



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:04 pm BST

PDB ID : 3PD6
Title : Crystal structure of mouse mitochondrial aspartate aminotransferase, a newly identified kynurenine aminotransferase-IV
Authors : Han, Q.; Robinson, H.; Cai, T.; Tagle, D.A.; Li, J.
Deposited on : 2010-10-22
Resolution : 2.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

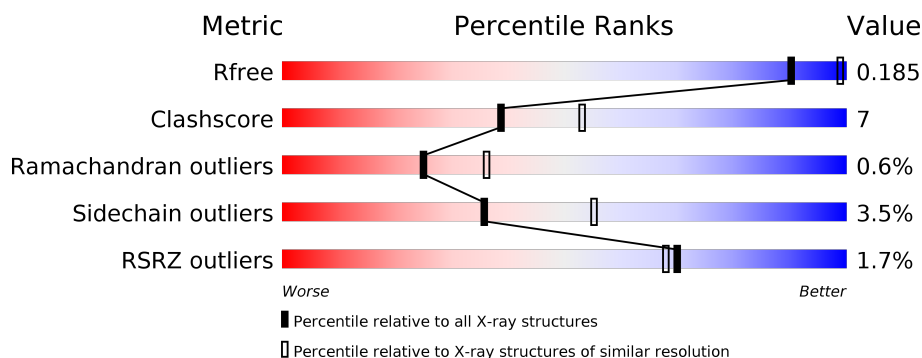
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	<div> <div>86%</div> <div>13%</div> </div>
1	C	401	<div> <div>86%</div> <div>13%</div> </div>
2	B	401	<div> <div>2%</div> <div>81%</div> <div>18%</div> </div>
2	D	401	<div> <div>4%</div> <div>80%</div> <div>19%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LLP	B	279	-	X	-	-
3	PMP	A	1	-	-	X	-
4	GOL	C	433	-	X	-	-
4	GOL	D	1	-	-	X	-
5	KYN	B	1	X	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13546 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.

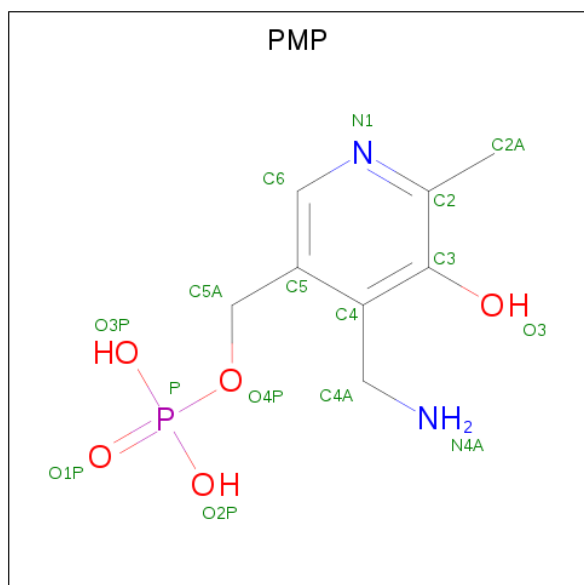
- Molecule 1 is a protein called Aspartate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3140	1997	550	577	16			
1	C	401	Total	C	N	O	S	0	0	0
			3140	1997	550	577	16			

- Molecule 2 is a protein called Aspartate aminotransferase, mitochondrial.

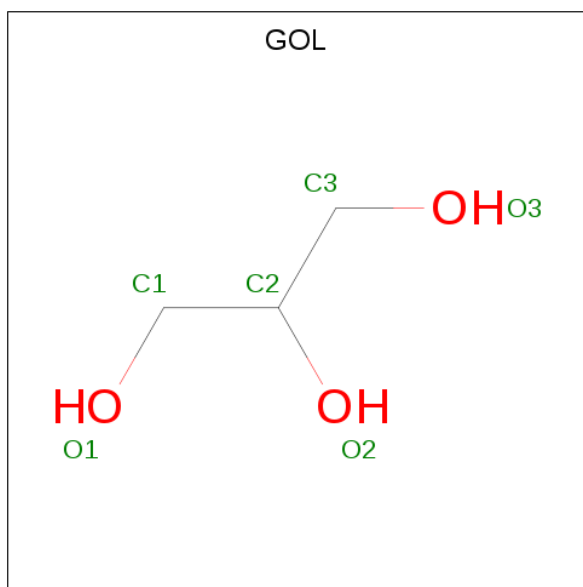
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	P	S	0	0
			3155	2005	551	582	1	16		
2	D	401	Total	C	N	O	P	S	0	0
			3155	2005	551	582	1	16		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



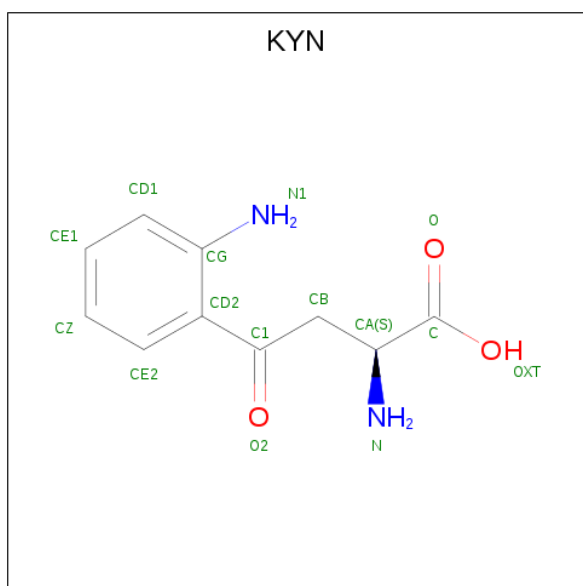
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (2S)-2-amino-4-(2-aminophenyl)-4-oxobutanoic acid (three-letter code: KYN) (formula: $C_{10}H_{12}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			15	10	2	3		

