



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:33 AM GMT

PDB ID : 3C3D  
Title : Crystal structure of 2-phospho-(S)-lactatetransferase from Methanosarcina mazei in complex with Fo and phosphate. Northeast Structural Genomics Consortium target MaR46  
Authors : Forouhar, F.; Abashidze, M.; Xu, H.; Grochowski, L.L.; Seetharaman, J.; Hus-sain, M.; Kuzin, A.P.; Chen, Y.; Zhou, W.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Galinier, A.; White, R.H.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-01-28  
Resolution : 2.50 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>

---

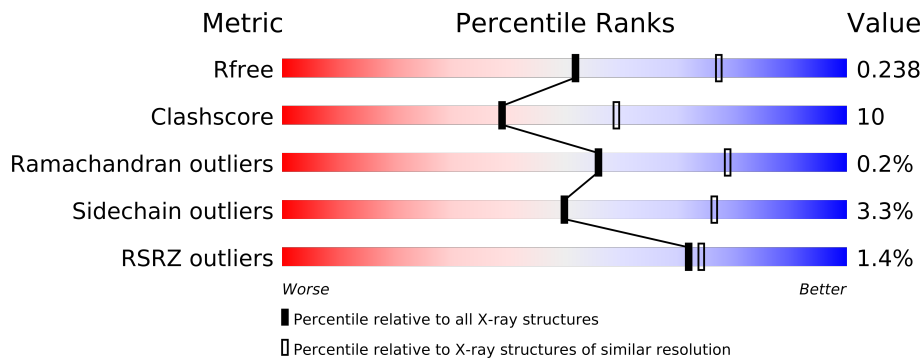
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	311	
1	B	311	
1	C	311	
1	D	311	

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	FO1	A	401	X	-
3	FO1	B	401	X	-
3	FO1	C	401	X	-
3	FO1	D	401	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10077 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 2-phospho-L-lactate transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	B	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	C	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	D	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			

There are 32 discrepancies between the modelled and reference sequences:

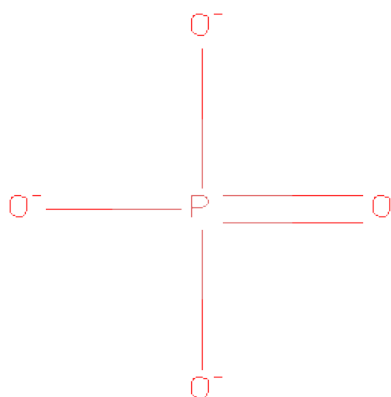
Chain	Residue	Modelled	Actual	Comment	Reference
A	304	LEU	-	EXPRESSION TAG	UNP Q8PVT6
A	305	GLU	-	EXPRESSION TAG	UNP Q8PVT6
A	306	HIS	-	EXPRESSION TAG	UNP Q8PVT6
A	307	HIS	-	EXPRESSION TAG	UNP Q8PVT6
A	308	HIS	-	EXPRESSION TAG	UNP Q8PVT6
A	309	HIS	-	EXPRESSION TAG	UNP Q8PVT6
A	310	HIS	-	EXPRESSION TAG	UNP Q8PVT6
A	311	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	304	LEU	-	EXPRESSION TAG	UNP Q8PVT6
B	305	GLU	-	EXPRESSION TAG	UNP Q8PVT6
B	306	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	307	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	308	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	309	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	310	HIS	-	EXPRESSION TAG	UNP Q8PVT6
B	311	HIS	-	EXPRESSION TAG	UNP Q8PVT6
C	304	LEU	-	EXPRESSION TAG	UNP Q8PVT6
C	305	GLU	-	EXPRESSION TAG	UNP Q8PVT6
C	306	HIS	-	EXPRESSION TAG	UNP Q8PVT6
C	307	HIS	-	EXPRESSION TAG	UNP Q8PVT6
C	308	HIS	-	EXPRESSION TAG	UNP Q8PVT6

*Continued on next page...*

Continued from previous page...

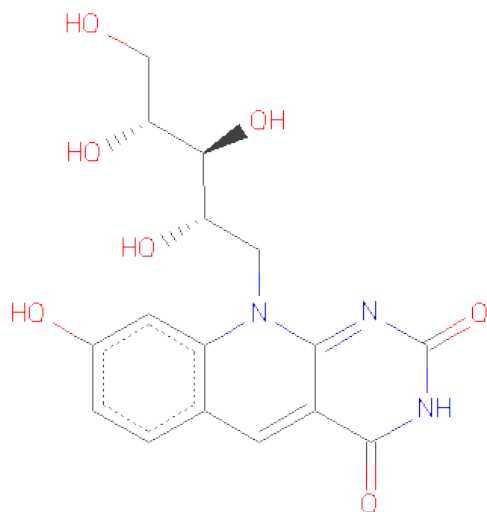
Chain	Residue	Modelled	Actual	Comment	Reference
C	309	HIS	-	EXPRESSION TAG	UNP Q8PVT6
C	310	HIS	-	EXPRESSION TAG	UNP Q8PVT6
C	311	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	304	LEU	-	EXPRESSION TAG	UNP Q8PVT6
D	305	GLU	-	EXPRESSION TAG	UNP Q8PVT6
D	306	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	307	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	308	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	309	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	310	HIS	-	EXPRESSION TAG	UNP Q8PVT6
D	311	HIS	-	EXPRESSION TAG	UNP Q8PVT6

