



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1ZAL  
Title : Fructose-1,6-bisphosphate aldolase from rabbit muscle in complex with partially disordered tagatose-1,6-bisphosphate, a weak competitive inhibitor  
Authors : St-Jean, M.; Lafrance-Vanasse, J.; Liotard, B.; Sygusch, J.  
Deposited on : 2005-04-06  
Resolution : 1.89 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

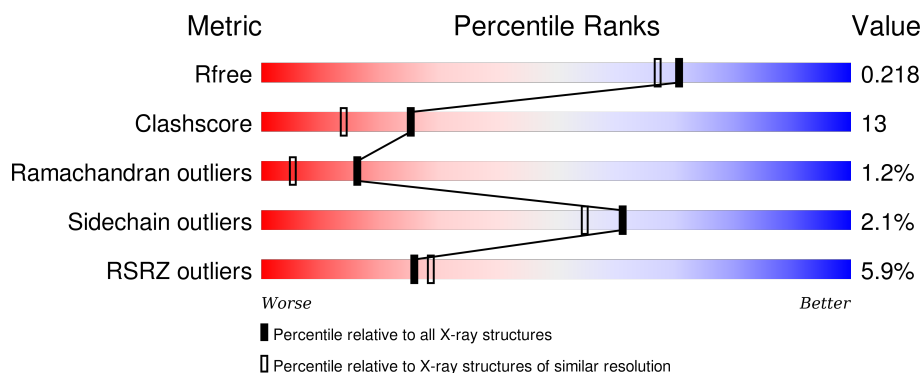
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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>5%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	B	363	<div> <div>5%</div> <div>81%</div> <div>19%</div> </div>
1	C	363	<div> <div>7%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
1	D	363	<div> <div>7%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	3002[A]	-	-	-	X
2	PO4	C	3006[A]	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13287 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	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	B	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	C	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	D	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			

- 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	1
			5	4	1		
2	A	1	Total	O	P	0	1
			5	4	1		

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

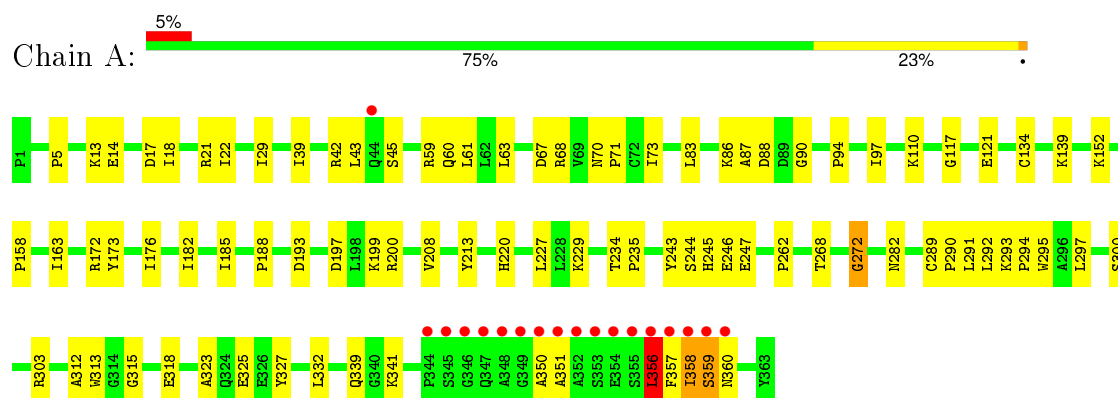
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	496	Total	O	0	7
			496	496		
3	B	538	Total	O	0	8
			538	538		
3	C	592	Total	O	0	8
			592	592		
3	D	589	Total	O	0	8
			589	589		

