



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:42 am BST

PDB ID : 6JIX
Title : The crystal structure of taurine:2-oxoglutarate aminotransferase from *Bifidobacterium kashiwanohense*, in complex with PLP and glutamate
Authors : Li, M.; Lin, L.; Zhang, Y.; Yuchi, Z.
Deposited on : 2019-02-23
Resolution : 2.65 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

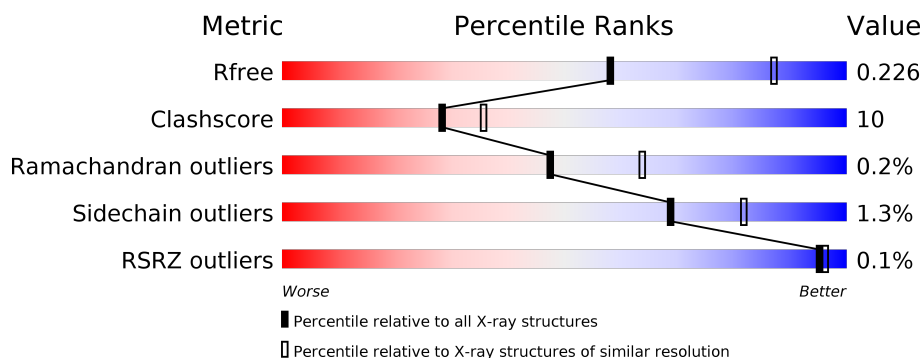
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	449	<div> <div style="width: 82%;"></div> <div style="width: 18%;"></div> </div> <div>82% 18%</div>
1	B	449	<div> <div style="width: 78%;"></div> <div style="width: 20%;"></div> <div style="width: 2%;"></div> </div> <div>78% 20% ..</div>
1	C	449	<div> <div style="width: 71%;"></div> <div style="width: 27%;"></div> <div style="width: 2%;"></div> </div> <div>71% 27% ..</div>
1	D	449	<div> <div style="width: 78%;"></div> <div style="width: 20%;"></div> <div style="width: 2%;"></div> </div> <div>78% 20% ..</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	GGL	B	501	-	-	X	-
2	GGL	B	502	-	-	X	-
2	GGL	C	502	-	-	-	X
2	GGL	C	503	-	-	X	-
2	GGL	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14305 atoms, of which 92 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.

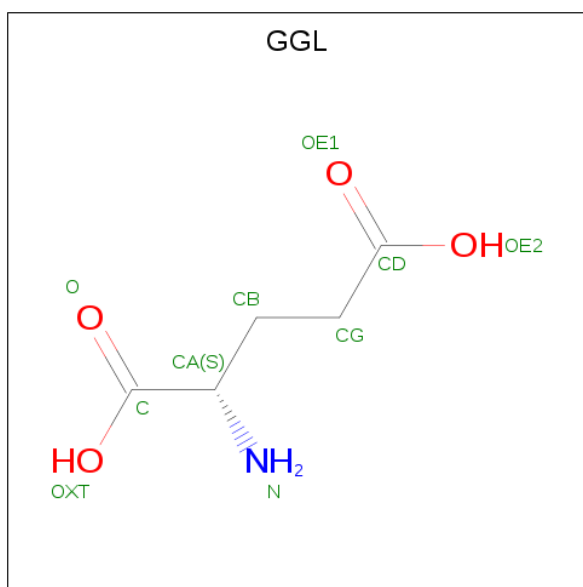
- Molecule 1 is a protein called taurine:2-oxoglutarate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	446	Total	C	N	O	S	0	0	0
			3428	2177	566	650	35			
1	A	447	Total	C	N	O	S	0	0	0
			3442	2185	571	651	35			
1	C	446	Total	C	N	O	S	0	0	0
			3421	2175	568	644	34			
1	D	446	Total	C	N	O	S	0	0	0
			3413	2169	566	644	34			

There are 8 discrepancies between the modelled and reference sequences:

