ARG:N	2.45	0.49
12:O:46:ARG:NH1	2:R:938:LEU:O	2.45	0.49
2:R:215:VAL:CG1	2:R:216:SER:N	2.74	0.49
2:B:1021:GLU:OE2	2:B:1022:GLY:N	2.45	0.49
5:T:123:VAL:O	5:T:124:ARG:O	2.30	0.49
5:E:136:ILE:CG2	5:E:137:GLN:N	2.75	0.49
2:B:136:TYR:CB	2:B:141:LEU:CD1	2.91	0.49
2:B:1091:LEU:O	2:B:1092:PHE:CG	2.66	0.49
1:W:426:HIS:CE1	3:Y:80:GLU:CD	2.86	0.49
13:X:5:ARG:CZ	13:X:6:CYS:O	2.61	0.49
1:W:879:LYS:NZ	3:Y:44:THR:O	2.45	0.49
5:T:84:VAL:CG1	6:U:75:ILE:CD1	2.90	0.49
1:A:304:GLY:C	1:A:306:GLU:N	2.65	0.49
7:V:102:LEU:O	7:V:103:VAL:C	2.51	0.49
9:K:49:ALA:O	9:K:50:LEU:C	2.50	0.49
5:T:132:SER:O	5:T:133:LYS:CG	2.60	0.49
2:R:404:GLY:O	2:R:405:ASN:O	2.31	0.49
2:B:604:SER:O	2:B:605:ILE:O	2.31	0.49
2:B:532:TYR:O	2:B:533:TYR:CB	2.60	0.49
2:B:1056:SER:CB	2:B:1057:ASP:OD1	2.60	0.49
2:B:599:LYS:O	2:B:600:LEU:C	2.50	0.49
8:Z:12:ARG:O	8:Z:14:HIS:N	2.45	0.49
9:I:51:ILE:O	9:I:52:ASP:CG	2.51	0.48
2:R:113:GLU:CB	2:R:114:PRO:CD	2.91	0.48
1:A:695:SER:O	1:A:699:TYR:CD2	2.66	0.48
4:S:40:SER:OG	4:S:156:PHE:CE1	2.66	0.48
1:A:45:MET:CG	1:A:45:MET:O	2.61	0.48
2:B:631:LEU:O	2:B:632:GLU:OE1	2.31	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:853:ASP:CB	3:C:311:ARG:NH1	2.76	0.48
12:O:61:HIS:O	12:O:62:TYR:CG	2.66	0.48
2:B:594:ARG:NH1	2:B:615:LYS:CB	2.76	0.48
13:X:5:ARG:NH1	13:X:6:CYS:O	2.46	0.48
5:E:30:LEU:CD1	5:E:72:PHE:CZ	2.96	0.48
5:E:30:LEU:CD2	5:E:72:PHE:CE2	2.96	0.48
5:T:30:LEU:CD1	5:T:72:PHE:CE2	2.96	0.48
3:C:133:ASP:O	3:C:249:TYR:CD2	2.66	0.48
1:W:818:TYR:CD2	1:W:822:ARG:NH1	2.81	0.48
4:S:84:ASP:O	4:S:85:CYS:C	2.51	0.48
2:B:502:GLU:O	2:B:506:ARG:N	2.46	0.48
3:Y:133:ASP:O	3:Y:249:TYR:CD2	2.66	0.48
3:C:163:MET:CB	3:C:164:SER:CA	2.91	0.48
4:S:38:VAL:CG1	4:S:39:MET:N	2.76	0.48
3:C:160:ILE:O	3:C:161:ALA:C	2.52	0.48
7:G:104:LYS:O	7:G:105:ILE:C	2.52	0.48
1:A:223:ILE:CG1	1:A:224:MET:N	2.76	0.48
1:A:73:GLY:O	1:A:74:HIS:ND1	2.47	0.48
1:A:99:ARG:NH1	1:A:147:PRO:CG	2.77	0.48
2:B:1069:TYR:CA	2:B:1070:ILE:CB	2.91	0.48
2:R:502:GLU:O	2:R:506:ARG:N	2.47	0.48
11:M:18:GLU:O	11:M:18:GLU:CG	2.60	0.48
1:W:45:MET:O	1:W:45:MET:CG	2.60	0.48
2:B:893:MET:CG	2:B:894:LEU:N	2.76	0.48
5:T:136:ILE:CG2	5:T:137:GLN:N	2.76	0.48
5:E:40:LYS:O	5:E:41:ASP:CG	2.52	0.48
1:A:640:GLU:OE1	2:B:977:ARG:NH1	2.46	0.48
3:C:28:ILE:CD1	9:K:14:HIS:CD2	2.97	0.48
4:D:38:VAL:CG1	4:D:39:MET:N	2.77	0.48
9:K:51:ILE:O	9:K:52:ASP:CG	2.51	0.48
2:B:330:LEU:O	2:B:332:ARG:N	2.46	0.48
2:B:984:SER:O	2:B:985:ARG:CB	2.61	0.48
2:R:599:LYS:O	2:R:600:LEU:C	2.52	0.47
3:Y:160:ILE:O	3:Y:161:ALA:C	2.53	0.47
1:A:28:ILE:CG2	1:A:29:THR:N	2.77	0.47
1:W:304:GLY:C	1:W:306:GLU:N	2.68	0.47
5:E:84:VAL:CG1	6:F:75:ILE:CD1	2.92	0.47
2:R:594:ARG:NH1	2:R:615:LYS:CB	2.77	0.47
3:Y:163:MET:CB	3:Y:164:SER:CA	2.92	0.47
2:B:109:ASN:O	2:B:109:ASN:CG	2.52	0.47
1:A:426:HIS:CG	3:C:80:GLU:CD	2.88	0.47
5:E:53:THR:O	5:E:54:SER:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:603:GLY:C	2:R:605:ILE:N	2.66	0.47
2:B:330:LEU:O	2:B:332:ARG:CG	2.62	0.47
3:Y:192:LYS:O	3:Y:194:GLY:N	2.47	0.47
2:B:370:TYR:O	2:B:370:TYR:CG	2.68	0.47
5:T:8:ARG:NE	5:T:69:GLU:OE2	2.48	0.47
2:B:372:LEU:CD2	2:B:376:LYS:CE	2.92	0.47
3:C:303:GLU:C	3:C:303:GLU:OE1	2.52	0.47
3:Y:80:GLU:N	3:Y:81:PRO:CD	2.78	0.47
1:A:103:ARG:CG	1:A:191:ASP:OD1	2.63	0.47
2:B:396:ARG:NH2	2:B:406:TRP:CZ2	2.83	0.47
2:R:1056:SER:CB	2:R:1057:ASP:OD1	2.62	0.47
2:R:370:TYR:CG	2:R:370:TYR:O	2.68	0.47
2:R:1009:ARG:NH2	1:W:385:ARG:NH1	2.62	0.47
1:A:241:ASP:OD2	1:A:289:HIS:NE2	2.48	0.47
2:B:786:TYR:CE2	2:B:788:GLY:CA	2.98	0.47
3:C:244:LYS:CA	3:C:245:LYS:CB	2.93	0.47
3:C:277:ILE:CG2	3:C:278:ARG:N	2.77	0.47
1:A:856:PHE:CE2	1:A:858:MET:CB	2.98	0.47
1:W:73:GLY:O	1:W:74:HIS:ND1	2.48	0.47
2:R:977:ARG:NH1	1:W:640:GLU:OE1	2.48	0.47
3:Y:176:ASP:O	3:Y:177:LYS:CG	2.62	0.47
3:C:277:ILE:C	3:C:279:GLU:N	2.67	0.47
13:P:4:TYR:O	13:P:4:TYR:CD1	2.67	0.47
3:C:192:LYS:O	3:C:194:GLY:N	2.48	0.47
2:R:532:TYR:O	2:R:533:TYR:CB	2.62	0.47
2:B:404:GLY:O	2:B:405:ASN:O	2.32	0.46
11:L:18:GLU:O	11:L:18:GLU:CG	2.62	0.46
1:A:67:ASN:OD1	2:B:1072:TRP:CZ3	2.68	0.46
2:R:1091:LEU:O	2:R:1092:PHE:CG	2.68	0.46
2:R:562:VAL:O	2:R:566:ILE:O	2.33	0.46
5:T:40:LYS:O	5:T:41:ASP:CG	2.53	0.46
2:B:103:MET:O	2:B:114:PRO:O	2.34	0.46
9:K:13:LEU:O	9:K:14:HIS:C	2.53	0.46
2:B:767:LYS:CB	2:B:768:TYR:CG	2.98	0.46
13:P:5:ARG:CZ	13:P:6:CYS:O	2.63	0.46
1:A:331:ASN:O	1:A:332:ILE:CG1	2.63	0.46
2:R:1069:TYR:CA	2:R:1070:ILE:CB	2.92	0.46
2:R:767:LYS:CE	2:R:767:LYS:CA	2.94	0.46
1:A:854:GLY:O	3:C:64:ILE:CG1	2.64	0.46
2:R:27:VAL:O	2:R:29:GLN:N	2.49	0.46
2:B:463:GLU:OE1	2:B:463:GLU:N	2.48	0.46
9:I:49:ALA:O	9:I:50:LEU:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:PRO:N	1:A:452:PRO:CD	2.79	0.46
3:Y:133:ASP:O	3:Y:249:TYR:CE2	2.69	0.46
1:A:181:ARG:NH1	1:A:210:THR:OG1	2.49	0.46
2:B:173:ASN:N	2:B:193:ILE:O	2.49	0.46
2:R:118:TYR:C	2:R:118:TYR:CD1	2.89	0.46
4:D:40:SER:OG	4:D:156:PHE:CE1	2.69	0.46
2:B:1007:ARG:CZ	2:B:1028:GLY:N	2.78	0.46
2:B:660:TYR:N	2:B:661:PRO:CD	2.79	0.46
1:W:331:ASN:O	1:W:332:ILE:CG1	2.64	0.46
2:R:622:GLU:O	2:R:625:GLU:CB	2.64	0.46
5:E:8:ARG:NE	5:E:69:GLU:OE2	2.49	0.45
2:R:1021:GLU:OE2	2:R:1022:GLY:N	2.49	0.45
9:I:14:HIS:CD2	3:Y:28:ILE:CD1	2.98	0.45
2:R:686:ASN:C	2:R:688:GLN:N	2.68	0.45
4:S:153:HIS:CG	4:S:153:HIS:O	2.69	0.45
3:Y:81:PRO:O	3:Y:83:THR:N	2.49	0.45
2:R:1007:ARG:CZ	2:R:1028:GLY:N	2.80	0.45
10:Q:61:VAL:C	10:Q:63:GLU:N	2.70	0.45
7:G:76:TYR:N	7:G:76:TYR:CD1	2.84	0.45
2:B:396:ARG:NH2	2:B:406:TRP:CZ3	2.85	0.45
1:W:682:GLY:O	1:W:683:GLU:C	2.55	0.45
3:C:133:ASP:O	3:C:249:TYR:CE2	2.69	0.45
2:R:1003:LYS:O	2:R:1004:ILE:C	2.54	0.45
1:W:599:ASP:N	1:W:599:ASP:OD1	2.49	0.45
3:Y:244:LYS:CA	3:Y:245:LYS:CB	2.93	0.45
