



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 07:41 am GMT

PDB ID : 3DFT  
Title : Phosphate ions in D33S mutant fructose-1,6-bisphosphate aldolase from rabbit muscle  
Authors : St-Jean, M.; Sygusch, J.  
Deposited on : 2008-06-12  
Resolution : 1.94 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

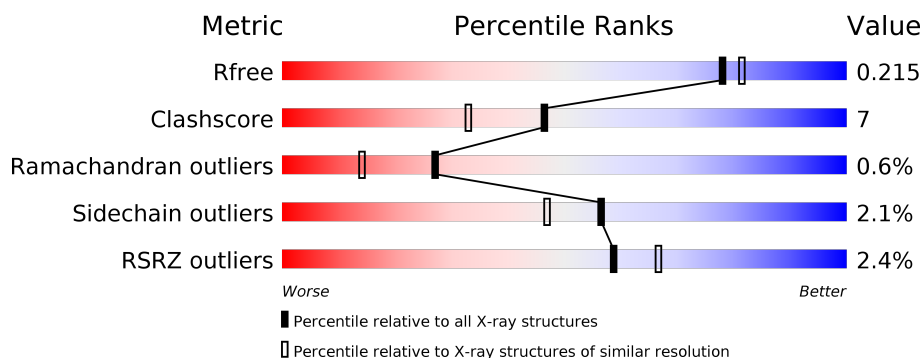
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	111664	3622 (1.96-1.92)
Clashscore	122126	3795 (1.96-1.92)
Ramachandran outliers	120053	3757 (1.96-1.92)
Sidechain outliers	120020	3757 (1.96-1.92)
RSRZ outliers	108989	3554 (1.96-1.92)

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. 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	363	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 82%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 87%; width: 13%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 100%; width: 2%; height: 10px; background-color: grey;"></div> </div> <div> <span style="float: left;">%</span> <span style="float: right;">82%13% . .</span> </div> </div>
1	B	363	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 2%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 2%; width: 79%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 81%; width: 15%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 100%; width: 4%; height: 10px; background-color: grey;"></div> </div> <div> <span style="float: left;">2%</span> <span style="float: right;">81%15% .</span> </div> </div>
1	C	363	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 79%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 84%; width: 13%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 100%; width: 3%; height: 10px; background-color: grey;"></div> </div> <div> <span style="float: left;">%</span> <span style="float: right;">84%13% .</span> </div> </div>
1	D	363	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 77%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 82%; width: 17%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 100%; width: 1%; height: 10px; background-color: grey;"></div> </div> <div> <span style="float: left;">5%</span> <span style="float: right;">82%17% .</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12993 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 Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2671	1679	475	506	11			
1	B	350	Total	C	N	O	S	0	0	0
			2671	1679	475	506	11			
1	C	352	Total	C	N	O	S	0	0	0
			2684	1686	478	509	11			
1	D	360	Total	C	N	O	S	0	0	0
			2728	1714	484	519	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	ASP	ENGINEERED	UNP P00883
B	33	SER	ASP	ENGINEERED	UNP P00883
C	33	SER	ASP	ENGINEERED	UNP P00883
D	33	SER	ASP	ENGINEERED	UNP P00883

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



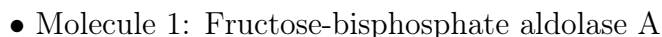
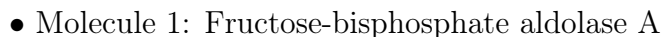
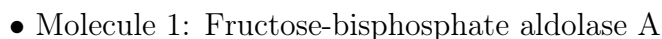
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	1
			5	4	1		