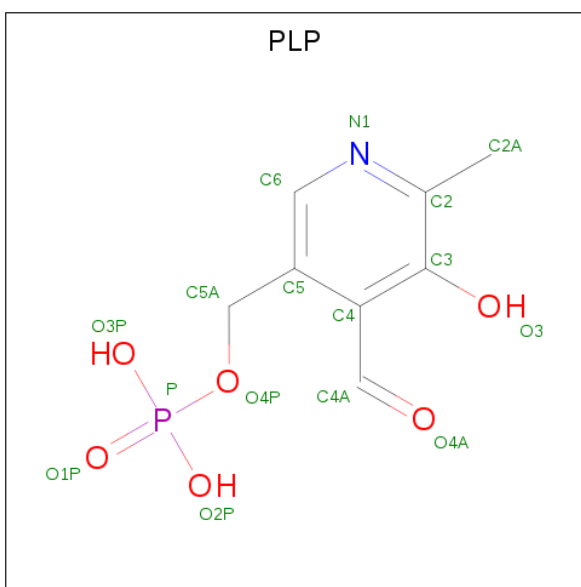
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP A0A0A7I435
B	0	ASN	-	expression tag	UNP A0A0A7I435
A	-1	SER	-	expression tag	UNP A0A0A7I435
A	0	ASN	-	expression tag	UNP A0A0A7I435
C	-1	SER	-	expression tag	UNP A0A0A7I435
C	0	ASN	-	expression tag	UNP A0A0A7I435
D	-1	SER	-	expression tag	UNP A0A0A7I435
D	0	ASN	-	expression tag	UNP A0A0A7I435

- Molecule 2 is GAMMA-L-GLUTAMIC ACID (three-letter code: GGL) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	B	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	A	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	C	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	C	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	C	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	D	1	Total	C	H	N	O	0	0
			17	5	7	1	4		
2	D	1	Total	C	H	N	O	0	0
			17	5	7	1	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	B	1	Total 25	C 8	H 9	N 1	O 6	P 1	0	0
3	A	1	Total 25	C 8	H 9	N 1	O 6	P 1	0	0
3	C	1	Total 25	C 8	H 9	N 1	O 6	P 1	0	0
3	D	1	Total 25	C 8	H 9	N 1	O 6	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	110	Total	O	0	0
			110	110		
4	A	119	Total	O	0	0
			119	119		
4	C	72	Total	O	0	0
			72	72		
4	D	64	Total	O	0	0
			64	64		

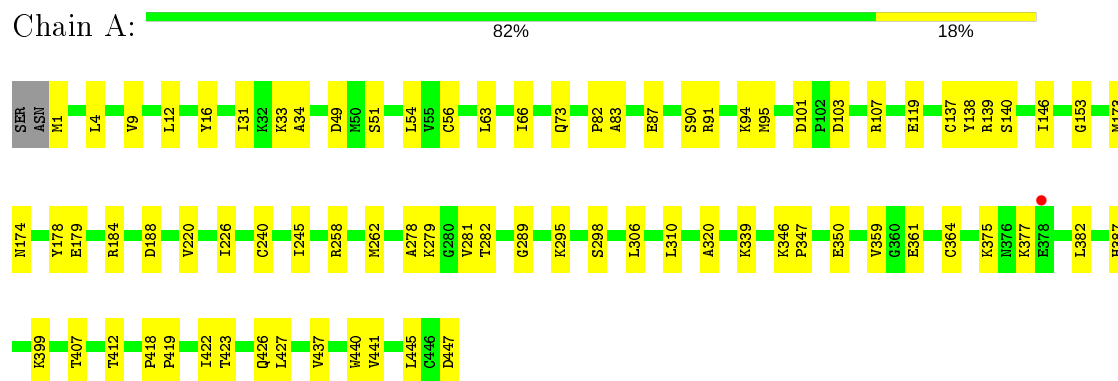
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

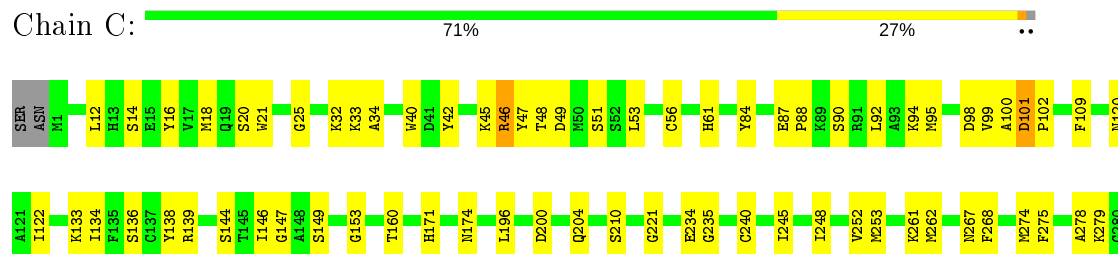
- Molecule 1: taurine:2-oxoglutarate aminotransferase