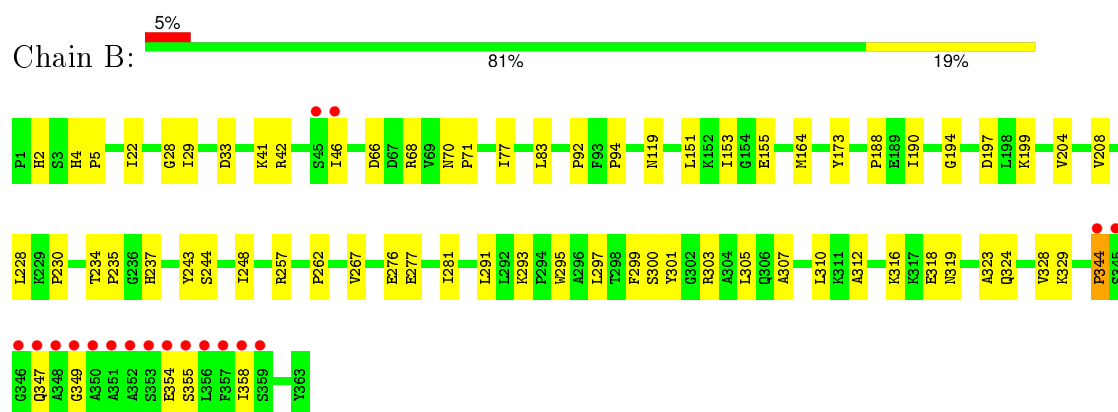
### 3 Residue-property plots

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

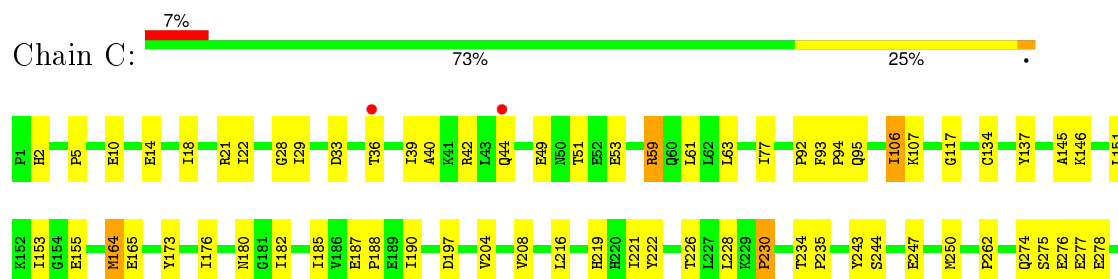
#### • Molecule 1: Fructose-bisphosphate aldolase A

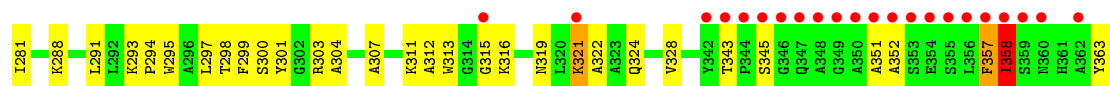


#### • Molecule 1: Fructose-bisphosphate aldolase A

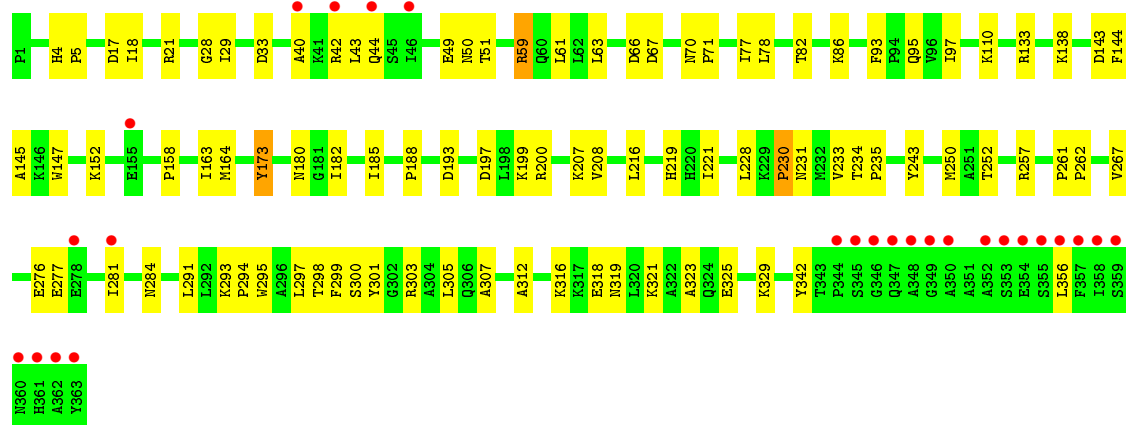
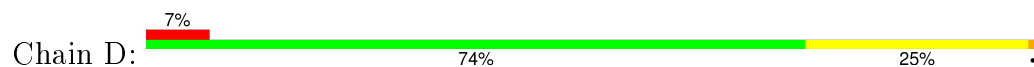


#### • Molecule 1: Fructose-bisphosphate aldolase A





● 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, $\alpha$ , $\beta$ , $\gamma$	83.05Å 103.22Å 84.55Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	50.00 – 1.89 48.31 – 1.68	Depositor EDS
% Data completeness (in resolution range)	85.4 (50.00-1.89) 76.0 (48.31-1.68)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.89 (at 1.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.168 , 0.211 0.176 , 0.218	Depositor DCC
$R_{free}$ test set	5302 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.5	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 134390 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.31	0/2812	0.64	3/3810 (0.1%)
1	B	0.30	0/2812	0.58	0/3810
1	C	0.31	0/2812	0.59	1/3810 (0.0%)
1	D	0.29	0/2812	0.57	0/3810
All	All	0.30	0/11248	0.60	4/15240 (0.0%)

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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	LEU	CA-CB-CG	7.20	131.86	115.30
1	A	350	ALA	N-CA-C	6.09	127.45	111.00
1	A	358	ILE	CG1-CB-CG2	-5.13	100.11	111.40
1	C	358	ILE	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	2758	0	2776	78	0
1	B	2758	0	2776	49	0
1	C	2758	0	2776	86	0
1	D	2758	0	2776	76	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	496	0	0	6	0
3	B	538	0	0	6	0
3	C	592	0	0	12	0
3	D	589	0	0	8	0
All	All	13287	0	11104	280	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 13.