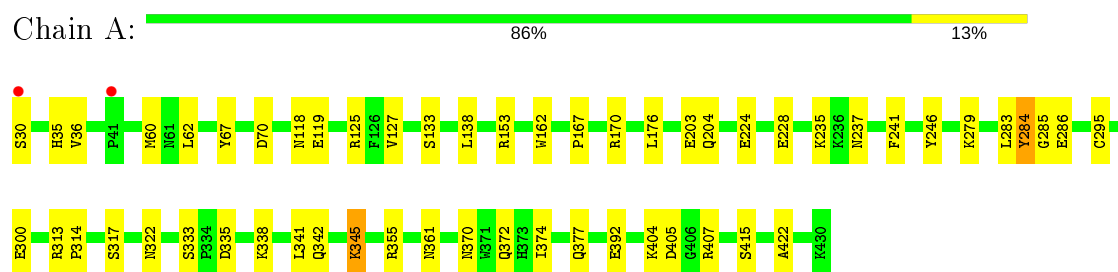
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	256	Total	O	0	0
			256	256		
6	B	172	Total	O	0	0
			172	172		
6	C	263	Total	O	0	0
			263	263		
6	D	140	Total	O	0	0
			140	140		

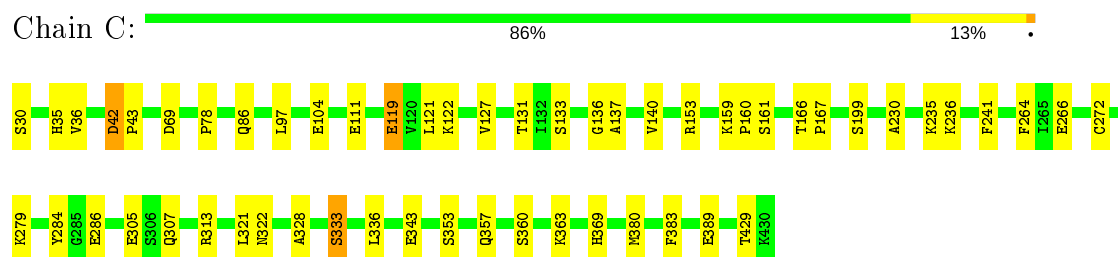
3 Residue-property plots [i](#)

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

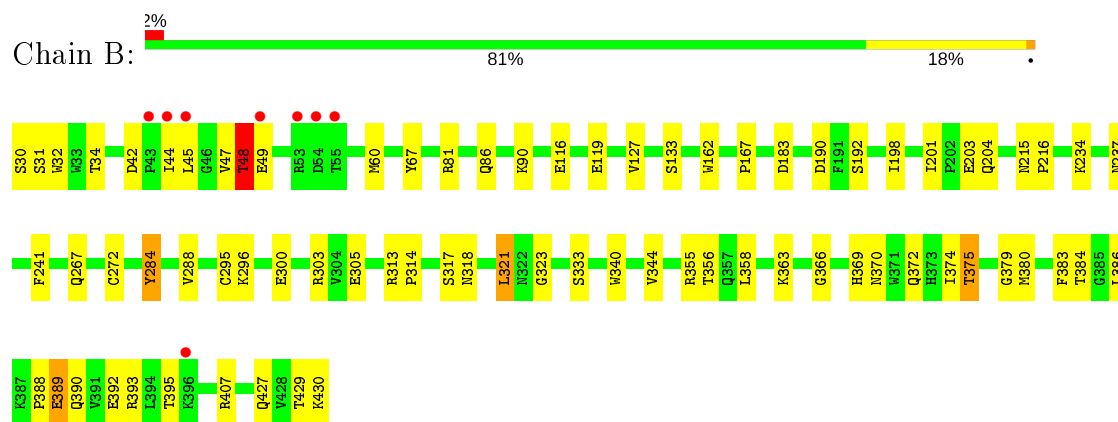
- Molecule 1: Aspartate aminotransferase, mitochondrial



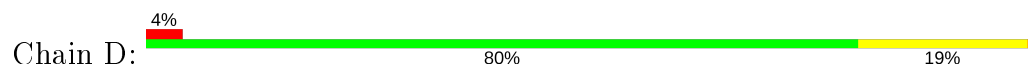
- Molecule 1: Aspartate aminotransferase, mitochondrial

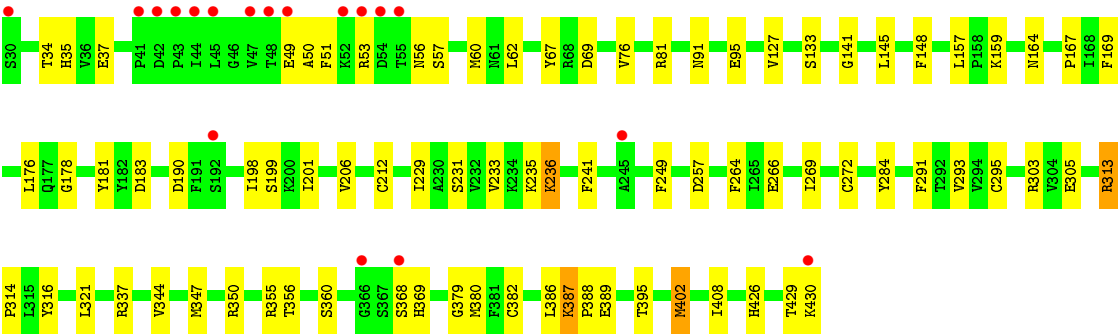


- Molecule 2: Aspartate aminotransferase, mitochondrial



- Molecule 2: Aspartate aminotransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	282.39 Å 78.11 Å 87.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 2.40 29.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.54-2.40) 93.9 (29.54-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.189 0.173 , 0.185	Depositor DCC
R_{free} test set	3603 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13546	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP, PMP, KYN

