



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:40 AM GMT

PDB ID : 3MLQ  
Title : Crystal structure of the Thermus thermophilus transcription-repair coupling factor RNA polymerase interacting domain with the Thermus aquaticus RNA polymerase beta1 domain  
Authors : Darst, S.A.; Westblade, L.F.; Campbell, E.A.  
Deposited on : 2010-04-18  
Resolution : 2.91 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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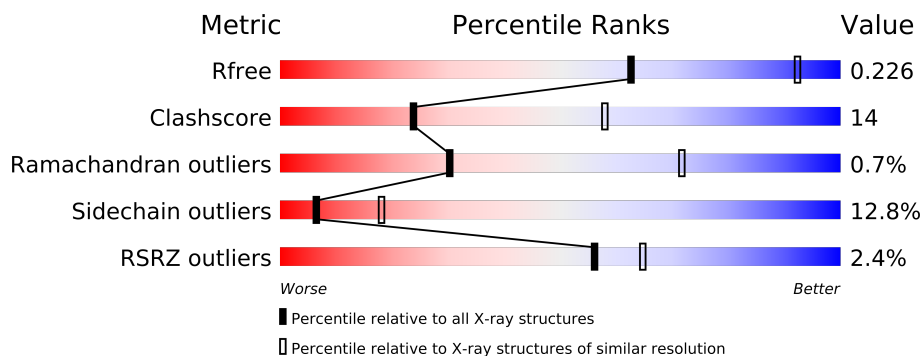
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.91 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	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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	188	
1	B	188	
1	C	188	
1	D	188	
2	E	71	
2	F	71	
2	G	71	
2	H	71	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6863 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 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1450	915	254	276	5			
1	B	180	Total	C	N	O	S	0	0	0
			1413	893	246	269	5			
1	C	182	Total	C	N	O	S	0	0	0
			1419	896	248	270	5			
1	D	185	Total	C	N	O	S	0	0	0
			1423	899	244	274	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	INITIATING METHIONINE	UNP Q9KWU7
A	332	GLY	-	LINKER	UNP Q9KWU7
A	333	GLY	-	LINKER	UNP Q9KWU7
B	16	MET	-	INITIATING METHIONINE	UNP Q9KWU7
B	332	GLY	-	LINKER	UNP Q9KWU7
B	333	GLY	-	LINKER	UNP Q9KWU7
C	16	MET	-	INITIATING METHIONINE	UNP Q9KWU7
C	332	GLY	-	LINKER	UNP Q9KWU7
C	333	GLY	-	LINKER	UNP Q9KWU7
D	16	MET	-	INITIATING METHIONINE	UNP Q9KWU7
D	332	GLY	-	LINKER	UNP Q9KWU7
D	333	GLY	-	LINKER	UNP Q9KWU7

- Molecule 2 is a protein called Transcription-repair coupling factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	38	Total	C	N	O	0	0	0
			290	192	50	48			
2	F	30	Total	C	N	O	0	0	0
			235	154	39	42			

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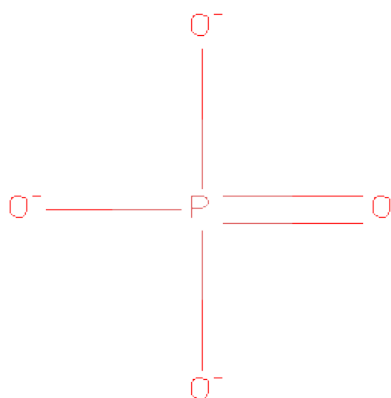
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	40	Total	C	N	O	0	0	0
			296	191	50	55			
2	H	42	Total	C	N	O	0	0	0
			332	217	58	57			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	317	GLY	-	EXPRESSION TAG	UNP Q72KB4
E	318	PRO	-	EXPRESSION TAG	UNP Q72KB4
E	319	HIS	-	EXPRESSION TAG	UNP Q72KB4
E	320	MET	-	EXPRESSION TAG	UNP Q72KB4
F	317	GLY	-	EXPRESSION TAG	UNP Q72KB4
F	318	PRO	-	EXPRESSION TAG	UNP Q72KB4
F	319	HIS	-	EXPRESSION TAG	UNP Q72KB4
F	320	MET	-	EXPRESSION TAG	UNP Q72KB4
G	317	GLY	-	EXPRESSION TAG	UNP Q72KB4
G	318	PRO	-	EXPRESSION TAG	UNP Q72KB4
G	319	HIS	-	EXPRESSION TAG	UNP Q72KB4
G	320	MET	-	EXPRESSION TAG	UNP Q72KB4
H	317	GLY	-	EXPRESSION TAG	UNP Q72KB4
H	318	PRO	-	EXPRESSION TAG	UNP Q72KB4
H	319	HIS	-	EXPRESSION TAG	UNP Q72KB4
H	320	MET	-	EXPRESSION TAG	UNP Q72KB4