All (280) 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:358:ILE:O	1:C:358:ILE:HG12	1.53	1.06
1:A:63:LEU:HD22	1:A:97:ILE:HD11	1.38	1.01
1:A:22:ILE:HG23	1:A:29:ILE:HD11	1.47	0.94
1:C:22:ILE:HG23	1:C:29:ILE:HD11	1.49	0.92
1:C:164:MET:HE3	1:C:165:GLU:HA	1.49	0.92
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.38	0.88
1:C:22:ILE:CG2	1:C:29:ILE:HD11	2.03	0.86
1:A:22:ILE:CG2	1:A:29:ILE:HD11	2.04	0.86
1:B:22:ILE:HG23	1:B:29:ILE:HD11	1.58	0.84
1:B:22:ILE:CG2	1:B:29:ILE:HD11	2.13	0.78
1:B:190:ILE:HD11	1:B:208:VAL:HG21	1.65	0.76
1:A:63:LEU:HD22	1:A:97:ILE:CD1	2.14	0.76
1:C:274:GLN:HB3	1:C:278:GLU:HG3	1.68	0.75
1:B:151:LEU:HB2	1:B:190:ILE:HD13	1.69	0.73
1:C:321:LYS:HA	1:C:321:LYS:HE3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:HE3	3:B:3054:HOH:O	1.89	0.73
1:A:60:GLN:HE22	1:A:88:ASP:H	1.37	0.72
1:D:63:LEU:HD22	1:D:97:ILE:HD11	1.72	0.71
1:A:341:LYS:HB3	1:A:351:ALA:O	1.89	0.71
1:A:39:ILE:HG13	1:A:43:LEU:HD23	1.71	0.70
1:A:60:GLN:NE2	1:A:88:ASP:H	1.90	0.70
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.07	0.70
1:D:277:GLU:O	1:D:281:ILE:HG12	1.92	0.69
1:C:153:ILE:HD11	1:C:204:VAL:HG11	1.74	0.69
1:A:185:ILE:HD13	1:A:227:LEU:HB2	1.74	0.69
1:B:153:ILE:HD12	1:B:204:VAL:HG21	1.74	0.68
1:A:163:ILE:HD12	1:A:208:VAL:HG22	1.75	0.68
1:B:155:GLU:O	1:C:2:HIS:HE1	1.76	0.68
1:C:95:GLN:HG2	3:C:3212:HOH:O	1.94	0.68
1:D:284:ASN:ND2	1:D:342:TYR:H	1.92	0.67
1:C:153:ILE:CD1	1:C:204:VAL:HG11	2.24	0.66
1:C:153:ILE:HD12	1:C:204:VAL:HG21	1.78	0.66
1:D:216:LEU:HA	1:D:221:ILE:HD13	1.78	0.65
1:C:358:ILE:CG1	1:C:358:ILE:O	2.40	0.65
1:A:200:ARG:HD2	3:D:3366:HOH:O	1.95	0.65
1:D:180:ASN:O	1:D:182:ILE:HD12	1.96	0.65
1:B:66:ASP:OD1	1:B:68:ARG:HD3	1.96	0.65
1:D:325:GLU:HG3	1:D:329:LYS:NZ	2.11	0.65
1:B:197:ASP:HB2	1:B:243:TYR:OH	1.97	0.65
1:C:146:LYS:HE2	1:C:187:GLU:OE1	1.97	0.64
1:C:288:LYS:HD3	3:C:3550:HOH:O	1.97	0.64
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.80	0.64
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.80	0.64
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.80	0.64
1:D:163:ILE:HD12	1:D:208:VAL:HG22	1.79	0.64
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.28	0.63
1:A:134:CYS:HB3	1:A:182:ILE:HD12	1.80	0.63
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.80	0.63
1:C:357:PHE:O	1:C:358:ILE:HG22	1.99	0.63
1:A:68:ARG:HG3	1:A:332:LEU:HD21	1.81	0.62
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.79	0.62
1:A:139:LYS:HB3	1:A:139:LYS:NZ	2.16	0.61
1:A:359:SER:O	1:A:360:ASN:HB3	2.00	0.61
1:B:194:GLY:H	1:B:237:HIS:CE1	2.18	0.61
1:D:321:LYS:HD3	1:D:321:LYS:C	2.21	0.61
1:C:106:ILE:HD13	1:C:107:LYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HG21	3:C:3275:HOH:O	2.02	0.60