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	0.95	0/3213	0.81	0/4340
1	C	0.91	0/3213	0.81	1/4340 (0.0%)
2	B	0.87	2/3203 (0.1%)	0.81	0/4326
2	D	0.84	1/3203 (0.0%)	0.80	2/4326 (0.0%)
All	All	0.89	3/12832 (0.0%)	0.81	3/17332 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	284	TYR	CD2-CE2	-5.71	1.30	1.39
2	B	284	TYR	CD1-CE1	-5.42	1.31	1.39
2	D	95	GLU	CD-OE1	-5.30	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	337	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	69	ASP	CB-CG-OD1	5.87	123.58	118.30
2	D	321	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3140	0	3125	41	0
1	C	3140	0	3125	33	0
2	B	3155	0	3128	54	0
2	D	3155	0	3128	60	0
3	A	16	0	10	8	0
3	C	16	0	10	1	0
4	A	18	0	24	4	0
4	B	18	0	24	5	0
4	C	36	0	48	4	0
4	D	6	0	8	6	0
5	B	15	0	11	15	0
6	A	256	0	0	10	0
6	B	172	0	0	4	0
6	C	263	0	0	4	0
6	D	140	0	0	2	0
All	All	13546	0	12641	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (190) 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)
2:B:375:THR:HG23	6:B:591:HOH:O	1.59	1.02
3:A:1:PMP:HNA2	5:B:1:KYN:HB	1.20	1.01
3:A:1:PMP:N4A	5:B:1:KYN:HB	1.77	0.99
3:C:1:PMP:H4A1	6:C:786:HOH:O	1.68	0.94
2:B:318:ASN:HD21	5:B:1:KYN:HD1	1.33	0.93
2:B:318:ASN:ND2	5:B:1:KYN:HD1	1.85	0.92
3:A:1:PMP:H4A1	6:A:785:HOH:O	1.68	0.92
2:D:198:ILE:HA	2:D:201:ILE:HD12	1.51	0.91
2:D:402:MET:HE1	2:D:408:ILE:HG23	1.56	0.87
2:D:164:ASN:O	2:D:167:PRO:HD2	1.76	0.86
2:D:350:ARG:HD3	4:D:1:GOL:H31	1.59	0.85
2:D:387:LYS:HB2	2:D:387:LYS:HZ3	1.41	0.85
1:C:119:GLU:HG2	6:C:497:HOH:O	1.79	0.82
1:C:357:GLN:HG2	6:C:553:HOH:O	1.82	0.79
1:C:279:LYS:HE2	1:C:380:MET:HE3	1.63	0.79
2:D:402:MET:CE	2:D:408:ILE:CG2	2.61	0.79
2:B:318:ASN:HD21	5:B:1:KYN:CD1	1.97	0.77
1:A:162:TRP:HE1	5:B:1:KYN:HBA	1.50	0.76
2:B:67:TYR:OH	4:B:432:GOL:H12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:MET:HE1	2:D:408:ILE:CG2	2.15	0.75
2:D:426:HIS:CE1	2:D:430:LYS:HB3	2.23	0.73
3:A:1:PMP:HNA2	5:B:1:KYN:CB	2.01	0.73
1:A:170:ARG:HD3	6:A:601:HOH:O	1.89	0.71
2:B:198:ILE:HA	2:B:201:ILE:HD12	1.73	0.70
3:A:1:PMP:N4A	5:B:1:KYN:HE2	2.07	0.70
1:A:246:TYR:CE1	1:A:279:LYS:HG3	2.28	0.69
2:D:313:ARG:CB	2:D:314:PRO:HD3	2.22	0.68
2:D:387:LYS:NZ	2:D:387:LYS:HB2	2.08	0.68
2:B:318:ASN:ND2	5:B:1:KYN:CD1	2.54	0.68
1:C:313:ARG:HD3	6:C:611:HOH:O	1.95	0.67
1:C:127:VAL:HG21	1:C:305:GLU:HB2	1.78	0.66
1:C:30:SER:O	4:C:435:GOL:H12	1.95	0.66
2:D:402:MET:HE2	2:D:408:ILE:HG22	1.79	0.65
1:A:370:ASN:HD21	1:A:372:GLN:HE21	1.43	0.64
1:C:279:LYS:CE	1:C:380:MET:HE3	2.27	0.64
1:A:237:ASN:OD1	4:A:433:GOL:H12	1.97	0.64
2:B:375:THR:CG2	6:B:591:HOH:O	2.31	0.63
2:D:60:MET:HE2	2:D:62:LEU:HD21	1.81	0.63
2:D:69:ASP:HB2	4:D:1:GOL:H32	1.81	0.63
1:A:67:TYR:OH	4:A:431:GOL:H12	2.00	0.62
1:C:199:SER:O	1:C:236:LYS:HE2	1.99	0.62
2:B:183:ASP:HB2	2:B:190:ASP:HB2	1.82	0.61
2:D:231:SER:O	2:D:235:LYS:HG2	2.00	0.61
1:A:203:GLU:HG3	1:A:204:GLN:HG3	1.81	0.61
1:C:35:HIS:CD2	1:C:35:HIS:H	2.17	0.61
1:C:307:GLN:NE2	2:D:37:GLU:O	2.31	0.60
2:B:234:LYS:HD2	2:B:267:GLN:O	2.02	0.59
2:B:369:HIS:HE1	2:B:429:THR:O	1.85	0.59
2:D:34:THR:HG22	2:D:35:HIS:HD2	1.66	0.59
2:B:370:ASN:HD21	2:B:372:GLN:HE21	1.52	0.58
2:D:389:GLU:OE2	2:D:389:GLU:N	2.29	0.57