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



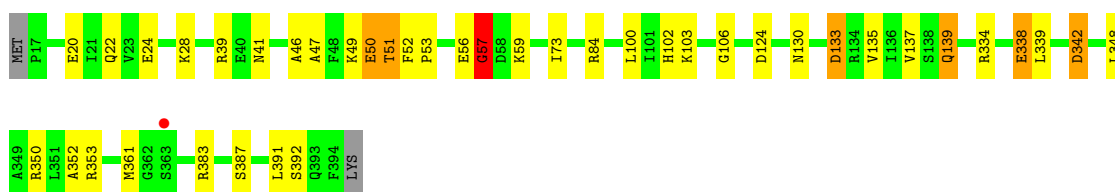
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

### 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.

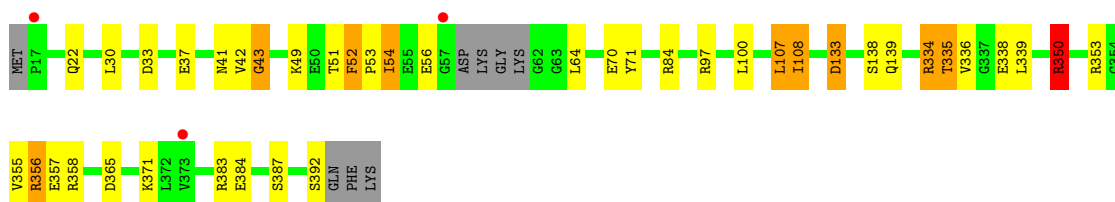
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain A: 



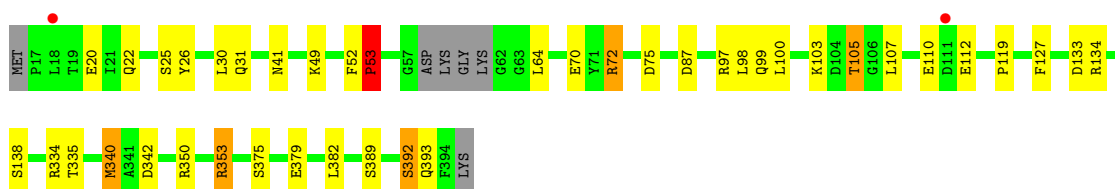
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain B: 



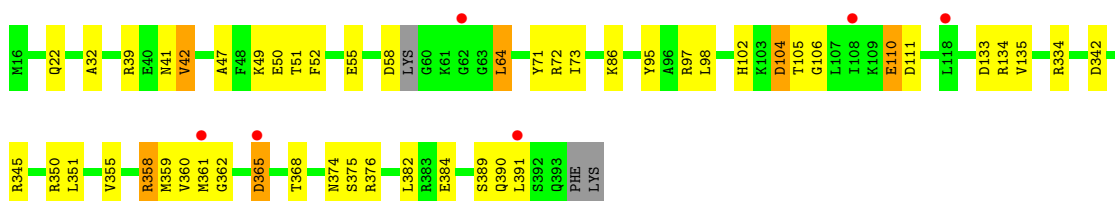
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain C: 



- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain D: 



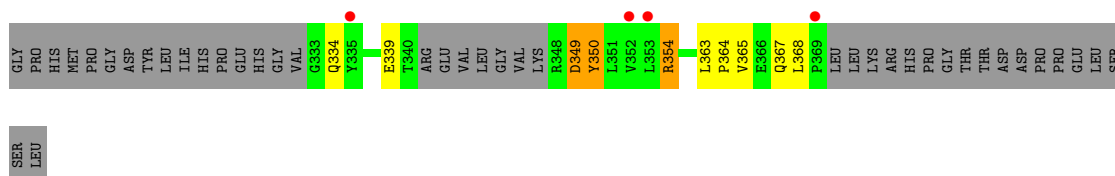
- Molecule 2: Transcription-repair coupling factor