2:R:136:TYR:CB	2:R:141:LEU:CD1	2.94	0.45
3:Y:394:LEU:O	3:Y:395:ARG:C	2.54	0.45
3:Y:112:ASP:O	3:Y:114:LYS:N	2.49	0.45
3:C:394:LEU:O	3:C:395:ARG:C	2.54	0.45
2:B:399:HIS:O	2:B:403:THR:CG2	2.65	0.45
3:Y:348:GLU:O	3:Y:349:VAL:C	2.54	0.45
7:G:102:LEU:O	7:G:103:VAL:C	2.55	0.45
1:A:421:ARG:CZ	1:A:454:ASN:O	2.64	0.45
2:R:722:GLY:O	2:R:992:TYR:CE1	2.70	0.45
4:D:153:HIS:O	4:D:153:HIS:CG	2.70	0.45
1:W:28:ILE:CG2	1:W:29:THR:N	2.80	0.45
1:A:426:HIS:NE2	3:C:80:GLU:CD	2.70	0.45
5:E:115:ASP:O	5:E:116:ASP:CG	2.55	0.45
9:K:27:LEU:CD2	9:K:78:ILE:CD1	2.94	0.45
2:B:75:GLU:N	2:B:79:GLY:O	2.50	0.45
1:W:426:HIS:CG	3:Y:80:GLU:CD	2.91	0.45
1:A:792:PRO:CD	2:B:948:PHE:CE1	3.00	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:46:ILE:CG1	2:B:66:ILE:CD1	2.94	0.45
9:I:61:VAL:O	9:I:62:ILE:C	2.55	0.45
1:A:502:TYR:O	1:A:503:ILE:C	2.54	0.45
1:W:871:ILE:CD1	3:Y:39:LYS:O	2.65	0.45
8:H:40:GLU:OE2	10:Q:66:ARG:NH1	2.50	0.44
3:Y:277:ILE:CG2	3:Y:278:ARG:N	2.80	0.44
2:R:660:TYR:N	2:R:661:PRO:CD	2.80	0.44
1:A:106:ILE:N	1:A:106:ILE:CD1	2.79	0.44
2:R:330:LEU:O	2:R:332:ARG:CG	2.65	0.44
7:V:104:LYS:O	7:V:106:ILE:N	2.50	0.44
2:R:463:GLU:OE1	2:R:463:GLU:N	2.50	0.44
2:R:396:ARG:NH2	2:R:406:TRP:CZ2	2.86	0.44
2:R:732:PHE:O	2:R:733:THR:CG2	2.66	0.44
9:K:56:ILE:N	9:K:57:SER:N	2.63	0.44
2:B:767:LYS:CE	2:B:767:LYS:CA	2.96	0.44
2:B:947:PRO:O	2:B:948:PHE:CD2	2.70	0.44
2:B:780:GLU:O	2:B:782:GLY:N	2.50	0.44
2:R:786:TYR:CE2	2:R:788:GLY:CA	3.00	0.44
2:B:628:TYR:CE2	2:B:640:HIS:ND1	2.85	0.44
4:D:108:MET:CG	4:D:110:TYR:CE2	3.00	0.44
4:D:108:MET:CG	4:D:110:TYR:CZ	3.01	0.44
2:B:622:GLU:O	2:B:625:GLU:CB	2.66	0.44
1:A:370:ASP:OD1	1:A:389:ARG:NH1	2.51	0.44
1:W:181:ARG:NH1	1:W:210:THR:OG1	2.51	0.44
1:W:241:ASP:OD2	1:W:289:HIS:NE2	2.50	0.44
1:W:856:PHE:CE2	1:W:858:MET:CB	3.01	0.44
2:B:317:TYR:OH	2:B:527:GLY:O	2.36	0.44
4:S:104:ASN:O	4:S:105:GLU:C	2.55	0.44
2:R:212:THR:O	2:R:213:PHE:CB	2.66	0.44
13:P:33:ILE:CD1	13:P:33:ILE:N	2.80	0.44
2:R:1074:ASP:CB	2:R:1075:LYS:CA	2.96	0.44
1:W:16:PRO:CD	1:W:206:TRP:CD1	3.01	0.44
2:B:947:PRO:C	2:B:948:PHE:CD2	2.91	0.44
7:G:22:SER:O	7:G:23:LEU:C	2.56	0.44
9:I:62:ILE:CD1	1:W:474:ALA:CB	2.96	0.44
7:V:76:TYR:N	7:V:76:TYR:CD1	2.85	0.44
1:A:474:ALA:CB	9:K:62:ILE:CD1	2.95	0.44
2:R:317:TYR:OH	2:R:527:GLY:O	2.36	0.44
7:V:75:GLY:C	7:V:76:TYR:CD1	2.91	0.43
2:R:460:GLU:OE1	2:R:472:ASN:ND2	2.51	0.43
2:R:372:LEU:CD2	2:R:376:LYS:CE	2.96	0.43
2:R:46:ILE:O	2:R:46:ILE:CG2	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:871:ILE:CD1	3:C:39:LYS:O	2.66	0.43
2:B:17:ILE:CG1	2:B:476:MET:SD	3.06	0.43
2:R:103:MET:O	2:R:114:PRO:O	2.36	0.43
2:B:252:GLN:O	2:B:256:PHE:CD2	2.71	0.43
3:C:76:GLN:O	3:C:80:GLU:N	2.51	0.43
2:B:946:THR:O	2:B:947:PRO:C	2.57	0.43
5:T:53:THR:O	5:T:54:SER:C	2.55	0.43
5:T:84:VAL:CG2	6:U:75:ILE:CD1	2.97	0.43
1:A:19:ILE:O	1:A:74:HIS:NE2	2.52	0.43
9:I:13:LEU:O	9:I:14:HIS:C	2.56	0.43
3:Y:213:ILE:O	3:Y:214:ASP:CG	2.57	0.43
7:V:22:SER:O	7:V:23:LEU:C	2.57	0.43
5:T:70:VAL:CG1	5:T:72:PHE:CE2	3.01	0.43
5:T:136:ILE:O	5:T:137:GLN:CB	2.66	0.43
2:B:699:HIS:CE1	4:D:57:ILE:CD1	3.01	0.43
3:C:213:ILE:O	3:C:214:ASP:CG	2.57	0.43
4:D:219:ILE:CD1	16:D:1001:F3S:S3	3.07	0.43
1:A:119:ASN:OD1	1:A:126:PRO:CB	2.67	0.43
1:A:16:PRO:CD	1:A:206:TRP:CD1	3.02	0.43
1:W:541:ALA:CB	1:W:542:PRO:CD	2.97	0.43
10:J:61:VAL:C	10:J:63:GLU:N	2.72	0.43
2:B:485:GLU:OE1	2:B:528:ARG:NH1	2.52	0.43
2:B:547:ARG:NH1	2:B:556:VAL:O	2.52	0.43
4:S:108:MET:CG	4:S:110:TYR:CE2	3.01	0.43
3:C:112:ASP:O	3:C:114:LYS:N	2.51	0.43
4:S:206:CYS:SG	4:S:207:GLU:N	2.91	0.43
2:R:17:ILE:CG1	2:R:476:MET:SD	3.07	0.43
4:S:108:MET:CG	4:S:110:TYR:CZ	3.02	0.43
1:A:753:ARG:NH2	2:B:447:ASP:OD2	2.52	0.43
1:W:426:HIS:NE2	3:Y:80:GLU:CD	2.72	0.43
1:W:45:MET:CE	1:W:46:ASP:OD1	2.67	0.43
2:R:547:ARG:NH1	2:R:556:VAL:O	2.51	0.43
2:R:948:PHE:CE1	1:W:792:PRO:CG	3.02	0.43
3:Y:127:THR:OG1	3:Y:129:GLU:O	2.35	0.43
1:W:103:ARG:CG	1:W:191:ASP:OD1	2.67	0.43
1:W:103:ARG:CB	1:W:191:ASP:CG	2.87	0.43
2:R:598:GLU:O	2:R:599:LYS:C	2.57	0.43
5:E:124:ARG:O	5:E:126:ILE:N	2.52	0.43
3:Y:277:ILE:C	3:Y:279:GLU:N	2.71	0.43
10:J:55:LEU:O	10:J:56:ASN:CB	2.67	0.43
2:R:173:ASN:N	2:R:193:ILE:O	2.52	0.43
1:W:412:THR:O	1:W:414:GLY:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:31:LEU:CA	2:R:125:MET:CE	2.97	0.43
1:A:390:TYR:O	1:A:391:VAL:C	2.58	0.43
2:B:562:VAL:O	2:B:566:ILE:O	2.37	0.43
12:O:64:ARG:CG	12:O:64:ARG:O	2.67	0.43
1:A:563:HIS:CD2	1:A:872:PHE:CE2	3.07	0.43
2:B:949:TYR:O	2:B:951:THR:N	2.52	0.43
4:S:219:ILE:CD1	16:S:1001:F3S:S3	3.07	0.42
1:A:682:GLY:O	1:A:683:GLU:C	2.57	0.42
1:A:683:GLU:OE1	1:A:683:GLU:N	2.52	0.42
2:B:46:ILE:O	2:B:46:ILE:CG2	2.67	0.42
1:W:870:ARG:CB	1:W:870:ARG:CZ	2.96	0.42
2:B:605:ILE:CG1	2:B:606:THR:N	2.81	0.42
3:C:163:MET:SD	3:C:206:LEU:CD2	3.07	0.42
12:O:61:HIS:O	12:O:62:TYR:CD2	2.72	0.42
5:T:40:LYS:O	5:T:41:ASP:OD1	2.37	0.42
4:D:154:ALA:C	4:D:156:PHE:N	2.72	0.42
10:J:57:GLY:C	10:J:61:VAL:CG1	2.88	0.42
9:I:27:LEU:CD2	9:I:78:ILE:CD1	2.97	0.42
2:R:1096:VAL:CG1	2:R:1097:SER:N	2.82	0.42
9:I:59:THR:O	9:I:60:ASP:CG	2.57	0.42
1:W:104:VAL:O	1:W:104:VAL:CG1	2.65	0.42
9:K:61:VAL:O	9:K:62:ILE:C	2.52	0.42
4:D:205:LEU:O	4:D:207:GLU:N	2.52	0.42
2:R:1025:ARG:O	2:R:1026:GLU:C	2.57	0.42
2:B:212:THR:O	2:B:213:PHE:CB	2.67	0.42
2:B:766:VAL:CG2	2:B:767:LYS:N	2.82	0.42
2:B:769:PRO:O	2:B:770:GLY:O	2.37	0.42
3:Y:163:MET:SD	3:Y:206:LEU:CD2	3.08	0.42
1:W:19:ILE:O	1:W:74:HIS:NE2	2.52	0.42
3:C:322:ARG:NH1	8:H:42:LEU:O	2.53	0.42
1:W:488:THR:CG2	1:W:493:GLY:O	2.67	0.42
4:S:46:PHE:CG	4:S:55:ASP:OD2	2.73	0.42
1:A:488:THR:CG2	1:A:493:GLY:O	2.68	0.42
5:T:115:ASP:O	5:T:116:ASP:CG	2.58	0.42
5:T:30:LEU:CD1	5:T:72:PHE:CZ	3.02	0.42
8:H:58:LYS:NZ	10:Q:51:TRP:CH2	2.88	0.42