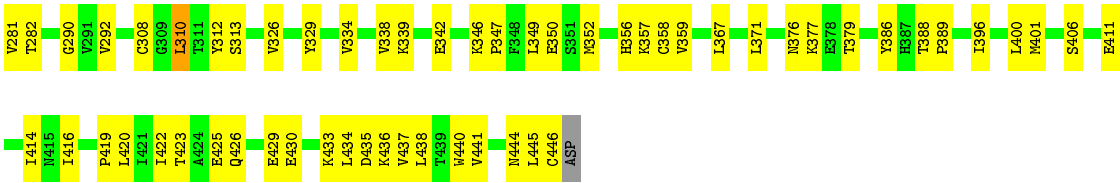


- Molecule 1: taurine:2-oxoglutarate aminotransferase

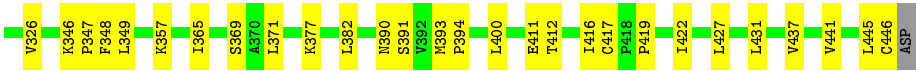
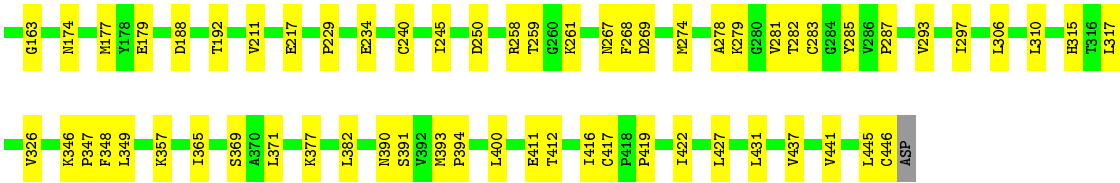
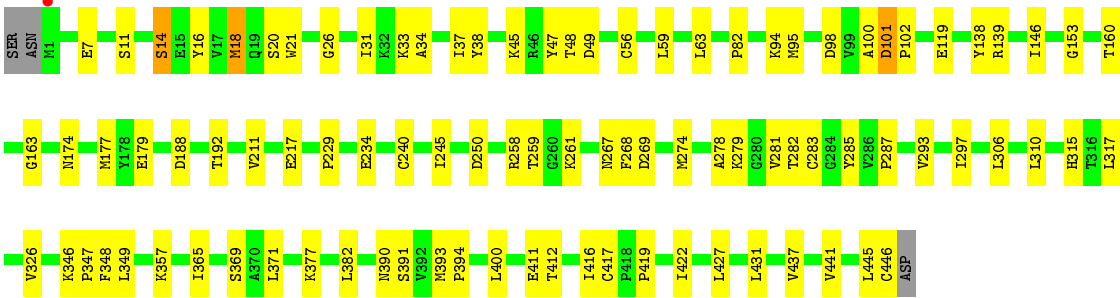
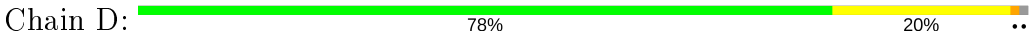


- Molecule 1: taurine:2-oxoglutarate aminotransferase





• Molecule 1: taurine:2-oxoglutarate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.39Å 164.54Å 109.24Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	44.29 – 2.65 44.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.29-2.65) 93.3 (44.29-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3247	Depositor
R, R_{free}	0.167 , 0.227 0.166 , 0.226	Depositor DCC
R_{free} test set	1996 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14305	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: GGL, PLP

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	0.43	0/3523	0.58	0/4775
1	B	0.41	0/3509	0.59	0/4758
1	C	0.40	0/3502	0.56	0/4748
1	D	0.42	0/3494	0.57	0/4740
All	All	0.42	0/14028	0.57	0/19021

There are no bond length outliers.

There are no bond angle outliers.

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	3442	0	3327	54	0
1	B	3428	0	3304	71	0
1	C	3421	0	3308	96	0
1	D	3413	0	3286	68	0
2	A	10	7	7	1	0
2	B	20	14	14	11	0
2	C	30	21	21	9	0
2	D	20	14	14	6	0
3	A	16	9	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	9	8	0	0
3	C	16	9	8	0	0
3	D	16	9	8	0	0
4	A	119	0	0	0	0
4	B	110	0	0	1	0
4	C	72	0	0	0	0
4	D	64	0	0	0	0
All	All	14213	92	13313	267	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 10.

