



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1ADO  
Title : FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM RABBIT MUSCLE  
Authors : Blom, N.S.; Sygusch, J.  
Deposited on : 1996-12-02  
Resolution : 1.90 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

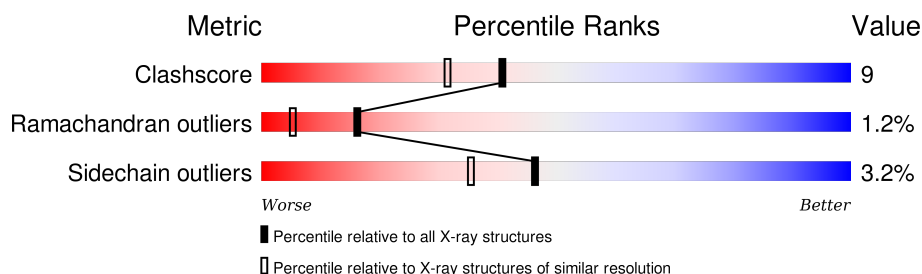
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16926 atoms, of which 2570 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 ALDOLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	H	N	O	S	0	0	0
			3398	1731	641	489	526	11			
1	B	363	Total	C	H	N	O	S	0	0	0
			3398	1731	641	489	526	11			
1	C	363	Total	C	H	N	O	S	0	0	0
			3398	1731	641	489	526	11			
1	D	363	Total	C	H	N	O	S	0	0	0
			3398	1731	641	489	526	11			

There are 4 discrepancies between the modelled and reference sequences:

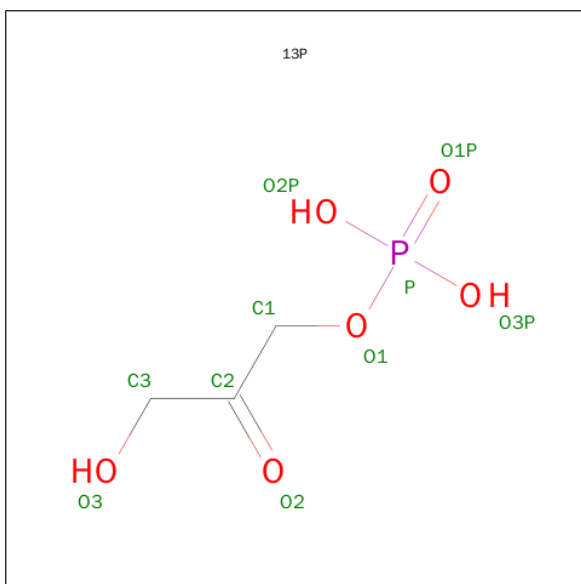
Chain	Residue	Modelled	Actual	Comment	Reference
A	344	SER	PRO	CONFLICT	UNP P00883
B	344	SER	PRO	CONFLICT	UNP P00883
C	344	SER	PRO	CONFLICT	UNP P00883
D	344	SER	PRO	CONFLICT	UNP P00883

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 3 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula:  $C_3H_7O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	1
			24	6	4	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	O	P	0	0
			12	3	2	6	1		

- Molecule 4 is water.

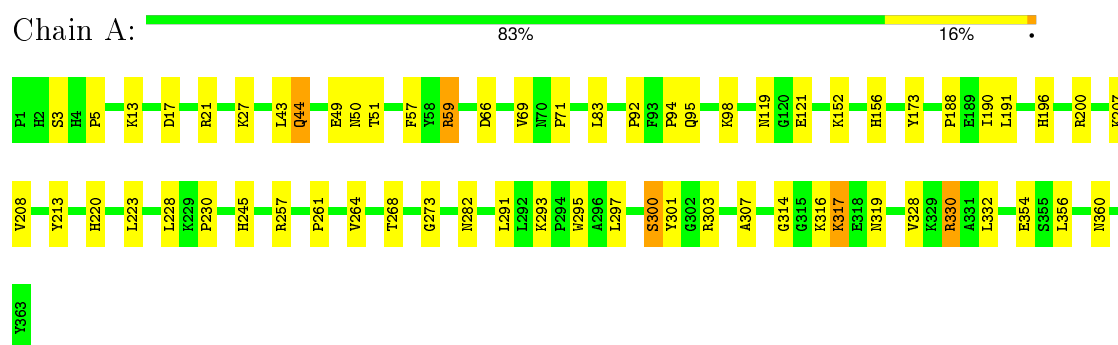
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	762	Total	O	0	0
			762	762		
4	B	682	Total	O	0	0
			682	682		
4	C	953	Total	O	0	0
			953	953		
4	D	891	Total	O	0	0
			891	891		

