



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:37 PM GMT

PDB ID : 4A01  
Title : Crystal Structure of the H-Translocating Pyrophosphatase  
Authors : Lin, S.-M.; Tsai, J.-Y.; Hsiao, C.-D.; Chiu, C.-L.; Pan, R.-L.; Sun, Y.-J.  
Deposited on : 2011-09-07  
Resolution : 2.35 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

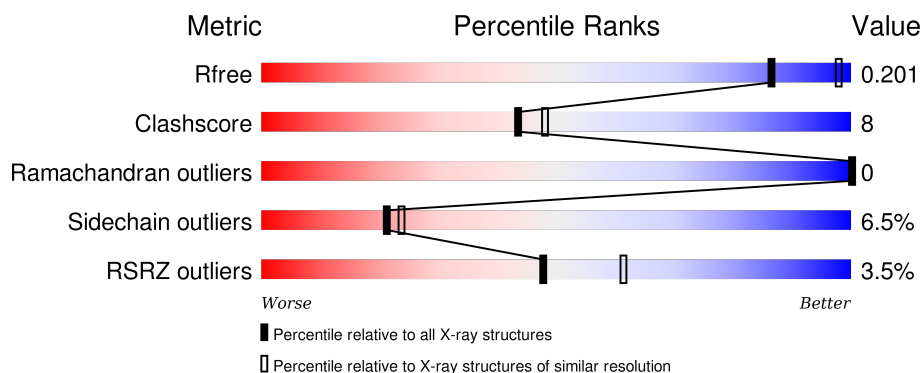
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	766	
1	B	766	

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
5	DMU	A	1774	X	-	-	X
5	DMU	A	1775	X	-	-	X
5	DMU	A	1776	X	-	-	X
5	DMU	A	1778	X	-	-	X
5	DMU	B	1774	X	-	-	X
5	DMU	B	1775	X	-	-	X
5	DMU	B	1777	X	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11759 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 PROTON PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5431	3540	862	1000	29			
1	B	740	Total	C	N	O	S	0	0	0
			5431	3540	862	1000	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	PHE	LEU	SEE REMARK 999	UNP O22124
B	476	PHE	LEU	SEE REMARK 999	UNP O22124

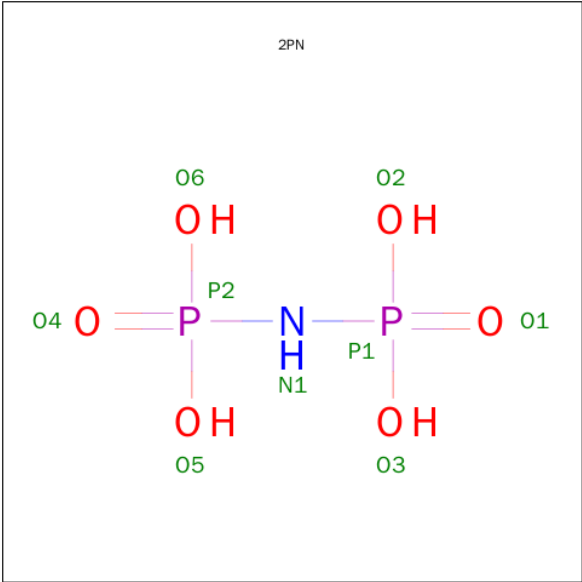
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Mg	0	0
			5	5		
2	A	5	Total	Mg	0	0
			5	5		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

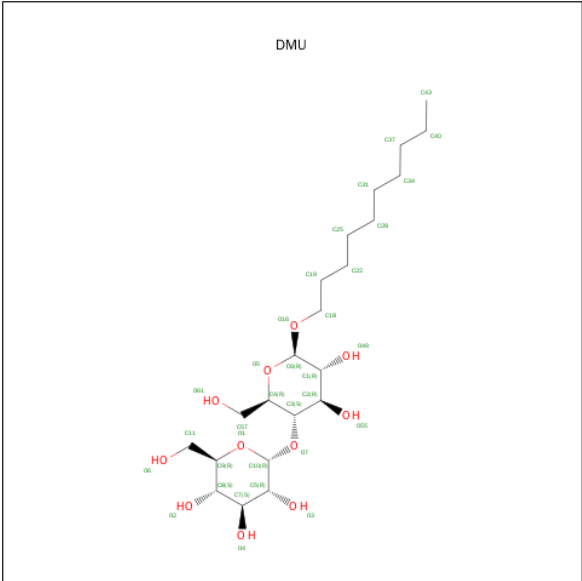
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is IMIDODIPHOSPHORIC ACID (three-letter code: 2PN) (formula: H<sub>5</sub>NO<sub>6</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	N	O	P	0	0
			9	1	6	2		
4	B	1	Total	N	O	P	0	0
			9	1	6	2		

- Molecule 5 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 22 16 6	0	0
5	A	1	Total C O 33 22 11	0	0
5	B	1	Total C O 33 22 11	0	0
5	B	1	Total C O 33 22 11	0	0
5	B	1	Total C O 22 16 6	0	0
5	B	1	Total C O 33 22 11	0	0