2:B:389:GLU:H	2:B:389:GLU:CD	2.08	0.57
1:C:97:LEU:HG	1:C:321:LEU:HD13	1.86	0.57
2:D:60:MET:CE	2:D:62:LEU:HD21	2.35	0.56
1:C:104:GLU:HG2	1:C:328:ALA:HB1	1.86	0.56
1:A:355:ARG:HD3	1:A:374:ILE:O	2.06	0.55
1:A:370:ASN:OD1	1:A:372:GLN:HG2	2.07	0.55
1:A:342:GLN:HG2	6:A:540:HOH:O	2.06	0.55
2:B:67:TYR:OH	4:B:432:GOL:C1	2.52	0.55
2:D:183:ASP:HB2	2:D:190:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:382:CYS:HB3	2:D:408:ILE:HG13	1.88	0.55
1:A:246:TYR:HE1	1:A:279:LYS:HG3	1.70	0.55
1:A:279:LYS:HD3	1:A:284:TYR:CE1	2.42	0.54
1:C:166:THR:HB	1:C:167:PRO:CD	2.37	0.54
2:B:241:PHE:CD1	2:B:272:CYS:SG	3.00	0.54
2:D:387:LYS:HB3	2:D:389:GLU:OE2	2.08	0.54
1:C:136:GLY:O	1:C:140:VAL:HG23	2.08	0.53
1:C:153:ARG:HE	1:C:153:ARG:HA	1.74	0.53
1:C:333:SER:OG	1:C:336:LEU:HB2	2.08	0.53
3:A:1:PMP:C4A	6:A:785:HOH:O	2.39	0.53
2:B:313:ARG:HB3	2:B:314:PRO:HD3	1.90	0.53
2:D:69:ASP:CB	4:D:1:GOL:H32	2.38	0.53
2:B:295:CYS:HB3	2:B:300:GLU:OE1	2.09	0.52
2:B:389:GLU:OE2	2:B:389:GLU:N	2.39	0.52
1:C:161:SER:H	4:C:432:GOL:H2	1.74	0.52
4:C:434:GOL:H12	2:D:76:VAL:HG23	1.90	0.52
2:D:402:MET:HE2	2:D:408:ILE:CG2	2.32	0.52
1:A:153:ARG:HD2	6:A:668:HOH:O	2.10	0.52
1:A:118:ASN:HA	6:A:507:HOH:O	2.10	0.52
2:D:355:ARG:NH2	2:D:379:GLY:O	2.43	0.52
1:C:78:PRO:HB2	1:C:343:GLU:OE1	2.09	0.52
2:B:45:LEU:HA	2:B:48:THR:HG22	1.92	0.52
2:D:313:ARG:HB3	2:D:314:PRO:HD3	1.89	0.52
2:B:31:SER:HB3	2:B:34:THR:HG23	1.93	0.50
3:A:1:PMP:P	5:B:1:KYN:HZ	2.51	0.50
2:B:31:SER:HB3	2:B:34:THR:CG2	2.42	0.50
1:C:35:HIS:HE1	2:D:148:PHE:O	1.94	0.50
4:A:433:GOL:H31	2:B:32:TRP:CE3	2.47	0.49
2:D:50:ALA:HA	2:D:53:ARG:NH2	2.28	0.49
2:D:49:GLU:HG2	2:D:53:ARG:HH12	1.78	0.49
2:B:215:ASN:OD1	2:B:216:PRO:HA	2.11	0.49
2:D:388:PRO:HD3	6:D:462:HOH:O	2.13	0.49
2:B:318:ASN:HD21	5:B:1:KYN:CE1	2.25	0.49
1:C:389:GLU:H	1:C:389:GLU:CD	2.16	0.49
2:D:127:VAL:HG21	2:D:305:GLU:HB2	1.95	0.49
1:A:279:LYS:HD3	1:A:284:TYR:HE1	1.77	0.49
5:B:1:KYN:HE2	5:B:1:KYN:HB	1.68	0.49
2:B:47:VAL:C	2:B:49:GLU:H	2.15	0.49
2:D:91:ASN:HB2	6:D:599:HOH:O	2.12	0.49
2:B:237:ASN:ND2	4:B:433:GOL:O2	2.42	0.48
1:A:167:PRO:HB2	2:B:314:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:LEU:HD13	2:D:206:VAL:HG21	1.94	0.48
2:B:81:ARG:O	6:B:504:HOH:O	2.20	0.48
2:D:293:VAL:HG12	2:D:295:CYS:SG	2.53	0.48
1:C:286:GLU:CD	1:C:322:ASN:ND2	2.67	0.48
2:D:199:SER:O	2:D:236:LYS:HD2	2.14	0.48
1:A:224:GLU:OE1	1:A:228:GLU:OE2	2.31	0.47
2:B:162:TRP:CD1	6:B:747:HOH:O	2.67	0.47
1:A:285:GLY:HA3	2:B:321:LEU:HD22	1.96	0.47
2:B:390:GLN:HE22	2:B:429:THR:HG22	1.78	0.47
2:D:169:PHE:HB2	2:D:176:LEU:HD11	1.97	0.47
2:D:402:MET:CE	2:D:408:ILE:HG22	2.37	0.47
2:B:384:THR:OG1	2:B:386:LEU:HD12	2.15	0.47
2:D:241:PHE:CD1	2:D:272:CYS:SG	3.07	0.47
1:A:162:TRP:HE1	5:B:1:KYN:CB	2.25	0.46
1:A:119:GLU:HB2	6:A:479:HOH:O	2.14	0.46
2:D:76:VAL:HG21	2:D:81:ARG:NH2	2.30	0.46
2:B:234:LYS:CD	2:B:267:GLN:O	2.64	0.46
2:D:157:LEU:O	2:D:178:GLY:HA2	2.16	0.46
1:A:176:LEU:HD22	1:A:176:LEU:N	2.31	0.45
2:D:387:LYS:HZ3	2:D:387:LYS:CB	2.17	0.45
1:A:60:MET:CE	1:A:62:LEU:HD21	2.46	0.45
1:A:138:LEU:HD23	1:A:241:PHE:HE2	1.80	0.45
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.84	0.45
1:C:230:ALA:HB2	1:C:264:PHE:CE1	2.52	0.45
1:C:266:GLU:O	1:C:266:GLU:HG2	2.15	0.45