### 3 Residue-property plots

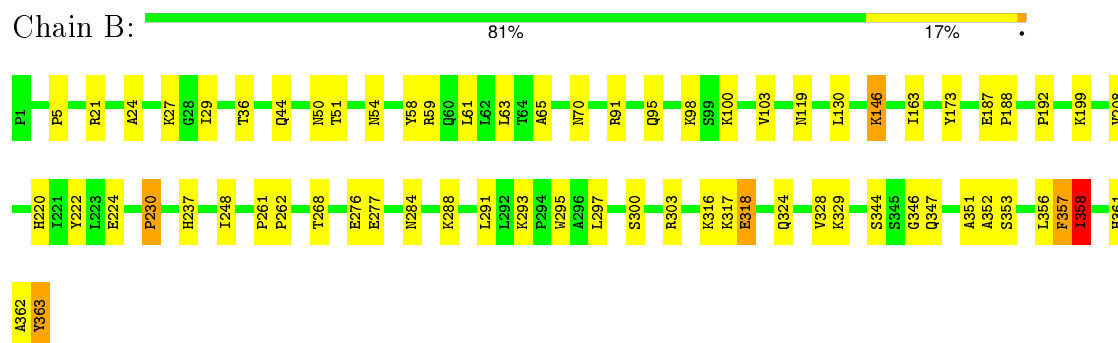
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

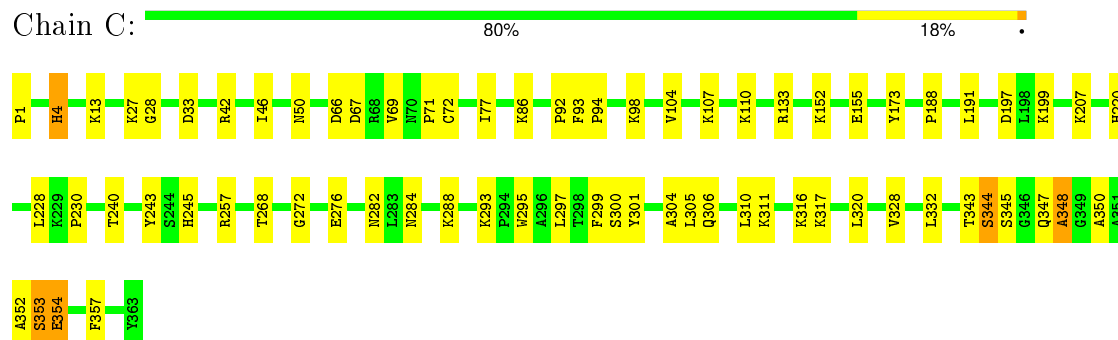
#### • Molecule 1: ALDOLASE




#### • Molecule 1: ALDOLASE

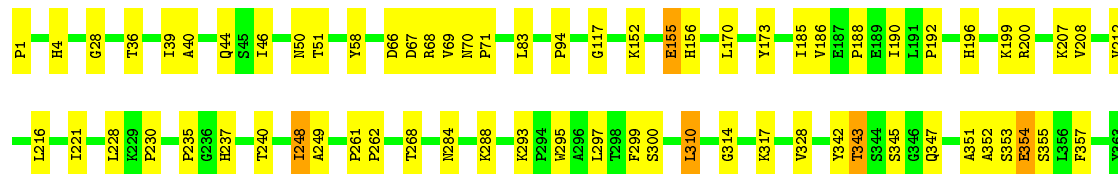


#### • Molecule 1: ALDOLASE



● Molecule 1: ALDOLASE

Chain D:  81% 18%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.88Å 57.47Å 85.03Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	12.00 – 1.90	Depositor
% Data completeness (in resolution range)	85.2 (12.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.162 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 13P, SO4

