



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 01:06 pm BST

PDB ID : 9GI4 / pdb\_00009gi4  
Title : TFIIC5 DNA binding domain  
Authors : Leen, E.; Bayliss, R.  
Deposited on : 2024-08-16  
Resolution : 2.63 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

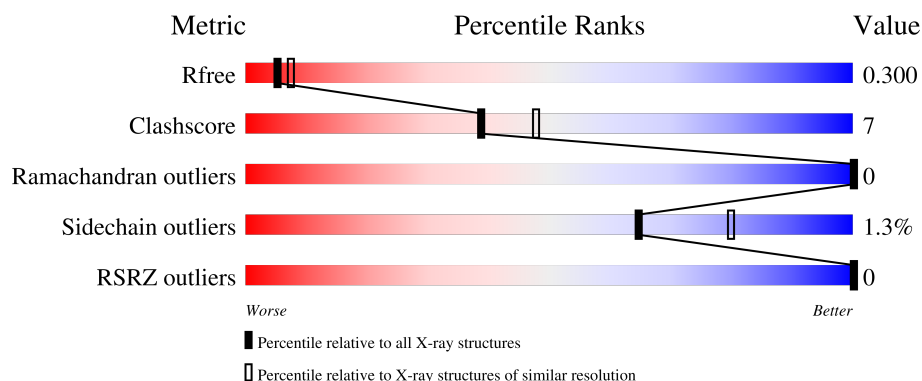
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*






The reported resolution of this entry is 2.63 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))
$R_{free}$	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	242	 64% 14% 22%
1	B	242	 66% 13% 21%
1	C	242	 69% 8% 22%
1	D	242	 64% 15% 20%
1	E	242	 58% 19% 23%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	242	 63% 15% 21%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called General transcription factor 3C polypeptide 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1532	984	269	271	8			
1	B	191	Total	C	N	O	S	0	1	0
			1560	1001	279	272	8			
1	C	188	Total	C	N	O	S	0	0	0
			1503	968	255	272	8			
1	D	193	Total	C	N	O	S	0	0	0
			1575	1009	281	277	8			
1	E	187	Total	C	N	O	S	0	1	0
			1531	981	269	273	8			
1	F	190	Total	C	N	O	S	0	0	0
			1540	988	272	272	8			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9Y5Q8
A	?	-	TYR	deletion	UNP Q9Y5Q8
A	?	-	ASN	deletion	UNP Q9Y5Q8
A	?	-	TYR	deletion	UNP Q9Y5Q8
A	?	-	SER	deletion	UNP Q9Y5Q8
A	?	-	LEU	deletion	UNP Q9Y5Q8
A	?	-	PRO	deletion	UNP Q9Y5Q8
A	?	-	ILE	deletion	UNP Q9Y5Q8
A	?	-	THR	deletion	UNP Q9Y5Q8
A	?	-	VAL	deletion	UNP Q9Y5Q8
A	?	-	LYS	deletion	UNP Q9Y5Q8
A	?	-	LYS	deletion	UNP Q9Y5Q8
A	?	-	THR	deletion	UNP Q9Y5Q8
A	?	-	SER	deletion	UNP Q9Y5Q8
A	?	-	SER	deletion	UNP Q9Y5Q8
A	?	-	GLN	deletion	UNP Q9Y5Q8
A	?	-	LEU	deletion	UNP Q9Y5Q8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q9Y5Q8
A	?	-	THR	deletion	UNP Q9Y5Q8
A	?	-	MET	deletion	UNP Q9Y5Q8
A	?	-	HIS	deletion	UNP Q9Y5Q8
A	?	-	ASP	deletion	UNP Q9Y5Q8
A	?	-	LEU	deletion	UNP Q9Y5Q8
B	1	GLY	-	expression tag	UNP Q9Y5Q8
B	?	-	TYR	deletion	UNP Q9Y5Q8
B	?	-	ASN	deletion	UNP Q9Y5Q8
B	?	-	TYR	deletion	UNP Q9Y5Q8
B	?	-	SER	deletion	UNP Q9Y5Q8
B	?	-	LEU	deletion	UNP Q9Y5Q8
B	?	-	PRO	deletion	UNP Q9Y5Q8
B	?	-	ILE	deletion	UNP Q9Y5Q8
B	?	-	THR	deletion	UNP Q9Y5Q8
B	?	-	VAL	deletion	UNP Q9Y5Q8
B	?	-	LYS	deletion	UNP Q9Y5Q8
B	?	-	LYS	deletion	UNP Q9Y5Q8
B	?	-	THR	deletion	UNP Q9Y5Q8
B	?	-	SER	deletion	UNP Q9Y5Q8
B	?	-	SER	deletion	UNP Q9Y5Q8
B	?	-	GLN	deletion	UNP Q9Y5Q8
B	?	-	LEU	deletion	UNP Q9Y5Q8
B	?	-	VAL	deletion	UNP Q9Y5Q8
B	?	-	THR	deletion	UNP Q9Y5Q8
B	?	-	MET	deletion	UNP Q9Y5Q8
B	?	-	HIS	deletion	UNP Q9Y5Q8
B	?	-	ASP	deletion	UNP Q9Y5Q8
B	?	-	LEU	deletion	UNP Q9Y5Q8
C	1	GLY	-	expression tag	UNP Q9Y5Q8
C	?	-	TYR	deletion	UNP Q9Y5Q8
C	?	-	ASN	deletion	UNP Q9Y5Q8
C	?	-	TYR	deletion	UNP Q9Y5Q8
C	?	-	SER	deletion	UNP Q9Y5Q8
C	?	-	LEU	deletion	UNP Q9Y5Q8
C	?	-	PRO	deletion	UNP Q9Y5Q8
C	?	-	ILE	deletion	UNP Q9Y5Q8
C	?	-	THR	deletion	UNP Q9Y5Q8
C	?	-	VAL	deletion	UNP Q9Y5Q8
C	?	-	LYS	deletion	UNP Q9Y5Q8
C	?	-	LYS	deletion	UNP Q9Y5Q8
C	?	-	THR	deletion	UNP Q9Y5Q8