2:B:215:ASN:HD21	4:B:431:GOL:H32	1.81	0.45
1:A:286:GLU:CD	1:A:322:ASN:HD22	2.20	0.45
1:C:166:THR:HG1	4:C:432:GOL:C3	2.30	0.45
1:C:36:VAL:O	2:D:303:ARG:HD2	2.17	0.45
2:D:313:ARG:CB	2:D:314:PRO:CD	2.95	0.45
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.82	0.44
1:A:392:GLU:HG3	1:A:404:LYS:HE2	1.99	0.44
2:B:389:GLU:O	2:B:393:ARG:HG3	2.18	0.44
2:D:49:GLU:HG2	2:D:53:ARG:NH1	2.31	0.44
2:B:388:PRO:O	2:B:392:GLU:HG3	2.18	0.44
2:D:344:VAL:HA	2:D:347:MET:HE3	2.00	0.44
2:B:313:ARG:HA	2:B:317:SER:HA	2.00	0.44
2:D:56:ASN:OD1	2:D:56:ASN:C	2.56	0.44
1:C:86:GLN:HE21	1:C:86:GLN:HB3	1.53	0.43
2:B:127:VAL:HG21	2:B:305:GLU:HB2	1.99	0.43
2:B:358:LEU:HD23	2:B:374:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:HA	4:D:1:GOL:H32	2.00	0.43
2:D:249:PHE:CZ	2:D:380:MET:CE	3.02	0.43
2:D:369:HIS:HE1	2:D:429:THR:O	2.02	0.43
1:C:241:PHE:CD1	1:C:272:CYS:SG	3.12	0.43
1:C:369:HIS:HE1	1:C:429:THR:O	2.02	0.43
2:B:427:GLN:O	2:B:430:LYS:HG2	2.19	0.43
1:C:131:THR:HG21	1:C:137:ALA:HA	2.01	0.43
1:A:407:ARG:NH1	5:B:1:KYN:O	2.49	0.43
2:B:198:ILE:HA	2:B:201:ILE:CD1	2.47	0.42
1:C:35:HIS:CE1	2:D:148:PHE:O	2.71	0.42
2:D:159:LYS:O	2:D:181:TYR:HB3	2.18	0.42
2:B:288:VAL:HG22	2:B:323:GLY:HA3	2.01	0.42
2:B:369:HIS:CE1	2:B:429:THR:O	2.68	0.42
2:D:141:GLY:HA2	2:D:291:PHE:CZ	2.54	0.42
1:C:42:ASP:HA	1:C:43:PRO:HD3	1.81	0.42
2:D:212:CYS:SG	2:D:257:ASP:HB3	2.60	0.42
1:A:283:LEU:O	1:A:284:TYR:C	2.58	0.42
2:B:288:VAL:CG2	2:B:323:GLY:HA3	2.49	0.42
2:B:363:LYS:O	2:B:366:GLY:N	2.52	0.42
2:B:372:GLN:O	2:B:375:THR:HG22	2.20	0.42
1:A:36:VAL:O	2:B:303:ARG:HD2	2.19	0.42
3:A:1:PMP:N4A	5:B:1:KYN:CB	2.66	0.41
1:A:35:HIS:CD2	1:A:35:HIS:H	2.38	0.41
1:A:67:TYR:OH	4:A:431:GOL:C1	2.66	0.41
2:B:203:GLU:O	2:B:204:GLN:HB2	2.21	0.41
2:D:229:ILE:HG22	2:D:264:PHE:HZ	1.85	0.41
2:B:355:ARG:NH2	2:B:379:GLY:O	2.30	0.41
2:D:67:TYR:OH	4:D:1:GOL:H12	2.20	0.41
2:D:344:VAL:HA	2:D:347:MET:CE	2.50	0.41
1:C:111:GLU:HA	1:C:121:LEU:HD11	2.02	0.41
1:C:159:LYS:HA	1:C:160:PRO:HA	1.74	0.41
2:D:233:VAL:CG1	2:D:269:ILE:HD13	2.50	0.41
1:A:153:ARG:NH1	6:A:668:HOH:O	2.39	0.41
2:B:86:GLN:O	2:B:90:LYS:HG3	2.21	0.41
1:A:295:CYS:HB3	1:A:300:GLU:OE1	2.21	0.41
2:B:340:TRP:O	2:B:344:VAL:HG23	2.21	0.41
2:D:386:LEU:HA	2:D:386:LEU:HD23	1.94	0.41
1:A:345:LYS:HE3	6:A:761:HOH:O	2.20	0.41
1:A:314:PRO:CG	2:B:167:PRO:HB2	2.51	0.41
1:A:338:LYS:NZ	6:A:580:HOH:O	2.54	0.40
2:B:162:TRP:HE1	4:B:431:GOL:H31	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ASN:OD1	2:D:57:SER:N	2.54	0.40
1:A:361:ASN:HB3	1:A:422:ALA:CB	2.51	0.40
2:B:47:VAL:C	2:B:49:GLU:N	2.75	0.40
1:A:355:ARG:NH1	1:A:377:GLN:HB2	2.36	0.40
2:D:69:ASP:HB2	4:D:1:GOL:C3	2.49	0.40
1:A:125:ARG:O	1:A:125:ARG:HG3	2.21	0.40
1:A:405:ASP:OD1	1:A:405:ASP:N	2.54	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	399/401 (100%)	388 (97%)	9 (2%)	2 (0%)	29	41
1	C	399/401 (100%)	385 (96%)	13 (3%)	1 (0%)	41	55
2	B	398/401 (99%)	379 (95%)	15 (4%)	4 (1%)	15	23
2	D	398/401 (99%)	376 (94%)	20 (5%)	2 (0%)	29	41
All	All	1594/1604 (99%)	1528 (96%)	57 (4%)	9 (1%)	25	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	TYR
1	C	284	TYR
2	D	284	TYR
1	A	317	SER
2	B	44	ILE
2	B	48	THR
2	B	119	GLU
2	B	284	TYR

