



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:06 AM EDT

PDB ID : 2QUU  
Title : Dihydroxyacetone phosphate Schiff base intermediate in mutant fructose-1,6-bisphosphate aldolase from rabbit muscle  
Authors : St-Jean, M.; Sygusch, J.  
Deposited on : 2007-08-06  
Resolution : 1.98 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

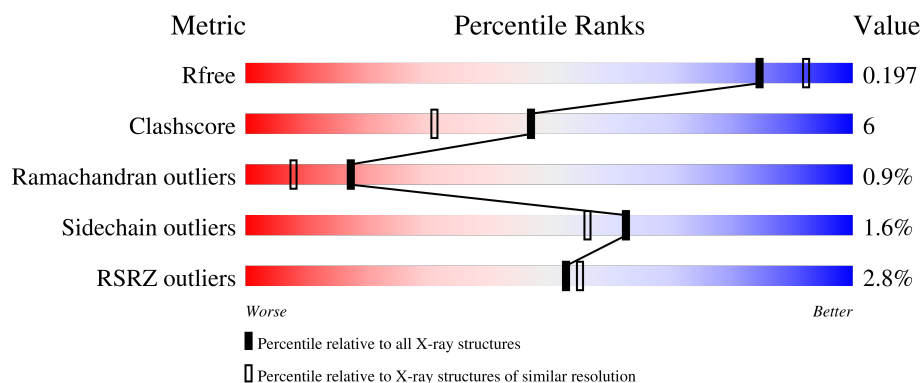
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>0%</div> <div>83% 13% .</div> </div>
1	B	363	<div> <div>2%</div> <div>84% 13% .</div> </div>
1	C	363	<div> <div>4%</div> <div>80% 17% .</div> </div>
1	D	363	<div> <div>4%</div> <div>81% 18% .</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13086 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.

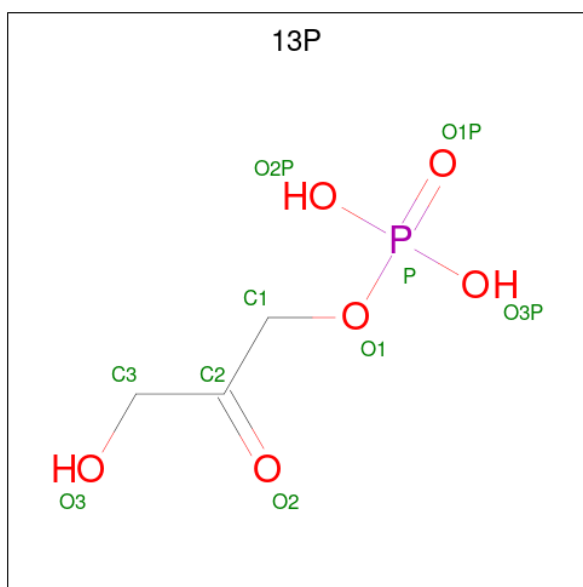
- Molecule 1 is a protein called Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2666	1676	473	505	12			
1	B	351	Total	C	N	O	S	0	0	0
			2680	1685	475	508	12			
1	C	353	Total	C	N	O	S	0	0	0
			2690	1689	478	511	12			
1	D	363	Total	C	N	O	S	0	8	0
			2784	1749	493	530	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	LYS	engineered mutation	UNP P00883
B	146	MET	LYS	engineered mutation	UNP P00883
C	146	MET	LYS	engineered mutation	UNP P00883
D	146	MET	LYS	engineered mutation	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		