*Continued on next page...*

*Continued from previous page...*

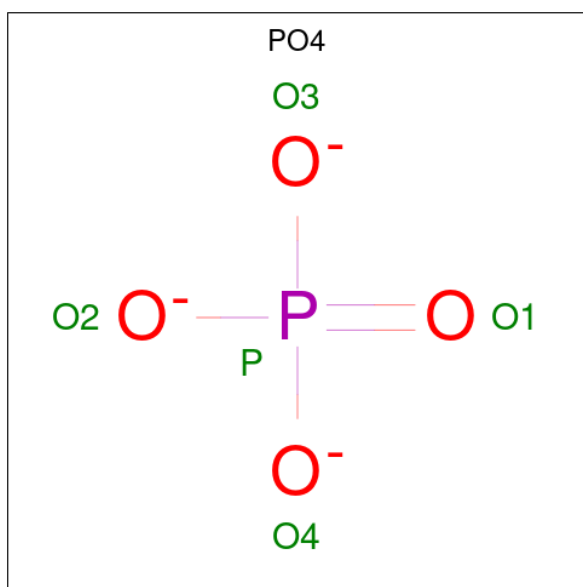
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q9Y5Q8
C	?	-	SER	deletion	UNP Q9Y5Q8
C	?	-	GLN	deletion	UNP Q9Y5Q8
C	?	-	LEU	deletion	UNP Q9Y5Q8
C	?	-	VAL	deletion	UNP Q9Y5Q8
C	?	-	THR	deletion	UNP Q9Y5Q8
C	?	-	MET	deletion	UNP Q9Y5Q8
C	?	-	HIS	deletion	UNP Q9Y5Q8
C	?	-	ASP	deletion	UNP Q9Y5Q8
C	?	-	LEU	deletion	UNP Q9Y5Q8
D	1	GLY	-	expression tag	UNP Q9Y5Q8
D	?	-	TYR	deletion	UNP Q9Y5Q8
D	?	-	ASN	deletion	UNP Q9Y5Q8
D	?	-	TYR	deletion	UNP Q9Y5Q8
D	?	-	SER	deletion	UNP Q9Y5Q8
D	?	-	LEU	deletion	UNP Q9Y5Q8
D	?	-	PRO	deletion	UNP Q9Y5Q8
D	?	-	ILE	deletion	UNP Q9Y5Q8
D	?	-	THR	deletion	UNP Q9Y5Q8
D	?	-	VAL	deletion	UNP Q9Y5Q8
D	?	-	LYS	deletion	UNP Q9Y5Q8
D	?	-	LYS	deletion	UNP Q9Y5Q8
D	?	-	THR	deletion	UNP Q9Y5Q8
D	?	-	SER	deletion	UNP Q9Y5Q8
D	?	-	SER	deletion	UNP Q9Y5Q8
D	?	-	GLN	deletion	UNP Q9Y5Q8
D	?	-	LEU	deletion	UNP Q9Y5Q8
D	?	-	VAL	deletion	UNP Q9Y5Q8
D	?	-	THR	deletion	UNP Q9Y5Q8
D	?	-	MET	deletion	UNP Q9Y5Q8
D	?	-	HIS	deletion	UNP Q9Y5Q8
D	?	-	ASP	deletion	UNP Q9Y5Q8
D	?	-	LEU	deletion	UNP Q9Y5Q8
E	1	GLY	-	expression tag	UNP Q9Y5Q8
E	?	-	TYR	deletion	UNP Q9Y5Q8
E	?	-	ASN	deletion	UNP Q9Y5Q8
E	?	-	TYR	deletion	UNP Q9Y5Q8
E	?	-	SER	deletion	UNP Q9Y5Q8