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	0/2810	0.61	1/3806 (0.0%)
1	B	0.36	0/2810	0.63	1/3806 (0.0%)
1	C	0.35	0/2810	0.62	1/3806 (0.0%)
1	D	0.35	0/2810	0.60	0/3806
All	All	0.35	0/11240	0.61	3/15224 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	SER	N-CA-C	-5.79	95.35	111.00
1	A	300	SER	N-CA-C	-5.35	96.56	111.00
1	B	356	LEU	CA-CB-CG	5.21	127.27	115.30

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	2757	641	2774	42	0
1	B	2757	641	2774	42	0
1	C	2757	641	2774	57	0
1	D	2757	641	2774	56	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	4	10	2	0
3	B	10	2	5	1	0
4	A	762	0	0	12	0
4	B	682	0	0	13	1
4	C	953	0	0	27	1
4	D	891	0	0	30	0
All	All	14356	2570	11111	191	1

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 9.

All (191) 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:D:170:LEU:HB3	4:D:1994:HOH:O	1.75	0.86
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.64	0.80
1:A:264:VAL:HG23	4:A:1314:HOH:O	1.83	0.78
1:D:208:VAL:HG13	4:D:2108:HOH:O	1.83	0.77
1:D:353:SER:HA	4:D:2066:HOH:O	1.89	0.72
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.71	0.71
1:C:301:TYR:HB2	1:C:305:LEU:HG	1.73	0.70
1:C:152:LYS:HD2	4:C:1472:HOH:O	1.93	0.69
1:D:343:THR:HG22	1:D:347:GLN:HA	1.76	0.68
1:D:314:GLY:HA2	4:D:1368:HOH:O	1.92	0.68
1:B:51:THR:HG23	1:B:54:ASN:H	1.59	0.67
1:A:354:GLU:HA	4:A:1196:HOH:O	1.94	0.67
1:C:245:HIS:HE1	1:C:348:ALA:HB2	1.58	0.67
1:D:248:ILE:HG22	4:D:2028:HOH:O	1.94	0.67
1:C:245:HIS:CE1	1:C:348:ALA:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.76	0.66
1:D:67:ASP:HB2	4:D:1784:HOH:O	1.96	0.65
1:A:121:GLU:HA	4:A:1773:HOH:O	1.96	0.65
1:C:94:PRO:O	1:C:98:LYS:HG3	1.96	0.65
1:C:86:LYS:HE3	4:C:2245:HOH:O	1.97	0.64
1:C:199:LYS:HE3	4:C:1590:HOH:O	1.96	0.64
1:D:185:ILE:HD13	4:D:1981:HOH:O	1.96	0.64
1:C:245:HIS:HB2	4:C:1418:HOH:O	1.98	0.63
1:B:146:LYS:HD3	1:B:187:GLU:OE1	1.98	0.63
1:C:13:LYS:HE2	4:C:1534:HOH:O	2.00	0.62
1:B:163:ILE:HG21	4:B:1131:HOH:O	1.99	0.62
1:B:248:ILE:HD11	4:B:1223:HOH:O	1.98	0.62
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.80	0.61
1:C:317:LYS:HD2	4:C:2047:HOH:O	2.00	0.61
1:A:356:LEU:HD23	4:A:1457:HOH:O	2.00	0.61
1:A:190:ILE:HD11	1:A:208:VAL:HG21	1.83	0.61
1:A:17:ASP:O	1:A:21:ARG:HG3	2.01	0.61
1:B:70:ASN:OD1	1:B:100:LYS:HE2	2.00	0.61
1:D:208:VAL:HG21	4:D:1990:HOH:O	2.00	0.61
