



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:30 PM UTC

PDB ID : 3PD6 / pdb_00003pd6
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 types of validation reports are described at

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

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

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

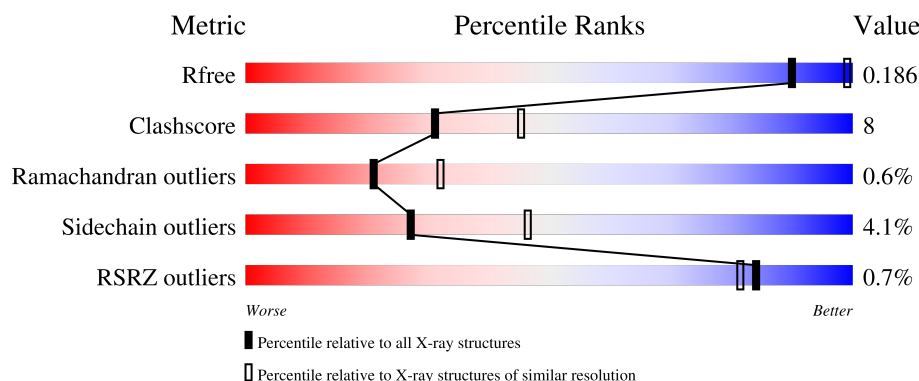
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of 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	 84% 15% .
1	C	401	 85% 13% .
2	B	401	 2% 78% 21% ..
2	D	401	 % 77% 21% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	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.

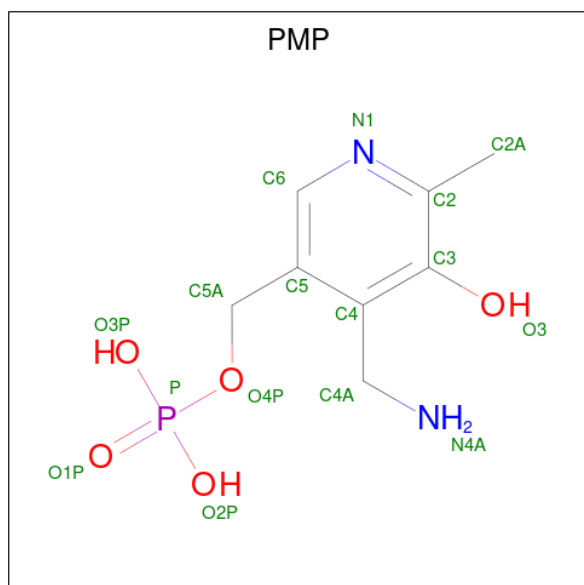
- Molecule 1 is a protein called Aspartate aminotransferase, mitochondrial.

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.

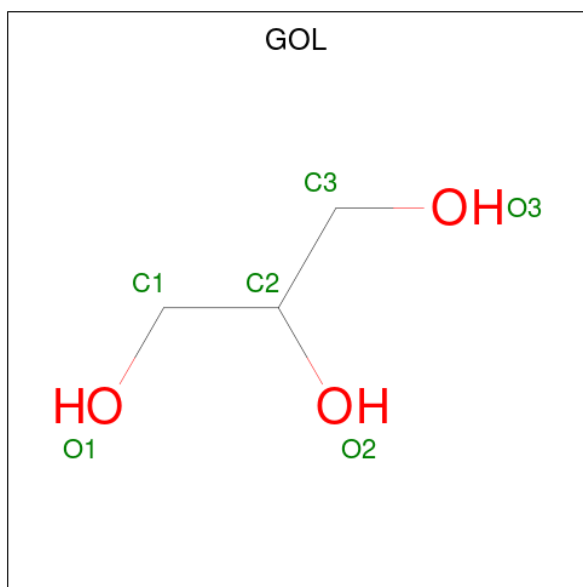
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	P	S	0	0
			3155	2005	551	582	1	16		
2	D	401	Total	C	N	O	P	S	0	0
			3155	2005	551	582	1	16		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