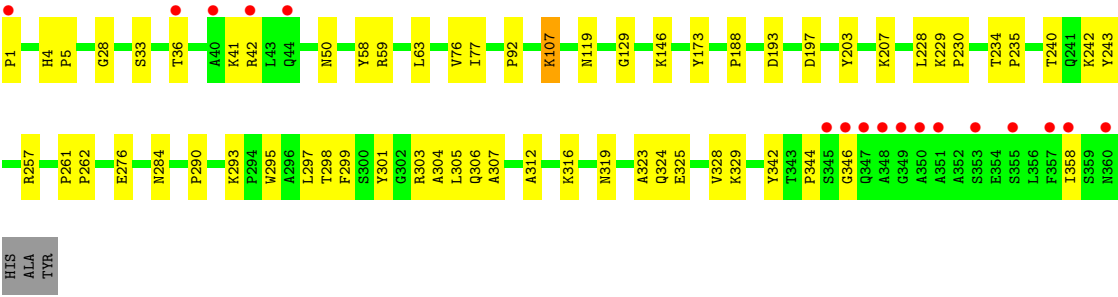
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	562	Total	O	0	1
			562	562		
3	B	551	Total	O	0	0
			551	551		
3	C	545	Total	O	0	0
			545	545		
3	D	561	Total	O	0	1
			561	561		



- Molecule 1: Fructose-bisphosphate aldolase A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.93Å 103.61Å 84.95Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	50.00 – 1.94 43.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.2 (50.00-1.94) 83.6 (43.94-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.149 , 0.205 0.161 , 0.215	Depositor DCC
$R_{free}$ test set	11985 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/2723	0.56	0/3688
1	B	0.28	0/2723	0.56	0/3688
1	C	0.28	0/2736	0.56	0/3705
1	D	0.27	0/2780	0.55	0/3767
All	All	0.28	0/10962	0.56	0/14848

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 [i](#)