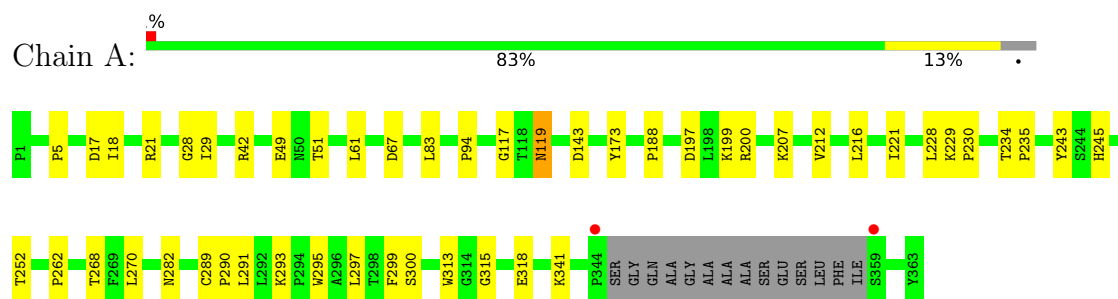
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	583	Total	O	0	0
			583	583		
3	B	555	Total	O	0	0
			555	555		
3	C	524	Total	O	0	0
			524	524		
3	D	568	Total	O	0	14
			568	568		

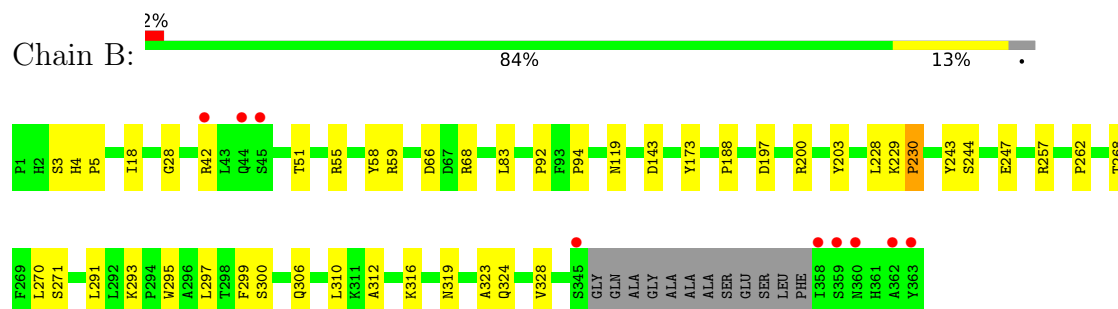
### 3 Residue-property plots [i](#)

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

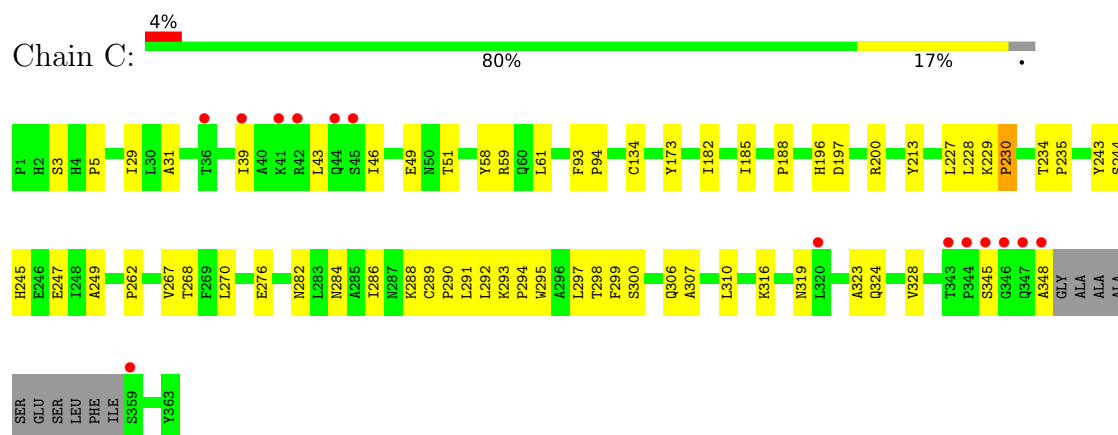
#### • Molecule 1: Fructose-bisphosphate aldolase A



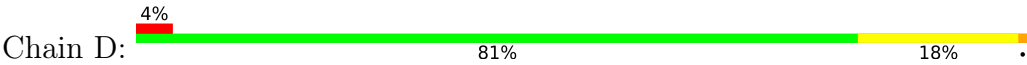
#### • Molecule 1: Fructose-bisphosphate aldolase A