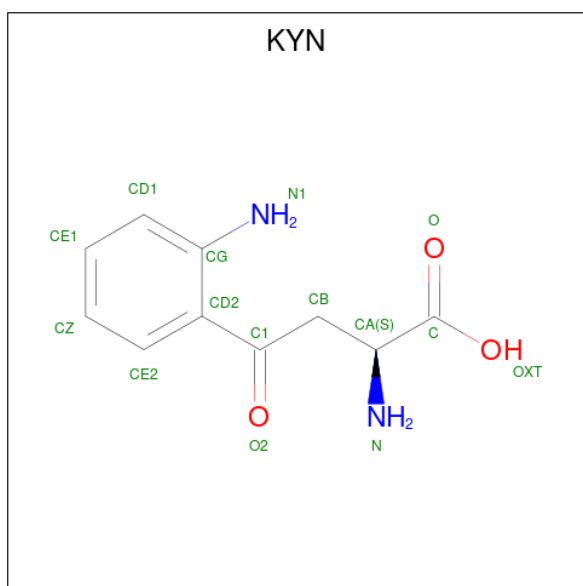
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

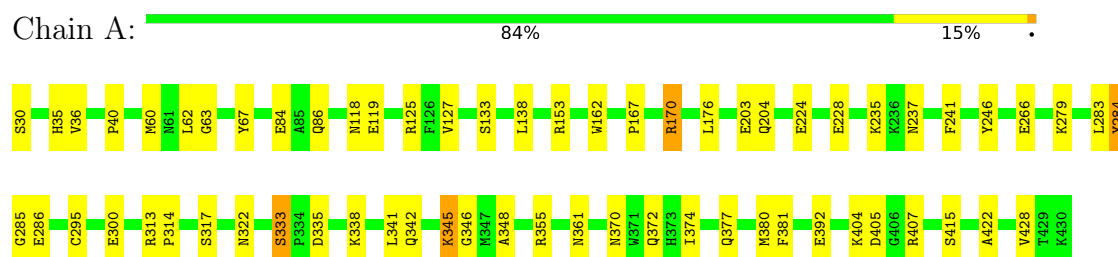
- Molecule 6 is water.

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		

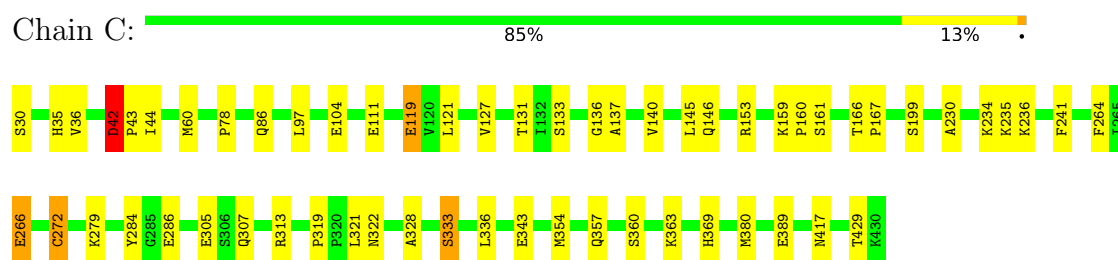
3 Residue-property plots

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

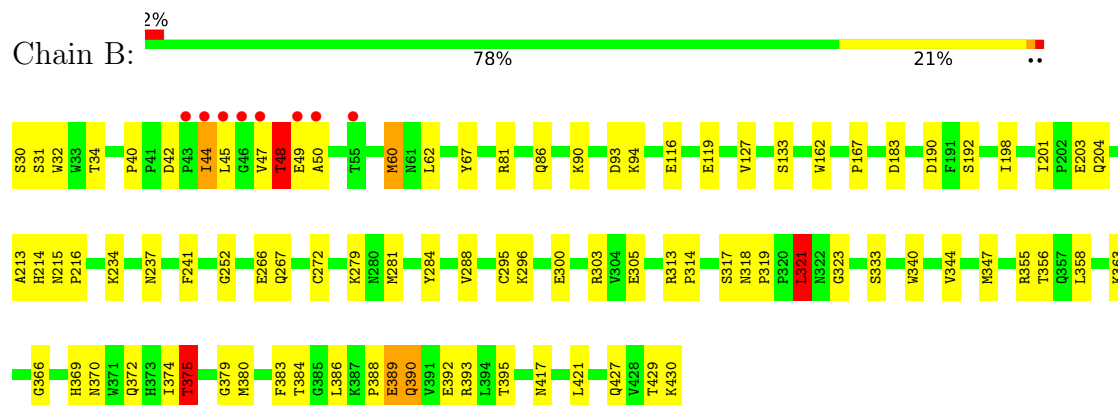
- Molecule 1: Aspartate aminotransferase, mitochondrial