1:A:185:ILE:HD11	1:A:227:LEU:HD12	1.83	0.60
3:A:3134:HOH:O	1:D:200:ARG:HD2	2.01	0.60
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.21	0.59
1:A:185:ILE:CD1	1:A:227:LEU:HD12	2.32	0.59
1:D:219:HIS:HB2	1:D:221:ILE:CD1	2.33	0.59
1:C:316:LYS:HD3	3:C:3557:HOH:O	2.02	0.59
1:A:29:ILE:HB	1:A:300:SER:HA	1.83	0.59
1:D:219:HIS:HB2	1:D:221:ILE:HD11	1.85	0.59
1:A:18:ILE:HD13	1:A:21:ARG:NH1	2.18	0.59
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.85	0.58
1:A:290:PRO:CG	1:A:356:LEU:O	2.52	0.58
1:C:250:MET:HE3	1:C:358:ILE:HG13	1.85	0.58
1:B:153:ILE:CD1	1:B:204:VAL:HG11	2.33	0.58
1:C:250:MET:CE	1:C:358:ILE:HG13	2.34	0.57
1:C:14:GLU:O	1:C:18:ILE:HG12	2.03	0.57
1:C:40:ALA:O	1:C:44:GLN:HG2	2.05	0.57
1:B:277:GLU:O	1:B:281:ILE:HG12	2.05	0.57
1:B:316:LYS:HB2	1:B:319:ASN:ND2	2.20	0.57
1:C:180:ASN:O	1:C:182:ILE:HD12	2.05	0.56
1:D:133:ARG:HD2	3:D:3398:HOH:O	2.04	0.56
1:A:199:LYS:HD3	3:A:3022:HOH:O	2.06	0.56
1:C:244:SER:OG	1:C:247:GLU:HG3	2.06	0.56
1:B:257:ARG:O	1:C:262:PRO:HD2	2.06	0.55
1:C:164:MET:CE	1:C:165:GLU:HA	2.31	0.55
1:A:339:GLN:CB	1:A:341:LYS:HZ3	2.12	0.55
1:A:13:LYS:HE3	1:A:17:ASP:OD1	2.07	0.55
1:C:221:ILE:HD12	1:C:221:ILE:N	2.22	0.55
1:B:291:LEU:O	1:B:293:LYS:HD3	2.06	0.55
1:C:219:HIS:HB2	1:C:221:ILE:CD1	2.37	0.55
1:B:153:ILE:HD11	1:B:204:VAL:HG11	1.89	0.54
1:C:190:ILE:HD11	1:C:208:VAL:HG21	1.88	0.54
1:A:290:PRO:HG3	1:A:356:LEU:O	2.06	0.54
1:D:356:LEU:HD22	1:D:356:LEU:N	2.23	0.54
1:B:155:GLU:HG3	3:B:3251:HOH:O	2.07	0.54
1:C:176:ILE:HD11	3:D:3208:HOH:O	2.08	0.54
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.42	0.54
1:D:325:GLU:HG3	1:D:329:LYS:HZ2	1.71	0.53
1:A:42:ARG:O	1:A:45:SER:HB3	2.08	0.53
1:C:29:ILE:HB	1:C:300:SER:HA	1.91	0.53
1:A:39:ILE:HG13	1:A:43:LEU:CD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HG3	3:A:3194:HOH:O	2.09	0.53
3:C:3463:HOH:O	1:D:110:LYS:HE3	2.08	0.53
1:D:63:LEU:HD22	1:D:97:ILE:CD1	2.39	0.53
1:A:358:ILE:HG22	1:A:359:SER:H	1.73	0.53
1:C:312:ALA:HB1	3:C:3552:HOH:O	2.09	0.53
1:C:234:THR:HB	1:C:235:PRO:HD2	1.91	0.53
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.43	0.52
1:C:277:GLU:O	1:C:281:ILE:HG12	2.09	0.52
1:D:221:ILE:HD12	1:D:221:ILE:N	2.23	0.52
1:C:311:LYS:HD3	3:C:3582:HOH:O	2.08	0.52
1:D:298:THR:OG1	1:D:299:PHE:N	2.43	0.52
1:D:250:MET:CE	1:D:291:LEU:HD11	2.39	0.52
1:A:70:ASN:HB2	1:A:71:PRO:HD3	1.92	0.52
1:B:29:ILE:HB	1:B:300:SER:HA	1.92	0.52
1:D:216:LEU:O	1:D:221:ILE:HD13	2.10	0.52
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.92	0.51
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.93	0.51
1:C:216:LEU:HA	1:C:221:ILE:HD13	1.93	0.51
1:A:246:GLU:HB3	1:A:358:ILE:CD1	2.41	0.51
1:C:324:GLN:O	1:C:328:VAL:HG23	2.11	0.51