- Molecule 2 is PHOSPHATE ION (three-letter code: 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		

- Molecule 3 is 1-DEOXY-1-(8-HYDROXY-2,4-DIOXO-3,4-DIHYDROPYRIMIDO[4,5-B]QUINOLIN-10(2H)-YL)-D-RIBITOL (three-letter code: FO1) (formula: C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	13	3	4		
3	B	1	Total	C	N	O	0	0
			20	13	3	4		
3	C	1	Total	C	N	O	0	0
			20	13	3	4		
3	D	1	Total	C	N	O	0	0
			20	13	3	4		

- Molecule 4 is water.

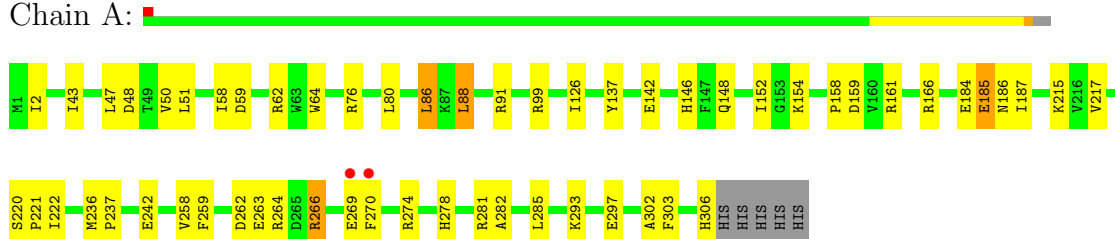
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	85	Total	O	0	0
			85	85		
4	C	90	Total	O	0	0
			90	90		
4	D	156	Total	O	0	0
			156	156		

### 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.

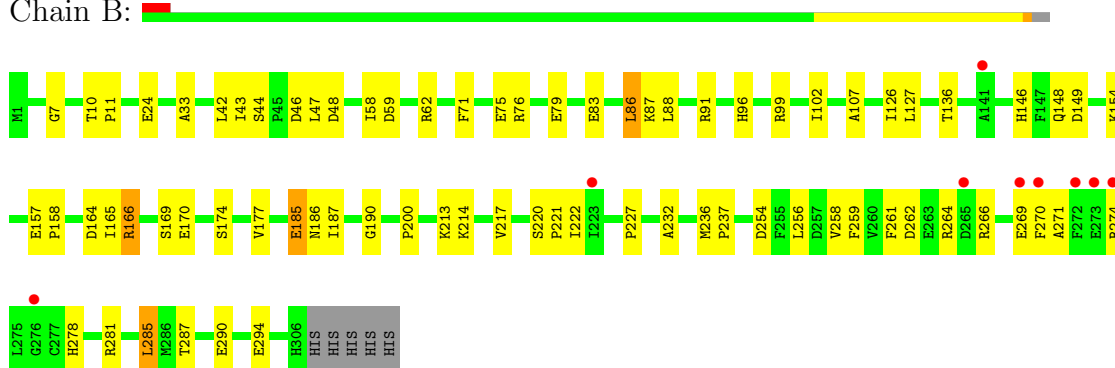
- Molecule 1: 2-phospho-L-lactate transferase

Chain A:



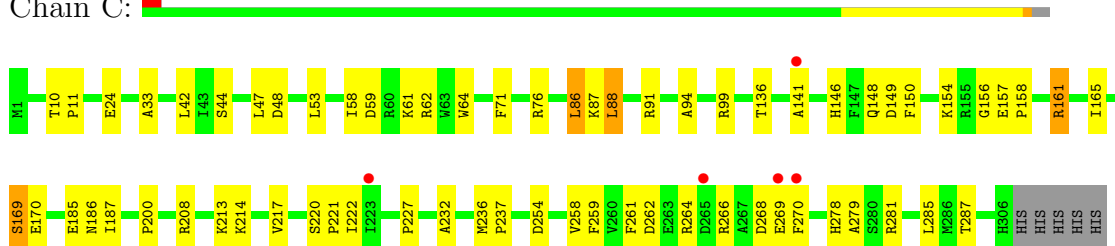
- Molecule 1: 2-phospho-L-lactate transferase

Chain B:



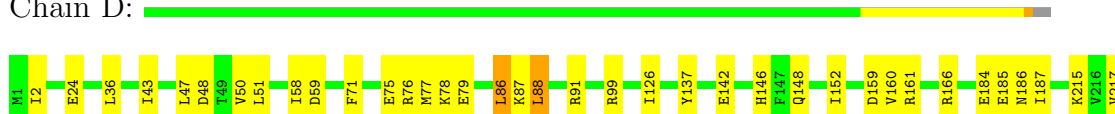
- Molecule 1: 2-phospho-L-lactate transferase