2:B:1046:MET:CG	5:E:61:PHE:CD1	3.03	0.42
2:B:31:LEU:CA	2:B:125:MET:CE	2.98	0.42
2:R:782:GLY:O	2:R:783:VAL:C	2.58	0.42
7:G:36:PHE:CE1	7:G:96:ILE:CG1	3.03	0.42
1:A:45:MET:CE	1:A:46:ASP:OD1	2.67	0.42
2:B:951:THR:O	2:B:951:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:855:ILE:O	13:X:34:ILE:CG2	2.68	0.42
2:R:734:GLY:CA	2:R:735:TYR:CB	2.97	0.42
2:B:938:LEU:O	12:N:46:ARG:NH1	2.52	0.42
2:B:773:GLU:CG	2:B:774:ASP:N	2.82	0.42
4:D:203:CYS:SG	4:D:204:THR:N	2.93	0.42
1:W:119:ASN:OD1	1:W:126:PRO:CB	2.67	0.42
8:H:29:TYR:CE1	10:Q:60:SER:CB	3.03	0.42
2:R:252:GLN:O	2:R:256:PHE:CD2	2.73	0.42
11:L:82:HIS:NE2	11:L:86:GLU:OE2	2.52	0.42
1:A:141:MET:O	1:A:141:MET:CG	2.67	0.42
1:W:102:GLY:O	1:W:103:ARG:C	2.58	0.42
1:W:108:GLU:O	1:W:109:ASP:C	2.57	0.42
1:A:645:THR:OG1	1:A:646:MET:N	2.53	0.42
1:W:645:THR:OG1	1:W:646:MET:N	2.53	0.42
9:I:56:ILE:N	9:I:57:SER:N	2.66	0.41
5:E:40:LYS:O	5:E:41:ASP:OD1	2.38	0.41
2:R:947:PRO:C	2:R:948:PHE:CD2	2.93	0.41
2:R:880:LYS:C	2:R:881:PHE:CD1	2.94	0.41
2:B:401:LEU:O	2:B:401:LEU:CG	2.68	0.41
7:G:34:ASN:OD1	7:G:34:ASN:N	2.53	0.41
3:C:127:THR:OG1	3:C:129:GLU:O	2.39	0.41
2:B:808:LYS:NZ	2:B:847:MET:CE	2.83	0.41
2:B:1112:ILE:O	2:B:1114:PRO:CD	2.68	0.41
13:X:4:TYR:O	13:X:4:TYR:CD1	2.73	0.41
1:A:736:SER:O	1:A:739:ASN:N	2.53	0.41
1:A:45:MET:O	1:A:45:MET:CE	2.68	0.41
1:A:23:SER:CB	1:A:74:HIS:NE2	2.83	0.41
5:T:39:LEU:O	5:T:40:LYS:C	2.58	0.41
2:R:786:TYR:CE1	2:R:792:TYR:CE2	3.08	0.41
2:R:780:GLU:O	2:R:782:GLY:N	2.53	0.41
2:R:176:LEU:CD2	2:R:343:ASN:OD1	2.68	0.41
2:B:1074:ASP:CB	2:B:1075:LYS:CA	2.98	0.41
2:R:808:LYS:O	2:R:809:GLY:C	2.59	0.41
2:B:598:GLU:OE2	2:B:605:ILE:CG1	2.68	0.41
2:B:108:ASN:C	2:B:110:ILE:N	2.72	0.41
2:B:594:ARG:NH1	2:B:615:LYS:CG	2.83	0.41
4:D:46:PHE:CG	4:D:55:ASP:OD2	2.73	0.41
3:C:193:LEU:O	3:C:195:GLU:N	2.53	0.41
2:R:485:GLU:OE1	2:R:528:ARG:NH1	2.54	0.41
2:B:767:LYS:CG	2:B:768:TYR:CA	2.98	0.41
2:B:732:PHE:O	2:B:733:THR:CG2	2.69	0.41
2:B:1096:VAL:CG1	2:B:1097:SER:N	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:41:LYS:O	2:B:43:GLN:N	2.53	0.41
3:C:174:LEU:N	3:C:174:LEU:CD1	2.84	0.41
5:T:124:ARG:O	5:T:126:ILE:N	2.54	0.41
10:Q:57:GLY:C	10:Q:61:VAL:CG1	2.89	0.41
6:F:8:GLU:OE1	6:F:10:HIS:ND1	2.54	0.41
2:B:161:GLU:OE1	2:B:419:ARG:NH1	2.54	0.41
4:S:154:ALA:C	4:S:156:PHE:N	2.74	0.41
1:W:45:MET:O	1:W:45:MET:CE	2.68	0.41
2:R:46:ILE:CG1	2:R:66:ILE:CD1	2.99	0.41
7:V:70:ASP:O	1:W:541:ALA:CB	2.69	0.41
3:Y:32:LEU:O	3:Y:33:LYS:C	2.59	0.41
3:Y:70:ILE:CD1	3:Y:70:ILE:N	2.84	0.41
1:A:108:GLU:O	1:A:109:ASP:C	2.58	0.41
3:Y:322:ARG:NH1	8:Z:42:LEU:O	2.54	0.41
5:E:84:VAL:CG2	6:F:75:ILE:CD1	2.99	0.41
2:R:732:PHE:CG	2:R:733:THR:N	2.89	0.41
2:B:782:GLY:O	2:B:783:VAL:C	2.59	0.41
2:R:66:ILE:CG2	2:R:67:ARG:N	2.83	0.41
1:A:420:ASN:O	1:A:463:ASN:N	2.54	0.41
11:M:82:HIS:NE2	11:M:86:GLU:OE2	2.54	0.41
3:C:70:ILE:CD1	3:C:70:ILE:N	2.84	0.41
2:R:808:LYS:NZ	2:R:847:MET:CE	2.84	0.41
2:B:971:GLU:OE2	12:N:43:TYR:OH	2.39	0.41
2:R:699:HIS:CE1	4:S:57:ILE:CD1	3.04	0.41
4:D:37:PRO:CG	4:D:78:TRP:CZ3	3.04	0.41
1:W:109:ASP:O	1:W:112:GLU:C	2.59	0.40
2:R:767:LYS:CG	2:R:768:TYR:CD1	3.04	0.40
5:T:123:VAL:CG1	5:T:123:VAL:O	2.69	0.40
1:W:876:VAL:C	1:W:878:TRP:N	2.75	0.40
13:X:33:ILE:N	13:X:33:ILE:CD1	2.83	0.40
4:S:203:CYS:SG	4:S:204:THR:N	2.94	0.40
3:Y:322:ARG:O	3:Y:323:THR:CB	2.69	0.40
2:B:25:GLY:O	2:B:27:VAL:N	2.54	0.40
2:R:598:GLU:OE2	2:R:605:ILE:CG1	2.69	0.40
2:B:31:LEU:CD2	2:B:125:MET:CE	2.98	0.40
2:R:631:LEU:O	2:R:632:GLU:OE1	2.37	0.40
1:A:555:PHE:CD1	1:A:626:TRP:CH2	3.09	0.40
2:R:398:ARG:O	2:R:401:LEU:N	2.54	0.40
2:B:535:ASP:OD2	2:B:538:GLU:OE2	2.39	0.40
2:R:759:ARG:CG	2:R:760:LEU:N	2.83	0.40
2:R:399:HIS:O	2:R:403:THR:CG2	2.69	0.40
5:T:101:LEU:N	5:T:101:LEU:CD1	2.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:555:PHE:CD1	1:W:626:TRP:CH2	3.09	0.40
2:R:947:PRO:O	2:R:948:PHE:CD2	2.75	0.40
1:W:552:VAL:CG1	1:W:598:PHE:CE2	3.05	0.40
1:A:552:VAL:CG1	1:A:598:PHE:CE2	3.04	0.40
1:A:598:PHE:CE1	1:A:611:ILE:CD1	3.05	0.40
3:Y:303:GLU:C	3:Y:303:GLU:OE1	2.59	0.40
1:W:563:HIS:CD2	1:W:872:PHE:CE2	3.10	0.40
3:Y:170:ASP:O	3:Y:174:LEU:CD1	2.70	0.40
2:B:367:ASP:O	2:B:371:GLN:N	2.55	0.40
2:R:873:ARG:NH2	2:R:1002:ASP:OD2	2.54	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	823/880 (94%)	669 (81%)	120 (15%)	34 (4%)	4	50
1	W	823/880 (94%)	672 (82%)	111 (14%)	40 (5%)	3	45
2	B	1077/1131 (95%)	887 (82%)	118 (11%)	72 (7%)	2	36
2	R	1077/1131 (95%)	881 (82%)	122 (11%)	74 (7%)	2	34
3	C	364/395 (92%)	278 (76%)	63 (17%)	23 (6%)	2	38
3	Y	364/395 (92%)	282 (78%)	54 (15%)	28 (8%)	1	30
4	D	258/265 (97%)	219 (85%)	31 (12%)	8 (3%)	7	59
4	S	258/265 (97%)	220 (85%)	30 (12%)	8 (3%)	7	59
5	E	160/180 (89%)	127 (79%)	21 (13%)	12 (8%)	2	31
5	T	160/180 (89%)	125 (78%)	24 (15%)	11 (7%)	2	34
6	F	88/113 (78%)	75 (85%)	11 (12%)	2 (2%)	10	65
6	U	88/113 (78%)	77 (88%)	9 (10%)	2 (2%)	10	65
7	G	108/132 (82%)	89 (82%)	15 (14%)	4 (4%)	5	54
7	V	108/132 (82%)	88 (82%)	16 (15%)	4 (4%)	5	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	72/84 (86%)	59 (82%)	9 (12%)	4 (6%)	3	41
8	Z	72/84 (86%)	59 (82%)	7 (10%)	6 (8%)	1	28
9	I	80/95 (84%)	64 (80%)	9 (11%)	7 (9%)	1	26
9	K	80/95 (84%)	64 (80%)	9 (11%)	7 (9%)	1	26
10	J	37/104 (36%)	27 (73%)	8 (22%)	2 (5%)	3	42
10	Q	37/104 (36%)	27 (73%)	8 (22%)	2 (5%)	3	42
11	L	89/92 (97%)	78 (88%)	9 (10%)	2 (2%)	10	66
11	M	89/92 (97%)	79 (89%)	8 (9%)	2 (2%)	10	66
12	N	62/66 (94%)	50 (81%)	10 (16%)	2 (3%)	6	58
12	O	62/66 (94%)	50 (81%)	9 (14%)	3 (5%)	4	45
13	P	43/48 (90%)	33 (77%)	7 (16%)	3 (7%)	2	34
13	X	43/48 (90%)	33 (77%)	7 (16%)	3 (7%)	2	34
All	All	6522/7170 (91%)	5312 (81%)	845 (13%)	365 (6%)	3	41