1:C:240:THR:HG22	1:C:357:PHE:O	2.01	0.61
1:D:66:ASP:O	1:D:69:VAL:HG22	2.01	0.61
1:C:110:LYS:HE2	4:C:1629:HOH:O	2.02	0.60
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.32	0.60
1:C:305:LEU:HD22	4:C:1496:HOH:O	2.01	0.59
1:A:261:PRO:HB2	4:A:1314:HOH:O	2.02	0.59
1:D:83:LEU:HD12	1:D:94:PRO:HG3	1.84	0.59
1:C:66:ASP:HB3	4:C:2203:HOH:O	2.03	0.58
1:D:212:VAL:HG13	4:D:1613:HOH:O	2.02	0.58
1:B:237:HIS:HD2	4:B:1221:HOH:O	1.85	0.58
1:B:276:GLU:HB2	1:B:351:ALA:HB2	1.86	0.57
1:B:344:SER:HA	4:B:1622:HOH:O	2.04	0.57
1:B:291:LEU:O	1:B:293:LYS:HD3	2.04	0.57
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.87	0.56
1:A:291:LEU:O	1:A:293:LYS:HD3	2.06	0.56
1:A:303:ARG:HG2	3:A:1104[A]:13P:H11	1.87	0.56
1:A:66:ASP:O	1:A:69:VAL:HG22	2.05	0.56
1:D:352:ALA:HA	4:D:1618:HOH:O	2.04	0.56
1:D:196:HIS:HB2	1:D:200:ARG:HG2	1.88	0.56
1:D:199:LYS:HE3	4:D:1733:HOH:O	2.06	0.55
1:C:104:VAL:HG12	4:C:1655:HOH:O	2.06	0.55
1:B:329:LYS:HE2	4:B:1366:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LEU:HD23	4:C:1992:HOH:O	2.06	0.55
1:D:4:HIS:HD2	4:D:1315:HOH:O	1.90	0.55
1:C:348:ALA:HA	4:C:2121:HOH:O	2.07	0.55
1:A:57:PHE:CE1	1:A:317:LYS:HE2	2.42	0.55
1:D:355:SER:HA	4:D:2000:HOH:O	2.06	0.55
1:B:208:VAL:HG13	4:B:1092:HOH:O	2.06	0.55
1:C:284:ASN:ND2	1:C:288:LYS:HE2	2.22	0.55
1:C:268:THR:HB	1:C:300:SER:HB2	1.89	0.54
1:B:268:THR:HB	1:B:300:SER:HB2	1.89	0.54
1:D:46:ILE:HG21	1:D:310:LEU:HD13	1.89	0.54
1:A:307:ALA:HB2	4:A:1800:HOH:O	2.07	0.54
1:D:317:LYS:HD2	4:D:1968:HOH:O	2.07	0.54
1:D:240:THR:HG22	1:D:357:PHE:O	2.08	0.54
1:D:235:PRO:HD3	4:D:2028:HOH:O	2.08	0.54
1:A:268:THR:HB	1:A:300:SER:HB2	1.89	0.54
1:C:276:GLU:HG2	1:C:304:ALA:O	2.08	0.53
1:C:354:GLU:HB3	4:C:1671:HOH:O	2.07	0.53
1:A:316:LYS:HE3	1:A:319:ASN:OD1	2.09	0.53
1:D:186:VAL:HG13	4:D:1994:HOH:O	2.07	0.53
1:A:196:HIS:HB2	1:A:200:ARG:HG2	1.91	0.53
1:D:44:GLN:HB2	4:D:1351:HOH:O	2.08	0.53
1:D:355:SER:HB3	4:D:1754:HOH:O	2.09	0.53
1:A:59:ARG:HG3	4:A:1666:HOH:O	2.08	0.53
1:D:354:GLU:HG3	4:D:1375:HOH:O	2.09	0.53
1:A:43:LEU:HD12	1:A:50:ASN:HA	1.91	0.53
1:B:36:THR:HG22	1:B:50:ASN:HD21	1.74	0.52
1:B:346:GLY:HA2	4:B:1680:HOH:O	2.09	0.52
1:B:358:ILE:HG23	4:B:1653:HOH:O	2.10	0.52
1:B:303:ARG:HB2	3:B:1053:13P:H12	1.91	0.52
1:B:59:ARG:O	1:B:63:LEU:HD13	2.10	0.51
1:A:94:PRO:O	1:A:98:LYS:HG3	2.10	0.51
1:C:42:ARG:NH2	1:C:306:GLN:OE1	2.44	0.51