#### • Molecule 1: Fructose-bisphosphate aldolase A



#### • 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, $\alpha$ , $\beta$ , $\gamma$	83.86Å 103.72Å 84.88Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 48.54 – 1.84	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-1.98) 84.0 (48.54-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.157 , 0.195 0.158 , 0.197	Depositor DCC
$R_{free}$ test set	10978 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13086	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 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/2718	0.57	0/3682
1	B	0.30	0/2732	0.57	0/3701
1	C	0.30	0/2742	0.55	0/3714
1	D	0.29	0/2838	0.56	0/3844
All	All	0.30	0/11030	0.56	0/14941

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	213	TYR	Sidechain
1	D	213	TYR	Sidechain



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2666	0	2682	31	0
1	B	2680	0	2698	27	0
1	C	2690	0	2703	36	0
1	D	2784	0	2799	47	0
2	A	9	0	5	0	0
2	B	9	0	5	1	0
2	C	9	0	5	1	0
2	D	9	0	5	3	0
3	A	583	0	0	9	0
3	B	555	0	0	2	0
3	C	524	0	0	1	0
3	D	568	0	0	9	0
All	All	13086	0	10902	135	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 6.

All (135) 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:49:GLU:HG2	1:C:51:THR:HG23	1.69	0.73
1:D:347:GLN:HG2	1:D:348:ALA:H	1.55	0.70
1:D:36:THR:HG22	1:D:50:ASN:HD21	1.59	0.68
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.76	0.66
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.77	0.66
1:D:284:ASN:ND2	1:D:342:TYR:H	1.93	0.66
1:D:316:LYS:HB2	1:D:319:ASN:ND2	2.11	0.66
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.77	0.64
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.79	0.63
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.83	0.60
1:D:363[A]:TYR:CE2	2:D:3004:13P:H32	2.36	0.59
1:C:268:THR:HB	1:C:300:SER:HB2	1.84	0.59
1:D:350:ALA:O	1:D:354:GLU:HG3	2.04	0.58
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.87	0.57
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.20	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363[A]:TYR:CZ	2:D:3004:13P:H32	2.40	0.56
1:D:36:THR:HG21	3:D:3215:HOH:O	2.05	0.56
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.06	0.56
1:A:252:THR:HG23	3:A:3536:HOH:O	2.06	0.56
1:C:324:GLN:O	1:C:328:VAL:HG23	2.06	0.56
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.88	0.55
1:A:199:LYS:HE2	3:A:3166:HOH:O	2.07	0.54
1:B:291:LEU:O	1:B:293:LYS:HD3	2.07	0.54
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.28	0.54
1:A:212:VAL:HG13	3:A:3254:HOH:O	2.09	0.53
1:A:200:ARG:HD2	3:D:3293:HOH:O	2.08	0.53
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.92	0.52
1:B:268:THR:HB	1:B:300:SER:HB2	1.91	0.52