E	?	-	LEU	deletion	UNP Q9Y5Q8
E	?	-	PRO	deletion	UNP Q9Y5Q8
E	?	-	ILE	deletion	UNP Q9Y5Q8
E	?	-	THR	deletion	UNP Q9Y5Q8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP Q9Y5Q8
E	?	-	LYS	deletion	UNP Q9Y5Q8
E	?	-	LYS	deletion	UNP Q9Y5Q8
E	?	-	THR	deletion	UNP Q9Y5Q8
E	?	-	SER	deletion	UNP Q9Y5Q8
E	?	-	SER	deletion	UNP Q9Y5Q8
E	?	-	GLN	deletion	UNP Q9Y5Q8
E	?	-	LEU	deletion	UNP Q9Y5Q8
E	?	-	VAL	deletion	UNP Q9Y5Q8
E	?	-	THR	deletion	UNP Q9Y5Q8
E	?	-	MET	deletion	UNP Q9Y5Q8
E	?	-	HIS	deletion	UNP Q9Y5Q8
E	?	-	ASP	deletion	UNP Q9Y5Q8
E	?	-	LEU	deletion	UNP Q9Y5Q8
F	1	GLY	-	expression tag	UNP Q9Y5Q8
F	?	-	TYR	deletion	UNP Q9Y5Q8
F	?	-	ASN	deletion	UNP Q9Y5Q8
F	?	-	TYR	deletion	UNP Q9Y5Q8
F	?	-	SER	deletion	UNP Q9Y5Q8
F	?	-	LEU	deletion	UNP Q9Y5Q8
F	?	-	PRO	deletion	UNP Q9Y5Q8
F	?	-	ILE	deletion	UNP Q9Y5Q8
F	?	-	THR	deletion	UNP Q9Y5Q8
F	?	-	VAL	deletion	UNP Q9Y5Q8
F	?	-	LYS	deletion	UNP Q9Y5Q8
F	?	-	LYS	deletion	UNP Q9Y5Q8
F	?	-	THR	deletion	UNP Q9Y5Q8
F	?	-	SER	deletion	UNP Q9Y5Q8
F	?	-	SER	deletion	UNP Q9Y5Q8
F	?	-	GLN	deletion	UNP Q9Y5Q8
F	?	-	LEU	deletion	UNP Q9Y5Q8
F	?	-	VAL	deletion	UNP Q9Y5Q8
F	?	-	THR	deletion	UNP Q9Y5Q8
F	?	-	MET	deletion	UNP Q9Y5Q8
F	?	-	HIS	deletion	UNP Q9Y5Q8
F	?	-	ASP	deletion	UNP Q9Y5Q8
F	?	-	LEU	deletion	UNP Q9Y5Q8