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	2671	0	2695	40	0
1	B	2671	0	2695	37	0
1	C	2684	0	2706	36	0
1	D	2728	0	2756	47	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	562	0	0	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	551	0	0	4	0
3	C	545	0	0	4	0
3	D	561	0	0	7	0
All	All	12993	0	10852	146	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 (146) 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:C:146:LYS:HZ3	1:C:229:LYS:HZ3	1.24	0.84
1:A:146:LYS:HZ3	1:A:229:LYS:HZ3	1.27	0.81
1:A:39:ILE:HD12	1:A:42:ARG:HD2	1.63	0.79
1:B:41:LYS:HA	1:B:44:GLN:HE21	1.46	0.79
1:B:8:THR:H	1:B:11:GLN:HE21	1.33	0.76
1:B:41:LYS:HA	1:B:44:GLN:HG2	1.69	0.73
1:C:146:LYS:NZ	1:C:229:LYS:HZ3	1.88	0.72
1:D:284:ASN:ND2	1:D:342:TYR:H	1.88	0.71
1:C:146:LYS:NZ	1:C:229:LYS:NZ	2.39	0.70
1:A:146:LYS:HZ3	1:A:229:LYS:NZ	1.89	0.70
1:D:146:LYS:HZ3	1:D:229:LYS:HZ3	1.39	0.70
1:D:107:LYS:HG3	3:D:3762:HOH:O	1.92	0.70
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.72	0.69
1:D:146:LYS:HZ3	1:D:229:LYS:NZ	1.90	0.69
1:C:146:LYS:HZ3	1:C:229:LYS:NZ	1.91	0.68
1:A:146:LYS:NZ	1:A:229:LYS:NZ	2.41	0.68
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.77	0.67
1:D:316:LYS:HB2	1:D:319:ASN:ND2	2.10	0.67
1:C:8:THR:H	1:C:11:GLN:HE21	1.42	0.67
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.78	0.66
1:D:301:TYR:HB3	1:D:304:ALA:HB3	1.77	0.65
1:A:146:LYS:NZ	1:A:229:LYS:HZ3	1.94	0.64
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.79	0.64
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.82	0.62
1:A:34:GLU:HG2	1:A:42:ARG:NH1	2.14	0.61
1:B:291:LEU:O	1:B:293:LYS:HD3	2.00	0.61
1:C:4:HIS:HB3	3:D:3704:HOH:O	2.00	0.61
1:B:316:LYS:HB2	1:B:319:ASN:ND2	2.15	0.61
1:B:152:LYS:HE2	3:B:3587:HOH:O	2.01	0.61
1:D:146:LYS:NZ	1:D:229:LYS:NZ	2.48	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.83	0.60
1:D:41:LYS:HE2	1:D:358:ILE:HD13	1.82	0.59
1:C:125:GLN:HE22	1:D:129:GLY:H	1.50	0.59
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.84	0.59
1:B:41:LYS:HG3	3:B:3666:HOH:O	2.03	0.58
1:A:39:ILE:HD12	1:A:42:ARG:CD	2.33	0.56
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.87	0.56
1:B:146:LYS:HZ3	1:B:229:LYS:NZ	2.03	0.56
1:B:146:LYS:HZ3	1:B:229:LYS:HZ3	1.54	0.56
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.21	0.56
1:B:146:LYS:NZ	1:B:229:LYS:NZ	2.54	0.55
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.06	0.55
1:D:325:GLU:O	1:D:329:LYS:HG3	2.07	0.54
1:C:199:LYS:HG3	3:C:3144:HOH:O	2.05	0.54
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.43	0.54
1:A:301:TYR:HB3	1:A:304:ALA:HB3	1.89	0.54
1:A:311:LYS:HE2	3:A:3534:HOH:O	2.07	0.53
1:B:316:LYS:HB2	1:B:319:ASN:HD22	1.71	0.53
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.44	0.53
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.91	0.53
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.90	0.53
1:B:41:LYS:HA	1:B:44:GLN:NE2	2.18	0.52
1:C:200:ARG:HG3	1:C:200:ARG:HH11	1.73	0.52
1:C:318:GLU:H	1:C:318:GLU:CD	2.13	0.52
1:D:92:PRO:HB3	3:D:3557:HOH:O	2.10	0.51
3:C:3348:HOH:O	1:D:1:PRO:HG3	2.11	0.51
1:C:291:LEU:O	1:C:293:LYS:HE2	2.10	0.50
1:C:324:GLN:O	1:C:328:VAL:HG23	2.10	0.50
1:A:324:GLN:O	1:A:328:VAL:HG23	2.12	0.50
1:C:234:THR:HB	1:C:235:PRO:HD2	1.93	0.50
1:B:203:TYR:CD1	1:C:3:SER:HB2	2.47	0.49
1:C:339:GLN:HG2	3:C:3370:HOH:O	2.12	0.49
1:A:312:ALA:HB3	1:A:323:ALA:HA	1.95	0.49
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.48	0.48
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.95	0.48
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.42	0.48
1:D:324:GLN:O	1:D:328:VAL:HG23	2.13	0.48
1:D:346:GLY:HA3	3:D:3473:HOH:O	2.13	0.48
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.13	0.48
1:C:61:LEU:HD12	1:C:320:LEU:HD12	1.96	0.48
1:A:291:LEU:O	1:A:293:LYS:HD3	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:HB3	1:B:318:GLU:OE2	2.13	0.48
1:A:39:ILE:O	1:A:42:ARG:HG3	2.13	0.48
1:B:234:THR:HB	1:B:235:PRO:HD2	1.95	0.47
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.96	0.47
1:D:42:ARG:HD2	1:D:303:ARG:HD3	1.96	0.47
1:A:262:PRO:HD2	1:D:257:ARG:O	2.15	0.47
1:D:298:THR:OG1	1:D:299:PHE:N	2.48	0.47
1:C:58:TYR:OH	1:C:306:GLN:HB3	2.15	0.47
1:D:234:THR:HB	1:D:235:PRO:HD2	1.95	0.47
1:D:284:ASN:HD21	1:D:342:TYR:H	1.59	0.47
1:B:301:TYR:HB3	1:B:304:ALA:HB3	1.96	0.46
1:B:51:THR:O	1:B:55:ARG:HG3	2.16	0.46
1:C:125:GLN:NE2	1:D:129:GLY:H	2.13	0.46
1:A:242:LYS:HE3	3:A:3468:HOH:O	2.16	0.46
1:C:293:LYS:HD2	1:C:297:LEU:HD12	1.98	0.46
1:A:61:LEU:HD11	1:A:323:ALA:HB3	1.98	0.46
1:B:324:GLN:O	1:B:328:VAL:HG23	2.16	0.46
1:D:207:LYS:HE2	3:D:3586:HOH:O	2.17	0.45
1:D:63:LEU:HD21	1:D:76:VAL:HG11	1.97	0.45
1:B:361:HIS:HB2	3:B:3884:HOH:O	2.16	0.45
1:B:203:TYR:CG	1:C:3:SER:HB2	2.51	0.45
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.98	0.45
1:D:240:THR:O	1:D:242:LYS:HD2	2.16	0.45
1:D:312:ALA:HB3	1:D:323:ALA:HA	1.99	0.45
1:D:36:THR:CG2	1:D:50:ASN:HD21	2.29	0.45
1:C:66:ASP:OD1	1:C:68:ARG:HB2	2.17	0.45
1:B:216:LEU:HD22	1:B:221:ILE:HG13	1.98	0.45
1:A:98:LYS:HE2	3:A:3397:HOH:O	2.17	0.44
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.48	0.44
1:D:146:LYS:NZ	1:D:229:LYS:HZ1	2.15	0.44
1:A:294:PRO:HG3	1:D:262:PRO:CG	2.47	0.44
1:B:318:GLU:CD	1:B:318:GLU:H	2.19	0.44
1:A:200:ARG:HD2	3:D:3479:HOH:O	2.17	0.44
1:A:29:ILE:HB	1:A:300:SER:HA	1.99	0.44
1:A:133:ARG:HD3	3:A:3225:HOH:O	2.17	0.44
1:B:146:LYS:NZ	1:B:229:LYS:HZ1	2.15	0.44
1:B:8:THR:H	1:B:11:GLN:NE2	2.08	0.44
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.92	0.43
1:D:33:SER:HB3	1:D:77:ILE:HG22	2.00	0.43
1:A:61:LEU:HD23	1:A:61:LEU:C	2.39	0.43
1:B:360:ASN:HB2	3:B:3707:HOH:O	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:O	1:A:324:GLN:HG3	2.19	0.43
1:C:330:ARG:HA	1:C:330:ARG:NE	2.34	0.43
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.18	0.43
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.00	0.43
1:A:146:LYS:NZ	1:A:229:LYS:HZ1	2.14	0.43
1:D:41:LYS:HE2	1:D:358:ILE:CD1	2.49	0.43
1:C:107:LYS:HE3	3:C:3528:HOH:O	2.18	0.42
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.55	0.42
1:B:58:TYR:OH	1:B:306:GLN:HB3	2.20	0.42
1:A:3:SER:HB2	1:D:203:TYR:CG	2.53	0.42
1:A:1:PRO:HB2	1:D:203:TYR:HE2	1.85	0.42
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.20	0.42
1:A:294:PRO:HG3	1:D:262:PRO:HG3	2.01	0.42
1:D:290:PRO:HB2	3:D:3735:HOH:O	2.19	0.42
1:C:222:TYR:CZ	1:C:224:GLU:HB2	2.55	0.42
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.40	0.41
1:B:98:LYS:NZ	1:B:141:GLY:HA2	2.36	0.41
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.54	0.41
1:A:3:SER:HB2	1:D:203:TYR:CD1	2.56	0.41
1:D:293:LYS:HD2	1:D:297:LEU:HD12	2.02	0.41
1:A:262:PRO:HG3	1:D:262:PRO:HG3	2.02	0.41
1:B:18:ILE:HD13	1:B:143:ASP:HB3	2.02	0.41
1:C:117:GLY:HA2	1:D:4:HIS:O	2.20	0.41
1:C:4:HIS:CD2	1:D:119:ASN:HB2	2.55	0.41
1:B:41:LYS:HA	1:B:44:GLN:CG	2.46	0.40
1:A:245:HIS:HD2	1:A:282:ASN:OD1	2.05	0.40
1:A:277:GLU:O	1:A:281:ILE:HG13	2.21	0.40
1:C:93:PHE:N	1:C:94:PRO:CD	2.84	0.40
1:D:325:GLU:HG3	1:D:329:LYS:HE3	2.04	0.40
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.89	0.40
1:A:276:GLU:CD	1:A:307:ALA:HB3	2.42	0.40
1:A:98:LYS:NZ	3:A:3286:HOH:O	2.54	0.40
1:B:268:THR:HB	1:B:300:SER:HB2	2.03	0.40
1:D:58:TYR:OH	1:D:306:GLN:HB3	2.22	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	346/363 (95%)	329 (95%)	15 (4%)	2 (1%)	27	14
1	B	346/363 (95%)	330 (95%)	14 (4%)	2 (1%)	27	14
1	C	348/363 (96%)	336 (97%)	10 (3%)	2 (1%)	27	14
1	D	358/363 (99%)	342 (96%)	13 (4%)	3 (1%)	21	9
All	All	1398/1452 (96%)	1337 (96%)	52 (4%)	9 (1%)	27	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	344	PRO
1	A	5	PRO
1	B	5	PRO
1	C	5	PRO
1	C	188	PRO
1	D	5	PRO
1	D	188	PRO
1	A	188	PRO
1	B	188	PRO