All (365) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	103	ARG
1	A	108	GLU
1	A	683	GLU
1	A	737	VAL
2	B	28	ARG
2	B	108	ASN
2	B	213	PHE
2	B	331	GLY
2	B	405	ASN
2	B	460	GLU
2	B	521	SER
2	B	590	PRO
2	B	591	LEU
2	B	600	LEU
2	B	602	SER
2	B	605	ILE
2	B	735	TYR
2	B	766	VAL
2	B	768	TYR
2	B	770	GLY

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Mol	Chain	Res	Type
2	B	835	LYS
2	B	950	LYS
2	B	1061	ILE
2	B	1070	ILE
3	C	162	SER
3	C	177	LYS
3	C	192	LYS
3	C	193	LEU
3	C	217	ALA
3	C	236	GLY
3	C	324	GLY
4	D	90	GLU
5	E	114	THR
5	E	116	ASP
5	E	124	ARG
5	E	126	ILE
5	E	133	LYS
5	E	167	PRO
7	G	17	SER
7	G	105	ILE
8	H	13	ILE
9	I	51	ILE
9	I	52	ASP
9	I	53	ILE
9	I	56	ILE
10	J	56	ASN
9	K	51	ILE
9	K	52	ASP
9	K	53	ILE
9	K	56	ILE
13	P	6	CYS
10	Q	56	ASN
2	R	108	ASN
2	R	213	PHE
2	R	405	ASN
2	R	460	GLU
2	R	521	SER
2	R	533	TYR
2	R	590	PRO
2	R	591	LEU
2	R	600	LEU
2	R	602	SER