1:A:156:HIS:HB3	4:A:1809:HOH:O	2.11	0.51
1:D:155:GLU:HG2	1:D:156:HIS:CD2	2.46	0.51
1:B:199:LYS:HE3	4:B:1124:HOH:O	2.10	0.51
1:A:152:LYS:HG2	1:A:191:LEU:HD12	1.92	0.51
1:D:310:LEU:HB2	4:D:1707:HOH:O	2.10	0.51
1:B:284:ASN:O	1:B:288:LYS:HG2	2.12	0.50
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.94	0.50
1:D:190:ILE:HG12	4:D:1990:HOH:O	2.10	0.50
1:C:293:LYS:HD2	1:C:297:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:HB	1:D:300:SER:HB2	1.93	0.50
1:B:21:ARG:NH2	1:B:103:VAL:HG22	2.26	0.50
1:C:4:HIS:O	1:D:117:GLY:HA2	2.12	0.49
1:D:248:ILE:HG13	1:D:249:ALA:N	2.27	0.49
1:C:92:PRO:HG2	4:C:2168:HOH:O	2.13	0.49
1:C:50:ASN:N	4:C:2021:HOH:O	2.46	0.49
1:A:223:LEU:HD13	4:A:1314:HOH:O	2.13	0.48
1:B:362:ALA:O	1:B:363:TYR:HB2	2.14	0.48
1:C:345:SER:HB2	4:C:2220:HOH:O	2.14	0.48
1:B:24:ALA:HB3	1:B:27:LYS:HD2	1.94	0.48
1:C:344:SER:HB3	4:C:1370:HOH:O	2.14	0.47
1:B:91:ARG:HG2	1:B:95:GLN:OE1	2.14	0.47
1:B:276:GLU:HB2	1:B:351:ALA:CB	2.43	0.47
1:D:69:VAL:HG13	1:D:328:VAL:HG22	1.97	0.47
1:C:133:ARG:HD3	4:C:1832:HOH:O	2.14	0.47
1:D:284:ASN:ND2	1:D:342:TYR:H	2.13	0.47
1:A:273:GLY:HA2	1:A:303:ARG:HE	1.78	0.47
1:C:67:ASP:HB2	4:C:1647:HOH:O	2.13	0.47
1:C:316:LYS:HD3	4:C:1518:HOH:O	2.14	0.47
1:D:46:ILE:CG2	1:D:310:LEU:HD13	2.44	0.46
1:D:216:LEU:HD22	1:D:221:ILE:HG13	1.97	0.46
1:C:72:CYS:SG	1:C:332:LEU:HD23	2.55	0.46
1:B:65:ALA:O	1:B:100:LYS:NZ	2.43	0.46
1:C:50:ASN:HB2	4:C:2021:HOH:O	2.14	0.46
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.16	0.46
1:C:352:ALA:HB2	4:C:1941:HOH:O	2.15	0.46
1:C:46:ILE:HG21	1:C:310:LEU:HG	1.98	0.46
1:A:200:ARG:NH1	1:D:1:PRO:O	2.49	0.46
1:A:3:SER:HB3	4:A:1388:HOH:O	2.15	0.46
1:A:57:PHE:HE1	1:A:317:LYS:HE2	1.81	0.45
1:B:277:GLU:H	1:B:351:ALA:CB	2.30	0.45
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.99	0.45
1:C:245:HIS:HE1	1:C:347:GLN:O	1.99	0.45
1:D:288:LYS:HD2	4:D:1449:HOH:O	2.17	0.45
1:C:77:ILE:HG23	4:C:2190:HOH:O	2.16	0.45
1:A:190:ILE:HD11	1:A:208:VAL:CG2	2.47	0.44
1:D:155:GLU:HG2	1:D:156:HIS:CG	2.52	0.44
1:B:293:LYS:HG2	1:B:297:LEU:CD1	2.46	0.44
1:D:68:ARG:O	1:D:71:PRO:HD2	2.18	0.44
1:D:317:LYS:HD3	4:D:1803:HOH:O	2.17	0.44
1:B:316:LYS:HE2	1:B:318:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:TYR:HE2	4:D:1324:HOH:O	1.99	0.44
1:A:330:ARG:HD2	1:A:330:ARG:HA	1.74	0.44
1:A:92:PRO:HD2	1:A:95:GLN:HG3	2.00	0.44