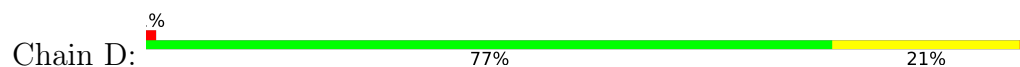
- Molecule 1: Aspartate aminotransferase, mitochondrial

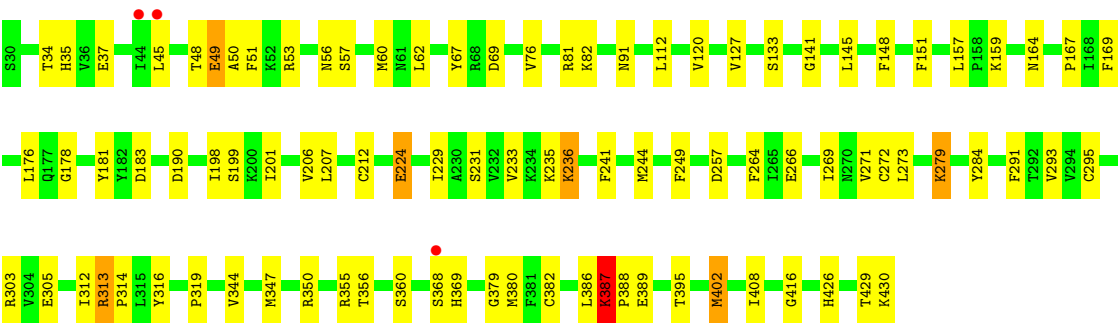


- Molecule 2: Aspartate aminotransferase, mitochondrial



- 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	282.39Å 78.11Å 87.51Å 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) 93.8 (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 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.189 0.173 , 0.186	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)	0.32 , 36.0	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: LLP, GOL, 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	1.14	4/3213 (0.1%)	1.09	3/4340 (0.1%)
1	C	1.08	0/3213	1.10	4/4340 (0.1%)
2	B	1.02	2/3203 (0.1%)	1.11	7/4326 (0.2%)
2	D	1.02	1/3203 (0.0%)	1.13	10/4326 (0.2%)
All	All	1.07	7/12832 (0.1%)	1.11	24/17332 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLY	C-O	-5.88	1.20	1.24
1	A	170	ARG	C-O	-5.85	1.17	1.24
1	A	40	PRO	CA-C	5.83	1.55	1.51
2	B	44	ILE	CA-CB	5.44	1.61	1.54
1	A	348	ALA	CA-CB	-5.30	1.45	1.53
2	B	281	MET	C-O	-5.12	1.17	1.24
2	D	319	PRO	CA-C	5.10	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	321	LEU	N-CA-C	8.29	120.39	111.36
2	D	416	GLY	N-CA-C	6.32	121.84	113.37
1	C	319	PRO	N-CA-C	5.79	117.76	110.70
2	B	252	GLY	N-CA-C	-5.79	107.40	114.92
2	D	151	PHE	N-CA-C	5.66	119.29	112.38
2	B	50	ALA	N-CA-C	-5.64	106.44	113.38
1	A	346	GLY	N-CA-C	5.44	119.26	112.73
1	A	333	SER	CA-C-N	-5.41	113.45	119.19
1	A	333	SER	C-N-CA	-5.41	113.45	119.19
2	D	112	LEU	N-CA-C	-5.33	105.38	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ASP	CA-C-N	5.29	124.80	119.19
1	C	42	ASP	C-N-CA	5.29	124.80	119.19
2	D	387	LYS	CA-C-N	5.24	124.42	118.97
2	D	387	LYS	C-N-CA	5.24	124.42	118.97
1	C	272	CYS	N-CA-C	-5.20	101.63	109.85
2	D	207	LEU	N-CA-C	5.19	117.19	108.73
2	B	319	PRO	CA-C-N	5.15	125.07	119.76
2	B	319	PRO	C-N-CA	5.15	125.07	119.76
2	D	120	VAL	N-CA-C	5.11	115.72	110.36
2	D	45	LEU	N-CA-C	-5.07	105.18	113.19
2	B	40	PRO	O-C-N	5.06	123.64	121.31
2	B	375	THR	CB-CA-C	5.05	117.21	109.03
2	D	319	PRO	CA-C-N	5.00	125.00	119.90
2	D	319	PRO	C-N-CA	5.00	125.00	119.90