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Mol	Chain	Res	Type
2	D	316	TYR

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	334/334 (100%)	325 (97%)	9 (3%)	44	65
1	C	334/334 (100%)	324 (97%)	10 (3%)	41	61
2	B	333/333 (100%)	316 (95%)	17 (5%)	24	39
2	D	333/333 (100%)	322 (97%)	11 (3%)	38	57
All	All	1334/1334 (100%)	1287 (96%)	47 (4%)	36	55

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	70	ASP
1	A	127	VAL
1	A	133	SER
1	A	235	LYS
1	A	333	SER
1	A	335	ASP
1	A	345	LYS
1	A	415	SER
2	B	30	SER
2	B	42	ASP
2	B	48	THR
2	B	60	MET
2	B	116	GLU
2	B	133	SER
2	B	192	SER
2	B	296	LYS
2	B	321	LEU
2	B	333	SER
2	B	356	THR

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Mol	Chain	Res	Type
2	B	375	THR
2	B	380	MET
2	B	383	PHE
2	B	389	GLU
2	B	395	THR
2	B	407	ARG
1	C	42	ASP
1	C	119	GLU
1	C	122	LYS
1	C	133	SER
1	C	235	LYS
1	C	333	SER
1	C	353	SER
1	C	360	SER
1	C	363	LYS
1	C	383	PHE
2	D	51	PHE
2	D	133	SER
2	D	236	LYS
2	D	266	GLU
2	D	313	ARG
2	D	356	THR
2	D	360	SER
2	D	368	SER
2	D	387	LYS
2	D	395	THR
2	D	402	MET

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	35	HIS
1	A	117	ASN
1	A	204	GLN
1	A	275	GLN
1	A	322	ASN
1	A	369	HIS
1	A	372	GLN
2	B	86	GLN
2	B	91	ASN
2	B	237	ASN
2	B	318	ASN

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Mol	Chain	Res	Type
2	B	361	ASN
2	B	369	HIS
2	B	372	GLN
1	C	35	HIS
1	C	86	GLN
1	C	322	ASN
1	C	361	ASN
1	C	369	HIS
2	D	35	HIS
2	D	86	GLN
2	D	91	ASN
2	D	237	ASN
2	D	369	HIS
2	D	372	GLN
2	D	426	HIS
2	D	427	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	LLP	B	279	2	23,24,25	3.33	11 (47%)	25,32,34	2.64	8 (32%)
2	LLP	D	279	2	23,24,25	2.56	9 (39%)	25,32,34	2.84	9 (36%)

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	LLP	B	279	2	-	12/16/17/19	0/1/1/1
2	LLP	D	279	2	-	8/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	279	LLP	O3-C3	-7.63	1.19	1.37
2	D	279	LLP	O3-C3	-7.37	1.19	1.37
2	B	279	LLP	CE-NZ	7.08	1.62	1.46
2	B	279	LLP	P-OP3	-4.87	1.36	1.54
2	B	279	LLP	P-OP2	-4.77	1.36	1.54
2	B	279	LLP	C4-C4'	4.33	1.54	1.46
2	D	279	LLP	P-OP3	-4.19	1.38	1.54
2	D	279	LLP	P-OP2	-4.05	1.39	1.54
2	D	279	LLP	P-OP1	-4.03	1.37	1.50
2	B	279	LLP	P-OP1	-3.98	1.37	1.50
2	B	279	LLP	P-OP4	-3.68	1.48	1.60
2	B	279	LLP	CD-CE	3.55	1.63	1.51
2	B	279	LLP	C3-C2	-3.20	1.37	1.40
2	D	279	LLP	P-OP4	-2.96	1.50	1.60
2	B	279	LLP	C4'-NZ	2.96	1.37	1.27
2	D	279	LLP	C4-C4'	2.81	1.52	1.46
2	D	279	LLP	CE-NZ	2.52	1.52	1.46
2	D	279	LLP	C3-C2	-2.39	1.38	1.40
2	B	279	LLP	C4-C3	-2.29	1.37	1.40
2	D	279	LLP	C4-C3	-2.08	1.37	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	279	LLP	OP4-C5'-C5	10.12	128.63	109.35
2	B	279	LLP	CD-CE-NZ	6.68	127.29	110.93
2	B	279	LLP	C3-C4-C5	-6.22	113.49	118.26
2	D	279	LLP	OP4-P-OP1	-4.81	92.97	106.47
2	D	279	LLP	C3-C4-C5	-4.12	115.10	118.26
2	B	279	LLP	OP4-C5'-C5	4.07	117.10	109.35
2	D	279	LLP	C5'-C5-C6	-3.84	113.06	119.37
2	B	279	LLP	C4-C3-C2	3.81	122.55	120.19
2	B	279	LLP	OP2-P-OP4	-3.43	97.60	106.73
2	B	279	LLP	OP3-P-OP2	3.33	120.35	107.64
2	B	279	LLP	C5'-C5-C6	-3.24	114.05	119.37
2	B	279	LLP	C6-C5-C4	2.66	123.04	118.15
2	D	279	LLP	OP3-P-OP4	-2.66	99.67	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	279	LLP	C6-C5-C4	2.28	122.34	118.15
2	D	279	LLP	OP3-P-OP2	2.17	115.93	107.64
2	D	279	LLP	C4-C3-C2	2.09	121.48	120.19
2	D	279	LLP	C5-C4-C4'	2.07	124.97	121.56

