



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:42 AM GMT

PDB ID : 2ISS  
Title : Structure of the PLP synthase Holoenzyme from *Thermotoga maritima*  
Authors : Zein, F.; Zhang, Y.; Kang, Y.N.; Burns, K.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2006-10-18  
Resolution : 2.90 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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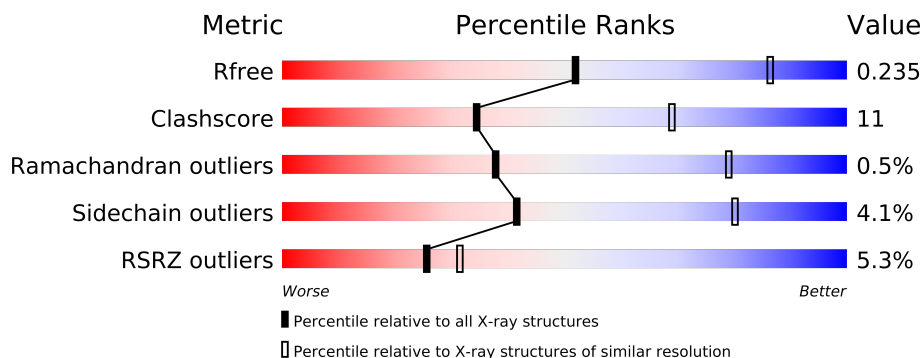
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	313	
1	B	313	
1	C	313	
2	D	208	
2	E	208	
2	F	208	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	5RP	B	294	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10860 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 Pyridoxal biosynthesis lyase pdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2129	1349	373	389	18			
1	B	285	Total	C	N	O	S	0	0	0
			2157	1365	380	394	18			
1	C	280	Total	C	N	O	S	0	0	0
			2119	1343	370	388	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU4
A	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU4
A	-17	SER	-	EXPRESSION TAG	UNP Q9WYU4
A	-16	SER	-	EXPRESSION TAG	UNP Q9WYU4
A	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU4
A	-9	SER	-	EXPRESSION TAG	UNP Q9WYU4
A	-8	SER	-	EXPRESSION TAG	UNP Q9WYU4
A	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU4
A	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU4
A	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU4
A	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU4
A	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU4
A	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU4
A	-1	SER	-	EXPRESSION TAG	UNP Q9WYU4
A	0	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU4
B	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU4
B	-17	SER	-	EXPRESSION TAG	UNP Q9WYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q9WYU4
B	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU4
B	-9	SER	-	EXPRESSION TAG	UNP Q9WYU4
B	-8	SER	-	EXPRESSION TAG	UNP Q9WYU4
B	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU4
B	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU4
B	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU4
B	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU4
B	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU4
B	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU4
B	-1	SER	-	EXPRESSION TAG	UNP Q9WYU4
B	0	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU4
C	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU4
C	-17	SER	-	EXPRESSION TAG	UNP Q9WYU4
C	-16	SER	-	EXPRESSION TAG	UNP Q9WYU4
C	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU4
C	-9	SER	-	EXPRESSION TAG	UNP Q9WYU4
C	-8	SER	-	EXPRESSION TAG	UNP Q9WYU4
C	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU4
C	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU4
C	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU4
C	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU4
C	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU4
C	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU4
C	-1	SER	-	EXPRESSION TAG	UNP Q9WYU4
C	0	HIS	-	EXPRESSION TAG	UNP Q9WYU4

- Molecule 2 is a protein called Glutamine amidotransferase subunit pdxT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	185	Total	C	N	O	S	0	0	0
			1461	937	248	268	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	184	Total	C	N	O	S	0	0	0
			1451	931	245	267	8			
2	F	184	Total	C	N	O	S	0	0	0
			1451	931	245	267	8			

There are 60 discrepancies between the modelled and reference sequences:

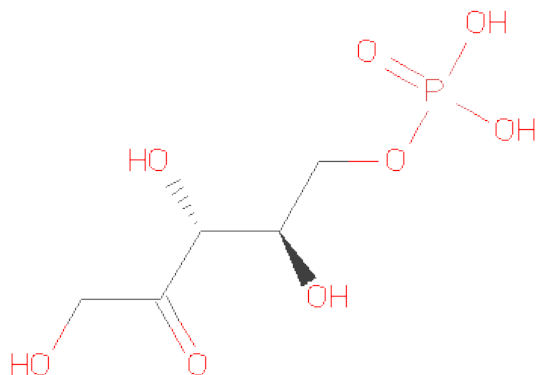
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU3
D	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU3
D	-17	SER	-	EXPRESSION TAG	UNP Q9WYU3
D	-16	SER	-	EXPRESSION TAG	UNP Q9WYU3
D	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU3
D	-9	SER	-	EXPRESSION TAG	UNP Q9WYU3
D	-8	SER	-	EXPRESSION TAG	UNP Q9WYU3
D	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU3
D	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU3
D	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU3
D	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU3
D	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU3
D	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU3
D	-1	SER	-	EXPRESSION TAG	UNP Q9WYU3
D	0	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU3
E	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU3
E	-17	SER	-	EXPRESSION TAG	UNP Q9WYU3
E	-16	SER	-	EXPRESSION TAG	UNP Q9WYU3
E	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU3
E	-9	SER	-	EXPRESSION TAG	UNP Q9WYU3
E	-8	SER	-	EXPRESSION TAG	UNP Q9WYU3
E	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU3
E	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU3