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Mol	Chain	Res	Type
2	R	605	ILE
2	R	735	TYR
2	R	766	VAL
2	R	768	TYR
2	R	835	LYS
2	R	950	LYS
2	R	1026	GLU
2	R	1061	ILE
2	R	1070	ILE
4	S	90	GLU
5	T	114	THR
5	T	116	ASP
5	T	124	ARG
5	T	126	ILE
5	T	133	LYS
5	T	167	PRO
7	V	17	SER
7	V	105	ILE
1	W	23	SER
1	W	103	ARG
1	W	108	GLU
1	W	683	GLU
1	W	737	VAL
13	X	6	CYS
3	Y	177	LYS
3	Y	192	LYS
3	Y	193	LEU
3	Y	217	ALA
3	Y	324	GLY
8	Z	13	ILE
1	A	96	ALA
1	A	280	GLU
1	A	310	ARG
1	A	332	ILE
1	A	391	VAL
1	A	734	ARG
1	A	812	ARG
1	A	876	VAL
2	B	24	LYS
2	B	46	ILE
2	B	418	ASP
2	B	533	TYR

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Mol	Chain	Res	Type
2	B	598	GLU
2	B	599	LYS
2	B	771	GLY
2	B	772	GLN
2	B	797	ASP
2	B	809	GLY
2	B	877	ILE
2	B	1026	GLU
2	B	1072	TRP
3	C	12	TYR
3	C	194	GLY
3	C	245	LYS
3	C	365	GLU
4	D	206	CYS
5	E	125	GLY
5	E	137	GLN
7	G	103	VAL
9	I	14	HIS
9	I	61	VAL
9	K	61	VAL
13	P	5	ARG
2	R	24	LYS
2	R	49	GLN
2	R	331	GLY
2	R	418	ASP
2	R	598	GLU
2	R	599	LYS
2	R	770	GLY
2	R	771	GLY
2	R	797	ASP
2	R	809	GLY
2	R	877	ILE
2	R	943	VAL
2	R	1029	LEU
2	R	1072	TRP
4	S	117	GLU
5	T	137	GLN
7	V	99	PHE
7	V	103	VAL
1	W	96	ALA
1	W	256	GLY
1	W	308	ARG

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Mol	Chain	Res	Type
1	W	310	ARG
1	W	332	ILE
1	W	391	VAL
1	W	605	ASN
1	W	734	ARG
1	W	812	ARG
1	W	876	VAL
13	X	13	PHE
3	Y	12	TYR
3	Y	82	GLY
3	Y	162	SER
3	Y	194	GLY
3	Y	245	LYS
3	Y	349	VAL
1	A	109	ASP
1	A	148	HIS
1	A	290	ARG
1	A	532	ILE
1	A	536	GLU
1	A	849	ALA
2	B	49	GLN
2	B	116	GLU
2	B	250	GLU
2	B	256	PHE
2	B	375	SER
2	B	407	VAL
2	B	417	LEU
2	B	606	THR
2	B	734	GLY
2	B	918	LEU
2	B	943	VAL
2	B	982	ILE
2	B	985	ARG
2	B	1029	LEU
3	C	53	ASP
3	C	113	ALA
3	C	114	LYS
3	C	171	ASN
3	C	211	ALA
4	D	83	ILE
4	D	85	CYS
4	D	117	GLU

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Mol	Chain	Res	Type
5	E	40	LYS
7	G	99	PHE
10	J	57	GLY
9	K	14	HIS
9	K	91	SER
11	L	19	GLY
11	M	19	GLY
13	P	13	PHE
10	Q	57	GLY
2	R	26	LEU
2	R	28	ARG
2	R	250	GLU
2	R	256	PHE
2	R	375	SER
2	R	406	TRP
2	R	417	LEU
2	R	453	TRP
2	R	772	GLN
2	R	918	LEU
2	R	985	ARG
4	S	83	ILE
4	S	85	CYS
4	S	206	CYS
5	T	40	LYS
5	T	82	GLN
1	W	107	SER
1	W	109	ASP
1	W	148	HIS
1	W	280	GLU
1	W	290	ARG
1	W	393	ASP
1	W	541	ALA
1	W	682	GLY
1	W	849	ALA
13	X	5	ARG
3	Y	53	ASP
3	Y	114	LYS
3	Y	127	THR
3	Y	170	ASP
3	Y	201	SER
3	Y	365	GLU
8	Z	15	TYR

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Mol	Chain	Res	Type
1	A	79	ARG
1	A	256	GLY
1	A	308	ARG
1	A	393	ASP
1	A	541	ALA
1	A	601	LYS
2	B	26	LEU
2	B	437	ALA
2	B	453	TRP
2	B	738	GLU
2	B	781	PRO
2	B	949	TYR
2	B	951	THR
3	C	161	ALA
3	C	170	ASP
3	C	201	SER
3	C	216	ILE
3	C	234	ILE
4	D	193	GLY
5	E	82	GLN
8	H	15	TYR
8	H	81	VAL
9	I	91	SER
12	N	41	LYS
12	O	41	LYS
2	R	116	GLU
2	R	210	ASP
2	R	437	ALA
2	R	535	ASP
2	R	606	THR
2	R	734	GLY
2	R	738	GLU
2	R	839	SER
2	R	949	TYR
2	R	951	THR
2	R	982	ILE
2	R	1053	LEU
2	R	1073	TYR
5	T	125	GLY
1	W	46	ASP
1	W	79	ARG
1	W	287	SER

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Mol	Chain	Res	Type
1	W	413	ASP
1	W	536	GLU
3	Y	113	ALA
3	Y	171	ASN
3	Y	216	ILE
3	Y	234	ILE
8	Z	81	VAL
1	A	46	ASP
1	A	47	PRO
1	A	287	SER
1	A	682	GLY
2	B	71	PRO
2	B	74	ARG
2	B	183	GLY
2	B	210	ASP
2	B	334	GLU
2	B	535	ASP
2	B	706	VAL
2	B	839	SER
2	B	907	VAL
2	B	1044	THR
3	C	44	THR
3	C	349	VAL
4	D	9	ASP
4	D	79	PRO
5	E	120	TYR
11	L	10	SER
11	M	10	SER
12	N	6	ARG
12	O	6	ARG
2	R	78	ARG
2	R	334	GLU
2	R	706	VAL
2	R	1051	ARG
2	R	1079	LYS
4	S	9	ASP
4	S	193	GLY
1	W	62	GLY
1	W	305	LYS
1	W	429	SER
1	W	656	ASP
3	Y	30	GLU