All (267) 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:502:GGL:HG3	1:D:82:PRO:HB2	1.52	0.92
1:C:423:THR:OG1	1:C:426:GLN:HG3	1.71	0.90
1:C:99:VAL:CG1	1:C:262:MET:HG2	2.07	0.85
1:C:99:VAL:HG11	1:C:262:MET:HG2	1.61	0.82
1:B:278:ALA:O	1:B:281:VAL:HG12	1.82	0.80
1:A:281:VAL:HG13	1:A:282:THR:HG23	1.64	0.80
1:C:346:LYS:HB3	1:C:347:PRO:HD3	1.63	0.80
1:C:352:MET:HE3	1:C:438:LEU:HD12	1.62	0.79
1:C:334:VAL:O	1:C:338:VAL:HG23	1.82	0.79
1:A:54:LEU:O	1:A:279:LYS:HE2	1.85	0.76
1:C:281:VAL:HG13	1:C:282:THR:HG23	1.66	0.75
1:C:278:ALA:O	1:C:281:VAL:HG12	1.87	0.75
1:C:352:MET:CE	1:C:435:ASP:HA	2.16	0.74
1:C:56:CYS:CB	1:C:279:LYS:HB3	2.18	0.73
1:A:278:ALA:O	1:A:281:VAL:HG12	1.89	0.73
1:B:220:VAL:HG11	1:B:226:ILE:HD12	1.69	0.73
1:B:54:LEU:O	1:B:279:LYS:HE2	1.90	0.72
1:B:21:TRP:HD1	2:B:502:GGL:HA	1.55	0.71
1:B:425:GLU:O	1:B:429:GLU:HG3	1.90	0.71
1:C:21:TRP:HD1	2:C:503:GGL:HB2	1.54	0.70
1:C:430:GLU:O	1:C:433:LYS:HG3	1.92	0.70
1:A:83:ALA:HB2	2:C:503:GGL:OE2	1.93	0.69
2:B:502:GGL:CG	1:D:82:PRO:HB2	2.21	0.69
1:D:259:THR:HB	1:D:365:ILE:HG12	1.73	0.68
1:C:352:MET:HE2	1:C:435:ASP:HA	1.76	0.68
1:D:357:LYS:O	1:D:377:LYS:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:O	1:D:419:PRO:HD3	1.93	0.68
1:C:261:LYS:HD2	1:C:267:ASN:HB3	1.77	0.67
1:C:422:ILE:HG12	1:C:426:GLN:HB2	1.77	0.67
1:A:54:LEU:HD21	2:C:501:GGL:HG3	1.75	0.66
1:C:21:TRP:HD1	2:C:503:GGL:CB	2.08	0.66
1:D:45:LYS:HD3	1:D:47:TYR:CZ	2.31	0.66
1:B:281:VAL:HG13	1:B:282:THR:HG23	1.78	0.65
1:C:352:MET:CE	1:C:438:LEU:HD12	2.25	0.64
1:D:441:VAL:HG13	1:D:445:LEU:HD12	1.78	0.64
1:C:98:ASP:HA	1:C:102:PRO:HG3	1.78	0.64
1:A:49:ASP:O	1:A:419:PRO:HD3	1.98	0.62
1:B:16:TYR:CE2	1:D:94:LYS:HD2	2.33	0.62
1:C:376:ASN:OD1	1:C:379:THR:HG23	2.00	0.62
1:B:220:VAL:CG1	1:B:226:ILE:HD12	2.30	0.62
1:C:444:ASN:O	1:C:445:LEU:HD23	1.99	0.62
1:C:388:THR:HG22	1:C:389:PRO:O	2.00	0.61
1:B:87:GLU:HB3	1:B:88:PRO:HD3	1.81	0.61
1:C:396:ILE:HG21	1:C:414:ILE:HD11	1.80	0.61
1:D:281:VAL:HG13	1:D:282:THR:HG23	1.81	0.61
1:D:240:CYS:HB3	1:D:245:ILE:O	2.01	0.61
1:B:51:SER:HB3	1:B:407:THR:HA	1.82	0.61
1:A:31:ILE:HG12	1:C:84:TYR:HB3	1.83	0.60
1:C:329:TYR:HA	1:C:334:VAL:CG2	2.32	0.60
1:C:352:MET:HE1	1:C:435:ASP:OD1	2.00	0.60
1:A:240:CYS:HB3	1:A:245:ILE:O	2.02	0.60