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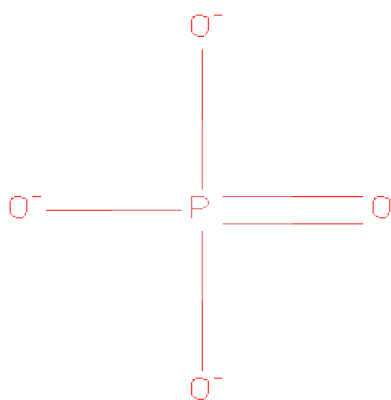
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU3
E	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU3
E	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU3
E	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU3
E	-1	SER	-	EXPRESSION TAG	UNP Q9WYU3
E	0	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-19	MET	-	INITIATING METHIONINE	UNP Q9WYU3
F	-18	GLY	-	EXPRESSION TAG	UNP Q9WYU3
F	-17	SER	-	EXPRESSION TAG	UNP Q9WYU3
F	-16	SER	-	EXPRESSION TAG	UNP Q9WYU3
F	-15	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-14	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-13	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-12	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-11	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-10	HIS	-	EXPRESSION TAG	UNP Q9WYU3
F	-9	SER	-	EXPRESSION TAG	UNP Q9WYU3
F	-8	SER	-	EXPRESSION TAG	UNP Q9WYU3
F	-7	GLY	-	EXPRESSION TAG	UNP Q9WYU3
F	-6	LEU	-	EXPRESSION TAG	UNP Q9WYU3
F	-5	VAL	-	EXPRESSION TAG	UNP Q9WYU3
F	-4	PRO	-	EXPRESSION TAG	UNP Q9WYU3
F	-3	ARG	-	EXPRESSION TAG	UNP Q9WYU3
F	-2	GLY	-	EXPRESSION TAG	UNP Q9WYU3
F	-1	SER	-	EXPRESSION TAG	UNP Q9WYU3
F	0	HIS	-	EXPRESSION TAG	UNP Q9WYU3

- Molecule 3 is SUGAR (RIBULOSE-5-PHOSPHATE) (three-letter code: 5RP) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			13	5	7	1		
3	B	1	Total	C	O	P	0	0
			13	5	7	1		
3	C	1	Total	C	O	P	0	0
			13	5	7	1		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	14	Total	O	0	0
			14	14		
5	C	9	Total	O	0	0
			9	9		
5	D	3	Total	O	0	0
			3	3		
5	E	3	Total	O	0	0
			3	3		
5	F	1	Total	O	0	0
			1	1		

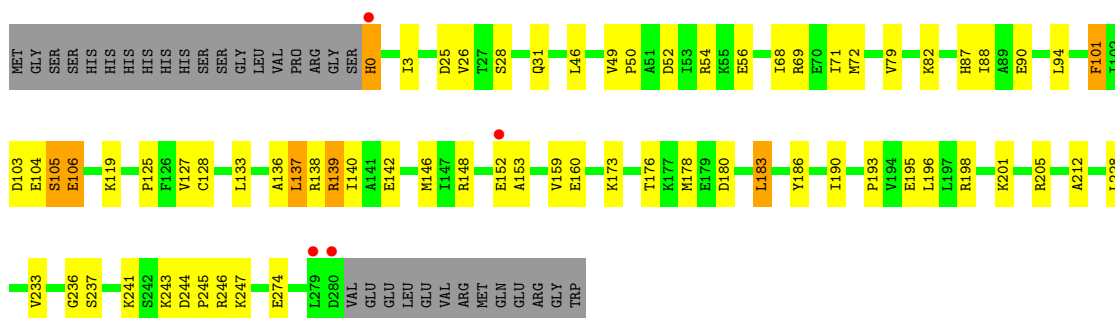


### 3 Residue-property plots

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.

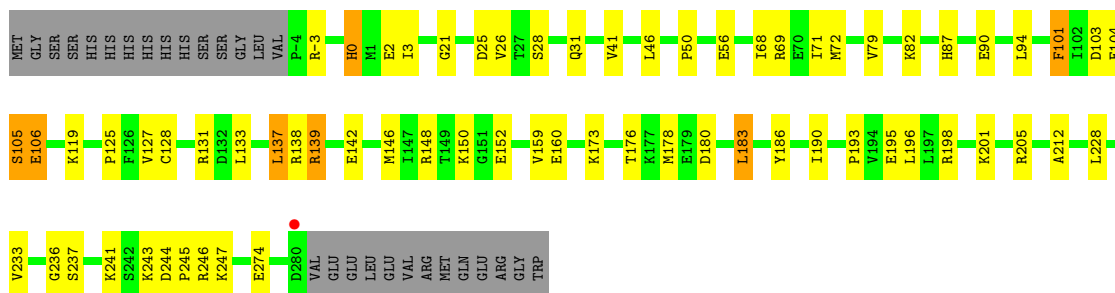
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain A: 



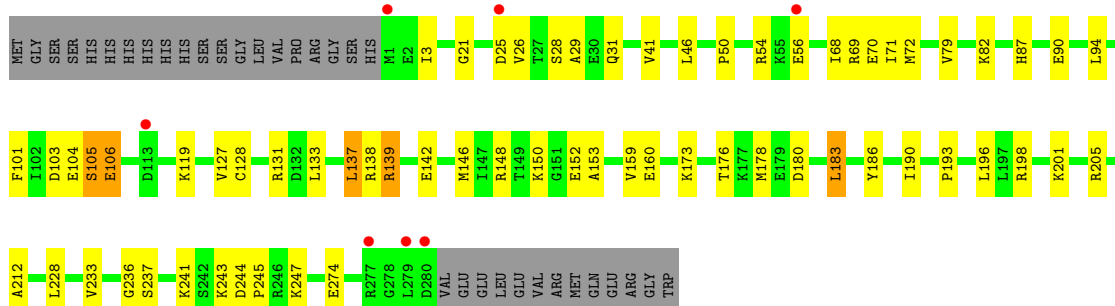
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain B: 