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Mol	Chain	Res	Type
3	Y	161	ALA
3	Y	196	PHE
3	Y	306	LEU
8	Z	10	ASP
8	Z	56	ASN
1	A	62	GLY
1	A	656	ASP
2	B	56	ILE
2	B	438	ARG
2	B	1079	LYS
5	E	166	GLN
8	H	10	ASP
12	O	63	THR
2	R	56	ILE
2	R	183	GLY
2	R	407	VAL
2	R	781	PRO
2	R	783	VAL
2	R	907	VAL
5	T	166	GLN
6	U	4	VAL
3	Y	132	HIS
3	Y	146	TYR
3	Y	210	PHE
1	A	145	VAL
2	R	46	ILE
2	R	1114	PRO
4	S	79	PRO
1	W	282	PRO
1	W	689	GLY
1	A	689	GLY
2	B	769	PRO
1	W	47	PRO
1	W	145	VAL
1	W	532	ILE
1	W	654	GLY
1	A	29	THR
2	B	588	GLY
2	B	901	PRO
2	B	1114	PRO
6	F	25	ILE
2	R	71	PRO

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Mol	Chain	Res	Type
2	R	588	GLY
2	B	783	VAL
6	F	4	VAL
2	R	769	PRO
2	R	901	PRO
6	U	63	ILE
8	Z	11	PRO
1	W	449	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	723/766 (94%)	683 (94%)	40 (6%)	30	79
1	W	723/766 (94%)	678 (94%)	45 (6%)	26	75
2	B	937/975 (96%)	880 (94%)	57 (6%)	26	75
2	R	937/975 (96%)	871 (93%)	66 (7%)	21	70
3	C	316/341 (93%)	290 (92%)	26 (8%)	17	63
3	Y	316/341 (93%)	294 (93%)	22 (7%)	21	70
4	D	233/238 (98%)	227 (97%)	6 (3%)	59	90
4	S	233/238 (98%)	226 (97%)	7 (3%)	53	89
5	E	144/158 (91%)	136 (94%)	8 (6%)	30	78
5	T	144/158 (91%)	135 (94%)	9 (6%)	25	74
6	F	84/107 (78%)	81 (96%)	3 (4%)	47	87
6	U	84/107 (78%)	81 (96%)	3 (4%)	47	87
7	G	104/125 (83%)	96 (92%)	8 (8%)	18	66
7	V	104/125 (83%)	99 (95%)	5 (5%)	35	82
8	H	67/75 (89%)	67 (100%)	0	100	100
8	Z	67/75 (89%)	67 (100%)	0	100	100
9	I	72/83 (87%)	70 (97%)	2 (3%)	56	89
9	K	72/83 (87%)	70 (97%)	2 (3%)	56	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	37/96 (38%)	35 (95%)	2 (5%)	31	79
10	Q	37/96 (38%)	35 (95%)	2 (5%)	31	79
11	L	79/80 (99%)	79 (100%)	0	100	100
11	M	79/80 (99%)	79 (100%)	0	100	100
12	N	58/60 (97%)	53 (91%)	5 (9%)	15	61
12	O	58/60 (97%)	54 (93%)	4 (7%)	22	70
13	P	41/43 (95%)	38 (93%)	3 (7%)	20	69
13	X	41/43 (95%)	38 (93%)	3 (7%)	20	69
All	All	5790/6294 (92%)	5462 (94%)	328 (6%)	29	77

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	49	LEU
1	A	61	CYS
1	A	64	THR
1	A	84	VAL
1	A	88	LYS
1	A	91	TYR
1	A	101	CYS
1	A	104	VAL
1	A	105	LYS
1	A	106	ILE
1	A	107	SER
1	A	220	ARG
1	A	223	ILE
1	A	224	MET
1	A	238	LYS
1	A	254	ASP
1	A	284	LEU
1	A	288	LYS
1	A	296	ARG
1	A	314	SER
1	A	326	ILE
1	A	366	ILE
1	A	425	LEU
1	A	438	LEU
1	A	464	LEU

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Mol	Chain	Res	Type
1	A	470	GLU
1	A	488	THR
1	A	551	VAL
1	A	593	LEU
1	A	603	ILE
1	A	653	LEU
1	A	708	ARG
1	A	723	ASN
1	A	763	THR
1	A	764	ARG
1	A	787	ARG
1	A	823	LEU
1	A	868	VAL
1	A	876	VAL
2	B	54	THR
2	B	104	ILE
2	B	111	GLU
2	B	118	TYR
2	B	119	ILE
2	B	166	THR
2	B	170	LEU
2	B	195	SER
2	B	203	VAL
2	B	213	PHE
2	B	215	VAL
2	B	216	SER
2	B	259	LEU
2	B	318	LEU
2	B	344	LYS
2	B	345	ARG
2	B	346	LEU
2	B	418	ASP
2	B	419	ARG
2	B	426	LEU
2	B	436	LEU
2	B	444	GLU
2	B	448	LEU
2	B	456	MET
2	B	470	VAL
2	B	471	LYS
2	B	481	VAL
2	B	525	LEU

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Mol	Chain	Res	Type
2	B	529	LEU
2	B	563	THR
2	B	579	ARG
2	B	591	LEU
2	B	610	LEU
2	B	653	ILE
2	B	662	GLU
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	735	TYR
2	B	742	ILE
2	B	767	LYS
2	B	874	ILE
2	B	884	ARG
2	B	905	LYS
2	B	913	LEU
2	B	924	LEU
2	B	950	LYS
2	B	951	THR
2	B	953	ILE
2	B	977	ARG
2	B	994	GLN
2	B	1013	GLN
2	B	1051	ARG
2	B	1070	ILE
2	B	1079	LYS
2	B	1081	VAL
2	B	1118	LEU
3	C	47	GLU
3	C	49	ASP
3	C	52	PHE
3	C	64	ILE
3	C	70	ILE
3	C	107	LEU
3	C	111	VAL
3	C	119	THR
3	C	164	SER
3	C	174	LEU
3	C	180	THR
3	C	231	ILE
3	C	232	LYS

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Mol	Chain	Res	Type
3	C	237	ILE
3	C	238	LYS
3	C	278	ARG
3	C	292	ILE
3	C	311	ARG
3	C	315	LEU
3	C	327	ARG
3	C	331	ARG
3	C	338	LYS
3	C	365	GLU
3	C	369	VAL
3	C	380	LYS
3	C	389	THR
4	D	13	ILE
4	D	109	LEU
4	D	151	LYS
4	D	165	ARG
4	D	178	LYS
4	D	258	LYS
5	E	27	LEU
5	E	30	LEU
5	E	48	ILE
5	E	53	THR
5	E	59	LEU
5	E	114	THR
5	E	120	TYR
5	E	137	GLN
6	F	63	ILE
6	F	88	ILE
6	F	90	ASP
7	G	34	ASN
7	G	46	ILE
7	G	48	ILE
7	G	67	THR
7	G	79	THR
7	G	101	LEU
7	G	104	LYS
7	G	106	ILE
9	I	25	ASN
9	I	74	LEU
10	J	43	LEU
10	J	52	ASP

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Mol	Chain	Res	Type
9	K	25	ASN
9	K	74	LEU
12	N	3	ILE
12	N	5	ILE
12	N	40	VAL
12	N	45	CYS
12	N	63	THR
12	O	3	ILE
12	O	5	ILE
12	O	7	CYS
12	O	40	VAL
13	P	18	LEU
13	P	33	ILE
13	P	41	THR
10	Q	43	LEU
10	Q	52	ASP
2	R	49	GLN
2	R	54	THR
2	R	68	ILE
2	R	111	GLU
2	R	118	TYR
2	R	119	ILE
2	R	166	THR
2	R	170	LEU
2	R	195	SER
2	R	213	PHE
2	R	215	VAL
2	R	216	SER
2	R	229	LEU
2	R	259	LEU
2	R	318	LEU
2	R	341	TYR
2	R	344	LYS
2	R	345	ARG
2	R	418	ASP
2	R	419	ARG
2	R	425	MET
2	R	426	LEU
2	R	436	LEU
2	R	444	GLU
2	R	448	LEU
2	R	456	MET