1:B:240:CYS:HB3	1:B:245:ILE:O	2.02	0.60
1:D:422:ILE:HD13	1:D:427:LEU:HG	1.83	0.59
1:A:306:LEU:CD2	1:C:18:MET:HG2	2.33	0.59
1:D:59:LEU:HB3	1:D:63:LEU:HD22	1.85	0.59
1:B:138:TYR:O	1:B:153:GLY:HA3	2.04	0.58
1:C:359:VAL:O	1:C:377:LYS:HE2	2.04	0.58
1:A:56:CYS:CB	1:A:279:LYS:HB3	2.34	0.58
1:B:31:ILE:HD12	1:B:39:PHE:HD1	1.68	0.58
1:C:425:GLU:O	1:C:429:GLU:HG3	2.04	0.58
1:D:261:LYS:HD2	1:D:267:ASN:ND2	2.20	0.57
1:C:352:MET:HE1	1:C:435:ASP:HA	1.85	0.57
1:D:21:TRP:HD1	2:D:502:GGL:HA	1.69	0.57
1:B:94:LYS:HG3	1:D:16:TYR:CE2	2.39	0.57
1:D:33:LYS:HE3	1:D:34:ALA:O	2.04	0.56
1:A:423:THR:OG1	1:A:426:GLN:HG3	2.05	0.56
1:A:107:ARG:HD2	1:A:298:SER:OG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:MET:HE1	1:D:188:ASP:OD1	2.06	0.56
1:B:56:CYS:CB	1:B:279:LYS:HB3	2.36	0.56
1:B:346:LYS:HB3	1:B:347:PRO:HD3	1.86	0.56
1:C:56:CYS:HB3	1:C:279:LYS:HB3	1.88	0.56
1:C:252:VAL:HG12	1:C:279:LYS:HE3	1.88	0.55
1:D:179:GLU:HG2	1:D:382:LEU:HD11	1.86	0.55
1:B:184:ARG:NH1	1:B:227:LEU:O	2.39	0.55
1:A:107:ARG:NH2	1:C:14:SER:O	2.40	0.55
1:A:33:LYS:HE3	1:A:34:ALA:O	2.07	0.54
1:B:13:HIS:HA	1:B:17:VAL:HG23	1.89	0.54
1:B:84:TYR:HB3	1:D:31:ILE:HG12	1.90	0.54
1:B:100:ALA:O	1:B:101:ASP:HB2	2.07	0.54
1:B:334:VAL:O	1:B:338:VAL:HG23	2.07	0.54
1:B:434:LEU:O	1:B:438:LEU:HG	2.08	0.54
1:A:91:ARG:O	1:A:95:MET:HG3	2.08	0.53
1:B:123:LYS:HE3	1:D:160:THR:OG1	2.08	0.53
1:A:179:GLU:HG2	1:A:382:LEU:HD11	1.90	0.53
1:D:278:ALA:O	1:D:281:VAL:HG12	2.07	0.53
1:A:441:VAL:HG13	1:A:445:LEU:HD12	1.90	0.53
1:C:420:LEU:N	1:C:420:LEU:HD23	2.24	0.53
1:A:346:LYS:HB3	1:A:347:PRO:HD3	1.91	0.53
1:A:138:TYR:CD2	1:A:173:MET:HE2	2.44	0.52
1:D:369:SER:OG	1:D:416:ILE:HB	2.10	0.52
1:D:100:ALA:O	1:D:101:ASP:HB2	2.09	0.52
1:B:20:SER:HB2	2:B:502:GGL:HG2	1.92	0.52
1:B:18:MET:HG2	1:D:306:LEU:CD2	2.39	0.52
1:B:49:ASP:O	1:B:419:PRO:HD3	2.11	0.52
1:D:21:TRP:CD1	2:D:502:GGL:HA	2.44	0.52
1:C:133:LYS:HB2	1:C:210:SER:O	2.09	0.51
1:C:436:LYS:HB2	1:C:436:LYS:NZ	2.25	0.51
1:D:268:PHE:O	1:D:269:ASP:HB3	2.10	0.51
1:A:184:ARG:NH1	1:A:184:ARG:HB2	2.25	0.51
1:C:346:LYS:HE2	1:C:350:GLU:OE1	2.10	0.51
1:B:21:TRP:CD1	2:B:502:GGL:HA	2.41	0.51
1:C:329:TYR:HA	1:C:334:VAL:HG21	1.92	0.51
1:C:436:LYS:HZ3	1:C:436:LYS:HB2	1.76	0.51