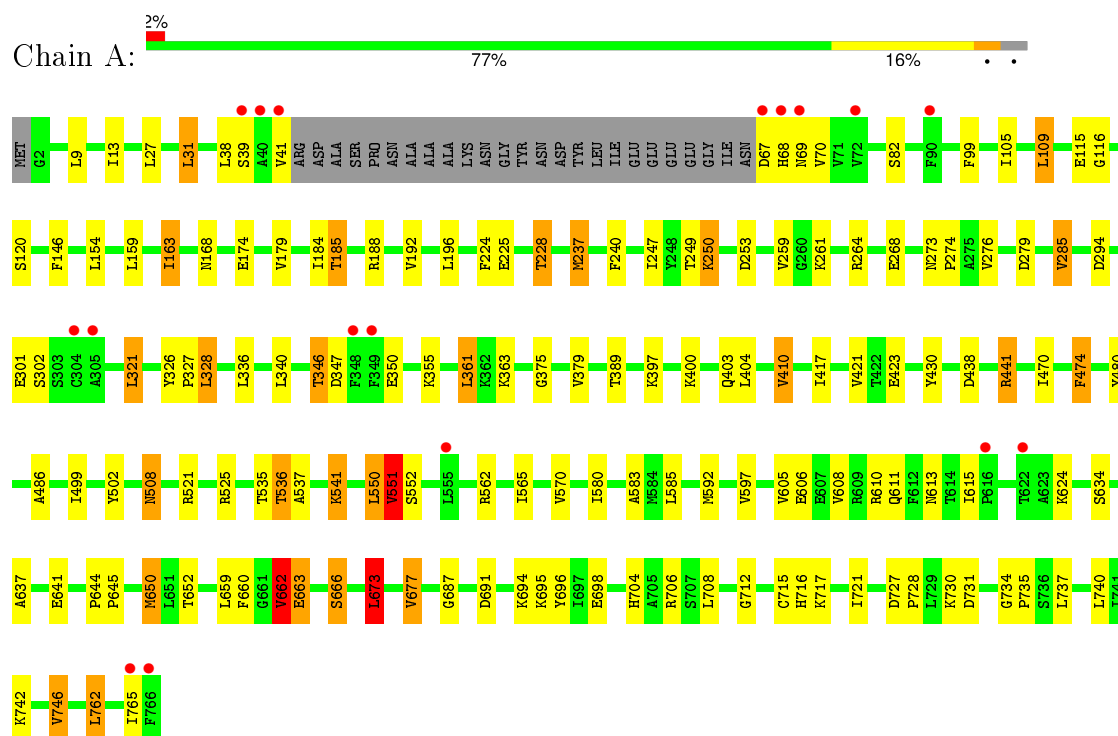
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	335	Total O 335 335	0	0
6	B	257	Total O 257 257	0	0

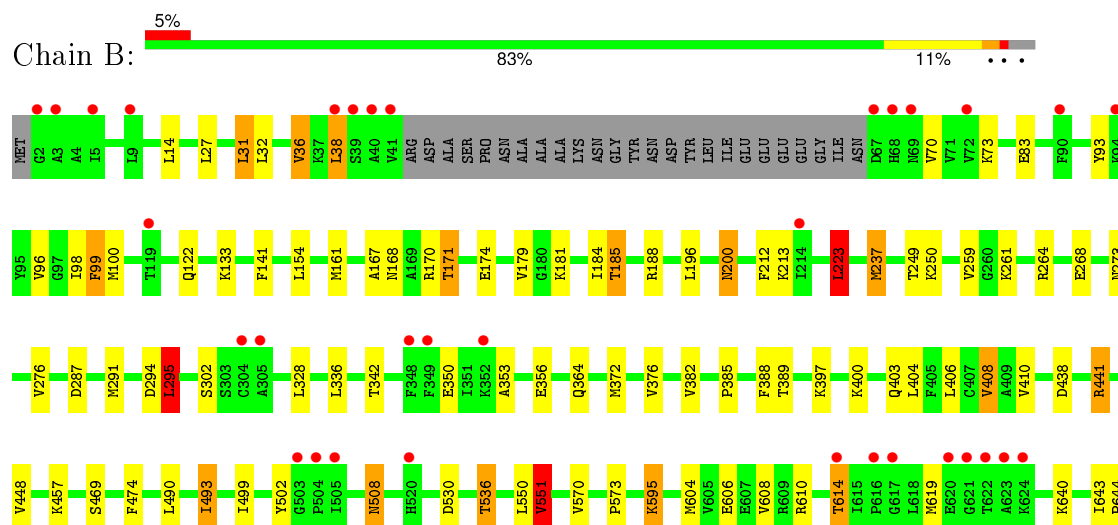
### 3 Residue-property plots

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: PROTON PYROPHOSPHATASE



#### • Molecule 1: PROTON PYROPHOSPHATASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.62Å 88.24Å 159.10Å 90.00° 125.53° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 29.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.35) 97.4 (29.97-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.168 , 0.203 0.168 , 0.201	Depositor DCC
$R_{free}$ test set	5013 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100208 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: MG, 2PN, K, DMU

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	1.12	4/5537 (0.1%)	0.99	28/7524 (0.4%)
1	B	1.05	2/5537 (0.0%)	0.93	15/7524 (0.2%)
All	All	1.09	6/11074 (0.1%)	0.96	43/15048 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	GLU	CG-CD	8.86	1.65	1.51
1	B	663	GLU	CG-CD	5.96	1.60	1.51
1	A	666	SER	CB-OG	-5.33	1.35	1.42
1	B	83	GLU	CG-CD	5.30	1.59	1.51
1	A	146	PHE	CE2-CZ	5.15	1.47	1.37
1	A	663	GLU	CD-OE1	5.00	1.31	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	LEU	CA-CB-CG	-10.44	91.28	115.30
1	B	441	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	706	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	525	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	746	VAL	CG1-CB-CG2	8.15	123.94	110.90
1	A	746	VAL	CB-CA-C	-7.98	96.24	111.40
1	B	294	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	441	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	595	LYS	CD-CE-NZ	-7.52	94.39	111.70
1	B	441	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	677	VAL	CG1-CB-CG2	6.98	122.06	110.90
1	A	441	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	551	VAL	CB-CA-C	-6.73	98.62	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	674	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	A	410	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	B	551	VAL	CB-CA-C	-6.28	99.46	111.40
1	A	321	LEU	CB-CG-CD2	6.23	121.59	111.00
1	A	551	VAL	CA-CB-CG2	6.21	120.22	110.90
1	B	551	VAL	CG1-CB-CG2	6.16	120.75	110.90
1	A	634	SER	CB-CA-C	6.00	121.50	110.10
1	B	674	VAL	CA-CB-CG1	5.99	119.89	110.90
1	A	551	VAL	CG1-CB-CG2	5.96	120.43	110.90
1	A	525	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	673	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	650	MET	CA-CB-CG	-5.71	103.59	113.30
1	A	662	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	A	285	VAL	CG1-CB-CG2	5.68	119.98	110.90
1	A	361	LEU	CB-CG-CD1	5.67	120.63	111.00
1	A	650	MET	CG-SD-CE	-5.63	91.19	100.20
1	A	673	LEU	CB-CG-CD1	5.51	120.36	111.00
1	A	410	VAL	CB-CA-C	-5.47	101.01	111.40
1	B	223	LEU	CA-CB-CG	5.42	127.77	115.30
1	B	31	LEU	CA-CB-CG	-5.38	102.92	115.30
1	B	746	VAL	CB-CA-C	-5.31	101.31	111.40
1	A	328	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	294	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	237	MET	CB-CG-SD	5.25	128.14	112.40
1	A	662	VAL	N-CA-CB	-5.25	99.96	111.50
1	A	31	LEU	CA-CB-CG	-5.24	103.24	115.30
1	B	38	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	253	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	441	ARG	CD-NE-CZ	5.09	130.73	123.60