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	44	0
1	C	3140	0	3125	37	0
2	B	3155	0	3128	62	0
2	D	3155	0	3129	64	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	3	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	5	0
6	C	263	0	0	4	0
6	D	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13546	0	12642	208	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 (208) 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
2:D:402:MET:HE2	2:D:408:ILE:CG2	1.90	1.01
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:HE2	2:D:408:ILE:HG22	1.54	0.89
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:HZ3	2:D:387:LYS:HB2	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
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
1:C:279:LYS:HE2	1:C:380:MET:HE3	1.68	0.75
2:D:402:MET:HE2	2:D:408:ILE:HG23	1.68	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:D:344:VAL:HA	2:D:347:MET:HE3	1.73	0.70
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:HB2	2:D:387:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:SER:O	4:C:435:GOL:H12	1.95	0.66
1:A:370:ASN:HD21	1:A:372:GLN:HE21	1.43	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: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:389:GLU:H	2:B:389:GLU:CD	2.08	0.62
1:C:60:MET:HE3	1:C:417:ASN:CG	2.25	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:H	1:C:35:HIS:CD2	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
1:A:60:MET:HE2	1:A:62:LEU:HD21	1.84	0.58
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:60:MET:HE3	2:B:417:ASN:CG	2.30	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
2:D:382:CYS:HB3	2:D:408:ILE:HG13	1.88	0.55
1:C:279:LYS:CE	1:C:380:MET:HE3	2.36	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:A:380:MET:HE3	1:A:381:PHE:CZ	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:B:162:TRP:NE1	6:B:747:HOH:O	2.40	0.54
2:D:60:MET:HE2	2:D:62:LEU:HD21	1.89	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:389:GLU:H	1:C:389:GLU:CD	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:VAL:C	2:B:49:GLU:H	2.15	0.53
1:C:153:ARG:HA	1:C:153:ARG:HE	1.74	0.53
1:C:333:SER:OG	1:C:336:LEU:HB2	2.08	0.53
2:B:60:MET:HE1	2:B:421:LEU:HD22	1.91	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:60:MET:HE2	2:B:62:LEU:HD21	1.90	0.53
1:C:286:GLU:CD	1:C:322:ASN:ND2	2.67	0.53
2:B:295:CYS:HB3	2:B:300:GLU:OE1	2.09	0.52
2:B:389:GLU:N	2:B:389:GLU:OE2	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:CE	2:D:408:ILE:HG23	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
1:A:286:GLU:CD	1:A:322:ASN:HD22	2.20	0.49
4:A:433:GOL:H31	2:B:32:TRP:CE3	2.47	0.49
2:D:49:GLU:HG2	2:D:53:ARG:HH12	1.78	0.49
2:D:50:ALA:HA	2:D:53:ARG:NH2	2.28	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
