



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 3DFT / pdb\_00003dft  
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

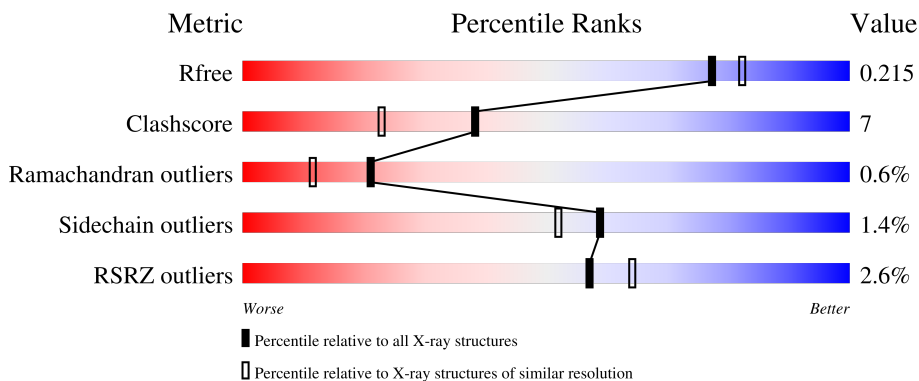
# 1 Overall quality at a glance i

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))
$R_{free}$	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">81%      15%      ..</p>
1	B	363	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">80%      16%      ..</p>
1	C	363	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">82%      14%      ..</p>
1	D	363	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">80%      18%      .</p>

## 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
			Total	C	N	O	S			
1	A	350	2671	1679	475	506	11	0	0	0
1	B	350	2671	1679	475	506	11	0	0	0
1	C	352	2684	1686	478	509	11	0	0	0
1	D	360	2728	1714	484	519	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

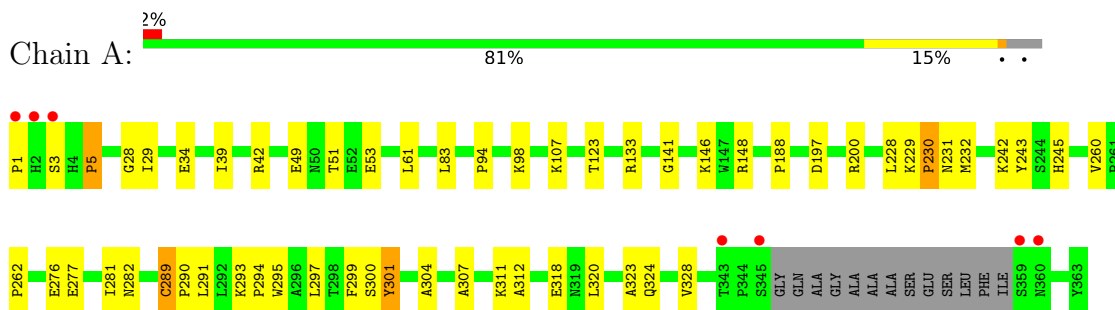
- Molecule 3 is water.

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

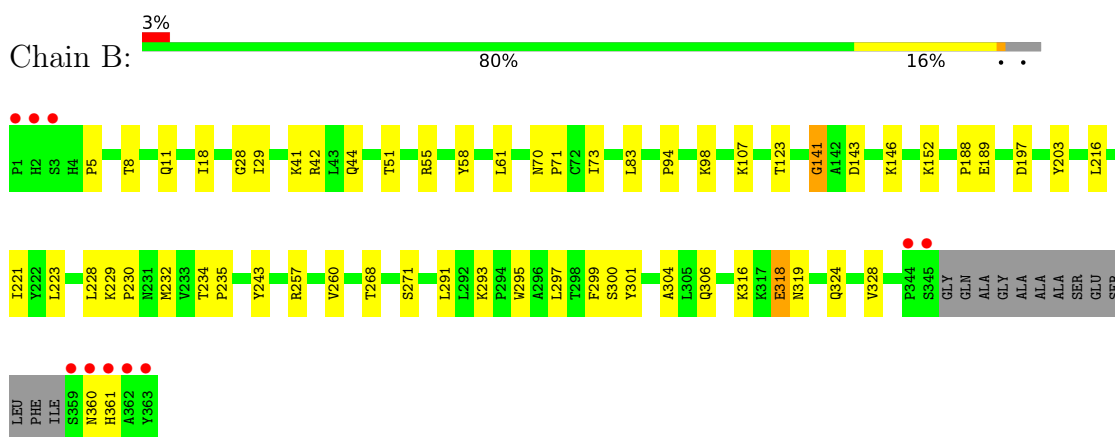
### 3 Residue-property plots [i](#)

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.