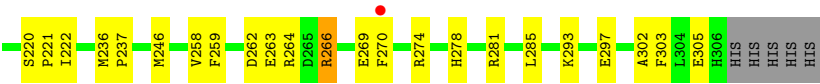
Chain C:



- Molecule 1: 2-phospho-L-lactate transferase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.28Å 185.28Å 67.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.50 29.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.59-2.50) 98.7 (29.59-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.195 , 0.231 0.203 , 0.238	Depositor DCC
$R_{free}$ test set	8660 reflections (9.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 22.8	EDS
Estimated twinning fraction	0.480 for -h,-k,l 0.021 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 178570 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, FO1

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	0.39	0/2408	0.58	0/3247
1	B	0.36	0/2408	0.55	0/3247
1	C	0.36	0/2408	0.55	0/3247
1	D	0.39	0/2408	0.59	0/3247
All	All	0.37	0/9632	0.57	0/12988

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	2371	0	2376	44	0
1	B	2371	0	2376	54	0
1	C	2371	0	2376	46	0
1	D	2371	0	2376	47	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	8	0	0
3	B	20	0	8	0	0
3	C	20	0	8	0	0
3	D	20	0	8	0	0
4	A	162	0	0	5	0
4	B	85	0	0	3	0
4	C	90	0	0	3	0
4	D	156	0	0	6	0
All	All	10077	0	9536	185	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 10.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ILE:HG13	1:A:184:GLU:HG3	1.38	1.05
1:C:221:PRO:HG2	1:C:222:ILE:HD12	1.45	0.94
1:D:2:ILE:HG13	1:D:184:GLU:HG3	1.53	0.91
1:B:227:PRO:HG3	1:B:232:ALA:HB3	1.52	0.91
1:B:221:PRO:HG2	1:B:222:ILE:HD12	1.50	0.91
1:C:227:PRO:HG3	1:C:232:ALA:HB3	1.55	0.89
1:A:159:ASP:HB3	1:A:161:ARG:NH1	1.96	0.80
1:B:266:ARG:HD3	1:B:281:ARG:NH2	1.97	0.79
1:C:266:ARG:HD3	1:C:281:ARG:NH2	1.98	0.78
1:A:221:PRO:HG2	1:A:222:ILE:HD12	1.64	0.77
1:D:266:ARG:HB2	1:D:266:ARG:HH11	1.51	0.76
1:D:221:PRO:HG2	1:D:222:ILE:HD12	1.67	0.75
1:D:146:HIS:HB2	4:D:527:HOH:O	1.87	0.74
1:A:146:HIS:HB2	4:A:511:HOH:O	1.86	0.74
1:A:266:ARG:HB2	1:A:266:ARG:HH11	1.52	0.74
1:B:278:HIS:HB3	4:B:486:HOH:O	1.87	0.73
1:B:266:ARG:HH11	1:B:281:ARG:HH22	1.39	0.69
1:C:48:ASP:OD2	1:C:99:ARG:NH2	2.26	0.68
1:D:146:HIS:CD2	1:D:148:GLN:H	2.12	0.68
1:D:48:ASP:OD2	1:D:99:ARG:NH2	2.26	0.67
1:B:48:ASP:OD2	1:B:99:ARG:NH2	2.29	0.66
1:A:146:HIS:CD2	1:A:148:GLN:H	2.14	0.66
1:B:86:LEU:N	1:B:86:LEU:HD23	2.12	0.65
1:A:48:ASP:OD2	1:A:99:ARG:NH2	2.29	0.64
1:D:278:HIS:HB3	4:D:556:HOH:O	1.97	0.64
1:C:221:PRO:HG2	1:C:222:ILE:CD1	2.25	0.64
1:D:159:ASP:HB3	1:D:161:ARG:NH1	2.13	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:146:HIS:CD2	1:B:148:GLN:H	2.17	0.63
1:A:262:ASP:OD1	1:A:264:ARG:HD3	2.01	0.61
1:D:266:ARG:NH1	1:D:281:ARG:HH22	1.99	0.61
1:A:184:GLU:HG2	4:A:461:HOH:O	2.00	0.60
1:A:217:VAL:HG22	1:A:258:VAL:HB	1.82	0.60
1:B:186:ASN:C	1:B:187:ILE:HD12	2.21	0.60
1:D:220:SER:HB2	1:D:259:PHE:CZ	2.36	0.60
1:C:86:LEU:HG	1:C:88:LEU:HD13	1.83	0.60
1:D:266:ARG:HH11	1:D:281:ARG:HH22	1.49	0.60
1:D:146:HIS:HD2	1:D:148:GLN:H	1.50	0.60
1:C:86:LEU:HD23	1:C:86:LEU:N	2.16	0.59
1:D:217:VAL:HG22	1:D:258:VAL:HB	1.84	0.59
1:C:24:GLU:H	1:C:24:GLU:CD	2.05	0.59
1:C:149:ASP:O	1:C:154:LYS:HG2	2.02	0.59
1:B:262:ASP:OD1	1:B:264:ARG:HD3	2.04	0.58
1:B:42:LEU:O	1:B:99:ARG:NH1	2.36	0.58
1:A:242:GLU:HG2	4:A:528:HOH:O	2.02	0.58
1:C:266:ARG:HD3	1:C:281:ARG:HH22	1.68	0.57
1:C:186:ASN:C	1:C:187:ILE:HD12	2.24	0.57