1:B:31:ILE:HD12	1:B:39:PHE:CD1	2.45	0.50
1:B:120:ASN:O	1:B:124:MET:HG3	2.10	0.50
1:C:430:GLU:OE1	1:C:433:LYS:HD2	2.11	0.50
1:B:33:LYS:HE3	1:B:34:ALA:O	2.10	0.50
1:C:434:LEU:O	1:C:438:LEU:HG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:SER:O	1:D:394:PRO:HD2	2.12	0.50
1:B:98:ASP:HA	1:B:102:PRO:HG3	1.94	0.50
1:D:400:LEU:HD23	1:D:437:VAL:HG21	1.93	0.50
1:C:357:LYS:HE3	1:C:446:CYS:HB2	1.92	0.50
1:A:139:ARG:HB2	1:A:174:ASN:OD1	2.12	0.49
1:C:49:ASP:O	1:C:419:PRO:HD3	2.11	0.49
1:C:425:GLU:O	1:C:429:GLU:CG	2.59	0.49
1:A:437:VAL:O	1:A:441:VAL:HG23	2.13	0.49
1:C:240:CYS:HB3	1:C:245:ILE:O	2.12	0.49
1:B:16:TYR:CZ	1:D:94:LYS:HD2	2.48	0.49
1:A:51:SER:HB3	1:A:407:THR:HA	1.95	0.49
1:C:40:TRP:NE1	1:C:46:ARG:HB2	2.28	0.49
1:C:51:SER:OG	2:C:502:GGL:N	2.46	0.49
1:A:12:LEU:HB2	1:C:90:SER:HB3	1.94	0.49
1:B:138:TYR:CD2	1:B:173:MET:HE2	2.48	0.48
1:C:339:LYS:O	1:C:342:GLU:HB3	2.13	0.48
2:D:501:GGL:OXT	2:D:501:GGL:HG2	2.14	0.48
1:A:178:TYR:HB2	1:A:361:GLU:OE2	2.13	0.48
1:C:367:LEU:HD12	1:C:420:LEU:HA	1.95	0.48
1:A:346:LYS:HE3	1:A:350:GLU:OE1	2.13	0.48
1:A:119:GLU:OE2	1:C:146:ILE:HG13	2.13	0.48
1:A:63:LEU:HD23	1:A:66:ILE:HG13	1.96	0.48
1:C:122:ILE:HG23	1:C:134:ILE:HG13	1.95	0.48
1:C:352:MET:HE3	1:C:356:HIS:CD2	2.48	0.48
1:C:401:MET:SD	1:C:406:SER:HB2	2.54	0.48
1:B:412:THR:O	1:B:412:THR:HG23	2.14	0.47
1:D:37:ILE:HD13	1:D:422:ILE:HG13	1.94	0.47
1:D:348:PHE:CZ	1:D:431:LEU:HB3	2.49	0.47
1:A:90:SER:HB3	1:C:12:LEU:HB2	1.95	0.47
1:B:48:THR:HG21	1:B:430:GLU:HG3	1.96	0.47
1:A:137:CYS:HB2	1:A:140:SER:HB3	1.96	0.47
1:A:220:VAL:HG11	1:A:226:ILE:HD12	1.95	0.47
1:A:422:ILE:HD13	1:A:427:LEU:HG	1.97	0.47
1:C:149:SER:HB3	1:C:160:THR:HG21	1.97	0.47
1:D:139:ARG:HB2	1:D:174:ASN:OD1	2.15	0.47
1:B:132:PRO:CB	1:D:163:GLY:HA2	2.45	0.47
1:B:132:PRO:HB3	1:D:163:GLY:HA2	1.96	0.47
1:C:33:LYS:HG3	1:C:34:ALA:N	2.30	0.47
1:B:349:LEU:HD22	1:B:371:LEU:HD21	1.97	0.47
1:C:21:TRP:CD1	2:C:503:GGL:HB2	2.43	0.47
1:A:278:ALA:HA	1:A:289:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:LEU:HB3	1:C:371:LEU:HD21	1.96	0.47
1:D:138:TYR:O	1:D:153:GLY:HA3	2.14	0.47
1:D:211:VAL:O	1:D:245:ILE:HG12	2.15	0.47
1:A:346:LYS:HG3	1:A:364:CYS:HB3	1.97	0.47
1:C:136:SER:O	1:C:171:HIS:HA	2.15	0.46
1:C:109:PHE:O	1:C:290:GLY:HA2	2.16	0.46