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	5431	0	5576	99	0
1	B	5431	0	5576	76	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	0	1	0
4	B	9	0	0	1	0
5	A	154	0	199	21	0
5	B	121	0	157	9	0
6	A	335	0	0	8	0
6	B	257	0	0	13	0
All	All	11759	0	11508	184	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 8.

All (184) 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:A:67:ASP:HB2	1:A:70:VAL:HG23	1.30	1.05
1:A:174:GLU:HG3	1:A:185:THR:HG21	1.37	1.04
1:B:174:GLU:HG3	1:B:185:THR:HG21	1.44	0.96
1:A:570:VAL:HG22	1:B:570:VAL:CG2	1.97	0.94
1:B:196:LEU:O	1:B:200:ASN:HB2	1.74	0.88
1:A:225:GLU:O	1:A:228:THR:HG23	1.75	0.88
1:A:154:LEU:HD23	6:A:2062:HOH:O	1.82	0.79
1:A:67:ASP:HB2	1:A:70:VAL:CG2	2.09	0.79
1:A:273:ASN:HB3	1:A:276:VAL:CG1	2.13	0.78
1:A:273:ASN:HB3	1:A:276:VAL:HG13	1.64	0.78
1:B:610:ARG:O	1:B:614:THR:HB	1.84	0.76
1:A:346:THR:HG22	1:A:347:ASP:OD2	1.88	0.74
5:A:1777:DMU:O55	6:A:2328:HOH:O	2.05	0.74
1:A:570:VAL:HG22	1:B:570:VAL:HG22	1.68	0.73
1:B:273:ASN:HB3	1:B:276:VAL:HG23	1.68	0.73
1:B:237:MET:HB3	6:B:2037:HOH:O	1.89	0.73
1:B:619:MET:HA	1:B:619:MET:CE	2.20	0.71
1:B:376:VAL:HG11	1:B:408:VAL:HG22	1.73	0.71
1:A:696:TYR:OH	1:A:704:HIS:HD2	1.74	0.71
1:A:592:MET:HE1	5:A:1775:DMU:H5	1.72	0.70
1:A:712:GLY:H	1:A:716:HIS:HD2	1.39	0.70
1:B:715:CYS:SG	6:B:2244:HOH:O	2.49	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1775:DMU:H41	6:B:2140:HOH:O	1.91	0.69
1:B:712:GLY:H	1:B:716:HIS:CD2	2.11	0.68
1:A:565:ILE:HD11	1:A:662:VAL:HG13	1.76	0.67
5:A:1777:DMU:C43	5:B:1777:DMU:H24	2.25	0.67
1:A:400:LYS:H	1:A:403:GLN:NE2	1.93	0.66
1:A:552:SER:HB2	1:A:673:LEU:HD22	1.77	0.66
1:A:606:GLU:OE2	1:B:441:ARG:NH2	2.28	0.66
1:A:570:VAL:HG22	1:B:570:VAL:HG23	1.75	0.66
1:A:240:PHE:HE2	1:A:650:MET:HE1	1.61	0.66
1:A:250:LYS:HG3	1:A:727:ASP:HB3	1.79	0.65
1:A:438:ASP:OD1	1:A:704:HIS:HE1	1.79	0.64
5:A:1777:DMU:H24	5:B:1777:DMU:H24	1.78	0.64
1:A:441:ARG:NH2	1:B:606:GLU:OE2	2.31	0.64
4:A:1773:2PN:P1	6:A:2105:HOH:O	2.56	0.63
1:B:530:ASP:OD2	1:B:695:LYS:HE2	1.98	0.62
1:A:499:ILE:O	1:A:536:THR:HG21	2.00	0.62
1:B:738:ASN:HB3	6:B:2245:HOH:O	1.99	0.62
4:B:1773:2PN:P1	6:B:2069:HOH:O	2.57	0.61
1:B:14:LEU:C	1:B:14:LEU:HD23	2.20	0.61
1:A:185:THR:HG22	6:A:2072:HOH:O	2.00	0.60
1:B:499:ILE:O	1:B:536:THR:HG21	2.02	0.60
1:B:184:ILE:O	1:B:188:ARG:HG3	2.02	0.60
1:B:302:SER:HA	1:B:551:VAL:CG1	2.32	0.59
1:B:712:GLY:H	1:B:716:HIS:HD2	1.50	0.59
1:A:274:PRO:HD2	1:A:608:VAL:HG13	1.86	0.58
1:A:470:ILE:O	1:A:474:PHE:HB2	2.04	0.58
1:A:521:ARG:NH2	6:A:2227:HOH:O	2.36	0.57
5:A:1777:DMU:H25	5:B:1777:DMU:C43	2.35	0.57
1:B:96:VAL:CG1	1:B:237:MET:HG3	2.33	0.57
1:A:698:GLU:OE2	1:A:716:HIS:HE1	1.87	0.57
1:A:712:GLY:H	1:A:716:HIS:CD2	2.22	0.57
1:A:430:TYR:HE1	5:A:1774:DMU:H35	1.69	0.57
1:A:499:ILE:O	1:A:536:THR:CG2	2.53	0.57
1:A:417:ILE:O	1:A:421:VAL:HG23	2.05	0.56
1:A:659:LEU:HB3	1:A:762:LEU:HD22	1.87	0.56
1:B:499:ILE:O	1:B:536:THR:CG2	2.53	0.56
1:B:696:TYR:OH	1:B:704:HIS:HD2	1.89	0.56
1:B:388:PHE:CZ	1:B:404:LEU:HD22	2.42	0.55
5:A:1775:DMU:C10	5:A:1775:DMU:H29	2.37	0.55
5:A:1775:DMU:H36	5:A:1775:DMU:H29	1.89	0.55
1:A:717:LYS:O	1:A:721:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HD23	6:B:2037:HOH:O	2.08	0.54
1:B:619:MET:HA	1:B:619:MET:HE3	1.90	0.54
1:A:159:LEU:O	1:A:163:ILE:HG22	2.09	0.53
1:A:597:VAL:HG11	1:A:728:PRO:HB3	1.90	0.53
1:A:249:THR:HG23	1:A:250:LYS:HD2	1.90	0.53
5:A:1778:DMU:H32	6:A:2331:HOH:O	2.09	0.53
1:A:67:ASP:CB	1:A:70:VAL:HG23	2.21	0.52
1:A:537:ALA:O	1:A:541:LYS:HD3	2.10	0.51
1:A:660:PHE:HE2	5:A:1777:DMU:H19	1.76	0.51
1:A:570:VAL:CG2	1:B:570:VAL:HG22	2.38	0.51
1:A:663:GLU:O	1:A:666:SER:HB2	2.10	0.51
1:B:259:VAL:HG21	1:B:608:VAL:HB	1.93	0.51
1:B:36:VAL:HG22	1:B:170:ARG:HG2	1.91	0.51
1:B:100:MET:HB2	1:B:237:MET:CE	2.42	0.50
1:B:389:THR:HA	1:B:397:LYS:O	2.11	0.50
1:B:259:VAL:HG11	1:B:608:VAL:HG12	1.94	0.50
1:B:619:MET:HA	1:B:619:MET:HE2	1.93	0.50
1:A:570:VAL:CG2	1:B:570:VAL:CG2	2.83	0.50
1:B:273:ASN:HB3	1:B:276:VAL:CG2	2.38	0.50
1:B:640:LYS:NZ	6:B:2224:HOH:O	2.44	0.50
1:B:167:ALA:O	1:B:171:THR:HG23	2.12	0.50
1:B:168:ASN:HB2	1:B:508:ASN:HB3	1.94	0.50
1:A:105:ILE:HG22	1:A:109:LEU:HD22	1.93	0.49
1:A:168:ASN:HB2	1:A:508:ASN:HB3	1.94	0.49
1:B:663:GLU:O	1:B:666:SER:HB2	2.13	0.49
1:A:610:ARG:HH21	1:A:611:GLN:HG2	1.76	0.49
1:A:250:LYS:HD3	1:A:731:ASP:HB2	1.95	0.49
1:A:250:LYS:HD3	1:A:731:ASP:CB	2.43	0.49