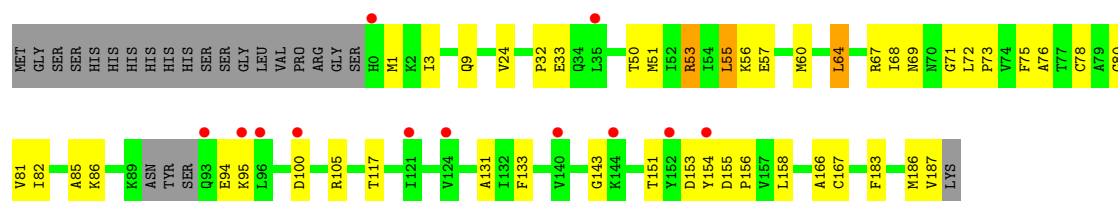
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain C: 



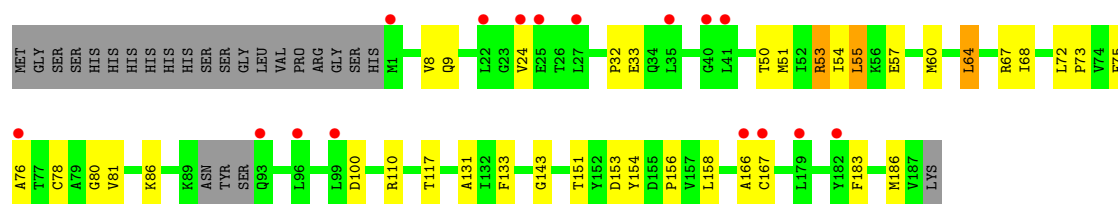
- Molecule 2: Glutamine amidotransferase subunit pdxT

Chain D: 



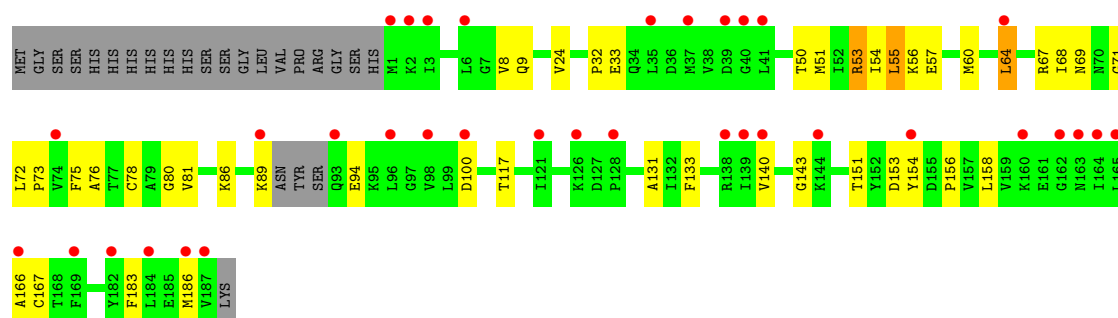
- Molecule 2: Glutamine amidotransferase subunit pdxT

Chain E: 



- Molecule 2: Glutamine amidotransferase subunit pdxT

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.53Å 204.10Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 2.90 49.12 – 2.89	Depositor EDS
% Data completeness (in resolution range)	92.7 (46.34-2.90) 92.1 (49.12-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.236 0.211 , 0.235	Depositor DCC
$R_{free}$ test set	2178 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 45755 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10860	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 3.96% 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, 5RP

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	0.38	0/2158	0.61	0/2898
1	B	0.39	0/2187	0.62	0/2936
1	C	0.37	0/2147	0.61	0/2883
2	D	0.33	0/1483	0.61	0/2003
2	E	0.35	0/1472	0.61	0/1988
2	F	0.33	0/1472	0.60	0/1988
All	All	0.36	0/10919	0.61	0/14696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2129	0	2205	53	0
1	B	2157	0	2233	54	0
1	C	2119	0	2198	50	0
2	D	1461	0	1514	33	0
2	E	1451	0	1507	27	0
2	F	1451	0	1507	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	9	2	0
3	B	13	0	9	2	0
3	C	13	0	9	2	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
5	A	8	0	0	1	0
5	B	14	0	0	2	0
5	C	9	0	0	1	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
All	All	10860	0	11191	238	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 11.