1:D:312:ALA:HB3	1:D:323:ALA:HA	1.93	0.50
1:A:244:SER:OG	1:A:247:GLU:HG3	2.11	0.50
1:D:29:ILE:HB	1:D:300:SER:HA	1.92	0.50
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.93	0.50
1:C:151:LEU:HB2	1:C:190:ILE:HD13	1.92	0.50
1:A:60:GLN:HE22	1:A:88:ASP:N	2.07	0.50
1:C:134:CYS:HB3	1:C:182:ILE:HD13	1.92	0.50
1:C:164:MET:HE3	1:C:165:GLU:CA	2.30	0.50
1:A:172:ARG:O	1:A:176:ILE:HG12	2.12	0.50
1:C:291:LEU:O	1:C:293:LYS:HE2	2.12	0.49
1:D:145:ALA:O	1:D:185:ILE:HD13	2.12	0.49
1:B:293:LYS:HG2	1:B:297:LEU:CD1	2.40	0.49
1:D:293:LYS:HD2	1:D:297:LEU:HD12	1.95	0.49
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.11	0.49
1:D:63:LEU:HD13	1:D:97:ILE:HD11	1.94	0.49
1:B:199:LYS:HG3	3:B:3105:HOH:O	2.13	0.49
1:C:250:MET:HG2	1:C:363:TYR:CE2	2.48	0.48
1:D:93:PHE:O	1:D:97:ILE:HG12	2.13	0.48
1:B:276:GLU:CD	1:B:307:ALA:HB3	2.33	0.48
1:B:324:GLN:O	1:B:328:VAL:HG23	2.13	0.48
1:D:42:ARG:HH11	1:D:42:ARG:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:O	1:A:293:LYS:HD3	2.13	0.48
1:A:14:GLU:O	1:A:18:ILE:HG12	2.14	0.48
1:A:73:ILE:HD11	1:A:327:TYR:OH	2.14	0.48
1:C:216:LEU:O	1:C:221:ILE:HD13	2.14	0.48
1:B:41:LYS:HD3	3:B:3358:HOH:O	2.13	0.48
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.20	0.48
1:A:290:PRO:HG2	1:A:356:LEU:O	2.12	0.48
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.49	0.48
1:D:147:TRP:HB3	1:D:173:TYR:CE2	2.48	0.48
1:A:152:LYS:NZ	1:A:193:ASP:OD1	2.46	0.48
1:B:312:ALA:HB3	1:B:323:ALA:HA	1.96	0.48
1:A:185:ILE:CD1	1:A:227:LEU:HB2	2.42	0.47
1:D:40:ALA:O	1:D:44:GLN:HG3	2.13	0.47
1:A:341:LYS:CB	1:A:351:ALA:O	2.59	0.47
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.96	0.47
1:C:357:PHE:O	1:C:358:ILE:CG2	2.62	0.47
1:C:343:THR:C	1:C:345:SER:H	2.17	0.47
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.14	0.47
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.97	0.47
1:A:139:LYS:HZ3	1:A:139:LYS:HB3	1.79	0.47
1:C:219:HIS:HB2	1:C:221:ILE:HD11	1.96	0.47
1:A:117:GLY:HA2	1:B:4:HIS:O	2.15	0.47
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.96	0.47
1:A:73:ILE:CD1	1:A:327:TYR:OH	2.63	0.47
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.50	0.47
1:B:244:SER:O	1:B:248:ILE:HD13	2.15	0.46
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.50	0.46
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.51	0.46
1:C:53:GLU:HB2	3:C:3112:HOH:O	2.14	0.46
1:A:134:CYS:CB	1:A:182:ILE:HD12	2.45	0.46
1:B:92:PRO:HB2	1:B:94:PRO:HD2	1.98	0.46
1:A:176:ILE:HD11	3:B:3017:HOH:O	2.15	0.46
1:C:298:THR:OG1	1:C:299:PHE:N	2.49	0.46
1:A:294:PRO:HG2	1:D:262:PRO:CG	2.46	0.46
1:D:86:LYS:HG3	3:D:3392:HOH:O	2.15	0.46
1:C:358:ILE:HD12	3:C:3275:HOH:O	2.16	0.46
1:D:250:MET:HE1	1:D:291:LEU:HD11	1.97	0.45