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.91	0.51
1:A:262:PRO:HD2	1:D:257:ARG:O	2.11	0.51
1:B:200:ARG:HD2	3:C:3270:HOH:O	2.09	0.51
1:C:46:ILE:HD13	1:C:310:LEU:HG	1.93	0.51
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.46	0.51
1:D:33:ASP:OD2	1:D:107[B]:LYS:HE2	2.11	0.51
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.94	0.51
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.10	0.50
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.93	0.50
1:D:107[A]:LYS:HD3	3:D:3019[A]:HOH:O	2.12	0.50
1:B:66:ASP:OD1	1:B:68:ARG:HB2	2.11	0.49
1:B:271:SER:OG	2:B:3002:13P:O3P	2.22	0.49
1:D:92:PRO:HB3	3:D:3366:HOH:O	2.13	0.49
1:D:268:THR:HB	1:D:300:SER:HB2	1.94	0.49
1:B:244:SER:OG	1:B:247:GLU:HG3	2.12	0.49
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.47	0.48
1:A:207:LYS:HD2	3:A:3583:HOH:O	2.13	0.48
1:D:234:THR:HB	1:D:235:PRO:HD2	1.93	0.48
1:C:293:LYS:HD2	1:C:297:LEU:HD12	1.94	0.48
1:C:345:SER:HB3	1:C:348:ALA:O	2.13	0.48
3:B:3044:HOH:O	1:C:200:ARG:HD2	2.13	0.48
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.96	0.48
1:D:324:GLN:O	1:D:328:VAL:HG23	2.13	0.48
1:D:360[A]:ASN:N	1:D:360[A]:ASN:HD22	2.11	0.48
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.49	0.47
1:B:229:LYS:HE2	1:B:270:LEU:HB3	1.95	0.47
1:A:199:LYS:HD3	3:A:3424:HOH:O	2.14	0.47
1:B:42:ARG:HG3	1:B:310:LEU:HD22	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ALA:HB1	2:C:3003:13P:H31	1.96	0.47
1:C:234:THR:HB	1:C:235:PRO:HD2	1.96	0.47
1:D:229:LYS:HE2	1:D:270:LEU:HB3	1.97	0.47
1:D:24:ALA:HB3	1:D:27:LYS:HD2	1.97	0.47
1:D:61:LEU:C	1:D:61:LEU:HD23	2.35	0.47
1:C:229:LYS:HE2	1:C:270:LEU:HB3	1.97	0.47
1:A:199:LYS:HG3	3:A:3401:HOH:O	2.14	0.46
1:C:29:ILE:HB	1:C:300:SER:HA	1.96	0.46
1:D:185:ILE:HG12	1:D:227:LEU:HB2	1.97	0.46
1:A:229:LYS:HE2	1:A:270:LEU:HB3	1.98	0.46
1:A:17:ASP:O	1:A:21:ARG:HG3	2.16	0.46
1:A:234:THR:HB	1:A:235:PRO:HD2	1.98	0.46
1:C:316:LYS:HB2	1:C:319:ASN:HD22	1.79	0.46
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.97	0.46
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.51	0.46
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.98	0.46
1:A:119:ASN:HB2	1:B:4:HIS:CE1	2.51	0.45
1:A:318:GLU:HG3	3:A:3341:HOH:O	2.17	0.45
1:A:268:THR:HB	1:A:300:SER:HB2	1.98	0.45
1:C:58:TYR:OH	1:C:306:GLN:HB3	2.16	0.45
1:D:351:ALA:HB3	3:D:3090:HOH:O	2.16	0.45
1:B:316:LYS:HB2	1:B:319:ASN:ND2	2.31	0.45
1:C:61:LEU:HD11	1:C:323:ALA:HB3	1.98	0.45
1:C:134:CYS:HB3	1:C:182:ILE:HD12	1.98	0.45
1:D:360[A]:ASN:N	1:D:360[A]:ASN:ND2	2.64	0.45
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.51	0.45
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.15	0.45
1:D:134:CYS:HB3	1:D:182:ILE:HD12	1.99	0.44
1:D:277:GLU:HG2	3:D:3200:HOH:O	2.17	0.44