1:C:400:LEU:HG	1:C:437:VAL:HG11	1.97	0.46
1:C:92:LEU:HD12	1:C:92:LEU:O	2.15	0.46
1:B:83:ALA:CB	2:B:501:GGL:HG2	2.45	0.46
1:D:56:CYS:HA	1:D:279:LYS:HB3	1.97	0.46
1:A:138:TYR:O	1:A:153:GLY:HA3	2.16	0.46
1:B:252:VAL:HG12	1:B:279:LYS:HD2	1.97	0.46
1:D:346:LYS:HB3	1:D:347:PRO:HD3	1.98	0.46
1:B:132:PRO:HD2	1:B:210:SER:O	2.16	0.46
1:A:412:THR:O	1:A:412:THR:HG23	2.16	0.45
1:B:119:GLU:OE2	1:D:146:ILE:HG13	2.16	0.45
1:B:309:GLY:HA2	1:D:20:SER:OG	2.16	0.45
1:B:107:ARG:HA	1:D:16:TYR:O	2.17	0.45
1:C:48:THR:HG21	1:C:430:GLU:HG3	1.97	0.45
1:D:437:VAL:O	1:D:441:VAL:HG23	2.16	0.45
1:B:261:LYS:HD2	1:B:266:GLN:HB3	1.98	0.45
1:C:386:TYR:HA	1:C:411:GLU:OE1	2.17	0.45
1:B:119:GLU:OE2	1:B:147:GLY:HA3	2.17	0.45
1:B:310:LEU:HG	1:B:313:SER:HB2	1.98	0.45
1:A:262:MET:HE2	1:A:262:MET:HA	1.99	0.45
1:B:177:MET:HE3	1:B:188:ASP:HA	1.99	0.45
1:C:310:LEU:HG	1:C:313:SER:HB2	1.99	0.45
1:D:192:THR:OG1	1:D:229:PRO:HB2	2.17	0.45
1:D:445:LEU:O	1:D:446:CYS:HB2	2.17	0.44
2:B:501:GGL:CD	2:D:502:GGL:HG2	2.47	0.44
1:A:258:ARG:NH2	1:A:418:PRO:O	2.51	0.44
1:B:306:LEU:HD22	1:D:18:MET:HG3	1.99	0.44
1:D:234:GLU:OE2	1:D:268:PHE:O	2.35	0.44
1:A:279:LYS:HA	1:C:312:TYR:OH	2.18	0.44
1:A:54:LEU:CD1	2:A:501:GGL:HB3	2.47	0.44
1:A:87:GLU:OE2	1:A:91:ARG:NH2	2.51	0.44
1:C:196:LEU:HD11	1:C:235:GLY:HA3	1.99	0.44
1:C:56:CYS:HB2	1:C:279:LYS:HB3	1.97	0.44
1:A:73:GLN:HG2	1:A:320:ALA:HB2	1.99	0.44
1:B:253:MET:HE2	1:B:253:MET:HB2	1.81	0.44
1:D:38:TYR:CE1	1:D:48:THR:HG23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:MET:HG2	1:D:306:LEU:HD22	1.99	0.44
1:B:33:LYS:HG3	1:B:34:ALA:N	2.33	0.44
1:C:32:LYS:HB2	1:C:42:TYR:CE1	2.53	0.44
1:A:146:ILE:HD12	1:C:147:GLY:HA3	2.00	0.43
1:B:82:PRO:HD2	2:B:501:GGL:OE2	2.18	0.43
1:C:87:GLU:HB3	1:C:88:PRO:HD3	2.00	0.43
1:A:107:ARG:HA	1:C:16:TYR:O	2.18	0.43
1:B:146:ILE:HG13	1:D:119:GLU:OE1	2.18	0.43
1:B:263:PHE:O	1:B:266:GLN:HB2	2.18	0.43
1:D:217:GLU:HA	1:D:250:ASP:HB3	2.00	0.43
1:D:274:MET:HG3	1:D:297:ILE:CD1	2.48	0.43
1:D:7:GLU:O	1:D:11:SER:HB2	2.19	0.43
1:B:56:CYS:HB3	1:B:279:LYS:HG2	2.01	0.43
1:B:73:GLN:HB3	1:B:317:LEU:HD12	2.01	0.43
1:B:369:SER:OG	1:B:416:ILE:HB	2.19	0.43
1:D:59:LEU:CB	1:D:63:LEU:HD22	2.48	0.43
1:C:221:GLY:CA	1:C:253:MET:HE2	2.49	0.43