1:A:580:ILE:HA	1:B:674:VAL:HG22	1.94	0.49
1:A:363:LYS:NZ	6:A:2165:HOH:O	2.46	0.49
1:A:163:ILE:HG12	1:A:192:VAL:HB	1.94	0.48
1:A:184:ILE:O	1:A:188:ARG:HG3	2.13	0.48
1:A:159:LEU:HD13	1:A:196:LEU:HD13	1.94	0.48
5:A:1777:DMU:C43	5:B:1777:DMU:C43	2.91	0.48
1:B:96:VAL:HG12	1:B:237:MET:HG3	1.96	0.48
1:A:474:PHE:CG	1:B:573:PRO:HG3	2.48	0.48
1:B:249:THR:HG23	1:B:250:LYS:HE3	1.96	0.48
1:A:67:ASP:HB3	1:A:69:ASN:H	1.79	0.48
1:A:583:ALA:HB2	1:B:674:VAL:HG13	1.95	0.48
1:A:687:GLY:HA3	1:A:730:LYS:HB3	1.96	0.47
1:A:224:PHE:O	1:A:228:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD21	1:A:480:TYR:HE2	1.78	0.47
1:A:174:GLU:HG3	1:A:185:THR:CG2	2.25	0.47
1:A:99:PHE:HE1	5:A:1776:DMU:H26	1.78	0.47
1:A:302:SER:HA	1:A:551:VAL:CG1	2.45	0.47
1:B:342:THR:HA	1:B:364:GLN:HE22	1.80	0.47
5:B:1777:DMU:H30	6:B:2256:HOH:O	2.15	0.46
5:A:1776:DMU:H36	5:A:1776:DMU:H4	1.46	0.46
1:A:400:LYS:H	1:A:403:GLN:HE21	1.62	0.46
1:A:644:PRO:HB2	1:A:645:PRO:HD3	1.97	0.46
5:A:1775:DMU:C57	5:A:1775:DMU:H36	2.46	0.45
1:B:604:MET:O	1:B:608:VAL:HG23	2.15	0.45
5:A:1775:DMU:O55	1:B:457:LYS:HE3	2.15	0.45
5:B:1775:DMU:H33	6:B:2140:HOH:O	2.15	0.45
5:A:1774:DMU:H29	6:A:2164:HOH:O	2.15	0.45
1:B:438:ASP:OD1	1:B:704:HIS:HE1	1.99	0.45
1:B:161:MET:SD	1:B:161:MET:C	2.95	0.45
1:A:302:SER:HA	1:A:551:VAL:HG13	1.99	0.45
1:B:353:ALA:O	1:B:356:GLU:HB2	2.15	0.45
1:A:611:GLN:HB3	1:A:615:ILE:HD12	1.98	0.45
1:B:99:PHE:CD1	1:B:99:PHE:C	2.90	0.45
1:A:734:GLY:N	1:A:735:PRO:HD2	2.31	0.45
1:A:67:ASP:HB3	1:A:69:ASN:N	2.32	0.45
1:B:167:ALA:O	1:B:171:THR:CG2	2.65	0.45
1:A:261:LYS:NZ	1:A:268:GLU:OE1	2.39	0.45
1:A:696:TYR:OH	1:A:704:HIS:CD2	2.62	0.45
1:A:116:GLY:HA3	5:A:1778:DMU:H3	1.99	0.45
1:A:240:PHE:HE2	1:A:650:MET:CE	2.29	0.45
1:B:400:LYS:H	1:B:403:GLN:NE2	2.15	0.44
1:B:448:VAL:HA	1:B:690:TRP:CZ2	2.51	0.44
5:B:1775:DMU:H29	5:B:1775:DMU:C10	2.47	0.44
1:A:99:PHE:CE1	5:A:1776:DMU:H26	2.53	0.44
1:A:39:SER:OG	1:A:41:VAL:HG22	2.17	0.44
1:B:174:GLU:HG3	1:B:185:THR:CG2	2.32	0.44
1:A:240:PHE:CE2	1:A:650:MET:CE	3.02	0.43
1:A:301:GLU:OE2	1:A:742:LYS:HG3	2.17	0.43
1:B:410:VAL:HG13	1:B:469:SER:HB2	2.01	0.43
1:B:141:PHE:HB3	1:B:212:PHE:CE2	2.54	0.43
1:A:264:ARG:NH2	1:A:613:ASN:OD1	2.51	0.43
1:A:740:LEU:C	1:A:740:LEU:HD23	2.38	0.43
1:A:592:MET:CE	5:A:1775:DMU:H5	2.46	0.43
5:A:1776:DMU:H36	5:A:1776:DMU:C57	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:HG3	1:A:535:THR:HG21	2.00	0.43
1:B:696:TYR:OH	1:B:704:HIS:CD2	2.71	0.43
1:B:376:VAL:HG11	1:B:408:VAL:CG2	2.44	0.43
1:B:213:LYS:HA	1:B:223:LEU:HD22	2.01	0.42
1:A:637:ALA:O	1:A:641:GLU:HG2	2.18	0.42
1:B:502:TYR:C	1:B:502:TYR:CD1	2.91	0.42
5:B:1775:DMU:H36	5:B:1775:DMU:C57	2.50	0.42
1:A:240:PHE:CE2	1:A:650:MET:HE1	2.48	0.42
1:B:328:LEU:HD12	1:B:328:LEU:N	2.33	0.42
1:B:295:LEU:HD13	6:B:2099:HOH:O	2.20	0.42
1:A:695:LYS:HD2	1:A:695:LYS:HA	1.95	0.42
1:B:643:ILE:HB	1:B:644:PRO:HD3	2.01	0.42
1:B:614:THR:HG21	6:B:2213:HOH:O	2.20	0.41
1:B:385:PRO:HD3	6:B:2107:HOH:O	2.19	0.41
1:B:490:LEU:O	1:B:493:ILE:HB	2.20	0.41
1:A:691:ASP:O	1:A:694:LYS:HB3	2.20	0.41
1:B:122:GLN:NE2	1:B:133:LYS:O	2.45	0.41
1:A:67:ASP:HB3	1:A:69:ASN:HB2	2.02	0.41
1:B:264:ARG:HA	1:B:264:ARG:HD3	1.57	0.41
1:A:375:GLY:O	1:A:379:VAL:HG23	2.19	0.41
1:B:100:MET:HB2	1:B:237:MET:SD	2.60	0.41
1:A:486:ALA:HB2	1:A:550:LEU:HB3	2.03	0.41
1:B:372:MET:O	1:B:376:VAL:HG23	2.21	0.41
1:A:247:ILE:HD13	1:A:641:GLU:HB2	2.02	0.41
1:A:585:LEU:CD1	1:A:652:THR:HG21	2.50	0.41
1:B:93:TYR:CD1	1:B:93:TYR:N	2.89	0.41
1:B:73:LYS:HG3	6:B:2172:HOH:O	2.21	0.41
1:A:326:TYR:N	1:A:327:PRO:HD2	2.35	0.41
1:A:259:VAL:CG2	1:A:605:VAL:HG13	2.50	0.41
1:A:67:ASP:HB2	1:A:70:VAL:H	1.86	0.41
1:A:163:ILE:O	1:A:163:ILE:HD12	2.21	0.41
1:A:389:THR:HA	1:A:397:LYS:O	2.21	0.40
1:A:346:THR:CG2	1:A:347:ASP:OD2	2.66	0.40
1:B:302:SER:HA	1:B:551:VAL:HG13	2.03	0.40
1:A:430:TYR:CE1	5:A:1774:DMU:H35	2.52	0.40
1:A:562:ARG:HA	1:A:562:ARG:HD2	1.76	0.40
1:B:261:LYS:NZ	1:B:268:GLU:OE1	2.43	0.40
1:A:9:LEU:HD13	1:A:13:ILE:HD12	2.02	0.40
1:A:708:LEU:O	1:A:715:CYS:HB2	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/766 (96%)	726 (99%)	10 (1%)	0	100	100
1	B	736/766 (96%)	715 (97%)	21 (3%)	0	100	100
All	All	1472/1532 (96%)	1441 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	568/588 (97%)	528 (93%)	40 (7%)	19	20
1	B	568/588 (97%)	534 (94%)	34 (6%)	24	28
All	All	1136/1176 (97%)	1062 (94%)	74 (6%)	21	24