1:D:49:GLU:HG3	1:D:51:THR:HG23	1.98	0.45
1:C:275:SER:H	1:C:278:GLU:CD	2.20	0.45
1:A:86:LYS:HD3	1:A:90:GLY:O	2.16	0.45
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLY:HA2	1:A:303:ARG:NH2	2.32	0.45
1:A:294:PRO:HG2	1:D:262:PRO:HG3	1.99	0.45
1:D:78:LEU:HD22	1:D:82:THR:HG21	1.98	0.45
1:D:163:ILE:CD1	1:D:208:VAL:HG22	2.46	0.45
1:C:59:ARG:O	1:C:63:LEU:HG	2.17	0.45
1:B:234:THR:HB	1:B:235:PRO:HD2	1.98	0.45
1:D:17:ASP:O	1:D:21:ARG:HG3	2.16	0.45
1:B:354:GLU:HG2	1:B:355:SER:N	2.31	0.45
1:A:59:ARG:O	1:A:63:LEU:HG	2.16	0.45
1:A:357:PHE:O	3:A:3306:HOH:O	2.21	0.44
1:B:316:LYS:HB2	1:B:319:ASN:HD22	1.80	0.44
1:A:234:THR:HB	1:A:235:PRO:HD2	1.99	0.44
1:C:2:HIS:HB3	3:C:3395:HOH:O	2.16	0.44
1:C:10:GLU:HG2	3:C:3270:HOH:O	2.17	0.44
1:B:42:ARG:HH21	1:B:303:ARG:HD3	1.81	0.44
1:B:316:LYS:HB3	1:B:318:GLU:OE1	2.16	0.44
1:A:61:LEU:HD23	1:A:61:LEU:C	2.38	0.44
3:A:3442:HOH:O	1:B:2:HIS:HD2	2.00	0.44
1:C:61:LEU:C	1:C:61:LEU:HD23	2.38	0.44
1:D:316:LYS:HB2	1:D:319:ASN:ND2	2.33	0.44
1:C:316:LYS:HD2	1:C:319:ASN:HD21	1.83	0.44
1:A:290:PRO:HG2	1:A:357:PHE:HA	1.99	0.44
1:A:325:GLU:HG2	3:A:3351:HOH:O	2.17	0.44
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.48	0.44
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.88	0.44
1:B:301:TYR:HA	3:B:3009[B]:HOH:O	2.17	0.44
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.53	0.43
1:B:46:ILE:HD13	1:B:310:LEU:HG	2.00	0.43
1:C:228:LEU:HG	1:C:230:PRO:HD3	2.00	0.43
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.99	0.43
1:D:138:LYS:HB2	1:D:182:ILE:HD11	2.00	0.43
1:D:152:LYS:HE2	3:D:3429:HOH:O	2.17	0.43
1:D:95:GLN:HG3	3:D:3050:HOH:O	2.17	0.43
1:A:262:PRO:HD2	1:D:257:ARG:O	2.19	0.43
1:C:18:ILE:CD1	1:C:21:ARG:HH22	2.31	0.43
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.00	0.43
1:A:292:LEU:C	1:A:292:LEU:HD23	2.39	0.43
1:A:60:GLN:NE2	1:A:88:ASP:N	2.63	0.43
1:A:139:LYS:NZ	1:A:139:LYS:CB	2.80	0.43
1:D:199:LYS:HG3	3:D:3167:HOH:O	2.17	0.43
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLU:OE2	1:D:307:ALA:HB3	2.17	0.42
1:C:293:LYS:HD2	1:C:297:LEU:HD12	2.00	0.42
1:C:301:TYR:HB3	1:C:304:ALA:HB3	2.00	0.42
1:C:164:MET:HG3	1:C:165:GLU:N	2.34	0.42
1:D:321:LYS:HD3	1:D:321:LYS:O	2.19	0.42
1:D:144:PHE:HD2	1:D:185:ILE:HD13	1.83	0.42
1:D:234:THR:HB	1:D:235:PRO:HD2	2.00	0.42
1:D:284:ASN:HD21	1:D:342:TYR:H	1.64	0.42
1:B:329:LYS:HB2	1:B:329:LYS:HE3	1.87	0.42
1:D:59:ARG:O	1:D:63:LEU:HG	2.20	0.42
1:C:276:GLU:CD	1:C:307:ALA:HB3	2.40	0.42
1:D:158:PRO:CG	1:D:163:ILE:HD11	2.49	0.42
1:A:313:TRP:CZ2	1:A:315:GLY:HA2	2.55	0.42
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.55	0.42
1:D:303:ARG:HD2	1:D:356:LEU:HB3	2.02	0.42
1:C:155:GLU:HA	1:C:155:GLU:OE1	2.20	0.42
1:A:163:ILE:CD1	1:A:208:VAL:HG22	2.47	0.42