1:B:221:PRO:HG2	1:B:222:ILE:CD1	2.30	0.57
1:D:186:ASN:C	1:D:187:ILE:HD12	2.26	0.57
1:C:278:HIS:HB3	4:C:486:HOH:O	2.05	0.56
1:A:86:LEU:HG	1:A:88:LEU:HD13	1.89	0.55
1:B:71:PHE:CE2	1:B:87:LYS:HG2	2.41	0.55
1:A:266:ARG:HH11	1:A:281:ARG:HH22	1.54	0.55
1:A:146:HIS:HD2	1:A:148:GLN:H	1.52	0.55
1:B:86:LEU:HG	1:B:88:LEU:HD13	1.89	0.55
1:B:266:ARG:HD3	1:B:281:ARG:HH22	1.71	0.54
1:D:274:ARG:HG3	1:D:274:ARG:HH11	1.72	0.54
1:C:146:HIS:CD2	1:C:148:GLN:H	2.24	0.54
1:A:186:ASN:C	1:A:187:ILE:HD12	2.28	0.54
1:C:165:ILE:HD13	1:C:200:PRO:HG3	1.90	0.54
1:A:266:ARG:NH1	1:A:281:ARG:HH22	2.05	0.53
1:C:261:PHE:HE1	1:C:279:ALA:HB1	1.74	0.53
1:D:86:LEU:HG	1:D:88:LEU:HD13	1.91	0.53
1:C:169:SER:HB2	1:C:170:GLU:OE2	2.09	0.53
1:B:164:ASP:OD1	1:B:166:ARG:HD3	2.10	0.52
1:B:220:SER:HB2	1:B:259:PHE:CZ	2.44	0.52
1:A:221:PRO:HG2	1:A:222:ILE:CD1	2.37	0.52
1:B:266:ARG:NH1	1:B:281:ARG:HH22	2.06	0.52
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.75	0.52
1:B:217:VAL:HG22	1:B:258:VAL:HB	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:146:HIS:HE1	4:D:485:HOH:O	1.93	0.51
1:D:51:LEU:HD23	1:D:126:ILE:HD12	1.93	0.51
1:D:24:GLU:H	1:D:24:GLU:CD	2.14	0.51
1:A:148:GLN:HG3	1:A:152:ILE:HD12	1.91	0.51
1:B:146:HIS:HD2	1:B:148:GLN:H	1.56	0.50
1:B:290:GLU:O	1:B:294:GLU:HG3	2.11	0.50
1:A:186:ASN:HB3	1:A:303:PHE:CE1	2.46	0.50
1:A:220:SER:HB2	1:A:259:PHE:CZ	2.46	0.50
1:A:76:ARG:HD3	1:B:91:ARG:CZ	2.41	0.50
1:B:44:SER:HB3	1:B:47:LEU:HB2	1.93	0.50
1:C:220:SER:HB2	1:C:259:PHE:CZ	2.47	0.50
1:D:50:VAL:HG12	1:D:126:ILE:HD13	1.95	0.49
1:C:187:ILE:HD11	1:C:214:LYS:HD2	1.94	0.49
1:D:184:GLU:HG2	4:D:464:HOH:O	2.12	0.49
1:D:78:LYS:HB3	1:D:78:LYS:NZ	2.27	0.49
1:B:59:ASP:OD2	1:B:62:ARG:HD3	2.13	0.48
1:B:146:HIS:HE1	4:B:469:HOH:O	1.96	0.48
1:C:213:LYS:O	1:C:214:LYS:HG2	2.13	0.48
1:B:24:GLU:H	1:B:24:GLU:CD	2.16	0.48
1:C:266:ARG:HH11	1:C:281:ARG:HH22	1.61	0.48
1:A:2:ILE:CG1	1:A:184:GLU:HG3	2.27	0.48
1:B:256:LEU:HD21	1:B:259:PHE:CD1	2.49	0.47
1:A:146:HIS:HE1	4:A:486:HOH:O	1.98	0.47
1:D:75:GLU:O	1:D:79:GLU:HG3	2.15	0.47
1:D:142:GLU:HG3	4:D:472:HOH:O	2.15	0.47
1:C:58:ILE:HG13	1:C:59:ASP:N	2.29	0.47
1:B:271:ALA:O	1:B:274:ARG:HB2	2.14	0.47
1:A:293:LYS:O	1:A:297:GLU:HG3	2.15	0.47
1:C:146:HIS:HE1	4:C:464:HOH:O	1.97	0.46
1:D:186:ASN:HB3	1:D:303:PHE:CE1	2.51	0.46
1:B:75:GLU:O	1:B:79:GLU:HG3	2.16	0.46
1:C:217:VAL:HG22	1:C:258:VAL:HB	1.98	0.46
1:B:157:GLU:N	1:B:158:PRO:CD	2.79	0.46
1:C:262:ASP:OD1	1:C:264:ARG:HD3	2.16	0.46
1:D:293:LYS:O	1:D:297:GLU:HG3	2.16	0.46
1:A:48:ASP:CG	1:A:99:ARG:HH22	2.19	0.46
1:B:213:LYS:O	1:B:214:LYS:HG2	2.15	0.46
1:B:102:ILE:HG22	1:B:107:ALA:HB3	1.98	0.46
1:B:165:ILE:HD13	1:B:200:PRO:HG3	1.98	0.46
1:B:187:ILE:HD11	1:B:214:LYS:HD2	1.98	0.46
1:B:169:SER:HB2	1:B:170:GLU:OE2	2.16	0.46
1:D:221:PRO:HG2	1:D:222:ILE:CD1	2.42	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:187:ILE:HD12	1:D:187:ILE:N	2.31	0.45
1:A:86:LEU:N	1:A:86:LEU:HD23	2.31	0.45
1:D:258:VAL:HG11	1:D:302:ALA:HB1	1.99	0.45
1:B:185:GLU:HA	1:B:214:LYS:HD3	1.98	0.45
1:D:236:MSE:N	1:D:237:PRO:HD2	2.31	0.45
1:C:185:GLU:HA	1:C:214:LYS:HD3	1.99	0.45
1:A:215:LYS:NZ	1:A:306:HIS:HA	2.32	0.45
1:A:137:TYR:CD2	1:A:166:ARG:HD2	2.51	0.45
1:A:185:GLU:N	1:A:185:GLU:CD	2.70	0.45
1:C:44:SER:HB3	1:C:47:LEU:HB2	1.97	0.45
1:C:266:ARG:HD3	1:C:281:ARG:CZ	2.46	0.45