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	LEU
1	A	38	LEU
1	A	68	HIS
1	A	82	SER
1	A	109	LEU
1	A	115	GLU
1	A	120	SER

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Mol	Chain	Res	Type
1	A	163	ILE
1	A	179	VAL
1	A	185	THR
1	A	228	THR
1	A	237	MET
1	A	250	LYS
1	A	279	ASP
1	A	285	VAL
1	A	321	LEU
1	A	328	LEU
1	A	336	LEU
1	A	340	LEU
1	A	346	THR
1	A	350	GLU
1	A	355	LYS
1	A	361	LEU
1	A	410	VAL
1	A	474	PHE
1	A	502	TYR
1	A	508	ASN
1	A	536	THR
1	A	541	LYS
1	A	550	LEU
1	A	551	VAL
1	A	624	LYS
1	A	662	VAL
1	A	673	LEU
1	A	677	VAL
1	A	737	LEU
1	A	746	VAL
1	A	762	LEU
1	A	765	ILE
1	B	27	LEU
1	B	31	LEU
1	B	32	LEU
1	B	36	VAL
1	B	38	LEU
1	B	70	VAL
1	B	98	ILE
1	B	99	PHE
1	B	171	THR
1	B	179	VAL

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Mol	Chain	Res	Type
1	B	181	LYS
1	B	185	THR
1	B	200	ASN
1	B	223	LEU
1	B	237	MET
1	B	287	ASP
1	B	291	MET
1	B	295	LEU
1	B	336	LEU
1	B	350	GLU
1	B	382	VAL
1	B	406	LEU
1	B	408	VAL
1	B	474	PHE
1	B	493	ILE
1	B	508	ASN
1	B	536	THR
1	B	550	LEU
1	B	551	VAL
1	B	595	LYS
1	B	614	THR
1	B	674	VAL
1	B	738	ASN
1	B	746	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	403	GLN
1	A	704	HIS
1	A	716	HIS
1	B	364	GLN
1	B	403	GLN
1	B	447	ASN
1	B	520	HIS
1	B	704	HIS
1	B	716	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

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$
4	2PN	A	1773	3,2	8,8,8	6.22	3 (37%)	8,13,13	2.35	5 (62%)
5	DMU	A	1774	-	34,34,34	0.75	0	45,45,45	2.32	15 (33%)
5	DMU	A	1775	-	34,34,34	0.76	0	45,45,45	2.34	13 (28%)
5	DMU	A	1776	-	34,34,34	0.79	1 (2%)	45,45,45	2.54	11 (24%)
5	DMU	A	1777	-	22,22,34	0.56	0	27,27,45	2.03	6 (22%)
5	DMU	A	1778	-	34,34,34	0.77	0	45,45,45	2.19	12 (26%)
4	2PN	B	1773	3,2	8,8,8	6.11	4 (50%)	8,13,13	2.71	3 (37%)
5	DMU	B	1774	-	34,34,34	0.81	0	45,45,45	2.55	12 (26%)
5	DMU	B	1775	-	34,34,34	0.94	2 (5%)	45,45,45	2.81	17 (37%)
5	DMU	B	1776	-	22,22,34	0.77	0	27,27,45	2.84	6 (22%)
5	DMU	B	1777	-	34,34,34	0.93	2 (5%)	45,45,45	2.57	11 (24%)

