



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:39 AM GMT

PDB ID : 3DFO  
Title : Dihydroxyacetone phosphate Schiff base and enamine intermediates in D33N 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 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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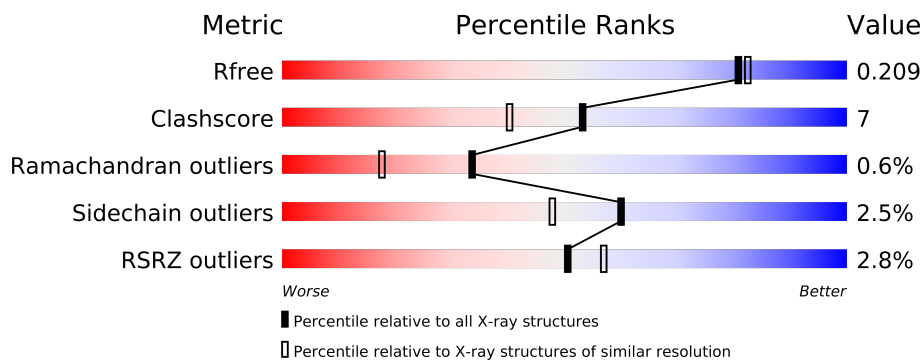
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (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. 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	363	
1	B	363	
1	C	363	
1	D	363	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12895 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.

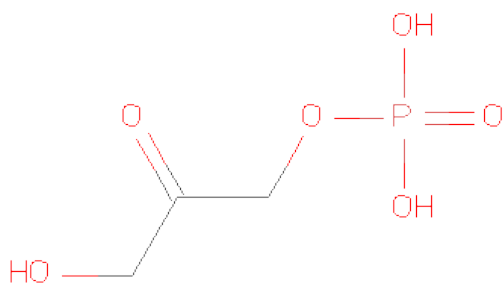
- Molecule 1 is a protein called Fructose-bisphosphatealdolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	1	0
			2682	1686	478	507	11			
1	B	350	Total	C	N	O	S	0	1	0
			2682	1686	478	507	11			
1	C	351	Total	C	N	O	S	0	0	0
			2677	1682	477	507	11			
1	D	360	Total	C	N	O	S	0	1	0
			2739	1721	487	520	11			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).

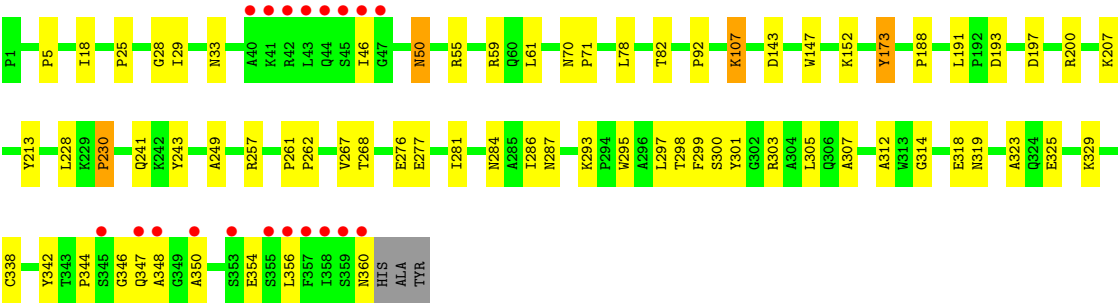


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	3	5	1		
2	B	1	Total	C	O	P	0	0
			9	3	5	1		
2	C	1	Total	C	O	P	0	0
			9	3	5	1		
2	D	1	Total	C	O	P	0	0
			9	3	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	541	Total	O	0	0
			541	541		
3	B	500	Total	O	0	0
			500	500		
3	C	532	Total	O	0	0
			532	532		
3	D	506	Total	O	0	0
			506	506		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.68Å 103.13Å 84.56Å 90.00° 98.71° 90.00°	Depositor
Resolution (Å)	43.76 – 1.94 43.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.5 (43.76-1.94) 83.4 (43.76-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.152 , 0.199 0.165 , 0.209	Depositor DCC
$R_{free}$ test set	9782 reflections (10.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.9	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 118053 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: 13P