1:D:164:MET:SD	1:D:164:MET:C	2.98	0.42
1:A:60:GLN:HE21	1:A:87:ALA:HB1	1.84	0.41
1:B:281:ILE:HD11	1:B:344:PRO:HB3	2.01	0.41
1:C:322:ALA:HB1	3:C:3552:HOH:O	2.19	0.41
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.01	0.41
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.20	0.41
1:A:268:THR:HB	1:A:300:SER:HB2	2.01	0.41
1:A:293:LYS:HE2	1:A:293:LYS:HB2	1.94	0.41
1:D:43:LEU:HD13	1:D:50:ASN:HA	2.01	0.41
1:C:18:ILE:HD13	1:C:21:ARG:HH22	1.85	0.41
1:D:318:GLU:OE1	1:D:318:GLU:N	2.50	0.41
1:B:33:ASP:HB3	1:B:77:ILE:HG22	2.02	0.41
1:C:106:ILE:C	1:C:106:ILE:HD13	2.41	0.41
1:C:106:ILE:HD12	1:C:137:TYR:CE2	2.56	0.41
1:C:343:THR:C	1:C:345:SER:N	2.73	0.41
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.93	0.41
1:B:164:MET:C	1:B:164:MET:SD	2.98	0.41
1:C:176:ILE:CD1	3:D:3208:HOH:O	2.67	0.41
1:C:93:PHE:N	1:C:94:PRO:CD	2.84	0.41
1:A:121:GLU:OE2	1:A:158:PRO:HA	2.21	0.41
1:C:92:PRO:HD2	1:C:95:GLN:HG3	2.02	0.41
1:D:43:LEU:CD1	1:D:50:ASN:HA	2.50	0.41
1:A:312:ALA:HB3	1:A:323:ALA:HA	2.01	0.41
1:A:229:LYS:HG3	1:A:268:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.02	0.41
1:D:61:LEU:HD23	1:D:61:LEU:C	2.41	0.41
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.20	0.41
1:C:357:PHE:C	1:C:358:ILE:CG2	2.89	0.41
1:D:250:MET:CE	1:D:291:LEU:CD1	2.99	0.41
1:C:222:TYR:O	1:C:226:THR:HG23	2.21	0.41
1:C:42:ARG:HH21	1:C:303:ARG:HD3	1.86	0.41
1:D:219:HIS:CB	1:D:221:ILE:HD11	2.48	0.41
1:C:36:THR:HA	1:C:39:ILE:HG22	2.02	0.40
1:D:293:LYS:HA	1:D:294:PRO:HD2	1.97	0.40
1:B:194:GLY:H	1:B:237:HIS:HE1	1.66	0.40
1:D:185:ILE:HD12	1:D:185:ILE:N	2.36	0.40
1:D:231:ASN:H	1:D:231:ASN:ND2	2.18	0.40
1:C:185:ILE:N	1:C:185:ILE:HD12	2.36	0.40
1:D:18:ILE:HD13	1:D:143:ASP:HB3	2.03	0.40
1:A:67:ASP:HA	1:A:70:ASN:OD1	2.21	0.40
1:D:233:VAL:CG2	1:D:252:THR:HA	2.51	0.40
1:C:145:ALA:O	1:C:185:ILE:HD13	2.22	0.40
1:C:117:GLY:HA2	1:D:4:HIS:O	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	361/363 (99%)	342 (95%)	15 (4%)	4 (1%)	17	6
1	B	361/363 (99%)	341 (94%)	15 (4%)	5 (1%)	14	4
1	C	361/363 (99%)	337 (93%)	19 (5%)	5 (1%)	14	4
1	D	361/363 (99%)	346 (96%)	12 (3%)	3 (1%)	24	11
All	All	1444/1452 (99%)	1366 (95%)	61 (4%)	17 (1%)	16	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	ILE
1	C	352	ALA
1	C	358	ILE
1	B	344	PRO
1	B	349	GLY
1	C	351	ALA
1	A	5	PRO
1	B	5	PRO
1	C	188	PRO
1	A	356	LEU
1	B	188	PRO
1	D	67	ASP
1	D	188	PRO
1	A	188	PRO
1	C	5	PRO
1	D	5	PRO
1	A	272	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	291/291 (100%)	286 (98%)	5 (2%)	68	64
1	B	291/291 (100%)	287 (99%)	4 (1%)	74	71
1	C	291/291 (100%)	282 (97%)	9 (3%)	47	37
1	D	291/291 (100%)	285 (98%)	6 (2%)	61	55
All	All	1164/1164 (100%)	1140 (98%)	24 (2%)	61	55