1:D:241:GLN:NE2	3:D:3336:HOH:O	2.50	0.44
1:B:3:SER:HB3	3:B:3372:HOH:O	2.17	0.44
1:D:38[A]:SER:HB2	1:D:363[A]:TYR:HA	2.00	0.44
1:D:363[A]:TYR:OH	2:D:3004:13P:H32	2.18	0.44
1:C:289:CYS:HA	1:C:290:PRO:HD3	1.86	0.44
1:B:324:GLN:O	1:B:328:VAL:HG23	2.18	0.44
1:D:229:LYS:HG3	1:D:268:THR:O	2.18	0.44
1:C:245:HIS:HD2	1:C:282:ASN:OD1	2.00	0.44
1:C:291:LEU:O	1:C:293:LYS:HE2	2.17	0.43
1:D:267:VAL:HB	1:D:297:LEU:HD23	2.00	0.43
1:D:298:THR:OG1	1:D:299:PHE:N	2.51	0.43
1:D:66:ASP:OD1	1:D:68:ARG:HB2	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HD13	1:B:143:ASP:HB3	2.01	0.43
1:D:25:PRO:HG2	3:D:3074:HOH:O	2.19	0.43
1:D:27:LYS:HG2	1:D:71:PRO:O	2.18	0.43
1:C:39:ILE:O	1:C:43:LEU:HG	2.19	0.43
1:C:185:ILE:HG12	1:C:227:LEU:HB2	2.01	0.43
1:A:18:ILE:HD13	1:A:143:ASP:HB3	2.00	0.43
1:C:276:GLU:CD	1:C:307:ALA:HB3	2.39	0.43
1:D:284:ASN:HD21	1:D:342:TYR:H	1.62	0.43
1:A:341:LYS:HE3	3:A:3120:HOH:O	2.19	0.43
1:C:93:PHE:N	1:C:94:PRO:HD2	2.33	0.42
1:C:244:SER:OG	1:C:247:GLU:HG3	2.18	0.42
1:D:29:ILE:HB	1:D:300:SER:HA	2.01	0.42
1:A:29:ILE:HB	1:A:300:SER:HA	2.01	0.42
1:B:92:PRO:HB2	1:B:94:PRO:HD2	2.02	0.42
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.55	0.42
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.50	0.42
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.92	0.42
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.90	0.41
1:D:196:HIS:HB2	1:D:200:ARG:HG2	2.01	0.41
1:A:61:LEU:C	1:A:61:LEU:HD23	2.41	0.41
1:B:58:TYR:OH	1:B:306:GLN:HB3	2.20	0.41
1:B:312:ALA:HB3	1:B:323:ALA:HA	2.02	0.41
1:C:196:HIS:HB2	1:C:200:ARG:HG2	2.02	0.41
1:B:203:TYR:CG	1:C:3:SER:HB2	2.54	0.41
1:D:207:LYS:HE2	3:D:3393:HOH:O	2.21	0.41
1:C:58:TYR:O	1:C:61:LEU:HB3	2.20	0.41
1:C:249:ALA:HB1	1:C:286:ILE:HA	2.02	0.41
1:D:38[B]:SER:O	1:D:42:ARG:NH2	2.54	0.41
1:A:42:ARG:HD2	3:A:3285:HOH:O	2.21	0.41
1:A:291:LEU:O	1:A:293:LYS:HD3	2.21	0.41
1:C:292:LEU:HD23	1:C:293:LYS:N	2.36	0.40
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.21	0.40
1:D:293:LYS:HD2	1:D:297:LEU:HD12	2.03	0.40
1:A:117:GLY:HA2	1:B:4:HIS:O	2.21	0.40
1:C:298:THR:OG1	1:C:299:PHE:N	2.54	0.40
1:B:51:THR:O	1:B:55:ARG:HG3	2.21	0.40
1:A:216:LEU:HD22	1:A:221:ILE:HG13	2.04	0.40
1:C:284:ASN:O	1:C:288:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	345/363 (95%)	333 (96%)	9 (3%)	3 (1%)	17	8
1	B	347/363 (96%)	331 (95%)	14 (4%)	2 (1%)	25	14
1	C	349/363 (96%)	335 (96%)	12 (3%)	2 (1%)	25	14
1	D	365/363 (101%)	344 (94%)	16 (4%)	5 (1%)	11	3
All	All	1406/1452 (97%)	1343 (96%)	51 (4%)	12 (1%)	17	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	349	GLY
1	B	5	PRO
1	D	188	PRO
1	A	5	PRO
1	A	67	ASP
1	A	188	PRO
1	C	5	PRO
1	C	188	PRO
1	D	5	PRO
1	D	348	ALA
1	D	346	GLY
1	B	188	PRO