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:HB	5:B:1:KYN:HE2	1.68	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
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
2:D:199:SER:O	2:D:236:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ASN:OD1	2:D:56:ASN:C	2.56	0.47
1:A:224:GLU:OE1	1:A:228:GLU:OE2	2.31	0.47
1:A:285:GLY:HA3	2:B:321:LEU:HD22	1.96	0.47
2:B:162:TRP:CD1	6:B:747:HOH:O	2.67	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: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:283:LEU:O	1:A:284:TYR:C	2.58	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: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
2:B:47:VAL:C	2:B:49:GLU:N	2.75	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
1:C:60:MET:HE3	1:C:417:ASN:ND2	2.33	0.44
2:B:313:ARG:HA	2:B:317:SER:HA	2.00	0.44
1:A:60:MET:CE	1:A:62:LEU:HD21	2.46	0.44
1:C:86:GLN:HE21	1:C:86:GLN:HB3	1.53	0.43
1:C:354:MET:HA	1:C:354:MET:HE2	1.98	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
2:D:69:ASP:HA	4:D:1:GOL:H32	2.00	0.43
2:D:279:LLP:HD3	2:D:279:LLP:H	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:279:LYS:CE	1:C:380:MET:CE	2.97	0.42
2:B:344:VAL:HA	2:B:347:MET:HE3	2.01	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
2:D:312:ILE:O	2:D:313:ARG:C	2.63	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
2:D:224:GLU:H	2:D:224:GLU:CD	2.27	0.42
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
3:A:1:PMP:N4A	5:B:1:KYN:CB	2.66	0.41
2:B:203:GLU:O	2:B:204:GLN:HB2	2.21	0.41
2:D:164:ASN:C	2:D:167:PRO:HD2	2.42	0.41
2:D:229:ILE:HG22	2:D:264:PHE:HZ	1.85	0.41
2:D:244:MET:HE2	2:D:273:LEU:HD11	2.01	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
1:C:145:LEU:O	1:C:146:GLN:C	2.61	0.41
1:A:84:GLU:CD	2:B:94:LYS:HZ1	2.29	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:213:ALA:O	2:B:214:HIS:C	2.63	0.41
2:B:340:TRP:O	2:B:344:VAL:HG23	2.21	0.41
2:D:386:LEU:HD23	2:D:386:LEU:HA	1.94	0.41
1:A:314:PRO:CG	2:B:167:PRO:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:HE3	6:A:761:HOH:O	2.20	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
2:D:56:ASN:OD1	2:D:57:SER:N	2.54	0.40
2:D:69:ASP:OD1	2:D:69:ASP:C	2.64	0.40
1:A:361:ASN:HB3	1:A:422:ALA:CB	2.51	0.40
1:A:355:ARG:NH1	1:A:377:GLN:HB2	2.36	0.40
2:B:93:ASP:OD1	2:B:93:ASP:C	2.63	0.40
2:D:69:ASP:HB2	4:D:1:GOL:C3	2.49	0.40
1:A:125:ARG:HG3	1:A:125:ARG:O	2.21	0.40
1:A:405:ASP:N	1:A:405:ASP:OD1	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%)	24	37
1	C	399/401 (100%)	385 (96%)	13 (3%)	1 (0%)	36	50
2	B	398/401 (99%)	379 (95%)	15 (4%)	4 (1%)	12	20
2	D	398/401 (99%)	376 (94%)	20 (5%)	2 (0%)	24	37
All	All	1594/1604 (99%)	1528 (96%)	57 (4%)	9 (1%)	21	32