All (238) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:53:ARG:HH11	2:D:53:ARG:HA	1.34	0.92
2:F:53:ARG:HA	2:F:53:ARG:HH11	1.35	0.92
2:E:53:ARG:HA	2:E:53:ARG:HH11	1.33	0.91
2:E:81:VAL:HG22	2:E:166:ALA:HB1	1.61	0.83
2:F:81:VAL:HG22	2:F:166:ALA:HB1	1.59	0.82
2:D:81:VAL:HG22	2:D:166:ALA:HB1	1.62	0.81
2:F:56:LYS:HE3	2:F:94:GLU:OE1	1.81	0.80
1:B:3:ILE:HG22	2:E:117:THR:HB	1.68	0.73
2:F:72:LEU:HD12	2:F:73:PRO:HD2	1.71	0.72
2:D:72:LEU:HD12	2:D:73:PRO:HD2	1.72	0.72
2:D:1:MET:HE3	2:D:187:VAL:HG11	1.71	0.71
2:E:72:LEU:HD12	2:E:73:PRO:HD2	1.73	0.70
2:E:53:ARG:HA	2:E:53:ARG:NH1	2.06	0.69
2:E:32:PRO:HG3	2:E:60:MET:HG2	1.75	0.69
2:D:53:ARG:NH1	2:D:53:ARG:HA	2.08	0.68
1:A:119:LYS:HE2	1:A:128:CYS:SG	2.34	0.67
1:B:119:LYS:HE2	1:B:128:CYS:SG	2.34	0.67
2:D:32:PRO:HG3	2:D:60:MET:HG2	1.76	0.67
1:C:119:LYS:HE2	1:C:128:CYS:SG	2.35	0.66
2:F:53:ARG:HA	2:F:53:ARG:NH1	2.08	0.66
2:F:32:PRO:HG3	2:F:60:MET:HG2	1.77	0.65
1:C:106:GLU:CD	1:C:106:GLU:H	2.00	0.65
1:B:25:ASP:HB2	1:B:236:GLY:HA2	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:100:ASP:OD2	2:E:143:GLY:HA3	1.97	0.64
1:B:106:GLU:CD	1:B:106:GLU:H	2.00	0.64
1:A:25:ASP:HB2	1:A:236:GLY:HA2	1.79	0.64
1:A:106:GLU:CD	1:A:106:GLU:H	2.00	0.64
1:A:87:HIS:CG	1:A:90:GLU:HG3	2.34	0.63
1:B:87:HIS:CG	1:B:90:GLU:HG3	2.33	0.63
2:D:100:ASP:OD2	2:D:143:GLY:HA3	1.99	0.63
2:E:158:LEU:HD13	2:E:167:CYS:HB3	1.81	0.62
2:D:56:LYS:HE3	2:D:94:GLU:OE2	1.99	0.62
2:F:151:THR:HG22	2:F:156:PRO:HA	1.80	0.62
1:C:87:HIS:CG	1:C:90:GLU:HG3	2.35	0.62
2:F:100:ASP:OD2	2:F:143:GLY:HA3	1.99	0.62
1:C:25:ASP:HB2	1:C:236:GLY:HA2	1.81	0.61
2:E:151:THR:HG22	2:E:156:PRO:HA	1.83	0.61
2:E:9:GLN:HG3	2:E:50:THR:HG21	1.83	0.61
2:D:151:THR:HG22	2:D:156:PRO:HA	1.82	0.61
1:C:128:CYS:CB	1:C:139:ARG:HG2	2.31	0.61
1:C:87:HIS:ND1	1:C:90:GLU:HG3	2.16	0.60
1:C:128:CYS:HB2	1:C:139:ARG:HG2	1.83	0.60
2:F:89:LYS:HD2	2:F:140:VAL:HG21	1.83	0.60
2:D:158:LEU:HD13	2:D:167:CYS:HB3	1.83	0.59
2:D:1:MET:HE2	2:D:3:ILE:HD11	1.85	0.59
2:D:9:GLN:HG3	2:D:50:THR:HG21	1.85	0.59
2:F:158:LEU:HD13	2:F:167:CYS:HB3	1.84	0.59
2:D:32:PRO:HG3	2:D:60:MET:CG	2.33	0.59
1:B:87:HIS:ND1	1:B:90:GLU:HG3	2.18	0.58
2:E:32:PRO:HG3	2:E:60:MET:CG	2.32	0.58
1:B:128:CYS:HB2	1:B:139:ARG:HG2	1.86	0.58
1:C:105:SER:HB2	1:C:148:ARG:NH2	2.18	0.58
1:A:87:HIS:ND1	1:A:90:GLU:HG3	2.18	0.58
1:A:128:CYS:CB	1:A:139:ARG:HG2	2.34	0.58
1:B:128:CYS:CB	1:B:139:ARG:HG2	2.34	0.57
2:F:32:PRO:HG3	2:F:60:MET:CG	2.33	0.57
1:A:128:CYS:HB2	1:A:139:ARG:HG2	1.87	0.57
2:F:9:GLN:HG3	2:F:50:THR:HG21	1.87	0.56
1:A:243:LYS:HG2	1:A:274:GLU:HB3	1.88	0.56
1:A:212:ALA:HB3	1:A:233:VAL:HG12	1.88	0.56
2:D:1:MET:HE3	2:D:187:VAL:CG1	2.35	0.56
1:B:212:ALA:HB3	1:B:233:VAL:HG12	1.89	0.55
1:B:105:SER:HB2	1:B:148:ARG:NH2	2.20	0.55
1:A:82:LYS:HE3	1:A:103:ASP:OD2	2.06	0.55
1:A:105:SER:HB2	1:A:148:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:LYS:HG2	1:B:274:GLU:HB3	1.88	0.55
1:C:212:ALA:HB3	1:C:233:VAL:HG12	1.89	0.55
1:C:243:LYS:HG2	1:C:274:GLU:HB3	1.87	0.55
1:A:237:SER:O	1:A:241:LYS:HB2	2.07	0.55
1:B:-3:ARG:HA	2:E:154:TYR:CD1	2.42	0.55
1:C:237:SER:O	1:C:241:LYS:HB2	2.06	0.55
1:B:28:SER:OG	1:B:31:GLN:HG3	2.07	0.55
1:A:25:ASP:OD2	3:A:294:5RP:H5	2.06	0.54
1:B:186:TYR:CE2	1:B:190:ILE:HD13	2.43	0.54
1:B:82:LYS:HE3	1:B:103:ASP:OD2	2.07	0.54
1:B:237:SER:O	1:B:241:LYS:HB2	2.07	0.54
1:B:50:PRO:HG2	3:B:294:5RP:H71	1.89	0.54
2:E:75:PHE:HB2	2:E:183:PHE:CD1	2.42	0.54
1:B:25:ASP:OD2	3:B:294:5RP:H5	2.07	0.54
1:C:50:PRO:HG2	3:C:294:5RP:H71	1.89	0.54
1:A:28:SER:OG	1:A:31:GLN:HG3	2.08	0.54
2:F:72:LEU:HD12	2:F:73:PRO:CD	2.37	0.54
1:A:50:PRO:HG2	3:A:294:5RP:H71	1.90	0.54