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	0/2734	0.57	0/3702
1	B	0.29	0/2734	0.58	0/3702
1	C	0.29	0/2729	0.57	0/3696
1	D	0.28	0/2791	0.56	0/3781
All	All	0.29	0/10988	0.57	0/14881

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	213	TYR	Sidechain

### 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	2682	0	2705	42	0
1	B	2682	0	2706	42	0
1	C	2677	0	2696	30	0
1	D	2739	0	2767	45	0
2	A	9	0	5	1	0
2	B	9	0	5	0	0
2	C	9	0	5	1	0
2	D	9	0	5	0	0
3	A	541	0	0	5	0
3	B	500	0	0	5	0
3	C	532	0	0	2	0
3	D	506	0	0	8	0
All	All	12895	0	10894	151	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 7.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:GLN:NE2	1:B:88:ASP:H	1.76	0.82
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.72	0.72
1:D:191:LEU:HD13	1:D:360:ASN:ND2	2.04	0.72
1:D:325:GLU:HG3	1:D:329:LYS:HE3	1.72	0.71
1:A:200:ARG:HD2	3:D:3263:HOH:O	1.92	0.69
1:B:33:ASN:HD22	1:B:107[B]:LYS:NZ	1.91	0.69
1:D:348:ALA:HB3	3:D:3222:HOH:O	1.92	0.69
1:D:284:ASN:ND2	1:D:342:TYR:H	1.94	0.66
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.77	0.66
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.78	0.66
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.80	0.64
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.80	0.63
1:B:311:LYS:HD2	3:B:3385:HOH:O	1.99	0.61
1:D:152:LYS:HE2	3:D:3317:HOH:O	2.02	0.60
1:B:60:GLN:HE22	1:B:88:ASP:H	1.45	0.60
1:A:110:LYS:HE3	3:B:3614:HOH:O	2.02	0.59
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.85	0.58
1:B:33:ASN:HD22	1:B:107[B]:LYS:HZ3	1.50	0.58
1:C:42:ARG:HD3	3:C:3664:HOH:O	2.03	0.57
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.40	0.57
1:A:107[A]:LYS:HD2	3:A:3002:HOH:O	2.05	0.56
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:50:ASN:ND2	1:D:55:ARG:HH11	2.05	0.55
1:A:33:ASN:HD22	1:A:107[B]:LYS:NZ	2.03	0.55
1:B:291:LEU:O	1:B:293:LYS:HD3	2.05	0.55
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.88	0.55
1:B:18:ILE:HD13	1:B:143:ASP:HB3	1.89	0.54
1:D:92:PRO:HB3	3:D:3339:HOH:O	2.08	0.54
1:C:318:GLU:H	1:C:318:GLU:CD	2.09	0.53
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.90	0.53
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.90	0.53
1:B:33:ASN:ND2	1:B:107[B]:LYS:HZ3	2.06	0.53
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.43	0.53
1:A:320:LEU:O	1:A:324:GLN:HG3	2.09	0.53
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.91	0.52
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.10	0.52
1:B:60:GLN:HE21	1:B:87:ALA:HA	1.75	0.52
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.44	0.52
1:B:89:ASP:OD1	1:B:91:ARG:HB2	2.10	0.52
1:B:60:GLN:NE2	1:B:88:ASP:N	2.52	0.52
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.44	0.52
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.92	0.51
1:C:152:LYS:HE2	3:C:3663:HOH:O	2.10	0.51
1:B:36:THR:HG23	1:B:50:ASN:HD21	1.75	0.51
1:B:152:LYS:HE2	3:B:3375:HOH:O	2.11	0.50
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.93	0.50
1:D:350:ALA:O	1:D:354:GLU:HG3	2.11	0.50
1:A:268:THR:HB	1:A:300:SER:HB2	1.94	0.50
1:C:234:THR:HB	1:C:235:PRO:HD2	1.93	0.50
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.43	0.49
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.47	0.49
1:C:93:PHE:N	1:C:94:PRO:HD2	2.27	0.49
1:C:40:ALA:HA	1:C:50:ASN:ND2	2.27	0.49
1:B:276:GLU:CD	1:B:307:ALA:HB3	2.34	0.48
3:B:3280:HOH:O	1:C:200:ARG:HD2	2.14	0.48
1:A:341:LYS:HE2	3:A:3099:HOH:O	2.13	0.48
1:A:40:ALA:O	1:A:44:GLN:HG3	2.13	0.48
1:D:50:ASN:HD21	1:D:55:ARG:HH11	1.62	0.48
1:B:324:GLN:O	1:B:328:VAL:HG23	2.14	0.48
1:D:325:GLU:O	1:D:329:LYS:HG3	2.13	0.47
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.34	0.47
1:A:291:LEU:O	1:A:293:LYS:HD3	2.14	0.47
1:D:298:THR:OG1	1:D:299:PHE:N	2.47	0.47
1:C:291:LEU:O	1:C:293:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.49	0.47
1:C:29:ILE:HB	1:C:300:SER:HA	1.96	0.47
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.50	0.47
1:D:287:ASN:ND2	1:D:338:CYS:HA	2.31	0.47
1:A:81:GLU:O	1:A:85:GLN:HG3	2.15	0.46
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.97	0.46
1:B:29:ILE:HB	1:B:300:SER:HA	1.97	0.46