1:C:76:ARG:HD3	1:D:91:ARG:CZ	2.46	0.45
1:C:157:GLU:N	1:C:158:PRO:CD	2.80	0.45
1:A:43:ILE:HD11	1:A:88:LEU:HD21	1.99	0.44
1:C:146:HIS:CE1	4:C:464:HOH:O	2.70	0.44
1:D:148:GLN:HG3	1:D:152:ILE:HD12	1.99	0.44
1:C:42:LEU:O	1:C:99:ARG:NH1	2.48	0.44
1:C:86:LEU:HG	1:C:88:LEU:CD1	2.48	0.44
1:D:36:LEU:HD11	1:D:146:HIS:CD2	2.53	0.44
1:B:43:ILE:HG12	1:B:96:HIS:CE1	2.53	0.44
1:B:149:ASP:O	1:B:154:LYS:HG2	2.18	0.44
1:B:58:ILE:HG13	1:B:59:ASP:N	2.32	0.44
1:C:62:ARG:HB3	1:C:64:TRP:NE1	2.32	0.44
1:C:236:MSE:N	1:C:237:PRO:HD2	2.33	0.44
1:D:262:ASP:OD1	1:D:264:ARG:HD3	2.17	0.44
1:C:91:ARG:CZ	1:D:76:ARG:HD3	2.48	0.44
1:A:58:ILE:HG13	1:A:59:ASP:N	2.32	0.44
1:A:263:GLU:H	1:A:263:GLU:HG3	1.65	0.43
1:B:10:THR:OG1	1:B:190:GLY:HA3	2.18	0.43
1:B:46:ASP:HA	4:B:455:HOH:O	2.18	0.43
1:B:266:ARG:HD3	1:B:281:ARG:CZ	2.48	0.43
1:A:236:MSE:N	1:A:237:PRO:HD2	2.33	0.43
1:D:71:PHE:CE2	1:D:87:LYS:HG2	2.54	0.43
1:D:160:VAL:O	1:D:161:ARG:HD2	2.19	0.43
1:A:91:ARG:CZ	1:B:76:ARG:HD3	2.49	0.43
1:B:187:ILE:HD12	1:B:187:ILE:N	2.33	0.43
1:C:86:LEU:CD2	1:C:86:LEU:N	2.81	0.42
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.84	0.42
1:C:61:LYS:HB2	1:C:61:LYS:HE3	1.87	0.42
1:C:48:ASP:CG	1:C:99:ARG:HH22	2.23	0.42
1:D:58:ILE:HG13	1:D:59:ASP:N	2.33	0.42
1:A:50:VAL:HG12	1:A:126:ILE:HD13	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:ASP:HA	1:A:282:ALA:O	2.19	0.42
1:B:10:THR:N	1:B:11:PRO:HD2	2.35	0.42
1:D:263:GLU:H	1:D:263:GLU:HG3	1.70	0.42
1:C:91:ARG:NH1	1:D:76:ARG:HD3	2.35	0.42
1:D:186:ASN:HD22	1:D:215:LYS:HB3	1.85	0.42
1:C:33:ALA:HB1	1:C:136:THR:OG1	2.19	0.42
1:A:258:VAL:HG11	1:A:302:ALA:HB1	2.02	0.42
1:B:126:ILE:O	1:B:127:LEU:HD23	2.20	0.42
1:A:215:LYS:CE	1:A:306:HIS:HA	2.49	0.42
1:D:43:ILE:HD11	1:D:88:LEU:HD21	2.02	0.41
1:A:154:LYS:HB3	1:A:158:PRO:HD3	2.02	0.41
1:D:266:ARG:HA	1:D:281:ARG:NH2	2.36	0.41
1:B:264:ARG:H	1:B:264:ARG:HD3	1.85	0.41
1:B:261:PHE:N	1:B:261:PHE:CD1	2.89	0.41
1:C:285:LEU:HD22	1:C:287:THR:HG23	2.03	0.41
1:D:246:MSE:HB2	4:D:523:HOH:O	2.20	0.41
1:B:285:LEU:HD22	1:B:287:THR:HG23	2.01	0.41
1:A:266:ARG:HD3	1:A:281:ARG:NH2	2.35	0.41
1:C:71:PHE:CE2	1:C:87:LYS:HG2	2.55	0.41
1:B:7:GLY:HA3	2:B:402:PO4:O3	2.21	0.41
1:C:94:ALA:HB1	1:D:77:MSE:HG3	2.03	0.41
1:A:142:GLU:HG3	4:A:445:HOH:O	2.21	0.41
1:B:33:ALA:HB1	1:B:136:THR:OG1	2.21	0.41
1:A:62:ARG:HB3	1:A:64:TRP:NE1	2.35	0.41
1:D:266:ARG:HD3	1:D:281:ARG:NH2	2.36	0.40
1:D:137:TYR:CD2	1:D:166:ARG:HD2	2.57	0.40
1:B:174:SER:HB3	1:B:177:VAL:HG23	2.02	0.40
1:A:51:LEU:HD23	1:A:126:ILE:HD12	2.04	0.40
1:C:141:ALA:HB2	1:C:161:ARG:HE	1.87	0.40
1:C:150:PHE:CE2	1:C:156:GLY:HA2	2.56	0.40
1:C:10:THR:N	1:C:11:PRO:HD2	2.36	0.40
1:B:236:MSE:N	1:B:237:PRO:HD2	2.36	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	304/311 (98%)	296 (97%)	8 (3%)	0	100	100
1	B	304/311 (98%)	293 (96%)	11 (4%)	0	100	100
1	C	304/311 (98%)	291 (96%)	12 (4%)	1 (0%)	50	73
1	D	304/311 (98%)	292 (96%)	11 (4%)	1 (0%)	50	73
All	All	1216/1244 (98%)	1172 (96%)	42 (4%)	2 (0%)	56	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	ASP
1	D	305	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	262/259 (101%)	252 (96%)	10 (4%)	44	71
1	B	262/259 (101%)	254 (97%)	8 (3%)	52	79
1	C	262/259 (101%)	253 (97%)	9 (3%)	49	75
1	D	262/259 (101%)	254 (97%)	8 (3%)	52	79
All	All	1048/1036 (101%)	1013 (97%)	35 (3%)	50	76