1:C:69:VAL:HG13	1:C:328:VAL:HG22	2.00	0.44
1:A:356:LEU:HD13	4:A:1461:HOH:O	2.18	0.44
1:D:40:ALA:HB2	1:D:50:ASN:ND2	2.33	0.44
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.53	0.44
1:B:262:PRO:HD2	1:C:257:ARG:O	2.18	0.44
1:B:324:GLN:O	1:B:328:VAL:HG23	2.18	0.43
1:A:44:GLN:HG3	4:A:1691:HOH:O	2.16	0.43
4:B:1724:HOH:O	1:C:1:PRO:HB2	2.18	0.43
1:D:355:SER:HA	4:D:1753:HOH:O	2.19	0.43
1:A:257:ARG:O	1:D:262:PRO:HD2	2.18	0.43
1:D:186:VAL:HG22	4:D:1994:HOH:O	2.19	0.43
1:D:351:ALA:HB3	4:D:1434:HOH:O	2.18	0.43
1:C:93:PHE:N	1:C:94:PRO:HD2	2.34	0.43
1:C:199:LYS:HA	1:C:199:LYS:HD3	1.80	0.43
1:A:95:GLN:HA	1:A:95:GLN:HE21	1.83	0.43
1:B:58:TYR:O	1:B:61:LEU:HB3	2.19	0.43
1:C:27:LYS:HG2	1:C:71:PRO:O	2.18	0.43
1:B:98:LYS:HG2	4:B:1259:HOH:O	2.17	0.43
1:C:220:HIS:HE1	4:D:1544:HOH:O	2.01	0.43
1:B:293:LYS:HE2	1:B:293:LYS:HB2	1.84	0.43
1:A:207:LYS:HD2	4:D:1668:HOH:O	2.19	0.43
1:C:207:LYS:HD2	4:C:1335:HOH:O	2.18	0.43
1:C:311:LYS:HD2	4:C:1805:HOH:O	2.19	0.42
1:D:152:LYS:HE2	4:D:1789:HOH:O	2.18	0.42
1:D:293:LYS:HD3	1:D:297:LEU:CD1	2.49	0.42
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.17	0.42
1:B:29:ILE:HB	1:B:300:SER:HA	2.01	0.42
1:A:301:TYR:HA	3:A:1104[A]:13P:O2P	2.20	0.42
1:D:192:PRO:HB2	1:D:237:HIS:CD2	2.55	0.42
1:B:220:HIS:HD2	1:C:207:LYS:NZ	2.18	0.42
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.55	0.42
1:C:343:THR:O	1:C:344:SER:HB2	2.20	0.41
1:B:222:TYR:CZ	1:B:224:GLU:HB2	2.55	0.41
1:C:350:ALA:HB3	4:C:1446:HOH:O	2.21	0.41
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.56	0.41
1:B:261:PRO:HA	1:B:262:PRO:HD3	1.94	0.41
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.55	0.41
1:B:357:PHE:CD1	1:B:357:PHE:C	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:332:LEU:HG	2.21	0.41
1:D:70:ASN:HB2	1:D:71:PRO:HD3	2.02	0.41
1:C:245:HIS:CB	4:C:1418:HOH:O	2.64	0.41
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.03	0.40
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.97	0.40
1:B:21:ARG:HD2	4:B:1313:HOH:O	2.20	0.40
1:B:95:GLN:HG3	4:B:1382:HOH:O	2.21	0.40
1:D:36:THR:HA	1:D:39:ILE:HG22	2.02	0.40
1:A:27:LYS:HG2	1:A:71:PRO:O	2.21	0.40
1:C:245:HIS:HD2	1:C:282:ASN:OD1	2.05	0.40
1:B:192:PRO:HB2	1:B:237:HIS:CD2	2.56	0.40
1:C:33:ASP:HB3	1:C:77:ILE:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1319:HOH:O	4:C:1454:HOH:O[2_645]	2.16	0.04