1:A:324:GLN:O	1:A:328:VAL:HG23	2.15	0.46
1:A:312:ALA:HB3	1:A:323:ALA:HA	1.97	0.46
1:A:61:LEU:HD11	1:A:323:ALA:HB3	1.96	0.46
1:A:317:LYS:HG3	3:A:3299:HOH:O	2.16	0.46
1:A:4:HIS:CD2	1:B:119:ASN:HB2	2.51	0.46
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.98	0.45
1:D:25:PRO:HG2	3:D:3055:HOH:O	2.16	0.45
1:D:318:GLU:HG2	1:D:319:ASN:OD1	2.17	0.45
1:D:46:ILE:HB	1:D:314:GLY:HA2	1.98	0.45
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.97	0.45
1:C:250:MET:HG2	1:C:363:TYR:CE2	2.51	0.45
1:A:316:LYS:HE3	3:A:3175:HOH:O	2.16	0.45
1:C:268:THR:HB	1:C:300:SER:HB2	1.99	0.45
1:D:293:LYS:HD3	1:D:297:LEU:CD1	2.47	0.45
1:D:33:ASN:HD22	1:D:107[A]:LYS:HG3	1.82	0.44
1:D:61:LEU:HD11	1:D:323:ALA:HB3	1.99	0.44
1:D:78:LEU:HD22	1:D:82:THR:HG21	1.99	0.44
1:B:234:THR:HB	1:B:235:PRO:HD2	1.99	0.44
1:D:29:ILE:HB	1:D:300:SER:HA	1.98	0.44
1:A:29:ILE:HB	1:A:300:SER:HA	1.97	0.44
1:B:320:LEU:O	1:B:324:GLN:HG3	2.17	0.44
1:D:268:THR:HB	1:D:300:SER:HB2	2.00	0.44
1:A:276:GLU:CD	1:A:307:ALA:HB3	2.38	0.44
1:A:196:HIS:HB2	1:A:200:ARG:HG2	2.00	0.44
1:A:58:TYR:O	1:A:61:LEU:HB3	2.18	0.44
1:A:121:GLU:OE2	1:A:158:PRO:HA	2.18	0.44
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.48	0.44
1:A:245:HIS:HD2	1:A:282:ASN:OD1	2.01	0.44
1:B:216:LEU:HD22	1:B:221:ILE:HG13	2.00	0.43
1:C:31:ALA:HB1	2:C:3003:13P:H31	1.99	0.43
1:A:262:PRO:HG3	1:D:262:PRO:HG3	2.00	0.43
1:C:333:ALA:HB1	1:C:342:TYR:CE1	2.54	0.43
1:B:42:ARG:HG2	1:B:42:ARG:HH11	1.84	0.43
1:A:229:LYS:HE2	1:A:270:LEU:HB3	2.00	0.43
1:B:66:ASP:OD1	1:B:68:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:51:THR:O	1:B:55:ARG:HG3	2.19	0.43
1:B:203:TYR:CD1	1:C:3:SER:HB2	2.53	0.43
1:D:241:GLN:NE2	3:D:3305:HOH:O	2.51	0.43
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.54	0.43
1:D:249:ALA:HB1	1:D:286:ILE:HA	2.00	0.43
1:D:207:LYS:HE2	3:D:3454:HOH:O	2.17	0.43
1:A:33:ASN:ND2	1:A:107[B]:LYS:NZ	2.66	0.43
1:A:292:LEU:HD23	1:A:292:LEU:C	2.39	0.42
1:B:316:LYS:HB2	1:B:319:ASN:ND2	2.33	0.42
1:B:121:GLU:OE2	1:B:158:PRO:HA	2.19	0.42
1:B:60:GLN:HE22	1:B:88:ASP:N	2.14	0.42
1:D:277:GLU:OE2	1:D:344:PRO:HB3	2.18	0.42
1:A:300:SER:O	2:A:3001:13P:H12	2.18	0.42
1:C:33:ASN:HD22	1:C:107:LYS:HG3	1.84	0.42
1:C:42:ARG:HG2	1:C:310:LEU:HD22	2.02	0.42
1:C:293:LYS:HD2	1:C:297:LEU:HD12	2.01	0.42
1:B:3:SER:HB3	3:B:3692:HOH:O	2.20	0.42
1:A:33:ASN:HD22	1:A:107[B]:LYS:HZ1	1.68	0.42
1:D:18:ILE:HD13	1:D:143:ASP:HB3	2.02	0.41
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.90	0.41
1:D:303:ARG:HB3	1:D:356:LEU:HD13	2.02	0.41
1:A:98:LYS:NZ	3:A:3262:HOH:O	2.53	0.41
1:A:33:ASN:ND2	1:A:107[B]:LYS:HZ1	2.19	0.41
1:A:262:PRO:HD2	1:D:257:ARG:O	2.21	0.41
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.93	0.41
1:B:36:THR:CG2	1:B:50:ASN:HD21	2.33	0.41
1:D:312:ALA:HB3	1:D:323:ALA:HA	2.02	0.41
1:D:200:ARG:HH11	1:D:200:ARG:HG2	1.85	0.41
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.20	0.41
1:A:4:HIS:NE2	1:B:119:ASN:HB2	2.35	0.41
1:D:61:LEU:HD11	1:D:323:ALA:CB	2.50	0.41
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.21	0.41
1:B:17:ASP:O	1:B:21:ARG:HG3	2.21	0.41
1:B:60:GLN:HE21	1:B:87:ALA:CA	2.33	0.41
1:A:294:PRO:HG3	1:D:262:PRO:CG	2.51	0.41
1:D:277:GLU:O	1:D:281:ILE:HG13	2.21	0.41
1:C:282:ASN:HA	1:C:282:ASN:HD22	1.66	0.40
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.56	0.40
1:B:261:PRO:HA	1:B:262:PRO:HD3	1.94	0.40
1:C:222:TYR:CZ	1:C:224:GLU:HB2	2.56	0.40
1:C:316:LYS:HB3	1:C:318:GLU:OE1	2.22	0.40
1:D:319:ASN:HA	3:D:3129:HOH:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:61:LEU:HD23	1:D:61:LEU:C	2.41	0.40
1:A:234:THR:HB	1:A:235:PRO:HD2	2.04	0.40
1:D:147:TRP:HB3	1:D:173:TYR:CE2	2.56	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	347/363 (96%)	336 (97%)	9 (3%)	2 (1%)	33	18
1	B	347/363 (96%)	332 (96%)	13 (4%)	2 (1%)	33	18
1	C	347/363 (96%)	335 (96%)	10 (3%)	2 (1%)	33	18
1	D	359/363 (99%)	344 (96%)	12 (3%)	3 (1%)	27	12
All	All	1400/1452 (96%)	1347 (96%)	44 (3%)	9 (1%)	33	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	B	5	PRO
1	C	5	PRO
1	A	188	PRO
1	B	188	PRO
1	D	188	PRO
1	C	188	PRO
1	D	5	PRO
1	D	346	GLY