Chain E:



- Molecule 2: Transcription-repair coupling factor

Chain F:



- Molecule 2: Transcription-repair coupling factor

Chain G:



- Molecule 2: Transcription-repair coupling factor

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.58Å 106.58Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.91 29.56 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.8 (29.56-2.91) 89.0 (29.56-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.227 , 0.250 0.227 , 0.226	Depositor DCC
$R_{free}$ test set	1144 reflections (4.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.2	EDS
Estimated twinning fraction	0.522 for H, K, L 0.478 for -H, K, -L 0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.522 for H, K, L 0.478 for -H, K, -L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26709 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PO4

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	0.47	0/1475	0.67	1/1989 (0.1%)
1	B	0.48	0/1437	0.68	1/1937 (0.1%)
1	C	0.50	0/1443	0.62	1/1947 (0.1%)
1	D	0.51	0/1447	0.63	1/1955 (0.1%)
2	E	0.53	0/295	0.96	3/400 (0.8%)
2	F	0.38	0/239	0.81	0/321
2	G	0.34	0/301	0.56	0/408
2	H	0.37	0/338	0.75	0/458
All	All	0.48	0/6975	0.68	7/9415 (0.1%)

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	3
1	B	0	3
1	C	0	2
2	E	0	2
2	F	0	1
2	H	0	1
All	All	0	12

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	357	GLY	N-CA-C	-7.54	94.25	113.10
1	C	353	ARG	NE-CZ-NH1	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	354	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	350	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	57	GLY	C-N-CA	5.59	135.68	121.70
2	E	360	LYS	N-CA-C	-5.32	96.64	111.00
1	D	358	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLN	Peptide
1	A	52	PHE	Peptide
1	A	57	GLY	Peptide
1	B	139	GLN	Peptide
1	B	51	THR	Peptide
1	B	52	PHE	Peptide
1	C	392	SER	Peptide
1	C	52	PHE	Peptide
2	E	347	LYS	Peptide
2	E	356	LYS	Peptide
2	F	367	GLN	Peptide
2	H	370	LEU	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	1450	0	0	19	1
1	B	1413	0	0	17	1
1	C	1419	0	0	19	0
1	D	1423	0	0	27	0
2	E	290	0	0	9	0
2	F	235	0	0	7	0
2	G	296	0	0	5	0
2	H	332	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
All	All	6863	0	0	98	1