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	279	LLP	C4-C5-C5'-OP4
2	B	279	LLP	C6-C5-C5'-OP4
2	B	279	LLP	C5'-OP4-P-OP1
2	B	279	LLP	C5'-OP4-P-OP2
2	B	279	LLP	C5'-OP4-P-OP3
2	B	279	LLP	N-CA-CB-CG
2	D	279	LLP	C5'-OP4-P-OP1
2	D	279	LLP	C5'-OP4-P-OP2
2	D	279	LLP	C5'-OP4-P-OP3
2	B	279	LLP	C3-C4-C4'-NZ
2	D	279	LLP	C4-C4'-NZ-CE
2	B	279	LLP	CA-CB-CG-CD
2	B	279	LLP	CG-CD-CE-NZ
2	B	279	LLP	C4-C4'-NZ-CE
2	D	279	LLP	C3-C4-C4'-NZ
2	B	279	LLP	C-CA-CB-CG
2	D	279	LLP	C5-C4-C4'-NZ
2	D	279	LLP	CD-CE-NZ-C4'
2	B	279	LLP	CD-CE-NZ-C4'
2	D	279	LLP	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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$
4	GOL	C	434	-	5,5,5	0.37	0	5,5,5	0.92	0
3	PMP	C	1	-	16,16,16	2.58	7 (43%)	21,23,23	1.31	3 (14%)
3	PMP	A	1	-	16,16,16	1.10	2 (12%)	21,23,23	2.15	9 (42%)
4	GOL	B	432	-	5,5,5	0.62	0	5,5,5	0.75	0
4	GOL	C	435	-	5,5,5	0.52	0	5,5,5	0.64	0
4	GOL	B	431	-	5,5,5	0.51	0	5,5,5	0.94	0
4	GOL	A	431	-	5,5,5	0.27	0	5,5,5	0.82	0
4	GOL	C	436	-	5,5,5	0.33	0	5,5,5	0.22	0
4	GOL	C	431	-	5,5,5	0.40	0	5,5,5	0.43	0
5	KYN	B	1	-	12,15,15	1.53	2 (16%)	14,20,20	1.63	2 (14%)
4	GOL	C	432	-	5,5,5	0.50	0	5,5,5	1.09	1 (20%)
4	GOL	A	432	-	5,5,5	0.32	0	5,5,5	0.32	0
4	GOL	B	433	-	5,5,5	0.37	0	5,5,5	0.45	0
4	GOL	D	1	-	5,5,5	0.56	0	5,5,5	0.48	0
4	GOL	C	433	-	5,5,5	1.02	1 (20%)	5,5,5	1.22	1 (20%)
4	GOL	A	433	-	5,5,5	0.48	0	5,5,5	0.85	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
4	GOL	C	434	-	-	2/4/4/4	-
3	PMP	C	1	-	-	4/8/8/8	0/1/1/1
3	PMP	A	1	-	-	3/8/8/8	0/1/1/1
4	GOL	B	432	-	-	4/4/4/4	-
4	GOL	C	435	-	-	0/4/4/4	-
4	GOL	B	431	-	-	3/4/4/4	-
4	GOL	A	431	-	-	0/4/4/4	-
4	GOL	C	436	-	-	2/4/4/4	-
4	GOL	C	431	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	432	-	-	2/4/4/4	-
4	GOL	A	432	-	-	4/4/4/4	-
4	GOL	C	433	-	-	4/4/4/4	-
4	GOL	B	433	-	-	2/4/4/4	-
4	GOL	D	1	-	-	2/4/4/4	-
5	KYN	B	1	-	1/1/3/3	4/8/12/12	0/1/1/1
4	GOL	A	433	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	PMP	C3-C2	-5.14	1.35	1.40
3	C	1	PMP	P-O3P	-4.24	1.38	1.54
5	B	1	KYN	CD2-CG	-4.02	1.36	1.41
3	C	1	PMP	P-O2P	-3.95	1.39	1.54
3	C	1	PMP	P-O1P	-3.72	1.38	1.50
3	C	1	PMP	C5-C4	-3.07	1.36	1.40
3	C	1	PMP	C3-C4	-2.73	1.35	1.40
5	B	1	KYN	CB-C1	-2.55	1.47	1.51
3	A	1	PMP	C2-N1	2.30	1.38	1.33
3	A	1	PMP	C6-N1	2.22	1.39	1.34
4	C	433	GOL	O2-C2	-2.11	1.37	1.43
3	C	1	PMP	O3-C3	-2.08	1.32	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PMP	O3P-P-O4P	4.47	118.63	106.73
3	A	1	PMP	C4A-C4-C3	-4.25	113.59	120.34
5	B	1	KYN	CA-CB-C1	3.86	118.61	113.70
3	C	1	PMP	O4P-C5A-C5	3.83	116.66	109.35
3	A	1	PMP	O4P-C5A-C5	3.81	116.61	109.35
3	C	1	PMP	O2P-P-O4P	2.98	114.66	106.73
3	A	1	PMP	C3-C4-C5	2.92	121.52	118.72
3	A	1	PMP	C3-C2-N1	-2.49	117.56	120.77
4	C	432	GOL	O3-C3-C2	2.30	121.22	110.20
3	A	1	PMP	C4A-C4-C5	2.26	124.89	120.19
3	A	1	PMP	C4-C4A-N4A	-2.24	104.11	115.38
5	B	1	KYN	O2-C1-CB	-2.23	118.18	120.76
3	A	1	PMP	O3-C3-C2	2.20	122.29	117.49
3	C	1	PMP	O4P-P-O1P	2.18	112.60	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PMP	C5-C6-N1	-2.13	120.26	123.82
4	C	433	GOL	O2-C2-C1	-2.00	100.30	109.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1	KYN	CA