### 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	285/291 (98%)	281 (99%)	4 (1%)	78	72
1	B	285/291 (98%)	275 (96%)	10 (4%)	48	31
1	C	284/291 (98%)	277 (98%)	7 (2%)	60	48
1	D	290/291 (100%)	281 (97%)	9 (3%)	52	37
All	All	1144/1164 (98%)	1114 (97%)	30 (3%)	60	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	173	TYR
1	A	230	PRO
1	A	295	TRP
1	B	5	PRO
1	B	59	ARG
1	B	91	ARG
1	B	107[A]	LYS
1	B	107[B]	LYS
1	B	119	ASN
1	B	173	TYR
1	B	193	ASP
1	B	230	PRO
1	B	295	TRP
1	C	5	PRO
1	C	42	ARG
1	C	59	ARG
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
1	C	320	LEU
1	D	50	ASN
1	D	59	ARG
1	D	107[A]	LYS
1	D	107[B]	LYS
1	D	173	TYR
1	D	193	ASP
1	D	230	PRO
1	D	295	TRP
1	D	347	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	119	ASN
1	A	180	ASN
1	A	241	GLN
1	A	245	HIS
1	A	319	ASN
1	B	33	ASN
1	B	54	ASN
1	B	60	GLN
1	B	95	GLN
1	B	119	ASN
1	B	319	ASN
1	C	54	ASN
1	C	241	GLN
1	C	282	ASN
1	C	319	ASN
1	D	44	GLN
1	D	50	ASN
1	D	180	ASN
1	D	241	GLN
1	D	284	ASN
1	D	360	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 ⓘ