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 14.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:64:LEU:CD1	1:D:359:MET:SD	2.46	1.04
2:E:355:TYR:O	2:E:357:GLY:O	1.83	0.97
1:A:334:ARG:NH2	1:A:342:ASP:OD1	2.03	0.92
1:A:47:ALA:O	1:A:51:THR:CG2	2.21	0.88
1:C:99:GLN:OE1	2:G:341:ARG:NH2	2.09	0.84
1:D:134:ARG:NH1	1:D:389:SER:OG	2.10	0.84
1:A:334:ARG:NH2	1:A:342:ASP:CG	2.40	0.75
1:D:351:LEU:CD1	1:D:374:ASN:O	2.35	0.74
1:B:41:ASN:OD1	1:B:49:LYS:NZ	2.22	0.73
1:B:30:LEU:O	1:B:71:TYR:OH	2.09	0.70
1:A:334:ARG:NH2	1:A:342:ASP:OD2	2.30	0.65
2:E:343:VAL:CG2	2:E:350:TYR:OH	2.46	0.64
1:D:72:ARG:N	1:D:95:TYR:O	2.31	0.63
2:E:349:ASP:OD1	2:E:349:ASP:N	2.33	0.61
1:C:70:GLU:OE2	1:D:86:LYS:NZ	2.34	0.60
1:C:375:SER:OG	1:C:379:GLU:OE1	2.20	0.59
1:B:383:ARG:O	1:B:387:SER:OG	2.20	0.59
2:G:346:VAL:CG1	2:G:347:LYS:O	2.51	0.58
1:A:137:VAL:CG1	1:A:139:GLN:OE1	2.52	0.58
1:B:334:ARG:CG	1:B:334:ARG:NH1	2.68	0.57
1:C:70:GLU:CG	1:D:86:LYS:NZ	2.68	0.56
1:A:41:ASN:OD1	1:A:49:LYS:NZ	2.39	0.56
1:B:42:VAL:CG1	1:B:43:GLY:N	2.69	0.56
1:A:383:ARG:O	1:A:387:SER:N	2.39	0.55
2:G:340:THR:CB	2:G:348:ARG:O	2.55	0.55
1:B:37:GLU:OE1	1:B:37:GLU:N	2.40	0.54
1:C:134:ARG:CB	1:C:389:SER:OG	2.55	0.54
2:F:339:GLU:N	2:F:350:TYR:O	2.41	0.53
2:H:365:VAL:O	2:H:365:VAL:CG1	2.56	0.53
1:A:41:ASN:OD1	1:A:49:LYS:CE	2.57	0.53
1:C:97:ARG:NE	1:C:110:GLU:OE1	2.42	0.53
1:C:25:SER:OG	1:C:335:THR:OG1	2.26	0.53
1:D:64:LEU:CD1	1:D:359:MET:CG	2.87	0.52
1:D:47:ALA:O	1:D:51:THR:OG1	2.28	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:358:ARG:CZ	1:B:371:LYS:O	2.59	0.51
1:D:104:ASP:OD1	1:D:104:ASP:C	2.49	0.51
1:D:58:ASP:OD1	1:D:360:VAL:CG2	2.59	0.51
1:B:54:ILE:CD1	1:B:355:VAL:CG1	2.89	0.51
2:E:341:ARG:O	2:E:348:ARG:N	2.45	0.50
1:A:57:GLY:O	1:A:59:LYS:O	2.30	0.49
1:A:338:GLU:O	1:A:342:ASP:OD2	2.30	0.49
1:A:130:ASN:O	2:F:354:ARG:NH2	2.45	0.49
1:C:112:GLU:OE1	1:D:86:LYS:O	2.31	0.49
1:C:53:PRO:O	1:C:53:PRO:CG	2.59	0.49
1:C:105:THR:CG2	1:C:107:LEU:CG	2.91	0.49
1:C:87:ASP:OD1	2:H:360:LYS:NZ	2.46	0.49
1:B:358:ARG:NH1	1:B:371:LYS:O	2.46	0.49
2:E:346:VAL:CG1	2:E:347:LYS:N	2.76	0.49
1:D:135:VAL:N	1:D:390:GLN:O	2.47	0.48
2:G:336:LEU:CD1	2:G:352:VAL:CG1	2.92	0.48
1:C:26:TYR:CE1	1:C:340:MET:CE	2.97	0.48
1:D:358:ARG:O	1:D:362:GLY:N	2.47	0.47
2:E:343:VAL:CG2	2:E:344:LEU:CD1	2.92	0.47
1:A:383:ARG:O	1:A:387:SER:CB	2.63	0.47
1:A:348:LEU:O	1:A:352:ALA:N	2.47	0.47
1:D:64:LEU:CD1	1:D:359:MET:CB	2.93	0.47
1:B:84:ARG:NE	1:B:133:ASP:OD1	2.48	0.47
1:D:73:ILE:O	1:D:73:ILE:CG2	2.61	0.47
2:G:366:GLU:OE1	2:G:366:GLU:N	2.48	0.47
1:A:46:ALA:O	1:A:50:GLU:CG	2.62	0.47
2:F:350:TYR:CD2	2:F:364:PRO:CA	2.98	0.46
1:A:46:ALA:O	1:A:47:ALA:C	2.53	0.46
2:H:353:LEU:O	2:H:361:LEU:N	2.49	0.46
1:A:135:VAL:CG2	1:A:392:SER:OG	2.64	0.46
1:C:72:ARG:CD	1:D:86:LYS:CE	2.93	0.46
2:E:340:THR:O	2:E:340:THR:CG2	2.64	0.46
1:A:84:ARG:NE	1:A:133:ASP:OD1	2.49	0.46
1:D:365:ASP:OD1	1:D:365:ASP:N	2.49	0.46
1:D:32:ALA:O	1:D:73:ILE:CG2	2.64	0.45
1:C:70:GLU:OE2	1:C:72:ARG:NH1	2.49	0.45
1:D:102:HIS:O	1:D:106:GLY:N	2.49	0.45
1:D:50:GLU:OE2	1:D:345:ARG:NH1	2.50	0.45
1:B:335:THR:OG1	1:B:336:VAL:N	2.50	0.44
1:B:350:ARG:CG	1:B:350:ARG:NH1	2.80	0.44
1:C:127:PHE:N	1:C:134:ARG:O	2.51	0.44
2:F:350:TYR:CB	2:F:363:LEU:O	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:HIS:O	1:A:106:GLY:N	2.50	0.44
1:A:391:LEU:CD2	2:F:334:GLN:OE1	2.66	0.44
1:C:97:ARG:CD	1:D:86:LYS:NZ	2.81	0.43
2:E:347:LYS:O	2:E:348:ARG:CG	2.67	0.43
1:B:107:LEU:C	1:B:108:ILE:CD1	2.87	0.43
2:F:349:ASP:OD1	2:F:349:ASP:N	2.52	0.43
1:C:26:TYR:OH	1:C:119:PRO:O	2.37	0.42
1:D:41:ASN:C	1:D:42:VAL:CG2	2.87	0.42
1:C:30:LEU:O	1:C:31:GLN:C	2.57	0.42
1:B:56:GLU:CG	1:B:356:ARG:CD	2.98	0.42
2:H:343:VAL:O	2:H:344:LEU:C	2.58	0.41
2:E:348:ARG:O	2:E:350:TYR:CE2	2.73	0.41
2:F:349:ASP:O	2:F:365:VAL:CB	2.67	0.41
1:D:39:ARG:CZ	1:D:71:TYR:CZ	3.03	0.41
1:B:353:ARG:O	1:B:357:GLU:N	2.53	0.41
1:D:97:ARG:NE	1:D:110:GLU:OE1	2.53	0.41
1:C:334:ARG:NH2	1:C:342:ASP:OD2	2.54	0.41
1:D:49:LYS:O	1:D:52:PHE:O	2.39	0.40
1:B:71:TYR:CD1	1:B:71:TYR:C	2.94	0.40
1:D:334:ARG:NH2	1:D:342:ASP:CG	2.74	0.40
1:D:98:LEU:N	1:D:98:LEU:CD1	2.83	0.40
1:B:70:GLU:O	1:B:97:ARG:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:ARG:NH2	1:B:392:SER:OG[4_665]	1.95	0.25