2:D:75:PHE:HB2	2:D:183:PHE:CD1	2.43	0.54
1:B:46:LEU:HD21	1:B:82:LYS:HD2	1.90	0.53
1:C:28:SER:OG	1:C:31:GLN:HG3	2.09	0.53
1:C:25:ASP:OD2	3:C:294:5RP:H5	2.07	0.53
1:C:105:SER:HB2	1:C:148:ARG:HH22	1.73	0.53
1:C:72:MET:HA	1:C:79:VAL:HG21	1.91	0.52
1:C:82:LYS:HE3	1:C:103:ASP:OD2	2.08	0.52
1:A:46:LEU:HD21	1:A:82:LYS:HD2	1.91	0.52
2:F:75:PHE:HB2	2:F:183:PHE:CD1	2.44	0.52
2:E:72:LEU:HD12	2:E:73:PRO:CD	2.40	0.52
1:A:72:MET:HA	1:A:79:VAL:HG21	1.92	0.52
1:B:72:MET:HB3	2:E:110:ARG:NH2	2.24	0.52
1:C:138:ARG:HH11	1:C:138:ARG:HG3	1.75	0.52
1:B:105:SER:HB2	1:B:148:ARG:HH22	1.74	0.51
1:A:243:LYS:O	1:A:245:PRO:HD3	2.11	0.51
1:A:105:SER:HB2	1:A:148:ARG:HH22	1.76	0.51
1:C:3:ILE:HG22	2:F:117:THR:HB	1.92	0.51
1:C:46:LEU:HD21	1:C:82:LYS:HD2	1.91	0.51
2:E:76:ALA:HB1	2:E:80:GLY:HA3	1.91	0.51
1:C:244:ASP:OD2	1:C:247:LYS:HB2	2.10	0.51
1:B:68:ILE:O	1:B:72:MET:HG3	2.10	0.51
1:B:183:LEU:HD23	1:B:198:ARG:HG2	1.92	0.51
1:B:104:GLU:OE2	1:B:119:LYS:HE3	2.11	0.50
1:A:186:TYR:CE2	1:A:190:ILE:HD13	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:GLU:OE2	1:A:119:LYS:HE3	2.11	0.50
1:C:243:LYS:O	1:C:245:PRO:HD3	2.12	0.50
1:B:72:MET:HA	1:B:79:VAL:HG21	1.94	0.50
1:A:3:ILE:HG22	2:D:117:THR:HB	1.93	0.50
2:F:53:ARG:O	2:F:57:GLU:HG3	2.11	0.50
1:B:2:GLU:HG2	1:B:3:ILE:N	2.25	0.50
1:C:186:TYR:CE2	1:C:190:ILE:HD13	2.46	0.50
2:F:76:ALA:HB1	2:F:80:GLY:HA3	1.93	0.50
1:C:183:LEU:HD23	1:C:198:ARG:HG2	1.93	0.50
1:B:244:ASP:OD2	1:B:247:LYS:HB2	2.12	0.50
1:A:26:VAL:HG23	1:A:71:ILE:HD13	1.94	0.49
1:B:159:VAL:HG13	1:B:160:GLU:N	2.27	0.49
1:B:26:VAL:HG23	1:B:71:ILE:HD13	1.94	0.49
1:A:159:VAL:HG13	1:A:160:GLU:N	2.26	0.49
2:D:76:ALA:HB1	2:D:80:GLY:HA3	1.93	0.49
1:C:159:VAL:HG13	1:C:160:GLU:N	2.27	0.49
2:E:53:ARG:O	2:E:57:GLU:HG3	2.11	0.49
1:C:178:MET:HB2	1:C:183:LEU:CD1	2.42	0.49
1:C:26:VAL:HG23	1:C:71:ILE:HD13	1.94	0.49
1:A:178:MET:HB2	1:A:183:LEU:CD1	2.42	0.49
1:C:68:ILE:O	1:C:72:MET:HG3	2.12	0.49
1:A:68:ILE:O	1:A:72:MET:HG3	2.13	0.49
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.77	0.49
1:B:243:LYS:O	1:B:245:PRO:HD3	2.13	0.48
1:A:183:LEU:HD23	1:A:198:ARG:HG2	1.94	0.48
1:B:178:MET:HB2	1:B:183:LEU:CD1	2.42	0.48
1:C:180:ASP:OD1	1:C:198:ARG:NH1	2.44	0.48
2:D:72:LEU:HD12	2:D:73:PRO:CD	2.40	0.48
1:C:104:GLU:OE2	1:C:119:LYS:HE3	2.12	0.48
1:B:180:ASP:OD1	1:B:198:ARG:NH1	2.44	0.48
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.78	0.48
1:C:127:VAL:HA	1:C:146:MET:O	2.14	0.48
1:A:127:VAL:HA	1:A:146:MET:O	2.14	0.47
2:F:67:ARG:HH11	2:F:67:ARG:HG3	1.78	0.47
1:A:244:ASP:OD2	1:A:247:LYS:HB2	2.14	0.47
2:D:53:ARG:O	2:D:57:GLU:HG3	2.15	0.47
1:B:127:VAL:HA	1:B:146:MET:O	2.15	0.47
1:A:0:HIS:O	1:A:0:HIS:CD2	2.68	0.46
1:C:133:LEU:HG	1:C:137:LEU:HD22	1.96	0.46
1:A:173:LYS:O	1:A:176:THR:HB	2.15	0.46
1:C:193:PRO:HG2	1:C:196:LEU:HD12	1.98	0.46
1:B:133:LEU:HG	1:B:137:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:PRO:HG2	1:A:196:LEU:HD12	1.98	0.46
2:D:67:ARG:HG3	2:D:67:ARG:HH11	1.80	0.45
2:E:67:ARG:HH11	2:E:67:ARG:HG3	1.81	0.45
1:A:139:ARG:HH21	1:A:142:GLU:CD	2.19	0.45
1:B:139:ARG:HH21	1:B:142:GLU:CD	2.20	0.45
1:A:137:LEU:HA	1:A:137:LEU:HD12	1.73	0.45
2:D:1:MET:CE	2:D:3:ILE:HD11	2.46	0.45
2:F:51:MET:O	2:F:55:LEU:HB2	2.17	0.45
1:C:138:ARG:NH1	1:C:138:ARG:HG3	2.30	0.45
1:A:133:LEU:HG	1:A:137:LEU:HD22	1.98	0.45
1:B:195:GLU:HB2	5:B:361:HOH:O	2.17	0.45
1:B:138:ARG:NH1	1:B:138:ARG:HG3	2.33	0.44
2:E:131:ALA:HB1	2:E:133:PHE:CE1	2.53	0.44
2:D:131:ALA:HB1	2:D:133:PHE:CE1	2.53	0.44
1:A:138:ARG:NH1	1:A:138:ARG:HG3	2.32	0.44
2:D:183:PHE:O	2:D:186:MET:HB2	2.18	0.44
1:C:139:ARG:HH12	4:C:302:PO4:P	2.41	0.44