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
4	2PN	A	1773	3,2	-	0/2/6/6	0/0/0/0
5	DMU	A	1774	-	2/2/10/10	0/19/59/59	0/2/2/2
5	DMU	A	1775	-	5/5/10/10	0/19/59/59	0/2/2/2
5	DMU	A	1776	-	4/4/10/10	0/19/59/59	0/2/2/2
5	DMU	A	1777	-	-	0/13/33/59	0/1/1/2
5	DMU	A	1778	-	2/2/10/10	0/19/59/59	0/2/2/2
4	2PN	B	1773	3,2	-	0/2/6/6	0/0/0/0
5	DMU	B	1774	-	2/2/10/10	0/19/59/59	0/2/2/2
5	DMU	B	1775	-	5/5/10/10	0/19/59/59	0/2/2/2
5	DMU	B	1776	-	-	0/13/33/59	0/1/1/2
5	DMU	B	1777	-	5/5/10/10	0/19/59/59	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1773	2PN	P2-O6	-2.65	1.49	1.56
5	B	1777	DMU	O49-C1	-2.28	1.37	1.43
5	B	1777	DMU	O55-C2	-2.22	1.37	1.43
5	A	1776	DMU	O55-C2	-2.18	1.37	1.43
5	B	1775	DMU	O55-C2	-2.09	1.38	1.43
5	B	1775	DMU	O16-C6	2.92	1.45	1.40
4	B	1773	2PN	P1-N1	3.85	1.73	1.63
4	A	1773	2PN	P1-N1	4.09	1.74	1.63
4	B	1773	2PN	P2-O4	10.45	1.58	1.46
4	A	1773	2PN	P2-O4	11.55	1.59	1.46
4	A	1773	2PN	P1-O1	12.47	1.60	1.46
4	B	1773	2PN	P1-O1	12.88	1.61	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1777	DMU	O5-C6-C1	-5.99	97.99	110.28
4	B	1773	2PN	O4-P2-N1	-5.00	104.23	111.90
5	A	1776	DMU	C10-O7-C3	-3.95	107.68	118.01
4	B	1773	2PN	O1-P1-N1	-3.24	106.93	111.90
5	A	1775	DMU	C10-O7-C3	-3.13	109.83	118.01
4	A	1773	2PN	O5-P2-O4	-3.07	105.33	113.49
4	A	1773	2PN	O6-P2-O4	-2.92	105.72	113.49
4	B	1773	2PN	O6-P2-O4	-2.74	106.20	113.49
5	A	1774	DMU	O4-C7-C8	-2.57	104.54	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1778	DMU	O5-C6-C1	-2.46	105.22	110.28
4	A	1773	2PN	O1-P1-N1	-2.35	108.30	111.90
5	A	1774	DMU	O5-C6-C1	-2.26	105.65	110.28
5	A	1775	DMU	O5-C6-C1	-2.24	105.67	110.28
5	A	1775	DMU	O49-C1-C2	-2.16	105.48	110.34
5	B	1774	DMU	O1-C9-C11	2.01	111.44	106.36
5	A	1776	DMU	O7-C3-C2	2.02	112.39	107.17
5	A	1775	DMU	O5-C6-O16	2.05	115.00	110.05
5	B	1776	DMU	O7-C3-C4	2.09	114.78	109.24
5	A	1777	DMU	O5-C6-O16	2.10	115.10	110.05
5	A	1778	DMU	O7-C3-C2	2.10	112.59	107.17
5	B	1777	DMU	C10-C5-C7	2.11	114.12	109.97
5	A	1777	DMU	C6-C1-C2	2.11	114.14	109.97
5	B	1776	DMU	C6-C1-C2	2.12	114.14	109.97
5	A	1774	DMU	O7-C10-C5	2.13	113.28	108.10
5	B	1774	DMU	O1-C10-C5	2.16	114.70	110.28
5	A	1775	DMU	O3-C5-C10	2.18	114.80	110.02
5	B	1777	DMU	O1-C9-C8	2.18	113.78	109.68
4	A	1773	2PN	O3-P1-O1	2.18	119.30	113.49
5	A	1778	DMU	O16-C6-C1	2.30	110.94	108.04
5	B	1775	DMU	O49-C1-C6	2.31	115.08	110.02
5	B	1777	DMU	C1-C2-C3	2.32	114.70	109.60
5	A	1775	DMU	C1-C2-C3	2.33	114.71	109.60
5	B	1775	DMU	C6-C1-C2	2.33	114.57	109.97
5	A	1775	DMU	O49-C1-C6	2.37	115.22	110.02
5	A	1774	DMU	O49-C1-C2	2.39	115.71	110.34
5	A	1778	DMU	O1-C9-C11	2.43	112.50	106.36
5	A	1776	DMU	O2-C8-C7	2.44	115.83	110.34
5	B	1777	DMU	C7-C8-C9	2.46	114.49	110.20
5	B	1775	DMU	C57-C4-C3	2.47	120.44	113.25
5	A	1776	DMU	C10-O1-C9	2.52	118.64	113.75
5	B	1775	DMU	O3-C5-C10	2.54	115.58	110.02
5	B	1775	DMU	C7-C8-C9	2.62	114.76	110.20
5	A	1774	DMU	O1-C9-C8	2.63	114.63	109.68
5	B	1775	DMU	O5-C4-C57	2.64	113.04	106.36