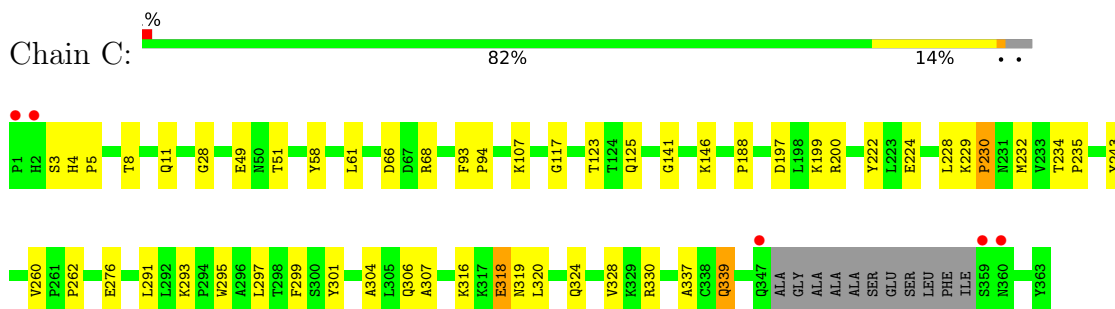
- Molecule 1: Fructose-bisphosphate aldolase A



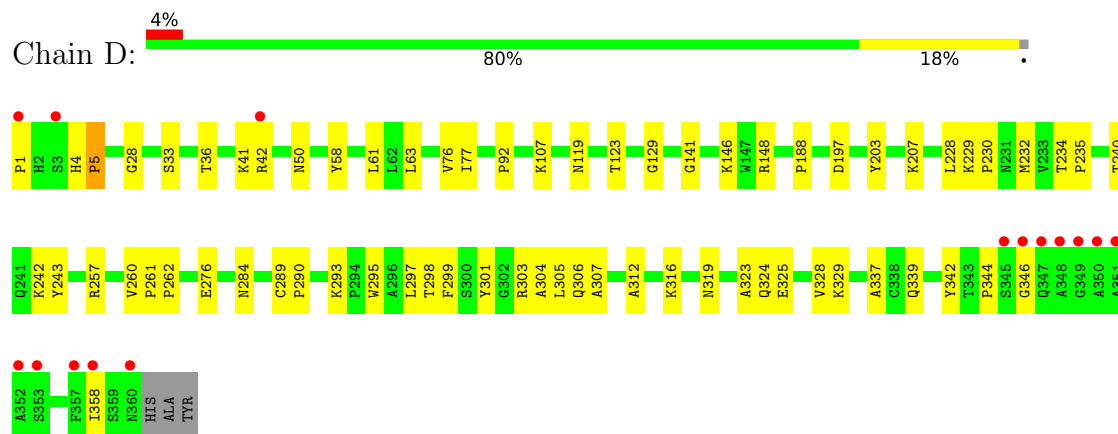
- Molecule 1: Fructose-bisphosphate aldolase A



- 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, $\alpha$ , $\beta$ , $\gamma$	83.93Å 103.61Å 84.95Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	50.00 – 1.94 50.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	86.2 (50.00-1.94) 93.5 (50.00-1.94)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.626	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage'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	0.34	0/2723	0.88	9/3688 (0.2%)
1	B	0.35	0/2723	0.88	8/3688 (0.2%)
1	C	0.35	0/2736	0.86	5/3705 (0.1%)
1	D	0.34	0/2780	0.86	7/3767 (0.2%)
All	All	0.34	0/10962	0.87	29/14848 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	VAL	N-CA-C	8.12	114.95	107.56
1	D	260	VAL	N-CA-C	7.82	114.68	107.56
1	C	260	VAL	N-CA-C	7.60	114.48	107.56
1	A	232	MET	N-CA-C	-7.45	100.49	110.55
1	B	260	VAL	N-CA-C	7.38	114.28	107.56
1	C	232	MET	N-CA-C	-6.85	101.30	110.55
1	D	232	MET	N-CA-C	-6.84	101.31	110.55
1	B	232	MET	N-CA-C	-6.82	101.53	110.53
1	C	123	THR	N-CA-C	-6.36	100.16	109.18
1	A	123	THR	N-CA-C	-6.28	100.27	109.18
1	B	73	ILE	N-CA-C	6.22	116.58	107.37
1	B	123	THR	N-CA-C	-6.04	100.61	109.18
1	A	289	CYS	CA-C-N	6.02	125.50	119.24
1	A	289	CYS	C-N-CA	6.02	125.50	119.24
1	B	141	GLY	N-CA-C	5.92	122.92	114.64
1	A	301	TYR	N-CA-C	5.88	119.67	110.32
1	C	141	GLY	N-CA-C	5.65	122.26	114.92
1	A	141	GLY	N-CA-C	5.40	122.20	114.64
1	D	148	ARG	N-CA-C	5.38	117.49	108.73
1	B	223	LEU	N-CA-C	5.37	117.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	141	GLY	N-CA-C	5.36	121.89	114.92
1	B	189	GLU	N-CA-C	5.34	117.44	109.59
1	A	148	ARG	N-CA-C	5.27	117.32	108.73
1	D	123	THR	N-CA-C	-5.25	101.45	108.86
1	D	289	CYS	CA-C-N	5.13	124.75	119.05
1	D	289	CYS	C-N-CA	5.13	124.75	119.05
1	B	29	ILE	N-CA-C	5.12	115.96	108.53
1	A	231	ASN	N-CA-C	-5.07	103.71	110.55
1	C	339	GLN	N-CA-C	-5.05	107.07	114.39