2:F:69:ASN:C	2:F:71:GLY:H	2.22	0.43
1:C:173:LYS:O	1:C:176:THR:HB	2.18	0.43
1:B:41:VAL:HG13	5:B:352:HOH:O	2.17	0.43
2:F:64:LEU:O	2:F:68:ILE:HG13	2.18	0.43
2:E:51:MET:O	2:E:55:LEU:HB2	2.18	0.43
2:F:183:PHE:O	2:F:186:MET:HB2	2.18	0.43
1:B:152:GLU:HG3	1:B:160:GLU:HG3	2.00	0.43
1:C:41:VAL:HG13	5:C:350:HOH:O	2.19	0.43
1:C:69:ARG:HH11	1:C:69:ARG:HG2	1.84	0.43
2:F:153:ASP:O	2:F:154:TYR:HB2	2.19	0.43
1:A:180:ASP:OD1	1:A:198:ARG:NH1	2.49	0.43
2:E:8:VAL:HB	2:E:54:ILE:HG21	2.01	0.43
1:B:173:LYS:O	1:B:176:THR:HB	2.19	0.43
2:E:183:PHE:O	2:E:186:MET:HB2	2.18	0.43
2:D:86:LYS:HD2	2:D:100:ASP:HA	2.01	0.43
2:D:69:ASN:C	2:D:71:GLY:H	2.22	0.43
2:D:56:LYS:HE3	2:D:94:GLU:CD	2.39	0.42
1:C:87:HIS:CE1	1:C:90:GLU:HG3	2.54	0.42
1:C:152:GLU:HG3	1:C:160:GLU:HG3	2.01	0.42
2:F:86:LYS:HD2	2:F:100:ASP:HA	2.02	0.42
1:A:195:GLU:HB2	5:A:380:HOH:O	2.20	0.42
1:B:139:ARG:HH12	4:B:301:PO4:P	2.42	0.42
1:C:139:ARG:HH21	1:C:142:GLU:CD	2.23	0.42
2:E:86:LYS:HD2	2:E:100:ASP:HA	2.00	0.42
1:B:21:GLY:HA3	1:B:41:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:131:ARG:HG3	1:C:150:LYS:HE3	2.02	0.42
2:F:55:LEU:HA	2:F:55:LEU:HD12	1.89	0.42
1:A:87:HIS:CE1	1:A:90:GLU:HG3	2.55	0.42
1:B:193:PRO:HG2	1:B:196:LEU:HD12	2.00	0.42
1:B:101:PHE:CZ	1:B:125:PRO:HB2	2.55	0.42
1:C:21:GLY:HA3	1:C:41:VAL:HG11	2.02	0.42
1:A:136:ALA:O	1:A:140:ILE:HG13	2.20	0.42
1:B:87:HIS:CE1	1:B:90:GLU:HG3	2.55	0.42
1:A:101:PHE:CZ	1:A:125:PRO:HB2	2.54	0.42
1:A:50:PRO:HB3	1:A:153:ALA:HB1	2.02	0.42
1:A:54:ARG:NH1	1:A:153:ALA:O	2.52	0.42
2:F:131:ALA:HB1	2:F:133:PHE:CE1	2.55	0.42
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.85	0.42
2:E:64:LEU:O	2:E:68:ILE:HG13	2.20	0.42
2:D:85:ALA:O	2:D:95:LYS:HD2	2.19	0.42
2:E:72:LEU:HA	2:E:73:PRO:HD3	1.94	0.41
1:B:-3:ARG:HB2	2:E:154:TYR:CE1	2.55	0.41
1:B:178:MET:HB2	1:B:183:LEU:HD13	2.02	0.41
1:C:54:ARG:NH1	1:C:153:ALA:O	2.53	0.41
2:E:153:ASP:O	2:E:154:TYR:HB2	2.20	0.41
1:C:128:CYS:HB3	1:C:139:ARG:HG2	2.02	0.41
2:D:51:MET:O	2:D:55:LEU:HB2	2.20	0.41
2:D:82:ILE:HD13	2:D:105:ARG:HG2	2.01	0.41
1:C:241:LYS:HA	1:C:241:LYS:HD3	1.96	0.41
1:A:152:GLU:HG3	1:A:160:GLU:HG3	2.01	0.41
1:B:133:LEU:O	1:B:137:LEU:HB2	2.19	0.41
1:A:49:VAL:HG22	1:A:52:ASP:OD2	2.21	0.41
2:D:72:LEU:HA	2:D:73:PRO:HD3	1.93	0.41
1:B:152:GLU:HG3	1:B:160:GLU:CG	2.51	0.41
2:D:64:LEU:O	2:D:68:ILE:HG13	2.20	0.41
2:F:8:VAL:HB	2:F:54:ILE:HG21	2.02	0.41
1:C:152:GLU:HG3	1:C:160:GLU:CG	2.51	0.41
1:A:133:LEU:O	1:A:137:LEU:HB2	2.21	0.41
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.36	0.41
1:A:139:ARG:HH12	4:A:300:PO4:P	2.44	0.40
1:A:178:MET:HB2	1:A:183:LEU:HD13	2.03	0.40
1:A:246:ARG:NH1	1:A:246:ARG:HG2	2.36	0.40
1:C:29:ALA:HB2	1:C:70:GLU:HG2	2.03	0.40
1:A:69:ARG:HG2	1:A:69:ARG:HH11	1.86	0.40
1:C:178:MET:HB2	1:C:183:LEU:HD13	2.03	0.40
2:D:153:ASP:O	2:D:154:TYR:HB2	2.21	0.40
2:D:155:ASP:HA	2:D:156:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:ILE:H	1:A:88:ILE:HG13	1.75	0.40
1:B:131:ARG:HG3	1:B:150:LYS:HE3	2.03	0.40
1:C:50:PRO:HB3	1:C:153:ALA:HB1	2.03	0.40
1:A:241:LYS:HA	1:A:241:LYS:HD3	1.95	0.40
1:B:137:LEU:HD12	1:B:137:LEU:HA	1.76	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	279/313 (89%)	267 (96%)	11 (4%)	1 (0%)	43	82
1	B	283/313 (90%)	270 (95%)	11 (4%)	2 (1%)	30	72
1	C	278/313 (89%)	266 (96%)	11 (4%)	1 (0%)	43	82
2	D	181/208 (87%)	167 (92%)	13 (7%)	1 (1%)	33	76
2	E	180/208 (86%)	166 (92%)	13 (7%)	1 (1%)	33	76
2	F	180/208 (86%)	167 (93%)	12 (7%)	1 (1%)	33	76
All	All	1381/1563 (88%)	1303 (94%)	71 (5%)	7 (0%)	38	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	HIS
2	D	78	CYS
2	E	78	CYS
2	F	78	CYS
1	B	56	GLU
1	C	56	GLU
1	A	56	GLU