5	A	1778	DMU	O5-C6-O16	2.65	116.44	110.05
5	A	1776	DMU	O7-C3-C4	2.69	116.40	109.32
5	A	1778	DMU	C7-C8-C9	2.74	114.97	110.20
5	B	1776	DMU	C18-O16-C6	2.77	118.79	113.94
5	A	1774	DMU	C10-C5-C7	2.79	115.47	109.97
5	A	1774	DMU	O4-C7-C5	2.89	116.84	110.34
5	B	1774	DMU	C10-C5-C7	2.89	115.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1774	DMU	C18-O16-C6	2.89	119.00	113.94
5	A	1776	DMU	O1-C9-C11	2.91	113.72	106.36
5	A	1774	DMU	O5-C4-C57	2.93	113.75	106.36
5	A	1775	DMU	O7-C3-C4	2.94	117.06	109.32
5	B	1774	DMU	C7-C8-C9	2.96	115.35	110.20
5	B	1777	DMU	O7-C10-C5	3.00	115.40	108.10
5	B	1777	DMU	O5-C6-O16	3.07	117.44	110.05
5	B	1774	DMU	C10-O7-C3	3.08	126.05	118.01
5	A	1778	DMU	C10-C5-C7	3.10	116.07	109.97
5	A	1775	DMU	O1-C9-C11	3.10	114.20	106.36
5	A	1778	DMU	O1-C9-C8	3.13	115.56	109.68
5	A	1777	DMU	O7-C3-C4	3.15	117.59	109.24
5	B	1776	DMU	O49-C1-C6	3.18	116.98	110.02
5	B	1777	DMU	C10-O1-C9	3.31	120.17	113.75
5	B	1775	DMU	O7-C3-C2	3.37	115.86	107.17
5	B	1775	DMU	O1-C10-C5	3.38	117.21	110.28
5	A	1778	DMU	O5-C4-C57	3.40	114.94	106.36
4	A	1773	2PN	O6-P2-O5	3.44	117.77	107.58
5	B	1775	DMU	O7-C10-C5	3.45	116.49	108.10
5	A	1777	DMU	O5-C4-C57	3.46	115.10	106.36
5	A	1776	DMU	O1-C10-C5	3.51	117.47	110.28
5	B	1774	DMU	O7-C3-C2	3.55	116.34	107.17
5	A	1775	DMU	O7-C10-C5	3.56	116.77	108.10
5	B	1775	DMU	O1-C9-C11	3.58	115.39	106.36
5	B	1774	DMU	C8-C7-C5	3.59	117.49	110.79
5	B	1775	DMU	O5-C6-O16	3.59	118.70	110.05
5	B	1774	DMU	C18-O16-C6	3.68	120.37	113.94
5	A	1774	DMU	C8-C7-C5	3.77	117.83	110.79
5	A	1774	DMU	O5-C6-O16	3.84	119.30	110.05
5	B	1774	DMU	O7-C10-C5	3.87	117.51	108.10
5	A	1778	DMU	C10-O1-C9	3.89	121.30	113.75
5	A	1775	DMU	C18-O16-C6	4.01	120.95	113.94
5	A	1777	DMU	O16-C6-C1	4.01	113.11	108.04
5	B	1774	DMU	O7-C3-C4	4.08	120.05	109.32
5	A	1774	DMU	O16-C6-C1	4.10	113.22	108.04
5	B	1775	DMU	C10-C5-C7	4.13	118.12	109.97
5	A	1776	DMU	C18-O16-C6	4.24	121.35	113.94
5	A	1774	DMU	C7-C8-C9	4.55	118.13	110.20
5	B	1775	DMU	C10-O1-C9	4.64	122.75	113.75
5	A	1776	DMU	O7-C10-C5	4.65	119.42	108.10
5	B	1775	DMU	C18-O16-C6	4.94	122.57	113.94
5	A	1774	DMU	O1-C9-C11	5.04	119.09	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1774	DMU	O16-C6-C1	5.24	114.66	108.04
5	B	1775	DMU	O7-C3-C4	5.62	124.08	109.32
5	A	1778	DMU	C18-O16-C6	5.69	123.89	113.94
5	B	1777	DMU	C18-O16-C6	5.80	124.09	113.94
5	B	1777	DMU	O16-C6-C1	6.18	115.84	108.04
5	A	1777	DMU	C6-O5-C4	6.46	126.29	113.75
5	A	1776	DMU	O16-C6-C1	6.62	116.39	108.04
5	A	1775	DMU	C6-O5-C4	6.92	127.18	113.75
5	B	1775	DMU	O16-C6-C1	7.57	117.60	108.04
5	A	1774	DMU	C6-O5-C4	7.60	128.49	113.75
5	A	1778	DMU	C6-O5-C4	8.76	130.75	113.75
5	B	1776	DMU	O16-C6-C1	8.77	119.11	108.04
5	A	1775	DMU	O16-C6-C1	9.13	119.56	108.04
5	B	1775	DMU	C6-O5-C4	9.17	131.53	113.75
5	B	1776	DMU	C6-O5-C4	9.93	133.03	113.75
5	A	1776	DMU	C6-O5-C4	10.26	133.65	113.75
5	B	1777	DMU	C6-O5-C4	10.36	133.84	113.75
5	B	1774	DMU	C6-O5-C4	11.12	135.33	113.75