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Mol	Chain	Res	Type
2	R	460	GLU
2	R	470	VAL
2	R	471	LYS
2	R	481	VAL
2	R	525	LEU
2	R	529	LEU
2	R	539	LEU
2	R	579	ARG
2	R	610	LEU
2	R	639	GLU
2	R	646	TRP
2	R	653	ILE
2	R	662	GLU
2	R	675	MET
2	R	688	GLN
2	R	711	LEU
2	R	735	TYR
2	R	742	ILE
2	R	767	LYS
2	R	768	TYR
2	R	772	GLN
2	R	773	GLU
2	R	840	ILE
2	R	874	ILE
2	R	884	ARG
2	R	905	LYS
2	R	913	LEU
2	R	924	LEU
2	R	950	LYS
2	R	951	THR
2	R	953	ILE
2	R	977	ARG
2	R	994	GLN
2	R	1013	GLN
2	R	1051	ARG
2	R	1070	ILE
2	R	1079	LYS
2	R	1081	VAL
2	R	1118	LEU
2	R	1121	ARG
4	S	13	ILE
4	S	109	LEU

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Mol	Chain	Res	Type
4	S	151	LYS
4	S	165	ARG
4	S	178	LYS
4	S	209	CYS
4	S	258	LYS
5	T	27	LEU
5	T	30	LEU
5	T	38	ILE
5	T	48	ILE
5	T	53	THR
5	T	59	LEU
5	T	114	THR
5	T	120	TYR
5	T	137	GLN
6	U	63	ILE
6	U	88	ILE
6	U	90	ASP
7	V	46	ILE
7	V	48	ILE
7	V	79	THR
7	V	104	LYS
7	V	106	ILE
1	W	24	VAL
1	W	61	CYS
1	W	64	THR
1	W	84	VAL
1	W	88	LYS
1	W	91	TYR
1	W	99	ARG
1	W	101	CYS
1	W	105	LYS
1	W	106	ILE
1	W	107	SER
1	W	108	GLU
1	W	191	ASP
1	W	220	ARG
1	W	223	ILE
1	W	224	MET
1	W	238	LYS
1	W	254	ASP
1	W	284	LEU
1	W	288	LYS

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Mol	Chain	Res	Type
1	W	296	ARG
1	W	314	SER
1	W	326	ILE
1	W	356	TRP
1	W	366	ILE
1	W	423	PRO
1	W	425	LEU
1	W	426	HIS
1	W	438	LEU
1	W	464	LEU
1	W	470	GLU
1	W	488	THR
1	W	551	VAL
1	W	593	LEU
1	W	603	ILE
1	W	653	LEU
1	W	708	ARG
1	W	723	ASN
1	W	763	THR
1	W	764	ARG
1	W	787	ARG
1	W	823	LEU
1	W	853	ASP
1	W	868	VAL
1	W	876	VAL
13	X	18	LEU
13	X	33	ILE
13	X	41	THR
3	Y	47	GLU
3	Y	49	ASP
3	Y	52	PHE
3	Y	70	ILE
3	Y	78	VAL
3	Y	119	THR
3	Y	174	LEU
3	Y	231	ILE
3	Y	232	LYS
3	Y	237	ILE
3	Y	238	LYS
3	Y	278	ARG
3	Y	292	ILE
3	Y	311	ARG