### 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	217/247 (88%)	206 (95%)	11 (5%)	33	72
1	B	220/247 (89%)	209 (95%)	11 (5%)	34	73
1	C	216/247 (87%)	206 (95%)	10 (5%)	37	76
2	D	161/181 (89%)	156 (97%)	5 (3%)	52	88
2	E	160/181 (88%)	155 (97%)	5 (3%)	52	88
2	F	160/181 (88%)	155 (97%)	5 (3%)	52	88
All	All	1134/1284 (88%)	1087 (96%)	47 (4%)	41	80

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	94	LEU
1	A	101	PHE
1	A	105	SER
1	A	106	GLU
1	A	137	LEU
1	A	139	ARG
1	A	183	LEU
1	A	201	LYS
1	A	205	ARG
1	A	228	LEU
1	B	0	HIS
1	B	94	LEU
1	B	101	PHE
1	B	105	SER
1	B	106	GLU
1	B	137	LEU
1	B	139	ARG
1	B	183	LEU
1	B	201	LYS
1	B	205	ARG
1	B	228	LEU
1	C	94	LEU

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Mol	Chain	Res	Type
1	C	101	PHE
1	C	105	SER
1	C	106	GLU
1	C	137	LEU
1	C	139	ARG
1	C	183	LEU
1	C	201	LYS
1	C	205	ARG
1	C	228	LEU
2	D	24	VAL
2	D	33	GLU
2	D	53	ARG
2	D	55	LEU
2	D	64	LEU
2	E	24	VAL
2	E	33	GLU
2	E	53	ARG
2	E	55	LEU
2	E	64	LEU
2	F	24	VAL
2	F	33	GLU
2	F	53	ARG
2	F	55	LEU
2	F	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	174	GLN
1	B	174	GLN
1	C	174	GLN
2	D	69	ASN