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	6	Total	O	0	0
			6	6		
3	C	1	Total	O	0	0
			1	1		
3	D	4	Total	O	0	0
			4	4		
3	E	8	Total	O	0	0
			8	8		

*Continued on next page...*



*Continued from previous page...*

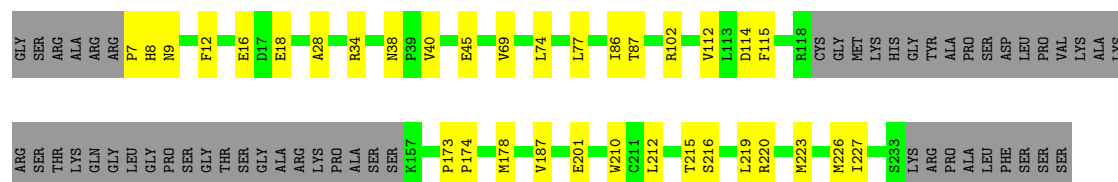
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	5	Total	O	0	0
			5	5		

### 3 Residue-property plots [i](#)

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

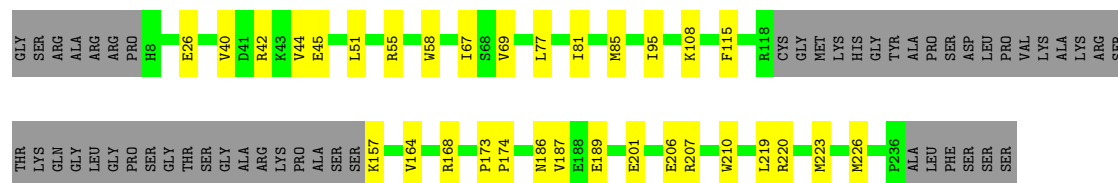
- Molecule 1: General transcription factor 3C polypeptide 5

Chain A: 



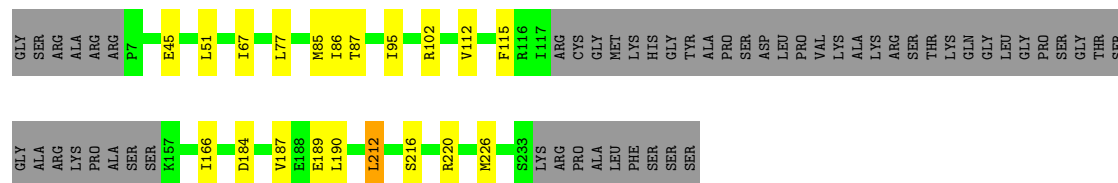
- Molecule 1: General transcription factor 3C polypeptide 5

Chain B: 



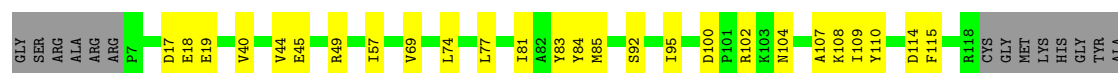
- Molecule 1: General transcription factor 3C polypeptide 5

Chain C: 



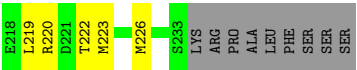
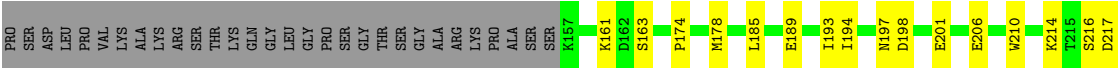
- Molecule 1: General transcription factor 3C polypeptide 5