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	13P	A	3001	1	6,8,9	0.65	0	7,10,12	0.44	0
2	13P	B	3002	1	6,8,9	0.60	0	7,10,12	0.43	0
2	13P	C	3003	1	6,8,9	0.68	0	7,10,12	0.43	0
2	13P	D	3004	1	6,8,9	0.67	0	7,10,12	0.43	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	13P	A	3001	1	-	0/4/6/8	0/0/0/0
2	13P	B	3002	1	-	0/4/6/8	0/0/0/0
2	13P	C	3003	1	-	0/4/6/8	0/0/0/0
2	13P	D	3004	1	-	0/4/6/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	350/363 (96%)	-0.25	6 (1%) 67 74	9, 18, 42, 56	2 (0%)
1	B	350/363 (96%)	-0.12	9 (2%) 53 59	8, 18, 43, 62	2 (0%)
1	C	351/363 (96%)	-0.19	5 (1%) 72 79	9, 18, 42, 62	2 (0%)
1	D	360/363 (99%)	0.08	19 (5%) 25 29	9, 21, 58, 88	0
All	All	1411/1452 (97%)	-0.12	39 (2%) 50 57	8, 19, 46, 88	6 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	SER	10.9
1	A	345	SER	8.6
1	D	345	SER	5.6
1	B	359	SER	4.4
1	C	359	SER	4.2
1	D	43	LEU	4.2
1	D	358	ILE	4.0
1	A	359	SER	3.9
1	D	348	ALA	3.5
1	D	359	SER	3.2
1	C	346	GLY	3.2
1	B	40	ALA	3.2
1	D	41	LYS	3.1
1	B	344	PRO	3.1
1	D	46	ILE	2.8
1	D	347	GLN	2.8
1	D	360	ASN	2.7
1	B	360	ASN	2.7
1	C	362	ALA	2.7
1	D	355	SER	2.6
1	A	344	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	357	PHE	2.5
1	D	42	ARG	2.5
1	D	40	ALA	2.5
1	D	44	GLN	2.4
1	B	42	ARG	2.4
1	B	43	LEU	2.4
1	D	47	GLY	2.3
1	C	345	SER	2.3
1	D	350	ALA	2.3
1	C	344	PRO	2.2
1	A	360	ASN	2.2
1	B	343	THR	2.2
1	D	356	LEU	2.1
1	D	353	SER	2.1
1	B	2	HIS	2.1
1	D	45	SER	2.1
1	A	1	PRO	2.0
1	A	44	GLN	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	13P	C	3003	9/10	0.10	0.84	21,26,30,35	0
2	13P	B	3002	9/10	0.10	0.19	24,30,36,36	0
2	13P	A	3001	9/10	0.09	-0.05	21,28,34,36	0
2	13P	D	3004	9/10	0.08	-1.77	24,28,38,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.