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	80	LEU
1	A	86	LEU
1	A	88	LEU
1	A	185	GLU
1	A	266	ARG
1	A	269	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	270	PHE
1	A	278	HIS
1	A	285	LEU
1	B	83	GLU
1	B	86	LEU
1	B	166	ARG
1	B	185	GLU
1	B	254	ASP
1	B	269	GLU
1	B	270	PHE
1	B	285	LEU
1	C	53	LEU
1	C	86	LEU
1	C	88	LEU
1	C	161	ARG
1	C	169	SER
1	C	208	ARG
1	C	254	ASP
1	C	269	GLU
1	C	270	PHE
1	D	47	LEU
1	D	86	LEU
1	D	88	LEU
1	D	185	GLU
1	D	266	ARG
1	D	269	GLU
1	D	270	PHE
1	D	285	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	125	ASN
1	A	146	HIS
1	A	186	ASN
1	A	253	GLN
1	B	57	GLN
1	B	125	ASN
1	B	146	HIS
1	B	186	ASN
1	B	253	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	301	GLN
1	C	57	GLN
1	C	125	ASN
1	C	146	HIS
1	C	186	ASN
1	C	253	GLN
1	C	301	GLN
1	D	57	GLN
1	D	125	ASN
1	D	146	HIS
1	D	186	ASN
1	D	253	GLN
1	D	301	GLN