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	434	GOL	O2-C2-C3-O3
3	C	1	PMP	C5A-O4P-P-O2P
3	C	1	PMP	C5A-O4P-P-O3P
3	A	1	PMP	C5A-O4P-P-O1P
3	A	1	PMP	C5A-O4P-P-O2P
3	A	1	PMP	C5A-O4P-P-O3P
4	B	431	GOL	C1-C2-C3-O3
4	C	436	GOL	C1-C2-C3-O3
4	A	432	GOL	C1-C2-C3-O3
4	B	433	GOL	C1-C2-C3-O3
4	D	1	GOL	C1-C2-C3-O3
4	D	1	GOL	O2-C2-C3-O3
4	C	433	GOL	C1-C2-C3-O3
4	C	436	GOL	O2-C2-C3-O3
4	A	432	GOL	O2-C2-C3-O3
4	C	434	GOL	C1-C2-C3-O3
4	B	432	GOL	O1-C1-C2-C3
4	B	432	GOL	C1-C2-C3-O3
4	C	432	GOL	C1-C2-C3-O3
4	A	432	GOL	O1-C1-C2-C3
4	C	433	GOL	O1-C1-C2-C3
3	C	1	PMP	C5-C4-C4A-N4A
4	B	432	GOL	O2-C2-C3-O3
4	B	431	GOL	O2-C2-C3-O3
4	C	432	GOL	O2-C2-C3-O3
4	B	433	GOL	O2-C2-C3-O3
4	C	433	GOL	O2-C2-C3-O3
5	B	1	KYN	N-CA-CB-C1
5	B	1	KYN	O2-C1-CB-CA
5	B	1	KYN	CD2-C1-CB-CA
4	C	433	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	1	PMP	C5A-O4P-P-O1P
5	B	1	KYN	C-CA-CB-C1
4	B	432	GOL	O1-C1-C2-O2
4	A	432	GOL	O1-C1-C2-O2
4	B	431	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	434	GOL	1	0
3	C	1	PMP	1	0
3	A	1	PMP	8	0
4	B	432	GOL	2	0
4	C	435	GOL	1	0
4	B	431	GOL	2	0
4	A	431	GOL	2	0
5	B	1	KYN	15	0
4	C	432	GOL	2	0
4	B	433	GOL	1	0
4	D	1	GOL	6	0
4	A	433	GOL	2	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, 95th 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 ²)	Q<0.9
1	A	401/401 (100%)	-0.61	2 (0%) 91 89	11, 19, 33, 44	0
1	C	401/401 (100%)	-0.60	0 100 100	12, 22, 37, 46	0
2	B	400/401 (99%)	-0.33	8 (2%) 65 63	14, 31, 64, 91	0
2	D	400/401 (99%)	-0.08	18 (4%) 33 31	16, 35, 70, 89	0
All	All	1602/1604 (99%)	-0.41	28 (1%) 70 68	11, 26, 55, 91	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	44	ILE	4.6
2	B	44	ILE	3.5
2	D	41	PRO	3.5
2	D	55	THR	3.4
2	B	53	ARG	3.4
2	D	52	LYS	3.3
2	D	42	ASP	3.2
2	D	45	LEU	3.2
2	D	30	SER	3.2
2	B	45	LEU	3.2
2	B	49	GLU	3.1
2	D	53	ARG	3.0
2	D	49	GLU	2.9
2	D	43	PRO	2.8
2	D	48	THR	2.6
2	B	55	THR	2.6
1	A	30	SER	2.5
2	D	47	VAL	2.5
2	D	430	LYS	2.4
2	D	366	GLY	2.3
1	A	41	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	192	SER	2.2
2	D	54	ASP	2.2
2	B	43	PRO	2.1
2	B	396	LYS	2.1
2	B	54	ASP	2.1
2	D	368	SER	2.1
2	D	245	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LLP	B	279	24/25	0.94	0.15	23,28,35,39	0
2	LLP	D	279	24/25	0.95	0.17	27,39,45,46	0

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	434	6/6	0.71	0.35	54,56,57,58	0
4	GOL	C	436	6/6	0.79	0.26	59,61,61,61	0
4	GOL	C	435	6/6	0.82	0.28	61,62,63,63	0
4	GOL	A	432	6/6	0.82	0.18	59,59,60,60	0
5	KYN	B	1	15/15	0.83	0.30	62,64,65,67	0
4	GOL	D	1	6/6	0.84	0.15	40,43,44,45	0
4	GOL	B	431	6/6	0.85	0.22	48,49,49,51	0
4	GOL	A	431	6/6	0.87	0.15	48,49,49,51	0
4	GOL	C	431	6/6	0.90	0.15	25,30,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	433	6/6	0.91	0.20	46,47,47,48	0
4	GOL	C	433	6/6	0.92	0.28	48,49,49,51	0
4	GOL	A	433	6/6	0.92	0.12	40,42,43,45	0
4	GOL	C	432	6/6	0.94	0.26	20,26,34,36	0
4	GOL	B	432	6/6	0.96	0.15	38,39,40,43	0
3	PMP	C	1	16/16	0.97	0.13	17,25,36,43	0
3	PMP	A	1	16/16	0.98	0.13	14,20,30,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.