There are no chirality outliers.

There are no planarity outliers.

## 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	2671	0	2695	40	0
1	B	2671	0	2695	38	0
1	C	2684	0	2706	37	0
1	D	2728	0	2756	49	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
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	150	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 (150) 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	1.05	0.97
1:C:146:LYS:NZ	1:C:229:LYS:HZ3	1.67	0.92
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:A:146:LYS:HZ3	1:A:229:LYS:HZ3	1.29	0.79
1:B:146:LYS:HZ3	1:B:229:LYS:HZ3	1.33	0.77
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: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:D:146:LYS:HZ3	1:D:229:LYS:NZ	1.89	0.70
1:D:107:LYS:HG3	3:D:3762:HOH:O	1.92	0.70
1:D:146:LYS:HZ3	1:D:229:LYS:HZ2	1.39	0.70
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.72	0.69
1:A:146:LYS:NZ	1:A:229:LYS:HZ3	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:A:146:LYS:HZ3	1:A:229:LYS:NZ	1.93	0.65
1:D:301:TYR:HB3	1:D:304:ALA:HB3	1.77	0.65
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
1:B:146:LYS:NZ	1:B:229:LYS:HZ3	1.97	0.60
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:C:316:LYS:HB2	1:C:319:ASN:ND2	2.21	0.56
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.06	0.55
1:C:318:GLU:H	1:C:318:GLU:CD	2.13	0.55
1:B:146:LYS:NZ	1:B:229:LYS:NZ	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:GLU:O	1:D:329:LYS:HG3	2.07	0.54
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.43	0.54
1:C:199:LYS:HG3	3:C:3144:HOH:O	2.05	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: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:B:318:GLU:H	1:B:318:GLU:CD	2.19	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:146:LYS:HZ3	1:B:229:LYS:NZ	2.06	0.49
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
1:B:316:LYS:HB3	1:B:318:GLU:OE2	2.13	0.48
1:A:61:LEU:C	1:A:61:LEU:HD23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:O	1:B:55:ARG:HG3	2.16	0.46
1:B:301:TYR:HB3	1:B:304:ALA:HB3	1.96	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:276:GLU:CD	1:D:307:ALA:HB3	2.40	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:83:LEU:HD12	1:B:94:PRO:HG3	1.98	0.45
1:B:203:TYR:CG	1:C:3:SER:HB2	2.51	0.45
1:A:276:GLU:CD	1:A:307:ALA:HB3	2.42	0.45
1:D:240:THR:O	1:D:242:LYS:HD2	2.16	0.45
1:B:61:LEU:C	1:B:61:LEU:HD23	2.42	0.45
1:D:36:THR:CG2	1:D:50:ASN:HD21	2.29	0.45
1:D:312:ALA:HB3	1:D:323:ALA:HA	1.99	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:A:294:PRO:HG3	1:D:262:PRO:CG	2.47	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:HZ3	2.15	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:D:61:LEU:C	1:D:61:LEU:HD23	2.42	0.44
1:A:133:ARG:HD3	3:A:3225:HOH:O	2.17	0.44
1:B:8:THR:H	1:B:11:GLN:NE2	2.08	0.44
1:D:337:ALA:C	1:D:339:GLN:H	2.24	0.44
1:D:33:SER:HB3	1:D:77:ILE:HG22	2.00	0.43
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.92	0.43
1:B:360:ASN:HB2	3:B:3707:HOH:O	2.19	0.43
1:A:320:LEU:O	1:A:324:GLN:HG3	2.19	0.43
1:C:330:ARG:NE	1:C:330:ARG:HA	2.34	0.43
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.18	0.43
1:C:276:GLU:CD	1:C:307:ALA:HB3	2.44	0.43
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:337:ALA:C	1:C:339:GLN:H	2.28	0.42
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.20	0.42
1:A:146:LYS:NZ	1:A:229:LYS:HZ2	2.18	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: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:4:HIS:CD2	1:D:119:ASN:HB2	2.55	0.41
1:C:117:GLY:HA2	1:D:4:HIS:O	2.20	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:98:LYS:NZ	3:A:3286:HOH:O	2.54	0.40
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.89	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 [\(i\)](#)