### 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	284/291 (98%)	276 (97%)	8 (3%)	47	34
1	B	284/291 (98%)	276 (97%)	8 (3%)	47	34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/291 (98%)	282 (99%)	3 (1%)	76	71
1	D	289/291 (99%)	284 (98%)	5 (2%)	63	56
All	All	1142/1164 (98%)	1118 (98%)	24 (2%)	56	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	42	ARG
1	A	53	GLU
1	A	59	ARG
1	A	173	TYR
1	A	230	PRO
1	A	295	TRP
1	A	318	GLU
1	B	42	ARG
1	B	59	ARG
1	B	107	LYS
1	B	119	ASN
1	B	173	TYR
1	B	193	ASP
1	B	271	SER
1	B	295	TRP
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
1	D	59	ARG
1	D	107	LYS
1	D	173	TYR
1	D	193	ASP
1	D	295	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	180	ASN
1	A	241	GLN
1	A	245	HIS
1	A	319	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	11	GLN
1	B	44	GLN
1	B	119	ASN
1	B	136	GLN
1	B	179	GLN
1	B	319	ASN
1	C	11	GLN
1	C	54	ASN
1	C	125	GLN
1	C	241	GLN
1	C	319	ASN
1	D	180	ASN
1	D	241	GLN
1	D	284	ASN
1	D	319	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