### 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 ⓘ

6 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	$\# Z  > 2$
3	5RP	A	294	1	11,12,13	1.47	2 (18%)	12,16,18	0.96	1 (8%)
4	PO4	A	300	-	4,4,4	0.97	0	6,6,6	0.31	0
3	5RP	B	294	1	11,12,13	1.47	2 (18%)	12,16,18	0.96	1 (8%)
4	PO4	B	301	-	4,4,4	0.91	0	6,6,6	0.31	0
3	5RP	C	294	1	11,12,13	1.46	2 (18%)	12,16,18	0.96	1 (8%)
4	PO4	C	302	-	4,4,4	0.83	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	5RP	A	294	1	-	0/10/13/16	0/0/0/0
4	PO4	A	300	-	-	0/0/0/0	0/0/0/0
3	5RP	B	294	1	-	0/10/13/16	0/0/0/0
4	PO4	B	301	-	-	0/0/0/0	0/0/0/0
3	5RP	C	294	1	-	0/10/13/16	0/0/0/0
4	PO4	C	302	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	294	5RP	P9-O12	3.04	1.61	1.51
3	B	294	5RP	P9-O12	3.03	1.61	1.51
3	A	294	5RP	P9-O12	3.02	1.61	1.51
3	B	294	5RP	C3-C5	2.23	1.53	1.50
3	A	294	5RP	C3-C5	2.22	1.53	1.50
3	C	294	5RP	C3-C5	2.16	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	294	5RP	O11-P9-O8	2.27	112.92	106.65
3	C	294	5RP	O11-P9-O8	2.26	112.89	106.65
3	A	294	5RP	O11-P9-O8	2.26	112.88	106.65

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	281/313 (89%)	-0.01	4 (1%)	72 80	29, 43, 78, 104	0
1	B	285/313 (91%)	-0.06	1 (0%)	90 94	29, 42, 76, 96	0
1	C	280/313 (89%)	0.01	7 (2%)	54 64	28, 43, 77, 97	0
2	D	185/208 (88%)	0.40	12 (6%)	18 22	37, 58, 76, 92	0
2	E	184/208 (88%)	0.58	16 (8%)	10 13	36, 57, 74, 80	0
2	F	184/208 (88%)	0.83	35 (19%)	2 2	39, 62, 79, 84	0
All	All	1399/1563 (89%)	0.23	75 (5%)	25 30	28, 50, 77, 104	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	7.2
1	A	280	ASP	5.4
1	C	279	LEU	5.1
2	F	163	ASN	4.4
2	D	93	GLN	4.4
2	F	1	MET	4.3
2	F	96	LEU	4.2
2	E	96	LEU	4.1
2	F	93	GLN	4.0
1	C	280	ASP	3.7
2	E	93	GLN	3.7
2	F	35	LEU	3.6
2	F	39	ASP	3.4
2	F	164	ILE	3.4
2	E	179	LEU	3.3
1	A	0	HIS	3.3
2	F	139	ILE	3.2
2	E	1	MET	3.2
2	F	154	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	140	VAL	3.1
2	F	126	LYS	3.1
2	D	154	TYR	3.0
2	F	166	ALA	3.0
2	F	6	LEU	2.9
2	F	144	LYS	2.9
2	D	121	ILE	2.8
2	F	37	MET	2.8
2	F	64	LEU	2.8
2	F	2	LYS	2.8
2	F	74	VAL	2.7
2	D	140	VAL	2.7
1	C	56	GLU	2.7
2	F	41	LEU	2.7
2	E	41	LEU	2.7
2	E	24	VAL	2.6
1	C	1	MET	2.6
2	F	89	LYS	2.6
2	F	165	LEU	2.6
1	A	152	GLU	2.6
2	F	40	GLY	2.5
2	F	162	GLY	2.5
2	E	25	GLU	2.4
2	F	182	TYR	2.4
2	D	144	LYS	2.4
2	D	124	VAL	2.4
2	F	184	LEU	2.3
2	D	96	LEU	2.3
2	D	152	TYR	2.3
2	F	186	MET	2.3
2	F	169	PHE	2.3
1	C	113	ASP	2.3
1	C	277	ARG	2.3
2	E	166	ALA	2.3
1	C	25	ASP	2.3
2	D	95	LYS	2.3
2	E	35	LEU	2.3
2	F	98	VAL	2.2
2	F	128	PRO	2.2
2	D	0	HIS	2.2
2	E	182	TYR	2.2
2	D	35	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	3	ILE	2.2
2	F	138	ARG	2.2
2	E	27	LEU	2.2
2	F	121	ILE	2.2
2	E	76	ALA	2.2
2	F	100	ASP	2.1
1	B	280	ASP	2.1
2	F	187	VAL	2.1
2	E	22	LEU	2.1
2	E	167	CYS	2.1
2	F	160	LYS	2.1
2	D	100	ASP	2.0
2	E	40	GLY	2.0
2	E	99	LEU	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	5RP	B	294	13/14	0.30	2.12	64,70,73,75	0
3	5RP	C	294	13/14	0.33	1.57	66,69,75,76	0
3	5RP	A	294	13/14	0.28	1.11	64,70,73,76	0
4	PO4	C	302	5/5	0.14	-1.53	56,57,58,59	0
4	PO4	B	301	5/5	0.15	-1.60	55,56,57,57	0
4	PO4	A	300	5/5	0.12	-2.68	55,56,56,57	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.