### 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 ⓘ

8 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	FO1	A	401	-	22,22,28	5.86	15 (68%)	26,32,41	3.15	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	A	402	-	4,4,4	0.93	0	6,6,6	0.31	0
3	FO1	B	401	-	22,22,28	5.76	17 (77%)	26,32,41	3.14	8 (30%)
2	PO4	B	402	-	4,4,4	0.88	0	6,6,6	0.31	0
3	FO1	C	401	-	22,22,28	5.72	17 (77%)	26,32,41	3.14	8 (30%)
2	PO4	C	402	-	4,4,4	0.85	0	6,6,6	0.31	0
3	FO1	D	401	-	22,22,28	5.84	15 (68%)	26,32,41	3.13	9 (34%)
2	PO4	D	402	-	4,4,4	0.93	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	FO1	A	401	-	-	0/2/3/14	0/0/3/3
2	PO4	A	402	-	-	0/0/0/0	0/0/0/0
3	FO1	B	401	-	-	0/2/3/14	0/0/3/3
2	PO4	B	402	-	-	0/0/0/0	0/0/0/0
3	FO1	C	401	-	-	0/2/3/14	0/0/3/3
2	PO4	C	402	-	-	0/0/0/0	0/0/0/0
3	FO1	D	401	-	-	0/2/3/14	0/0/3/3
2	PO4	D	402	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	FO1	O3-C15	19.93	1.47	1.25
3	A	401	FO1	O3-C15	19.91	1.47	1.25
3	B	401	FO1	O3-C15	19.06	1.46	1.25
3	C	401	FO1	O3-C15	18.64	1.46	1.25
3	C	401	FO1	C5-C12	9.30	1.58	1.42
3	B	401	FO1	C5-C12	9.18	1.58	1.42
3	A	401	FO1	C5-C12	9.12	1.58	1.42
3	D	401	FO1	C5-C12	9.07	1.58	1.42
3	A	401	FO1	C12-N3	7.85	1.50	1.38
3	C	401	FO1	C12-N3	7.80	1.50	1.38
3	D	401	FO1	C12-N3	7.54	1.50	1.38
3	B	401	FO1	C12-N3	7.52	1.50	1.38
3	D	401	FO1	C3-C13	7.10	1.52	1.41
3	B	401	FO1	C3-C13	7.04	1.52	1.41
3	A	401	FO1	C3-C13	7.01	1.52	1.41
3	C	401	FO1	C3-C13	6.83	1.52	1.41