4 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	A	3001	-	4,4,4	1.38	0	6,6,6	0.37	0
2	PO4	B	3002	-	4,4,4	1.37	0	6,6,6	0.39	0
2	PO4	C	3003	-	4,4,4	1.37	0	6,6,6	0.38	0
2	PO4	D	3004[A]	-	4,4,4	1.39	0	6,6,6	0.39	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
2	PO4	A	3001	-	-	0/0/0/0	0/0/0/0
2	PO4	B	3002	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3003	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3004[A]	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

### 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	350/363 (96%)	-0.28	4 (1%) 80 85	6, 15, 41, 56	2 (0%)
1	B	350/363 (96%)	-0.21	8 (2%) 60 68	7, 15, 38, 64	2 (0%)
1	C	352/363 (96%)	-0.19	5 (1%) 75 81	5, 16, 41, 62	2 (0%)
1	D	360/363 (99%)	-0.07	17 (4%) 31 39	7, 18, 51, 79	0
All	All	1412/1452 (97%)	-0.19	34 (2%) 59 66	5, 16, 45, 79	6 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	10.0
1	D	345	SER	8.0
1	B	345	SER	5.6
1	C	359	SER	4.9
1	B	362	ALA	4.0
1	D	348	ALA	4.0
1	B	1	PRO	3.9
1	D	347	GLN	3.8
1	D	1	PRO	3.7
1	D	346	GLY	3.5
1	A	359	SER	3.5
1	A	1	PRO	3.5
1	D	360	ASN	3.4
1	D	358	ILE	3.4
1	D	40	ALA	3.3
1	D	353	SER	3.3
1	B	360	ASN	3.2
1	D	349	GLY	3.2
1	C	360	ASN	3.1
1	B	344	PRO	3.0
1	A	2	HIS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	362	ALA	2.9
1	C	347	GLN	2.9
1	D	355	SER	2.9
1	D	351	ALA	2.9
1	B	359	SER	2.7
1	D	350	ALA	2.6
1	D	357	PHE	2.4
1	C	344	PRO	2.3
1	D	44	GLN	2.1
1	D	42	ARG	2.1
1	B	45	SER	2.1
1	B	2	HIS	2.0
1	D	36	THR	2.0

## 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	C	3003	5/5	0.95	0.14	49,53,60,63	0
2	PO4	B	3002	5/5	0.97	0.10	32,34,38,39	0
2	PO4	D	3004[A]	5/5	0.97	0.09	17,18,24,28	5
2	PO4	A	3001	5/5	0.98	0.08	25,26,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.