## 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	184/188 (98%)	173 (94%)	10 (5%)	1 (0%)	38 78
1	B	176/188 (94%)	170 (97%)	4 (2%)	2 (1%)	21 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	178/188 (95%)	171 (96%)	6 (3%)	1 (1%)	33	75
1	D	181/188 (96%)	168 (93%)	13 (7%)	0	100	100
2	E	36/71 (51%)	33 (92%)	2 (6%)	1 (3%)	8	28
2	F	26/71 (37%)	23 (88%)	3 (12%)	0	100	100
2	G	38/71 (54%)	35 (92%)	3 (8%)	0	100	100
2	H	40/71 (56%)	37 (92%)	2 (5%)	1 (2%)	9	32
All	All	859/1036 (83%)	810 (94%)	43 (5%)	6 (1%)	30	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	B	43	GLY
1	B	53	PRO
1	C	53	PRO
2	H	368	LEU
2	E	346	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	154/159 (97%)	136 (88%)	18 (12%)	8	22
1	B	152/159 (96%)	134 (88%)	18 (12%)	8	21
1	C	151/159 (95%)	131 (87%)	20 (13%)	6	16
1	D	150/159 (94%)	131 (87%)	19 (13%)	6	18
2	E	28/62 (45%)	23 (82%)	5 (18%)	2	7
2	F	22/62 (36%)	18 (82%)	4 (18%)	2	7
2	G	26/62 (42%)	23 (88%)	3 (12%)	8	23
2	H	33/62 (53%)	28 (85%)	5 (15%)	4	12
All	All	716/884 (81%)	624 (87%)	92 (13%)	6	18