### 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	346/363 (95%)	329 (95%)	15 (4%)	2 (1%)	21	11
1	B	346/363 (95%)	330 (95%)	14 (4%)	2 (1%)	21	11
1	C	348/363 (96%)	336 (97%)	10 (3%)	2 (1%)	21	11
1	D	358/363 (99%)	342 (96%)	13 (4%)	3 (1%)	16	7
All	All	1398/1452 (96%)	1337 (96%)	52 (4%)	9 (1%)	21	11

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 [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	284/291 (98%)	278 (98%)	6 (2%)	47	37
1	B	284/291 (98%)	279 (98%)	5 (2%)	51	43
1	C	285/291 (98%)	282 (99%)	3 (1%)	65	60
1	D	289/291 (99%)	287 (99%)	2 (1%)	76	74
All	All	1142/1164 (98%)	1126 (99%)	16 (1%)	59	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	53	GLU

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	230	PRO
1	A	295	TRP
1	A	318	GLU
1	B	42	ARG
1	B	107	LYS
1	B	271	SER
1	B	295	TRP
1	B	318	GLU
1	C	230	PRO
1	C	295	TRP
1	C	318	GLU
1	D	5	PRO
1	D	295	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	136	GLN
1	A	180	ASN
1	A	241	GLN
1	A	245	HIS
1	A	319	ASN
1	B	11	GLN
1	B	44	GLN
1	B	119	ASN
1	B	136	GLN
1	B	179	GLN
1	B	180	ASN
1	B	237	HIS
1	B	319	ASN
1	C	11	GLN
1	C	54	ASN
1	C	85	GLN
1	C	125	GLN
1	C	241	GLN
1	C	287	ASN
1	C	339	GLN
1	D	4	HIS
1	D	54	ASN
1	D	156	HIS

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Mol	Chain	Res	Type
1	D	180	ASN
1	D	237	HIS
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 oligosaccharides 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	PO4	B	3002	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
2	PO4	D	3004[A]	-	4,4,4	1.75	0	6,6,6	0.46	0
2	PO4	A	3001	-	4,4,4	1.74	0	6,6,6	0.44	0
2	PO4	C	3003	-	4,4,4	1.73	0	6,6,6	0.46	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	PO4	P-O4	-2.01	1.48	1.54

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%)	-0.25	7 (2%) 65 72	6, 15, 40, 56	2 (0%)
1	B	350/363 (96%)	-0.24	10 (2%) 53 60	7, 15, 37, 64	2 (0%)
1	C	352/363 (96%)	-0.24	5 (1%) 73 79	5, 16, 39, 62	2 (0%)
1	D	360/363 (99%)	-0.10	15 (4%) 40 46	7, 18, 51, 79	0
All	All	1412/1452 (97%)	-0.20	37 (2%) 57 64	5, 16, 44, 79	6 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	SER	5.7
1	B	359	SER	5.4
1	D	1	PRO	5.4
1	B	1	PRO	5.2
1	A	345	SER	4.9
1	C	359	SER	4.9
1	C	347	GLN	4.6
1	A	1	PRO	4.5
1	B	362	ALA	3.5
1	B	345	SER	3.4
1	D	358	ILE	3.2
1	D	348	ALA	3.2
1	D	345	SER	3.2
1	A	2	HIS	3.2
1	B	2	HIS	3.2
1	D	360	ASN	3.1
1	B	360	ASN	3.1
1	D	42	ARG	2.8
1	D	349	GLY	2.7
1	C	360	ASN	2.6
1	D	347	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	344	PRO	2.4
1	B	363	TYR	2.3
1	C	2	HIS	2.3
1	D	351	ALA	2.3
1	C	1	PRO	2.3
1	D	353	SER	2.3
1	A	360	ASN	2.3
1	D	352	ALA	2.2
1	B	3	SER	2.2
1	D	3	SER	2.2
1	A	3	SER	2.1
1	D	346	GLY	2.1
1	B	361	HIS	2.1
1	D	357	PHE	2.1
1	D	350	ALA	2.0
1	A	343	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	PO4	C	3003	5/5	0.90	0.12	49,53,60,63	0
2	PO4	B	3002	5/5	0.94	0.09	32,34,38,39	0
2	PO4	A	3001	5/5	0.96	0.07	25,26,31,31	0
2	PO4	D	3004[A]	5/5	0.97	0.08	17,18,24,28	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.