Chain D: 

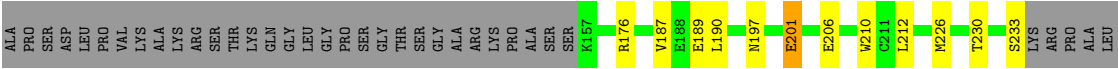
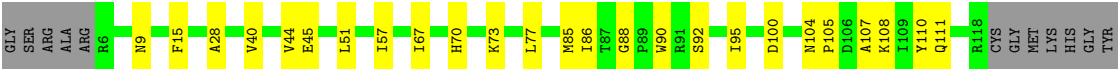
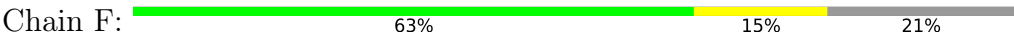




● Molecule 1: General transcription factor 3C polypeptide 5



● Molecule 1: General transcription factor 3C polypeptide 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.52Å 37.64Å 276.68Å 90.01° 90.02° 59.90°	Depositor
Resolution (Å)	46.11 – 2.63 46.11 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.11-2.63) 97.7 (46.11-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.244 , 0.300 0.244 , 0.300	Depositor DCC
$R_{free}$ test set	1828 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 68.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.009 for h-k,h,l 0.009 for k,-h+k,l 0.397 for -k,h-k,l 0.397 for -h+k,-h,l 0.417 for h,h-k,-l 0.407 for -k,-h,-l 0.013 for -h,-k,l 0.014 for h-k,-k,-l 0.418 for -h+k,k,-l 0.014 for -h,-h+k,-l 0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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	0.09	0/1571	0.24	0/2133
1	B	0.09	0/1606	0.24	0/2179
1	C	0.09	0/1543	0.23	0/2100
1	D	0.10	0/1615	0.27	0/2189
1	E	0.09	0/1569	0.26	0/2129
1	F	0.10	0/1579	0.26	0/2144
All	All	0.09	0/9483	0.25	0/12874