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	FO1	C7-C9	5.89	1.51	1.38
3	D	401	FO1	C7-C9	5.87	1.51	1.38
3	A	401	FO1	C7-C9	5.77	1.51	1.38
3	B	401	FO1	C7-C9	5.74	1.51	1.38
3	C	401	FO1	C6-C7	4.89	1.47	1.36
3	B	401	FO1	C6-C7	4.75	1.46	1.36
3	D	401	FO1	C6-C7	4.70	1.46	1.36
3	A	401	FO1	C6-C7	4.65	1.46	1.36
3	C	401	FO1	C4-C3	4.28	1.46	1.39
3	D	401	FO1	C4-C3	4.19	1.46	1.39
3	D	401	FO1	C1-N2	4.18	1.45	1.37
3	A	401	FO1	C4-C3	4.13	1.46	1.39
3	B	401	FO1	C4-C3	4.09	1.45	1.39
3	B	401	FO1	C1-N2	3.90	1.44	1.37
3	C	401	FO1	C11-C12	3.87	1.48	1.40
3	B	401	FO1	C11-C12	3.85	1.48	1.40
3	C	401	FO1	C1-N2	3.83	1.44	1.37
3	A	401	FO1	C1-N2	3.83	1.44	1.37
3	B	401	FO1	C2-C3	3.70	1.53	1.39
3	C	401	FO1	C2-C3	3.69	1.53	1.39
3	A	401	FO1	C11-C12	3.55	1.47	1.40
3	C	401	FO1	C13-N3	3.44	1.46	1.38
3	B	401	FO1	C13-N3	3.43	1.46	1.38
3	A	401	FO1	C2-C3	3.42	1.52	1.39
3	D	401	FO1	C2-C3	3.35	1.52	1.39
3	D	401	FO1	C11-C12	3.19	1.47	1.40
3	D	401	FO1	C13-N1	3.16	1.41	1.35
3	A	401	FO1	C13-N3	3.12	1.45	1.38
3	B	401	FO1	C13-N1	3.09	1.41	1.35
3	D	401	FO1	C2-N2	3.06	1.42	1.37
3	B	401	FO1	C2-N2	3.04	1.42	1.37
3	B	401	FO1	C15-C14	3.00	1.56	1.46
3	A	401	FO1	C15-C14	2.99	1.56	1.46
3	D	401	FO1	C13-N3	2.96	1.45	1.38
3	C	401	FO1	C13-N1	2.91	1.40	1.35
3	C	401	FO1	C2-N2	2.90	1.42	1.37
3	C	401	FO1	C15-C14	2.89	1.56	1.46
3	A	401	FO1	C13-N1	2.88	1.40	1.35
3	A	401	FO1	C2-N2	2.85	1.42	1.37
3	D	401	FO1	C15-C14	2.83	1.55	1.46
3	A	401	FO1	C4-C5	2.80	1.44	1.39
3	C	401	FO1	C4-C5	2.76	1.44	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	FO1	C4-C5	2.74	1.44	1.39
3	B	401	FO1	C14-N3	2.31	1.53	1.49
3	D	401	FO1	C4-C5	2.19	1.43	1.39
3	B	401	FO1	C11-C9	2.13	1.41	1.37
3	C	401	FO1	C14-N3	2.12	1.53	1.49
3	C	401	FO1	C11-C9	2.12	1.41	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	FO1	C1-N1-C13	10.89	125.95	114.98
3	C	401	FO1	C1-N1-C13	10.79	125.86	114.98
3	A	401	FO1	C1-N1-C13	10.77	125.84	114.98
3	D	401	FO1	C1-N1-C13	10.38	125.44	114.98
3	D	401	FO1	C3-C2-N2	8.42	122.49	115.40
3	A	401	FO1	C3-C2-N2	8.33	122.42	115.40
3	C	401	FO1	C3-C2-N2	8.21	122.32	115.40
3	B	401	FO1	C3-C2-N2	8.15	122.27	115.40
3	D	401	FO1	C4-C3-C13	3.87	120.71	117.03
3	B	401	FO1	C3-C13-N1	-3.62	118.94	123.55
3	A	401	FO1	C4-C3-C13	3.60	120.46	117.03
3	C	401	FO1	C3-C13-N1	-3.41	119.20	123.55
3	C	401	FO1	C4-C3-C13	3.32	120.19	117.03
3	A	401	FO1	C3-C13-N1	-3.30	119.34	123.55
3	B	401	FO1	C4-C3-C13	3.29	120.16	117.03
3	D	401	FO1	C3-C13-N1	-3.18	119.50	123.55
3	D	401	FO1	O10-C9-C11	-3.01	112.19	121.07
3	A	401	FO1	O10-C9-C11	-2.91	112.48	121.07
3	C	401	FO1	O10-C9-C11	-2.82	112.74	121.07
3	B	401	FO1	C2-N2-C1	-2.82	119.61	125.39
3	C	401	FO1	C2-N2-C1	-2.80	119.64	125.39
3	D	401	FO1	C2-N2-C1	-2.75	119.74	125.39
3	B	401	FO1	O10-C9-C11	-2.73	113.01	121.07
3	A	401	FO1	C2-N2-C1	-2.69	119.87	125.39
3	C	401	FO1	C4-C3-C2	2.39	126.38	121.89
3	A	401	FO1	C4-C3-C2	2.36	126.31	121.89
3	D	401	FO1	C3-C13-N3	-2.32	118.72	121.93
3	B	401	FO1	C4-C3-C2	2.31	126.22	121.89
3	D	401	FO1	N1-C13-N3	2.21	121.78	115.97
3	B	401	FO1	N1-C13-N3	2.19	121.73	115.97
3	A	401	FO1	N1-C13-N3	2.11	121.53	115.97
3	C	401	FO1	N1-C13-N3	2.11	121.52	115.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	FO1	C4-C3-C2	2.11	125.84	121.89
3	A	401	FO1	C3-C13-N3	-2.02	119.13	121.93

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	306/311 (98%)	0.09	2 (0%) 84 86	18, 31, 53, 89	0
1	B	306/311 (98%)	0.28	9 (2%) 49 51	22, 41, 76, 98	0
1	C	306/311 (98%)	0.28	5 (1%) 68 71	21, 41, 77, 99	0
1	D	306/311 (98%)	0.07	1 (0%) 91 93	18, 31, 53, 87	0
All	All	1224/1244 (98%)	0.18	17 (1%) 72 74	18, 35, 72, 99	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	GLU	4.6
1	B	141	ALA	3.8
1	C	270	PHE	3.8
1	C	141	ALA	3.1
1	B	274	ARG	3.0
1	B	269	GLU	3.0
1	B	223	ILE	2.9
1	B	270	PHE	2.8
1	D	270	PHE	2.4
1	B	265	ASP	2.3
1	B	276	GLY	2.2
1	C	223	ILE	2.2
1	A	269	GLU	2.1
1	B	273	GLU	2.1
1	C	265	ASP	2.1
1	A	270	PHE	2.0
1	B	272	PHE	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
2	PO4	D	402	5/5	0.19	1.89	70,70,71,72	0
2	PO4	A	402	5/5	0.18	1.88	64,64,64,66	0
2	PO4	B	402	5/5	0.19	1.58	72,73,74,75	0
2	PO4	C	402	5/5	0.18	1.45	70,71,72,73	0
3	FO1	B	401	20/26	0.19	0.74	25,33,39,40	20
3	FO1	C	401	20/26	0.18	0.63	28,34,39,42	20
3	FO1	A	401	20/26	0.17	0.16	16,20,30,32	20
3	FO1	D	401	20/26	0.16	-0.00	17,21,31,33	20

### 6.5 Other polymers ⓘ

There are no such residues in this entry.