## 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%)	341 (94%)	16 (4%)	4 (1%)	17	6
1	B	361/363 (99%)	343 (95%)	12 (3%)	6 (2%)	11	2
1	C	361/363 (99%)	337 (93%)	19 (5%)	5 (1%)	14	4
1	D	361/363 (99%)	345 (96%)	14 (4%)	2 (1%)	30	17
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	352	ALA
1	B	353	SER
1	B	358	ILE
1	C	348	ALA
1	C	354	GLU
1	A	360	ASN
1	C	344	SER
1	D	354	GLU
1	A	5	PRO
1	A	188	PRO
1	B	188	PRO
1	C	272	GLY
1	D	188	PRO
1	A	314	GLY
1	B	5	PRO
1	C	188	PRO
1	B	230	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/291 (100%)	283 (97%)	8 (3%)	52	43
1	B	291/291 (100%)	277 (95%)	14 (5%)	31	19
1	C	291/291 (100%)	284 (98%)	7 (2%)	57	49
1	D	291/291 (100%)	283 (97%)	8 (3%)	52	43
All	All	1164/1164 (100%)	1127 (97%)	37 (3%)	46	35

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	44	GLN
1	A	59	ARG
1	A	119	ASN
1	A	173	TYR

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Mol	Chain	Res	Type
1	A	295	TRP
1	A	317	LYS
1	A	330	ARG
1	B	44	GLN
1	B	119	ASN
1	B	130	LEU
1	B	146	LYS
1	B	173	TYR
1	B	230	PRO
1	B	295	TRP
1	B	317	LYS
1	B	318	GLU
1	B	347	GLN
1	B	357	PHE
1	B	358	ILE
1	B	361	HIS
1	B	363	TYR
1	C	4	HIS
1	C	107	LYS
1	C	155	GLU
1	C	173	TYR
1	C	191	LEU
1	C	295	TRP
1	C	353	SER
1	D	51	THR
1	D	155	GLU
1	D	173	TYR
1	D	248	ILE
1	D	295	TRP
1	D	310	LEU
1	D	343	THR
1	D	345	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	119	ASN
1	A	220	HIS
1	A	241	GLN
1	A	245	HIS
1	B	44	GLN

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Mol	Chain	Res	Type
1	B	119	ASN
1	B	179	GLN
1	B	220	HIS
1	B	237	HIS
1	C	220	HIS
1	C	241	GLN
1	C	245	HIS
1	C	361	HIS
1	D	85	GLN
1	D	241	GLN
1	D	284	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](#)

5 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
3	13P	A	1104[A]	-	9,9,9	1.86	2 (22%)	9,12,12	2.07	2 (22%)
3	13P	A	1104[B]	-	9,9,9	1.19	1 (11%)	9,12,12	1.42	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	13P	B	1053	-	9,9,9	1.06	1 (11%)	9,12,12	1.07	1 (11%)
2	SO4	C	1326	-	4,4,4	1.55	0	6,6,6	0.78	0
2	SO4	D	1261	-	4,4,4	1.56	1 (25%)	6,6,6	0.60	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
3	13P	A	1104[A]	-	-	1/7/8/8	0/0/0/0
3	13P	A	1104[B]	-	-	0/7/8/8	0/0/0/0
3	13P	B	1053	-	-	0/7/8/8	0/0/0/0
2	SO4	C	1326	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1261	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1261	SO4	O2-S	-2.16	1.39	1.47
3	B	1053	13P	P-O1P	2.71	1.60	1.51
3	A	1104[B]	13P	P-O1P	2.91	1.60	1.51
3	A	1104[A]	13P	P-O1P	3.51	1.62	1.51
3	A	1104[A]	13P	O1-C1	3.93	1.45	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1104[A]	13P	O2P-P-O1P	-3.73	98.57	110.58
3	B	1053	13P	O2P-P-O1	2.17	112.82	106.56
3	A	1104[B]	13P	O2P-P-O1	2.32	113.23	106.56
3	A	1104[B]	13P	O1-P-O1P	2.47	113.42	107.14
3	A	1104[A]	13P	O1-P-O1P	4.60	118.86	107.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1104[A]	13P	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1104[A]	13P	2	0
3	B	1053	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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.