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1532	0	1494	20	0
1	B	1560	0	1522	20	0
1	C	1503	0	1436	15	0
1	D	1575	0	1545	21	0
1	E	1531	0	1486	27	0
1	F	1540	0	1496	23	0
2	A	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	8	0	0	0	0
3	F	5	0	0	0	0
All	All	9306	0	8979	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:ARG:HD3	1:F:176:ARG:H	1.39	0.85
1:D:18:GLU:HG3	1:D:19:GLU:HG2	1.64	0.79
1:F:187:VAL:HG21	1:F:226:MET:HE1	1.64	0.79
1:C:187:VAL:HG21	1:C:226:MET:HE1	1.68	0.75
1:A:173:PRO:HD2	1:A:227:ILE:HD11	1.68	0.75
1:E:161:LYS:HE3	1:E:163:SER:HB3	1.72	0.71
1:C:86:ILE:HG22	1:C:87:THR:HG23	1.73	0.70
1:B:26:GLU:OE2	1:E:42[B]:ARG:NE	2.26	0.67
1:E:16:GLU:N	1:E:16:GLU:OE1	2.29	0.65
1:A:86:ILE:HG22	1:A:87:THR:HG23	1.80	0.63
1:E:189:GLU:O	1:E:193:ILE:HD12	1.99	0.63
1:E:219:LEU:O	1:E:223:MET:HG3	1.98	0.62
1:F:176:ARG:H	1:F:176:ARG:CD	2.12	0.62
1:B:206:GLU:HG2	1:B:207:ARG:HD2	1.80	0.61
1:B:187:VAL:HG11	1:B:226:MET:HE1	1.82	0.61
1:D:57:ILE:HG13	1:D:95:ILE:HG23	1.80	0.61
1:E:43:LYS:O	1:E:47:GLU:HG3	1.99	0.61
1:B:108:LYS:HB2	1:B:210:TRP:HB2	1.81	0.61
1:C:166:ILE:HG12	1:C:184:ASP:HB3	1.83	0.60
1:D:85:MET:HE3	1:D:95:ILE:HD12	1.84	0.60
1:C:216:SER:HB3	1:C:220:ARG:HH21	1.67	0.59
1:B:40:VAL:O	1:B:44:VAL:HG23	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PHE:HD1	1:B:220:ARG:HG2	1.66	0.59
1:D:69:VAL:HG11	1:D:74:LEU:HD13	1.86	0.57
1:C:45:GLU:HA	1:C:77:LEU:HD21	1.87	0.56
1:E:214:LYS:HE3	1:E:217:ASP:CG	2.30	0.56
1:A:219:LEU:O	1:A:223:MET:HG3	2.05	0.56
1:D:212:LEU:HD12	1:D:212:LEU:H	1.71	0.56
1:B:189:GLU:N	1:B:189:GLU:OE2	2.38	0.56
1:D:108:LYS:HB2	1:D:210:TRP:HB2	1.87	0.56
1:C:189:GLU:N	1:C:189:GLU:OE2	2.39	0.55
1:D:166:ILE:HG12	1:D:184:ASP:HB3	1.87	0.55
1:F:100:ASP:O	1:F:104:ASN:ND2	2.39	0.55
1:E:108:LYS:HB2	1:E:210:TRP:HB2	1.88	0.55
1:F:15:PHE:CD2	1:F:206:GLU:HG3	2.42	0.53
1:E:55:ARG:HD2	1:E:58:TRP:CE2	2.43	0.53
1:B:219:LEU:O	1:B:223:MET:HG3	2.09	0.53
1:F:88:GLY:HA2	1:F:206:GLU:HG2	1.90	0.52
1:C:85:MET:HG3	1:C:95:ILE:HD12	1.92	0.52
1:F:105:PRO:HB3	1:F:201:GLU:HG3	1.91	0.52
1:A:45:GLU:HA	1:A:77:LEU:HD21	1.92	0.52
1:F:57:ILE:HG23	1:F:95:ILE:HG13	1.92	0.52
1:B:201:GLU:HG2	1:B:210:TRP:HB3	1.92	0.52
1:A:115:PHE:HD1	1:A:220:ARG:HG2	1.74	0.51
1:E:197:ASN:ND2	1:E:210:TRP:O	2.44	0.51
1:C:115:PHE:HD2	1:C:220:ARG:HG3	1.76	0.51
1:D:17:ASP:O	1:D:102:ARG:NH1	2.38	0.50
1:B:85:MET:HE2	1:B:95:ILE:HD13	1.93	0.50
1:E:15:PHE:CD1	1:E:206:GLU:HG2	2.46	0.50
1:E:100:ASP:O	1:E:104:ASN:ND2	2.44	0.50
1:B:115:PHE:CD1	1:B:220:ARG:HG2	2.45	0.49
1:F:40:VAL:O	1:F:44:VAL:HG13	2.12	0.49
1:E:222:THR:O	1:E:226:MET:HG3	2.12	0.49
1:B:168:ARG:HG3	1:B:186:ASN:HB3	1.95	0.49
1:C:51:LEU:HD11	1:C:67:ILE:HG12	1.93	0.49
1:A:9:ASN:HB2	1:A:28:ALA:HB2	1.95	0.48