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

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Mol	Chain	Res	Type
2	B	44	ILE
2	B	48	THR
2	B	119	GLU
2	B	284	TYR
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%)	323 (97%)	11 (3%)	33	55
1	C	334/334 (100%)	324 (97%)	10 (3%)	36	58
2	B	333/333 (100%)	315 (95%)	18 (5%)	20	35
2	D	333/333 (100%)	317 (95%)	16 (5%)	23	40
All	All	1334/1334 (100%)	1279 (96%)	55 (4%)	27	46

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	86	GLN
1	A	127	VAL
1	A	133	SER
1	A	235	LYS
1	A	266	GLU
1	A	333	SER
1	A	335	ASP
1	A	345	LYS
1	A	415	SER
1	A	428	VAL
2	B	30	SER
2	B	42	ASP
2	B	48	THR
2	B	60	MET
2	B	116	GLU

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Mol	Chain	Res	Type
2	B	133	SER
2	B	192	SER
2	B	266	GLU
2	B	296	LYS
2	B	321	LEU
2	B	333	SER
2	B	356	THR
2	B	375	THR
2	B	380	MET
2	B	383	PHE
2	B	389	GLU
2	B	390	GLN
2	B	395	THR
1	C	42	ASP
1	C	44	ILE
1	C	119	GLU
1	C	133	SER
1	C	234	LYS
1	C	235	LYS
1	C	266	GLU
1	C	333	SER
1	C	360	SER
1	C	363	LYS
2	D	48	THR
2	D	49	GLU
2	D	51	PHE
2	D	82	LYS
2	D	133	SER
2	D	224	GLU
2	D	236	LYS
2	D	266	GLU
2	D	271	VAL
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

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

Mol	Chain	Res	Type
1	A	35	HIS
1	A	117	ASN
1	A	204	GLN
1	A	275	GLN
1	A	322	ASN
1	A	357	GLN
1	A	361	ASN
1	A	372	GLN
2	B	86	GLN
2	B	91	ASN
2	B	237	ASN
2	B	263	HIS
2	B	275	GLN
2	B	318	ASN
2	B	369	HIS
2	B	372	GLN
1	C	35	HIS
1	C	86	GLN
1	C	361	ASN
1	C	369	HIS
2	D	35	HIS
2	D	86	GLN
2	D	91	ASN
2	D	204	GLN
2	D	275	GLN
2	D	361	ASN
2	D	369	HIS
2	D	372	GLN
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	D	279	2	23,24,25	2.58	9 (39%)	25,32,34	2.88	9 (36%)
2	LLP	B	279	2	23,24,25	3.33	12 (52%)	25,32,34	2.61	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	D	279	2	-	8/16/17/19	0/1/1/1
2	LLP	B	279	2	-	12/16/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	279	LLP	O3-C3	-7.71	1.19	1.36
2	D	279	LLP	O3-C3	-7.45	1.19	1.36
2	B	279	LLP	CE-NZ	6.90	1.62	1.46
2	B	279	LLP	P-OP3	-5.04	1.36	1.54
2	B	279	LLP	P-OP2	-4.94	1.36	1.54
2	D	279	LLP	P-OP3	-4.33	1.38	1.54
2	D	279	LLP	P-OP2	-4.19	1.39	1.54
2	D	279	LLP	P-OP1	-4.16	1.37	1.50
2	B	279	LLP	P-OP1	-4.11	1.37	1.50
2	B	279	LLP	C4-C4'	3.86	1.54	1.46
2	B	279	LLP	P-OP4	-3.78	1.48	1.60
2	B	279	LLP	CD-CE	3.59	1.63	1.51
2	B	279	LLP	C3-C2	-3.15	1.37	1.41
2	D	279	LLP	P-OP4	-3.05	1.50	1.60
2	B	279	LLP	C4'-NZ	3.00	1.37	1.27
2	D	279	LLP	C4-C4'	2.51	1.52	1.46
2	D	279	LLP	CE-NZ	2.45	1.52	1.46
2	D	279	LLP	C3-C2	-2.37	1.38	1.41
2	B	279	LLP	C4-C3	-2.27	1.37	1.41
2	B	279	LLP	C2'-C2	-2.10	1.47	1.50
2	D	279	LLP	C4-C3	-2.08	1.37	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	279	LLP	OP4-C5'-C5	10.28	128.63	109.36
2	B	279	LLP	CD-CE-NZ	6.22	127.29	110.83
2	B	279	LLP	C3-C4-C5	-5.96	113.49	118.28
2	D	279	LLP	OP4-P-OP1	-4.98	92.97	106.44
2	B	279	LLP	C4-C3-C2	4.27	122.55	120.14
2	B	279	LLP	OP4-C5'-C5	4.13	117.10	109.36
2	D	279	LLP	C3-C4-C5	-3.96	115.10	118.28
2	D	279	LLP	C5'-C5-C6	-3.87	113.06	119.36
2	B	279	LLP	OP2-P-OP4	-3.48	97.60	106.67
2	B	279	LLP	OP3-P-OP2	3.35	120.35	107.80
2	B	279	LLP	C5'-C5-C6	-3.26	114.05	119.36
2	B	279	LLP	C6-C5-C4	2.81	123.04	118.21
2	D	279	LLP	OP3-P-OP4	-2.69	99.67	106.67
2	D	279	LLP	C6-C5-C4	2.40	122.34	118.21
2	D	279	LLP	C4-C3-C2	2.38	121.48	120.14
2	D	279	LLP	C5-C4-C4'	2.26	124.97	121.47
2	D	279	LLP	OP3-P-OP2	2.17	115.93	107.80
2	B	279	LLP	C5-C6-N1	-2.00	120.58	123.83