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Mol	Chain	Res	Type
3	Y	315	LEU
3	Y	327	ARG
3	Y	331	ARG
3	Y	338	LYS
3	Y	365	GLU
3	Y	369	VAL
3	Y	380	LYS
3	Y	389	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	F3S	D	1001	4	3,9,9	32.58	3 (100%)	0,15,15	0.00	-
16	F3S	S	1001	4	3,9,9	32.59	3 (100%)	0,15,15	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	F3S	D	1001	4	-	0/0/24/24	0/0/3/3
16	F3S	S	1001	4	-	0/0/24/24	0/0/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	1001	F3S	S3-FE4	-33.25	2.10	2.33
16	S	1001	F3S	S3-FE4	-33.18	2.10	2.33
16	S	1001	F3S	S3-FE1	-32.34	2.11	2.33
16	D	1001	F3S	S3-FE1	-32.32	2.11	2.33
16	S	1001	F3S	S3-FE3	-32.25	2.11	2.33
16	D	1001	F3S	S3-FE3	-32.15	2.11	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	831/880 (94%)	0.28	14 (1%) 67 46	28, 92, 200, 308	0
1	W	831/880 (94%)	0.42	41 (4%) 28 20	46, 106, 212, 378	0
2	B	1085/1131 (95%)	0.29	27 (2%) 54 36	29, 88, 181, 293	0
2	R	1085/1131 (95%)	0.32	33 (3%) 48 31	55, 93, 190, 334	0
3	C	368/395 (93%)	0.53	10 (2%) 52 34	33, 108, 214, 329	0
3	Y	368/395 (93%)	0.58	21 (5%) 23 16	56, 115, 224, 338	0
4	D	262/265 (98%)	0.32	0 100 100	59, 116, 219, 298	0
4	S	262/265 (98%)	0.50	14 (5%) 25 18	77, 134, 209, 265	0
5	E	164/180 (91%)	1.16	25 (15%) 3 4	70, 166, 254, 302	0
5	T	164/180 (91%)	1.12	20 (12%) 5 6	72, 164, 255, 300	0
6	F	90/113 (79%)	0.95	12 (13%) 4 4	98, 188, 257, 327	0
6	U	90/113 (79%)	1.03	12 (13%) 4 4	128, 184, 276, 323	0
7	G	110/132 (83%)	0.55	3 (2%) 52 34	66, 132, 226, 301	0
7	V	110/132 (83%)	0.82	10 (9%) 9 9	75, 145, 228, 295	0
8	H	74/84 (88%)	0.19	0 100 100	53, 82, 153, 205	0
8	Z	74/84 (88%)	0.24	0 100 100	83, 99, 171, 205	0
9	I	82/95 (86%)	0.27	0 100 100	57, 91, 160, 195	0
9	K	82/95 (86%)	0.24	0 100 100	35, 84, 181, 219	0
10	J	39/104 (37%)	1.02	3 (7%) 13 11	130, 183, 243, 268	0
10	Q	39/104 (37%)	0.81	4 (10%) 7 8	112, 162, 213, 265	0
11	L	91/92 (98%)	0.22	0 100 100	65, 99, 194, 250	0
11	M	91/92 (98%)	0.42	3 (3%) 44 29	95, 121, 175, 247	0
12	N	64/66 (96%)	0.31	0 100 100	59, 103, 177, 205	0
12	O	64/66 (96%)	0.13	0 100 100	91, 112, 168, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	P	45/48 (93%)	0.53	4 (8%)	10 10	71, 93, 189, 275	0
13	X	45/48 (93%)	0.51	3 (6%)	17 14	85, 105, 197, 249	0
All	All	6610/7170 (92%)	0.43	259 (3%)	36 26	28, 105, 217, 378	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	119	LYS	7.0
5	T	119	LYS	6.6
1	W	24	VAL	5.2
5	E	87	GLY	5.1
1	W	118	TYR	5.0
1	A	118	TYR	4.7
1	A	117	ILE	4.7
1	W	105	LYS	4.3
5	E	130	GLU	4.2
13	P	11	LYS	4.1
1	W	25	THR	4.1
5	T	88	GLU	3.9
2	R	279	VAL	3.9
5	T	8	ARG	3.9
1	W	293	ARG	3.9
3	C	234	ILE	3.8
1	W	194	ILE	3.7
1	W	75	ILE	3.7
5	E	124	ARG	3.7
5	T	131	LYS	3.7
3	Y	234	ILE	3.6
3	Y	224	ASP	3.6
1	W	191	ASP	3.6
6	F	50	GLU	3.6
5	T	107	LEU	3.5
6	F	57	GLU	3.5
5	E	131	LYS	3.5
2	B	838	THR	3.5
5	E	88	GLU	3.5
5	T	87	GLY	3.5
6	F	58	GLU	3.5
5	E	135	VAL	3.5
5	T	130	GLU	3.5
5	E	116	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	W	26	ALA	3.4
2	R	278	ARG	3.4
5	T	124	ARG	3.4
5	E	136	ILE	3.4
1	W	91	TYR	3.3
2	R	257	PRO	3.3
6	U	58	GLU	3.3
6	F	63	ILE	3.2
1	W	74	HIS	3.2
2	R	231	ARG	3.2
13	X	11	LYS	3.2
1	W	192	VAL	3.2
3	Y	212	ASN	3.2
2	R	790	GLU	3.2
2	R	247	LEU	3.2
1	W	291	SER	3.2
2	R	1072	TRP	3.1
5	E	86	GLU	3.1
3	Y	262	LEU	3.1
5	E	118	LEU	3.1
5	T	118	LEU	3.1
1	W	142	LYS	3.0
5	T	121	ASP	3.0
5	T	135	VAL	3.0
1	W	238	LYS	3.0
2	R	779	PRO	3.0
2	R	217	PHE	2.9
5	E	125	GLY	2.9
3	Y	229	THR	2.9
2	R	234	GLY	2.9
5	E	137	GLN	2.9
7	V	38	ILE	2.9
5	E	74	MET	2.8
1	W	665	ILE	2.8
6	U	63	ILE	2.8
3	Y	249	TYR	2.8
5	E	134	LYS	2.8
7	V	92	TYR	2.8
2	R	437	ALA	2.8
1	A	114	TYR	2.8
7	G	17	SER	2.8
3	C	190	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	92	TYR	2.7
1	W	288	LYS	2.7
4	S	143	ALA	2.7
1	A	80	PRO	2.7
13	X	30	GLY	2.7
10	J	73	LYS	2.7
4	S	191	LYS	2.7
1	W	27	ILE	2.7
1	W	531	LYS	2.7
3	C	213	ILE	2.7
2	R	771	GLY	2.7
3	Y	214	ASP	2.7
5	E	81	VAL	2.7
7	V	53	GLU	2.7
2	B	55	GLU	2.6
3	Y	192	LYS	2.6
2	B	769	PRO	2.6
2	R	53	PRO	2.6
1	W	195	LEU	2.6
2	R	769	PRO	2.6
5	E	158	PRO	2.6
6	U	88	ILE	2.6
2	B	279	VAL	2.6
6	U	89	MET	2.6
7	V	31	MET	2.6
1	A	237	HIS	2.6
5	T	136	ILE	2.6
6	F	78	ILE	2.6
6	U	90	ASP	2.6
1	A	137	LYS	2.6
2	R	136	TYR	2.6
4	S	94	THR	2.6
10	J	51	TRP	2.6
5	E	8	ARG	2.6
2	B	257	PRO	2.6
2	B	217	PHE	2.5
2	B	283	GLN	2.6
2	R	224	ILE	2.5
2	B	387	LEU	2.5
13	P	28	TYR	2.5
2	R	275	ILE	2.5
1	W	30	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	790	GLU	2.5
3	Y	211	ALA	2.5
2	R	603	GLY	2.5
7	V	14	GLU	2.5
1	A	293	ARG	2.5
5	T	72	PHE	2.5
1	W	398	ALA	2.5
2	R	283	GLN	2.5
2	R	838	THR	2.5
1	W	80	PRO	2.5
6	F	89	MET	2.5
6	U	77	PRO	2.5
10	Q	42	GLU	2.5
1	A	194	ILE	2.5
5	E	151	SER	2.5
1	W	187	VAL	2.5
1	W	193	GLU	2.5
2	B	600	LEU	2.5
2	R	436	LEU	2.5
3	C	229	THR	2.5
5	T	73	ASP	2.5
1	W	134	GLU	2.5
5	E	10	ILE	2.5
2	B	437	ALA	2.5
3	C	332	HIS	2.4
2	R	770	GLY	2.4
2	R	80	GLU	2.4
10	Q	51	TRP	2.4
6	U	78	ILE	2.4
1	W	274	ALA	2.4
5	E	97	VAL	2.4
3	Y	244	LYS	2.4
2	R	772	GLN	2.4
11	M	15	LEU	2.4
1	W	143	ALA	2.4
3	C	27	LYS	2.4
2	B	278	ARG	2.4
2	R	54	THR	2.4
2	B	436	LEU	2.4
3	C	131	LYS	2.4
3	C	194	GLY	2.4
10	Q	73	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	R	600	LEU	2.4
10	Q	75	TYR	2.4
1	W	260	LEU	2.3
2	R	280	ALA	2.3
1	W	116	ARG	2.3
3	Y	190	ARG	2.3
1	A	139	THR	2.3
2	B	770	GLY	2.3
3	C	189	ASN	2.3
4	S	145	LEU	2.3
1	W	182	GLU	2.3
5	T	97	VAL	2.3
6	F	47	CYS	2.3
13	X	28	TYR	2.3
1	W	135	TYR	2.3
2	R	781	PRO	2.3
3	C	192	LYS	2.3
4	S	86	THR	2.3
2	B	771	GLY	2.3
3	Y	189	ASN	2.3
11	M	89	GLY	2.3
3	Y	167	LEU	2.2
6	F	90	ASP	2.2
1	W	151	GLU	2.2
3	Y	168	GLN	2.2
2	R	60	LYS	2.2
2	B	1072	TRP	2.2
2	R	57	PRO	2.2
1	A	24	VAL	2.2
1	A	103	ARG	2.2
1	W	88	LYS	2.2
2	B	224	ILE	2.2
3	Y	124	ILE	2.2
2	B	814	ILE	2.2
1	A	142	LYS	2.2
4	S	109	LEU	2.2
1	W	359	GLU	2.2
3	Y	27	LYS	2.2
2	B	1062	TYR	2.2
6	F	28	GLY	2.2
5	T	122	ASN	2.2
6	F	62	ILE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	P	25	ARG	2.2
2	B	72	ARG	2.2
3	Y	213	ILE	2.2
1	W	18	GLU	2.2
1	A	263	GLU	2.1
3	Y	131	LYS	2.1
4	S	190	LEU	2.1
5	T	140	ASP	2.1
3	Y	267	VAL	2.1
1	W	576	LYS	2.1
6	U	19	LYS	2.1
6	U	42	ASN	2.1
2	R	306	THR	2.1
4	S	262	GLU	2.1
7	V	36	PHE	2.1
7	V	91	ARG	2.1
4	S	142	GLU	2.1
5	T	125	GLY	2.1
5	T	36	GLU	2.1
1	W	139	THR	2.1
2	B	54	THR	2.1
2	B	22	LYS	2.1
7	G	53	GLU	2.1
6	F	75	ILE	2.1
7	V	10	ILE	2.1
7	V	17	SER	2.1
5	E	107	LEU	2.1
11	M	71	LYS	2.1
6	U	12	ILE	2.1
4	S	174	GLY	2.1
5	E	106	GLY	2.1
2	R	52	ILE	2.1
2	B	234	GLY	2.1
5	E	72	PHE	2.1
1	W	184	LEU	2.1
2	B	60	LYS	2.1
6	U	70	ALA	2.1
1	W	130	ARG	2.1
2	B	779	PRO	2.1
13	P	30	GLY	2.1
2	R	387	LEU	2.0
6	U	76	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	116	ARG	2.0
2	B	280	ALA	2.0
2	B	840	ILE	2.0
4	S	93	TYR	2.0
4	S	240	ARG	2.0
6	F	77	PRO	2.0
1	W	112	GLU	2.0
5	T	114	THR	2.0
5	E	28	ASN	2.0
4	S	176	CYS	2.0
7	V	11	LEU	2.0
3	Y	39	LYS	2.0
3	Y	158	ILE	2.0
4	S	177	GLU	2.0
10	J	70	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	ZN	B	2125	1/1	0.69	20.43	246,246,246,246	0
14	ZN	R	2125	1/1	1.04	7.00	246,246,246,246	0
14	ZN	R	2124	1/1	0.51	5.18	246,246,246,246	0
14	ZN	B	2124	1/1	0.50	3.12	246,246,246,246	0
15	MG	W	1882	1/1	0.47	2.40	246,246,246,246	0
16	F3S	D	1001	7/7	0.35	1.76	232,235,241,245	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	F3S	S	1001	7/7	0.34	1.02	247,251,257,260	0
15	MG	A	1882	1/1	0.25	0.96	246,246,246,246	0
14	ZN	W	1881	1/1	0.19	-0.58	246,246,246,246	0
14	ZN	B	2123	1/1	0.27	-0.63	246,246,246,246	0
14	ZN	A	1880	1/1	0.14	-0.95	246,246,246,246	0
14	ZN	R	2123	1/1	0.21	-1.09	246,246,246,246	0
14	ZN	X	1049	1/1	0.12	-1.14	157,157,157,157	0
14	ZN	P	1049	1/1	0.09	-1.17	142,142,142,142	0
14	ZN	A	1881	1/1	0.07	-1.23	246,246,246,246	0
14	ZN	N	1065	1/1	0.12	-1.29	130,130,130,130	0
14	ZN	O	1065	1/1	0.10	-1.64	165,165,165,165	0
14	ZN	W	1880	1/1	0.08	-2.32	246,246,246,246	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.