1:D:83:TYR:HE1	1:D:85:MET:HE2	1.78	0.48
1:E:53:ASP:HA	1:E:96:ARG:HH11	1.77	0.48
1:F:108:LYS:O	1:F:111:GLN:HG3	2.13	0.48
1:F:45:GLU:HA	1:F:77:LEU:HD21	1.95	0.48
1:C:45:GLU:HG3	1:C:77:LEU:HD11	1.96	0.48
1:A:216:SER:HA	1:A:219:LEU:HD12	1.95	0.48
1:B:44:VAL:HG13	1:B:67:ILE:HG21	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ALA:HA	1:D:110:TYR:HD2	1.79	0.47
1:B:51:LEU:HD12	1:B:67:ILE:HD11	1.95	0.47
1:F:85:MET:HE3	1:F:90:TRP:HB2	1.96	0.47
1:F:70:HIS:HB3	1:F:73:LYS:HG3	1.96	0.47
1:A:173:PRO:HB3	1:A:178:MET:SD	2.54	0.47
1:D:207:ARG:HH22	1:D:214:LYS:HZ2	1.63	0.47
1:E:108:LYS:NZ	1:E:198:ASP:OD1	2.46	0.47
1:F:230:THR:O	1:F:233:SER:OG	2.31	0.47
1:F:9:ASN:HB2	1:F:28:ALA:HB2	1.97	0.47
1:E:38:ASN:HB3	1:E:40:VAL:HG12	1.96	0.46
1:E:86:ILE:HG23	1:E:87:THR:HG23	1.98	0.46
1:B:45:GLU:HA	1:B:77:LEU:HD21	1.97	0.46
1:F:187:VAL:HG12	1:F:190:LEU:H	1.79	0.46
1:B:157:LYS:HA	1:B:157:LYS:HD2	1.72	0.45
1:F:187:VAL:HB	1:F:190:LEU:HD12	1.98	0.45
1:B:55:ARG:O	1:B:58:TRP:NE1	2.49	0.45
1:C:187:VAL:HB	1:C:190:LEU:HD12	1.99	0.45
1:E:201:GLU:HG2	1:E:210:TRP:HB3	1.99	0.45
1:D:100:ASP:O	1:D:104:ASN:ND2	2.50	0.45
1:D:192:LYS:HD3	1:D:192:LYS:HA	1.61	0.44
1:E:174:PRO:HD2	1:E:178:MET:SD	2.57	0.44
1:A:114:ASP:OD1	1:A:114:ASP:N	2.45	0.44
1:A:69:VAL:HG21	1:A:74:LEU:HD13	2.00	0.44
1:C:216:SER:HB3	1:C:220:ARG:NH2	2.33	0.44
1:D:49:ARG:HG3	1:D:81:ILE:HD12	1.99	0.44
1:F:197:ASN:HB3	1:F:212:LEU:HG	2.00	0.44
1:F:108:LYS:HB2	1:F:210:TRP:HB2	2.00	0.44
1:D:219:LEU:O	1:D:223:MET:HG3	2.17	0.44
1:E:102:ARG:HE	1:E:102:ARG:HB2	1.62	0.44
1:A:18:GLU:O	1:A:102:ARG:NH2	2.50	0.43
1:A:212:LEU:O	1:A:215:THR:OG1	2.24	0.43
1:B:44:VAL:HG11	1:B:69:VAL:HB	1.99	0.43
1:B:173:PRO:HA	1:B:174:PRO:HD3	1.92	0.43
1:E:35:VAL:O	1:E:37:THR:HG23	2.18	0.43
1:D:84:TYR:CZ	1:D:92:SER:HA	2.53	0.43
1:D:109:ILE:HD12	1:D:183:CYS:HB3	2.01	0.43
1:B:26:GLU:HB2	1:E:42[B]:ARG:HG2	2.00	0.43
1:F:51:LEU:HD12	1:F:67:ILE:HD11	2.00	0.43
1:D:45:GLU:HA	1:D:77:LEU:HD21	2.01	0.43
1:E:8:HIS:C	1:E:10:ALA:H	2.27	0.42
1:A:34:ARG:HB2	1:D:19:GLU:OE1	2.18	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:GLU:HA	1:E:77:LEU:HD21	2.01	0.42
1:E:185:LEU:HD12	1:E:194:ILE:HD11	2.01	0.42
1:A:7:PRO:HB2	1:A:8:HIS:H	1.71	0.42
1:D:40:VAL:O	1:D:44:VAL:HG13	2.19	0.42
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.81	0.42
1:E:214:LYS:HD2	1:E:214:LYS:HA	1.81	0.42
1:E:216:SER:HB2	1:E:220:ARG:NH2	2.35	0.41
1:A:12:PHE:HD1	1:A:86:ILE:HD11	1.85	0.41
1:A:187:VAL:HG21	1:A:226:MET:HE1	2.01	0.41
1:A:215:THR:O	1:A:219:LEU:HD12	2.21	0.41
1:A:38:ASN:HB2	1:A:40:VAL:HG12	2.03	0.41
1:C:86:ILE:HD13	1:C:86:ILE:HA	1.98	0.41
1:F:107:ALA:HA	1:F:110:TYR:HD1	1.86	0.41
1:A:173:PRO:HA	1:A:174:PRO:HD3	1.85	0.41
1:A:201:GLU:HG2	1:A:210:TRP:HB3	2.02	0.41
1:D:114:ASP:OD1	1:D:115:PHE:N	2.54	0.40