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

Mol	Chain	Res	Type
1	A	173	TYR
1	A	295	TRP
1	A	318	GLU

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Mol	Chain	Res	Type
1	A	356	LEU
1	A	359	SER
1	B	119	ASN
1	B	173	TYR
1	B	295	TRP
1	B	347	GLN
1	C	59	ARG
1	C	106	ILE
1	C	164	MET
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
1	C	321	LYS
1	C	357	PHE
1	C	358	ILE
1	D	59	ARG
1	D	66	ASP
1	D	173	TYR
1	D	193	ASP
1	D	230	PRO
1	D	295	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	220	HIS
1	A	241	GLN
1	A	245	HIS
1	A	339	GLN
1	B	54	ASN
1	B	95	GLN
1	B	119	ASN
1	B	237	HIS
1	B	319	ASN
1	B	361	HIS
1	C	2	HIS
1	C	4	HIS
1	C	54	ASN
1	C	237	HIS
1	C	241	GLN
1	C	245	HIS

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Mol	Chain	Res	Type
1	C	319	ASN
1	D	44	GLN
1	D	54	ASN
1	D	85	GLN
1	D	180	ASN
1	D	231	ASN
1	D	241	GLN
1	D	284	ASN
1	D	319	ASN
1	D	360	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	3001[A]	-	4,4,4	1.13	0	6,6,6	0.27	0
2	PO4	A	3002[A]	-	4,4,4	1.16	0	6,6,6	0.27	0
2	PO4	B	3003[A]	-	4,4,4	1.12	0	6,6,6	0.27	0
2	PO4	B	3004[A]	-	4,4,4	1.12	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	C	3005[A]	-	4,4,4	1.14	0	6,6,6	0.27	0
2	PO4	C	3006[A]	-	4,4,4	1.13	0	6,6,6	0.27	0
2	PO4	D	3007[A]	-	4,4,4	1.14	0	6,6,6	0.27	0
2	PO4	D	3008[A]	-	4,4,4	1.15	0	6,6,6	0.27	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[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	A	3002[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	B	3003[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	B	3004[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3005[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3006[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3007[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3008[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	363/363 (100%)	0.17	18 (4%)	32	35	11, 22, 52, 79	16 (4%)
1	B	363/363 (100%)	0.14	18 (4%)	32	35	12, 23, 56, 79	16 (4%)
1	C	363/363 (100%)	0.38	24 (6%)	22	24	13, 24, 54, 77	16 (4%)
1	D	363/363 (100%)	0.20	26 (7%)	18	20	12, 25, 66, 103	4 (1%)
All	All	1452/1452 (100%)	0.22	86 (5%)	26	29	11, 23, 59, 103	52 (3%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	358	ILE	30.5
1	B	350	ALA	30.1
1	A	350	ALA	25.1
1	A	356	LEU	20.8
1	C	357	PHE	20.7
1	A	355	SER	18.9
1	D	362	ALA	18.7
1	A	351	ALA	16.6
1	C	352	ALA	15.5
1	B	358	ILE	15.1
1	A	353	SER	14.6
1	C	348	ALA	14.5
1	D	363	TYR	14.3
1	A	357	PHE	14.1
1	B	357	PHE	14.0
1	C	356	LEU	13.5
1	B	352	ALA	13.5
1	C	355	SER	13.4
1	A	352	ALA	13.1
1	A	354	GLU	13.0
1	B	356	LEU	12.8

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Mol	Chain	Res	Type	RSRZ
1	B	353	SER	12.2
1	B	349	GLY	10.9
1	C	354	GLU	10.6
1	D	361	HIS	9.9
1	D	348	ALA	9.8
1	C	350	ALA	8.4
1	B	354	GLU	8.3
1	B	351	ALA	8.3
1	C	349	GLY	8.0
1	A	358	ILE	8.0
1	C	351	ALA	7.4
1	D	358	ILE	7.3
1	A	347	GLN	7.1
1	D	349	GLY	6.9
1	C	353	SER	6.7
1	A	346	GLY	6.4
1	B	348	ALA	6.3
1	C	346	GLY	6.3
1	D	356	LEU	6.2
1	A	348	ALA	6.2
1	C	345	SER	6.1
1	B	345	SER	6.1
1	B	355	SER	6.0
1	D	353	SER	5.9
1	B	344	PRO	5.8
1	D	345	SER	5.7
1	D	360	ASN	5.3
1	D	359	SER	5.2
1	D	347	GLN	5.0
1	A	349	GLY	4.9
1	A	359	SER	4.9
1	B	347	GLN	4.9
1	D	355	SER	4.8
1	A	345	SER	4.8
1	C	344	PRO	4.7
1	D	350	ALA	4.6
1	D	352	ALA	4.4
1	D	344	PRO	4.4
1	D	357	PHE	4.1
1	C	44	GLN	3.8
1	D	346	GLY	3.7
1	B	359	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	45	SER	3.4
1	C	359	SER	3.4
1	A	344	PRO	3.3
1	B	346	GLY	3.2
1	A	360	ASN	3.2
1	D	46	ILE	3.1
1	C	347	GLN	2.8
1	D	44	GLN	2.7
1	C	315	GLY	2.7
1	C	321	LYS	2.7
1	D	354	GLU	2.7
1	C	343	THR	2.6
1	A	44	GLN	2.6
1	C	360	ASN	2.6
1	D	155	GLU	2.4
1	D	42	ARG	2.3
1	D	281	ILE	2.3
1	D	40	ALA	2.2
1	B	46	ILE	2.2
1	C	36	THR	2.2
1	C	362	ALA	2.1
1	D	278	GLU	2.1
1	C	342	TYR	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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	3002[A]	5/5	0.89	0.20	6.80	45,45,45,45	5
2	PO4	C	3006[A]	5/5	0.88	0.17	3.56	41,41,42,43	5
2	PO4	B	3004[A]	5/5	0.90	0.10	1.40	52,53,53,54	5
2	PO4	B	3003[A]	5/5	0.85	0.11	0.88	37,39,40,40	5
2	PO4	C	3005[A]	5/5	0.91	0.11	-0.00	37,38,39,40	5
2	PO4	A	3001[A]	5/5	0.93	0.08	-0.18	33,33,35,35	5
2	PO4	D	3008[A]	5/5	0.95	0.09	-0.29	41,42,42,42	5
2	PO4	D	3007[A]	5/5	0.96	0.08	-0.96	24,25,27,27	5

## 6.5 Other polymers

There are no such residues in this entry.