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	C4-C4'-NZ-CE
2	D	279	LLP	C3-C4-C4'-NZ
2	B	279	LLP	CG-CD-CE-NZ
2	B	279	LLP	CA-CB-CG-CD
2	B	279	LLP	C-CA-CB-CG
2	D	279	LLP	CD-CE-NZ-C4'
2	D	279	LLP	C5-C4-C4'-NZ
2	B	279	LLP	CD-CE-NZ-C4'
2	D	279	LLP	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	279	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	431	-	5,5,5	0.53	0	5,5,5	0.99	0
4	GOL	C	432	-	5,5,5	0.53	0	5,5,5	1.14	1 (20%)
4	GOL	A	431	-	5,5,5	0.28	0	5,5,5	0.87	0
4	GOL	C	434	-	5,5,5	0.39	0	5,5,5	0.96	0
4	GOL	A	432	-	5,5,5	0.33	0	5,5,5	0.33	0
4	GOL	C	435	-	5,5,5	0.54	0	5,5,5	0.65	0
4	GOL	D	1	-	5,5,5	0.58	0	5,5,5	0.50	0
4	GOL	B	433	-	5,5,5	0.39	0	5,5,5	0.47	0
3	PMP	C	1	-	16,16,16	2.63	7 (43%)	22,23,23	1.32	3 (13%)
4	GOL	C	436	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	B	432	-	5,5,5	0.63	0	5,5,5	0.81	0
4	GOL	C	433	-	5,5,5	1.05	1 (20%)	5,5,5	1.29	1 (20%)
4	GOL	A	433	-	5,5,5	0.50	0	5,5,5	0.93	0
3	PMP	A	1	-	16,16,16	1.15	2 (12%)	22,23,23	2.13	9 (40%)
4	GOL	C	431	-	5,5,5	0.42	0	5,5,5	0.47	0
5	KYN	B	1	-	14,15,15	1.75	3 (21%)	15,20,20	2.74	4 (26%)

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	B	431	-	-	3/4/4/4	-
4	GOL	C	432	-	-	2/4/4/4	-
4	GOL	A	431	-	-	0/4/4/4	-
3	PMP	A	1	-	-	3/8/8/8	0/1/1/1
4	GOL	A	432	-	-	4/4/4/4	-
4	GOL	C	434	-	-	2/4/4/4	-
4	GOL	C	435	-	-	0/4/4/4	-
4	GOL	D	1	-	-	2/4/4/4	-
4	GOL	B	433	-	-	2/4/4/4	-
3	PMP	C	1	-	-	4/8/8/8	0/1/1/1
4	GOL	C	436	-	-	2/4/4/4	-
4	GOL	B	432	-	-	4/4/4/4	-
4	GOL	C	433	-	-	4/4/4/4	-
4	GOL	A	433	-	-	0/4/4/4	-
5	KYN	B	1	-	1/1/3/3	7/12/12/12	0/1/1/1
4	GOL	C	431	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	PMP	C3-C2	-5.02	1.35	1.41
3	C	1	PMP	P-O3P	-4.39	1.38	1.54
3	C	1	PMP	P-O2P	-4.08	1.39	1.54
5	B	1	KYN	OXT-C	-3.87	1.18	1.30
3	C	1	PMP	P-O1P	-3.83	1.38	1.50
5	B	1	KYN	CD2-CG	-3.66	1.36	1.41
3	C	1	PMP	C5-C4	-3.10	1.36	1.40
3	C	1	PMP	C3-C4	-2.85	1.35	1.40
5	B	1	KYN	CB-C1	-2.77	1.47	1.51
3	A	1	PMP	C2-N1	2.44	1.38	1.33
3	A	1	PMP	C6-N1	2.31	1.39	1.34
4	C	433	GOL	O2-C2	-2.16	1.37	1.43
3	C	1	PMP	O3-C3	-2.08	1.32	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	KYN	OXT-C-O	-7.94	106.07	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	KYN	CA-CB-C1	5.20	118.61	113.06
3	A	1	PMP	O3P-P-O4P	4.59	118.63	106.67
3	A	1	PMP	C4A-C4-C3	-3.92	113.59	120.22
3	C	1	PMP	O4P-C5A-C5	3.90	116.66	109.36
3	A	1	PMP	O4P-C5A-C5	3.87	116.61	109.36
3	A	1	PMP	C3-C4-C5	3.08	121.52	118.73
3	C	1	PMP	O2P-P-O4P	3.06	114.66	106.67
3	A	1	PMP	C3-C2-N1	-2.70	117.56	120.96
4	C	432	GOL	O3-C3-C2	2.41	121.22	110.38
3	A	1	PMP	C4A-C4-C5	2.30	124.89	120.27
3	C	1	PMP	O4P-P-O1P	2.28	112.60	106.44
3	A	1	PMP	O3-C3-C2	2.27	122.29	117.58
3	A	1	PMP	C5-C6-N1	-2.19	120.26	123.83
4	C	433	GOL	O2-C2-C1	-2.14	100.30	109.18
5	B	1	KYN	O2-C1-CB	-2.12	118.18	120.70
5	B	1	KYN	O2-C1-CD2	2.07	124.18	120.79
3	A	1	PMP	C4-C4A-N4A	-2.07	104.11	114.85