1:F:197:ASN:ND2	1:F:210:TRP:O	2.54	0.40
1:C:102:ARG:HE	1:C:102:ARG:HB2	1.60	0.40
1:F:189:GLU:OE1	1:F:189:GLU:N	2.55	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	185/242 (76%)	178 (96%)	7 (4%)	0	100	100
1	B	188/242 (78%)	181 (96%)	7 (4%)	0	100	100
1	C	184/242 (76%)	180 (98%)	4 (2%)	0	100	100
1	D	189/242 (78%)	184 (97%)	5 (3%)	0	100	100
1	E	184/242 (76%)	178 (97%)	6 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	186/242 (77%)	180 (97%)	6 (3%)	0	100	100
All	All	1116/1452 (77%)	1081 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/214 (76%)	160 (99%)	2 (1%)	67	82
1	B	164/214 (77%)	160 (98%)	4 (2%)	44	64
1	C	157/214 (73%)	155 (99%)	2 (1%)	65	80
1	D	167/214 (78%)	166 (99%)	1 (1%)	84	92
1	E	161/214 (75%)	159 (99%)	2 (1%)	67	82
1	F	161/214 (75%)	158 (98%)	3 (2%)	52	71
All	All	972/1284 (76%)	958 (99%)	14 (1%)	65	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	112	VAL
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	81	ILE
1	B	164	VAL
1	C	112	VAL
1	C	212	LEU
1	D	204	CYS
1	E	34	ARG
1	E	103	LYS
1	F	86	ILE
1	F	92	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	201	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	177	GLN
1	A	191	GLN
1	B	181	GLN
1	C	66	ASN
1	D	66	ASN
1	E	14	ASN
1	F	66	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are 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	$\# Z  > 2$
2	PO4	E	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	A	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	D	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	C	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	B	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	F	301	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	D	302	-	4,4,4	0.91	0	6,6,6	0.43	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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	189/242 (78%)	-0.79	0 100 100	47, 68, 86, 105	0
1	B	191/242 (78%)	-0.81	0 100 100	42, 66, 88, 102	1 (0%)
1	C	188/242 (77%)	-0.65	0 100 100	51, 70, 89, 100	0
1	D	193/242 (79%)	-0.87	0 100 100	50, 66, 90, 97	0
1	E	187/242 (77%)	-0.81	0 100 100	32, 67, 88, 92	1 (0%)
1	F	190/242 (78%)	-0.66	0 100 100	52, 71, 89, 108	0
All	All	1138/1452 (78%)	-0.76	0 100 100	32, 68, 89, 108	2 (0%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	F	301	5/5	0.93	0.08	80,87,96,118	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	C	301	5/5	0.94	0.10	82,88,104,123	0
2	PO4	B	301	5/5	0.94	0.09	79,83,96,115	0
2	PO4	D	302	5/5	0.95	0.09	86,91,100,110	0
2	PO4	E	301	5/5	0.97	0.09	74,86,86,113	0
2	PO4	D	301	5/5	0.98	0.06	93,100,111,125	0
2	PO4	A	301	5/5	0.98	0.09	90,91,92,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.