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1774	DMU	C5
5	B	1774	DMU	C9
5	A	1774	DMU	C5
5	A	1774	DMU	C9
5	B	1775	DMU	C5
5	B	1775	DMU	C10
5	B	1775	DMU	C6
5	B	1775	DMU	C9
5	B	1775	DMU	C4
5	A	1775	DMU	C5
5	A	1775	DMU	C10
5	A	1775	DMU	C3
5	A	1775	DMU	C9
5	A	1775	DMU	C7
5	A	1776	DMU	C5
5	A	1776	DMU	C8
5	A	1776	DMU	C10
5	A	1776	DMU	C7
5	A	1778	DMU	C5
5	A	1778	DMU	C9

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Mol	Chain	Res	Type	Atom
5	B	1777	DMU	C5
5	B	1777	DMU	C10
5	B	1777	DMU	C9
5	B	1777	DMU	C4
5	B	1777	DMU	C7

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1773	2PN	1	0
5	A	1774	DMU	3	0
5	A	1775	DMU	6	0
5	A	1776	DMU	4	0
5	A	1777	DMU	6	0
5	A	1778	DMU	2	0
4	B	1773	2PN	1	0
5	B	1775	DMU	4	0
5	B	1777	DMU	5	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	740/766 (96%)	-0.32	17 (2%) 64 76	26, 37, 54, 84	0
1	B	740/766 (96%)	-0.10	35 (4%) 35 50	27, 42, 62, 94	0
All	All	1480/1532 (96%)	-0.21	52 (3%) 48 61	26, 39, 59, 94	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	8.6
1	B	40	ALA	6.0
1	B	766	PHE	6.0
1	A	41	VAL	5.9
1	B	68	HIS	5.8
1	A	766	PHE	5.3
1	B	2	GLY	4.8
1	A	40	ALA	4.6
1	A	68	HIS	4.4
1	B	622	THR	4.2
1	A	348	PHE	4.2
1	B	520	HIS	4.0
1	A	616	PRO	3.9
1	B	39	SER	3.9
1	B	69	ASN	3.8
1	A	67	ASP	3.8
1	A	349	PHE	3.6
1	B	348	PHE	3.5
1	B	349	PHE	3.5
1	B	38	LEU	3.5
1	B	67	ASP	3.4
1	B	72	VAL	3.4
1	A	765	ILE	3.4
1	B	623	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	352	LYS	3.0
1	A	72	VAL	3.0
1	B	616	PRO	2.9
1	B	765	ILE	2.9
1	A	90	PHE	2.9
1	B	214	ILE	2.9
1	B	624	LYS	2.8
1	A	39	SER	2.8
1	B	5	ILE	2.8
1	B	505	ILE	2.7
1	B	504	PRO	2.6
1	A	305	ALA	2.6
1	B	119	THR	2.6
1	B	614	THR	2.5
1	A	622	THR	2.5
1	B	9	LEU	2.4
1	B	620	GLU	2.3
1	B	3	ALA	2.3
1	B	90	PHE	2.3
1	B	621	GLY	2.2
1	B	304	CYS	2.2
1	A	69	ASN	2.2
1	A	555	LEU	2.2
1	B	94	LYS	2.1
1	B	503	GLY	2.1
1	A	304	CYS	2.1
1	B	617	GLY	2.0
1	B	305	ALA	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(Å <sup>2</sup> )	Q<0.9
5	DMU	A	1774	33/33	0.76	0.34	9.28	64,82,97,99	0
5	DMU	B	1777	33/33	0.68	0.32	8.81	68,111,119,119	0
5	DMU	B	1775	33/33	0.49	0.40	6.90	61,103,118,119	0
5	DMU	A	1776	33/33	0.71	0.40	6.58	81,92,96,97	0
5	DMU	A	1778	33/33	0.40	0.47	5.32	90,125,134,134	0
5	DMU	B	1774	33/33	0.81	0.28	4.78	51,93,105,106	0
5	DMU	A	1775	33/33	0.75	0.27	4.42	46,94,111,111	0
2	MG	A	1770	1/1	0.97	0.22	1.74	35,35,35,35	0
5	DMU	B	1776	22/33	0.81	0.31	1.63	62,82,93,93	0
2	MG	B	1770	1/1	0.99	0.23	1.00	41,41,41,41	0
2	MG	A	1769	1/1	0.98	0.18	0.86	33,33,33,33	0
2	MG	B	1767	1/1	0.99	0.20	0.81	41,41,41,41	0
5	DMU	A	1777	22/33	0.82	0.21	0.78	57,82,97,98	0
2	MG	B	1769	1/1	0.98	0.21	0.75	36,36,36,36	0
4	2PN	A	1773	9/9	0.98	0.17	0.68	30,32,37,42	0
3	K	A	1772	1/1	0.92	0.16	0.41	62,62,62,62	0
2	MG	A	1768	1/1	0.98	0.14	0.14	44,44,44,44	0
4	2PN	B	1773	9/9	0.98	0.17	-0.07	33,34,40,47	0
2	MG	B	1768	1/1	0.99	0.14	-0.53	40,40,40,40	0
2	MG	A	1767	1/1	0.97	0.13	-0.59	36,36,36,36	0
3	K	B	1772	1/1	0.93	0.11	-0.96	60,60,60,60	0
2	MG	A	1771	1/1	0.98	0.18	-	34,34,34,34	0
2	MG	B	1771	1/1	0.98	0.15	-	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.