### 5.3.2 Protein sidechains [i](#)

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	283/291 (97%)	280 (99%)	3 (1%)	73	70
1	B	285/291 (98%)	280 (98%)	5 (2%)	59	51
1	C	285/291 (98%)	281 (99%)	4 (1%)	67	62
1	D	294/291 (101%)	287 (98%)	7 (2%)	49	41
All	All	1147/1164 (98%)	1128 (98%)	19 (2%)	62	53

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	173	TYR
1	A	295	TRP
1	B	59	ARG
1	B	119	ASN
1	B	173	TYR
1	B	230	PRO
1	B	295	TRP
1	C	59	ARG
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
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	360[A]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	95	GLN
1	A	119	ASN
1	A	156	HIS
1	A	220	HIS
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	4	HIS
1	B	95	GLN
1	B	119	ASN
1	B	136	GLN
1	B	179	GLN
1	B	319	ASN
1	C	54	ASN
1	C	219	HIS
1	C	241	GLN
1	C	245	HIS
1	C	319	ASN
1	D	54	ASN
1	D	180	ASN
1	D	241	GLN
1	D	284	ASN
1	D	319	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	D	3004	1	8,8,9	0.83	0	10,10,12	1.07	1 (10%)
2	13P	C	3003	1	8,8,9	0.83	0	10,10,12	1.03	1 (10%)
2	13P	A	3001	1	8,8,9	0.79	0	10,10,12	1.01	1 (10%)
2	13P	B	3002	1	8,8,9	0.79	0	10,10,12	1.00	1 (10%)

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	D	3004	1	-	2/6/6/8	-
2	13P	C	3003	1	-	4/6/6/8	-
2	13P	A	3001	1	-	3/6/6/8	-
2	13P	B	3002	1	-	2/6/6/8	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3004	13P	C1-C2-C3	3.20	120.93	113.95
2	C	3003	13P	C1-C2-C3	3.03	120.56	113.95
2	A	3001	13P	C1-C2-C3	2.97	120.41	113.95
2	B	3002	13P	C1-C2-C3	2.95	120.39	113.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3003	13P	C1-O1-P-O2P
2	D	3004	13P	O1-C1-C2-C3
2	B	3002	13P	O1-C1-C2-C3
2	C	3003	13P	C1-O1-P-O1P
2	A	3001	13P	O1-C1-C2-C3
2	A	3001	13P	C1-O1-P-O3P
2	B	3002	13P	C1-O1-P-O3P
2	C	3003	13P	C1-O1-P-O3P
2	D	3004	13P	C1-O1-P-O3P
2	A	3001	13P	C1-O1-P-O1P

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	3003	13P	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3004	13P	3	0
2	C	3003	13P	1	0
2	B	3002	13P	1	0

## 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	349/363 (96%)	-0.34	2 (0%) 89 90	9, 17, 37, 69	1 (0%)
1	B	351/363 (96%)	-0.17	9 (2%) 56 58	9, 18, 43, 79	3 (0%)
1	C	353/363 (97%)	0.14	14 (3%) 38 40	10, 20, 47, 83	5 (1%)
1	D	363/363 (100%)	0.02	15 (4%) 37 39	10, 20, 48, 79	4 (1%)
All	All	1416/1452 (97%)	-0.09	40 (2%) 53 55	9, 19, 44, 83	13 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346	GLY	17.9
1	B	345	SER	13.7
1	B	358	ILE	12.1
1	C	348	ALA	10.3
1	C	347	GLN	8.1
1	C	359	SER	6.4
1	A	344	PRO	6.1
1	A	359	SER	5.9
1	D	345	SER	5.8
1	B	359	SER	5.2
1	C	345	SER	5.2
1	D	349	GLY	4.8
1	D	347	GLN	4.6
1	D	346	GLY	4.5
1	D	348	ALA	4.4
1	D	350	ALA	4.2
1	C	343	THR	3.6
1	B	45	SER	3.6
1	D	42	ARG	3.6
1	C	344	PRO	3.4
1	D	360[A]	ASN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	353	SER	3.1
1	D	358	ILE	3.1
1	B	360	ASN	3.1
1	C	41	LYS	3.0
1	C	42	ARG	3.0
1	B	42	ARG	2.9
1	C	44	GLN	2.8
1	B	44	GLN	2.7
1	B	362	ALA	2.6
1	C	320	LEU	2.6
1	B	363	TYR	2.5
1	D	351	ALA	2.5
1	C	39	ILE	2.3
1	C	36	THR	2.3
1	D	41	LYS	2.3
1	D	44	GLN	2.2
1	D	357	PHE	2.1
1	C	45	SER	2.1
1	D	361[A]	HIS	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 monosaccharides 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	13P	C	3003	9/10	0.96	0.12	19,23,26,27	0
2	13P	B	3002	9/10	0.97	0.08	21,23,24,25	0
2	13P	A	3001	9/10	0.97	0.07	18,19,22,23	0
2	13P	D	3004	9/10	0.98	0.10	19,20,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.