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	22	GLN
1	A	24	GLU
1	A	28	LYS
1	A	39	ARG
1	A	50	GLU
1	A	51	THR
1	A	56	GLU
1	A	73	ILE
1	A	100	LEU
1	A	103	LYS
1	A	124	ASP
1	A	133	ASP
1	A	338	GLU
1	A	339	LEU
1	A	342	ASP
1	A	350	ARG
1	A	361	MET
1	B	22	GLN
1	B	33	ASP
1	B	52	PHE
1	B	54	ILE
1	B	64	LEU
1	B	100	LEU
1	B	107	LEU
1	B	108	ILE
1	B	133	ASP
1	B	138	SER
1	B	334	ARG
1	B	335	THR
1	B	338	GLU
1	B	339	LEU
1	B	350	ARG
1	B	356	ARG
1	B	365	ASP
1	B	384	GLU
1	C	20	GLU
1	C	22	GLN
1	C	41	ASN
1	C	49	LYS
1	C	53	PRO
1	C	64	LEU

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Mol	Chain	Res	Type
1	C	72	ARG
1	C	75	ASP
1	C	98	LEU
1	C	100	LEU
1	C	103	LYS
1	C	105	THR
1	C	133	ASP
1	C	138	SER
1	C	340	MET
1	C	350	ARG
1	C	353	ARG
1	C	382	LEU
1	C	392	SER
1	C	393	GLN
1	D	22	GLN
1	D	42	VAL
1	D	55	GLU
1	D	64	LEU
1	D	104	ASP
1	D	105	THR
1	D	110	GLU
1	D	111	ASP
1	D	133	ASP
1	D	350	ARG
1	D	355	VAL
1	D	361	MET
1	D	365	ASP
1	D	368	THR
1	D	375	SER
1	D	376	ARG
1	D	382	LEU
1	D	384	GLU
1	D	391	LEU
2	E	346	VAL
2	E	349	ASP
2	E	354	ARG
2	E	361	LEU
2	E	365	VAL
2	F	349	ASP
2	F	350	TYR
2	F	354	ARG
2	F	368	LEU

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Mol	Chain	Res	Type
2	G	336	LEU
2	G	349	ASP
2	G	361	LEU
2	H	354	ARG
2	H	361	LEU
2	H	365	VAL
2	H	368	LEU
2	H	373	ARG

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 ⓘ

1 ligand is modelled in this entry.

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	$\# Z  > 2$
3	PO4	A	1	-	4,4,4	0.22	0	6,6,6	0.31	0

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
3	PO4	A	1	-	-	0/0/0/0	0/0/0/0

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.

## 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	186/188 (98%)	0.30	1 (0%) 88 93	38, 48, 62, 74	0
1	B	180/188 (95%)	0.31	3 (1%) 67 76	39, 46, 65, 69	0
1	C	182/188 (96%)	0.28	2 (1%) 77 84	38, 48, 61, 70	0
1	D	185/188 (98%)	0.34	6 (3%) 45 54	39, 47, 68, 78	0
2	E	38/71 (53%)	0.50	4 (10%) 7 8	54, 62, 83, 89	0
2	F	30/71 (42%)	0.60	4 (13%) 4 5	58, 65, 81, 85	0
2	G	40/71 (56%)	0.27	0 100 100	52, 61, 84, 89	0
2	H	42/71 (59%)	0.17	1 (2%) 56 65	58, 72, 118, 135	0
All	All	883/1036 (85%)	0.32	21 (2%) 56 65	38, 49, 72, 135	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	368	LEU	3.6
1	D	365	ASP	3.1
2	E	345	GLY	2.8
1	D	62	GLY	2.7
1	D	108	ILE	2.7
1	A	363	SER	2.7
1	B	373	VAL	2.5
2	H	347	LYS	2.5
2	F	352	VAL	2.5
1	B	57	GLY	2.4
1	C	111	ASP	2.3
1	D	118	LEU	2.3
2	E	369	PRO	2.2
1	D	391	LEU	2.2
1	D	361	MET	2.2
2	F	353	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	346	VAL	2.2
1	C	18	LEU	2.1
2	F	335	TYR	2.1
1	B	17	PRO	2.1
2	F	369	PRO	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
3	PO4	A	1	5/5	0.17	-1.21	53,53,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.