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1	KYN	CA

All (39) torsion outliers are listed below:

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

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

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	431	GOL	2	0
4	C	432	GOL	1	0
4	A	431	GOL	2	0
4	C	434	GOL	1	0
4	C	435	GOL	1	0
4	D	1	GOL	6	0
4	B	433	GOL	1	0
3	C	1	PMP	1	0
4	B	432	GOL	2	0
4	A	433	GOL	2	0
3	A	1	PMP	8	0
5	B	1	KYN	15	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%)	-0.85	0 100 100	11, 19, 33, 44	0
1	C	401/401 (100%)	-0.75	0 100 100	12, 22, 37, 46	0
2	B	400/401 (99%)	-0.42	8 (2%) 65 60	14, 31, 64, 91	0
2	D	400/401 (99%)	-0.11	3 (0%) 82 80	16, 35, 70, 89	0
All	All	1602/1604 (99%)	-0.53	11 (0%) 84 81	11, 26, 55, 91	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	47	VAL	3.5
2	B	44	ILE	3.4
2	D	45	LEU	2.8
2	B	50	ALA	2.7
2	D	44	ILE	2.6
2	B	45	LEU	2.6
2	D	368	SER	2.2
2	B	46	GLY	2.2
2	B	55	THR	2.1
2	B	49	GLU	2.1
2	B	43	PRO	2.0

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

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	0.91	0.12	23,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LLP	D	279	24/25	0.93	0.10	27,39,45,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	GOL	B	431	6/6	0.80	0.14	48,49,49,51	0
4	GOL	C	435	6/6	0.80	0.12	61,62,63,63	0
4	GOL	C	433	6/6	0.81	0.20	48,49,49,51	0
5	KYN	B	1	15/15	0.81	0.19	62,64,65,67	0
4	GOL	A	431	6/6	0.83	0.15	48,49,49,51	0
4	GOL	C	434	6/6	0.85	0.13	54,56,57,58	0
4	GOL	D	1	6/6	0.89	0.13	40,43,44,45	0
4	GOL	C	436	6/6	0.89	0.12	59,61,61,61	0
4	GOL	A	432	6/6	0.90	0.12	59,59,60,60	0
4	GOL	C	431	6/6	0.90	0.09	25,30,32,37	0
4	GOL	B	432	6/6	0.91	0.10	38,39,40,43	0
4	GOL	B	433	6/6	0.92	0.08	46,47,47,48	0
4	GOL	A	433	6/6	0.92	0.09	40,42,43,45	0
4	GOL	C	432	6/6	0.93	0.18	20,26,34,36	0
3	PMP	C	1	16/16	0.96	0.07	17,25,36,43	0
3	PMP	A	1	16/16	0.97	0.07	14,20,30,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.