1:B:400:LEU:HG	1:B:437:VAL:HG11	1.99	0.43
1:C:138:TYR:O	1:C:153:GLY:HA3	2.19	0.43
1:B:29:LYS:HB2	1:B:29:LYS:HE2	1.78	0.43
1:B:355:LYS:O	1:B:355:LYS:HG2	2.18	0.43
1:B:411:GLU:OE1	1:B:411:GLU:HA	2.18	0.43
1:C:358:CYS:SG	1:C:441:VAL:CG2	3.07	0.43
1:A:94:LYS:HD2	1:C:16:TYR:CE2	2.54	0.42
1:C:234:GLU:OE2	1:C:268:PHE:O	2.37	0.42
1:C:275:PHE:CE1	1:C:292:VAL:HB	2.54	0.42
1:D:369:SER:HG	1:D:416:ILE:HB	1.82	0.42
1:D:382:LEU:HD13	1:D:412:THR:HG21	2.01	0.42
1:B:91:ARG:HG3	1:B:91:ARG:NH1	2.34	0.42
1:C:196:LEU:CD1	1:C:235:GLY:HA3	2.50	0.42
1:A:82:PRO:HG2	2:C:503:GGL:H2	1.84	0.42
1:B:339:LYS:O	1:B:342:GLU:HB3	2.20	0.42
1:C:440:TRP:CE3	1:C:441:VAL:HG12	2.54	0.42
1:C:20:SER:HB2	2:C:503:GGL:HB3	2.01	0.42
1:D:315:HIS:CE1	1:D:317:LEU:HB3	2.54	0.42
1:A:56:CYS:HB2	1:A:279:LYS:HB3	2.02	0.42
1:C:200:ASP:O	1:C:204:GLN:HG3	2.20	0.42
1:D:14:SER:OG	1:D:26:GLY:O	2.34	0.42
1:A:375:LYS:O	1:A:447:ASP:N	2.46	0.42
1:D:56:CYS:CB	1:D:279:LYS:HB3	2.50	0.42
1:C:248:ILE:HA	1:C:274:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LYS:HD2	1:A:440:TRP:CE3	2.55	0.41
1:B:13:HIS:HA	1:B:17:VAL:CG2	2.49	0.41
2:B:501:GGL:HG3	2:D:502:GGL:HG2	2.01	0.41
1:A:306:LEU:HD22	1:C:18:MET:HG2	2.03	0.41
1:C:95:MET:HE2	1:C:326:VAL:CG1	2.49	0.41
1:B:312:TYR:CE2	1:D:287:PRO:HA	2.55	0.41
1:A:16:TYR:CE2	1:C:94:LYS:HG3	2.55	0.41
2:C:502:GGL:O	2:C:502:GGL:CG	2.66	0.41
1:B:411:GLU:HB3	4:B:667:HOH:O	2.20	0.41
1:B:340:GLU:HG2	1:B:341:MET:CE	2.50	0.41
1:C:346:LYS:HB3	1:C:347:PRO:CD	2.42	0.41
1:D:274:MET:HG2	1:D:293:VAL:HG12	2.02	0.41
1:D:98:ASP:HA	1:D:102:PRO:HG3	2.01	0.41
1:D:258:ARG:NH2	1:D:417:CYS:C	2.74	0.41
1:C:53:LEU:CD1	1:C:61:HIS:HE1	2.33	0.41
1:D:393:MET:HG3	1:D:411:GLU:O	2.21	0.41
1:A:4:LEU:HB3	1:A:9:VAL:HG23	2.01	0.41
1:B:83:ALA:HB3	2:B:501:GGL:HG2	2.03	0.41
1:D:285:TYR:CD1	1:D:285:TYR:N	2.89	0.41
1:D:349:LEU:HB3	1:D:371:LEU:HD21	2.02	0.41
1:C:139:ARG:HB2	1:C:174:ASN:OD1	2.20	0.41
1:C:100:ALA:O	1:C:101:ASP:HB2	2.21	0.40
1:C:14:SER:O	1:C:25:GLY:HA2	2.21	0.40
1:C:45:LYS:HD3	1:C:47:TYR:CZ	2.56	0.40
1:A:359:VAL:O	1:A:377:LYS:HE2	2.20	0.40
1:B:136:SER:O	1:B:171:HIS:HA	2.21	0.40
1:B:184:ARG:NH2	1:B:363:ARG:HD3	2.37	0.40
1:C:56:CYS:CA	1:C:279:LYS:HB3	2.52	0.40
1:C:120:ASN:ND2	1:C:308:CYS:HB3	2.35	0.40
1:C:329:TYR:HA	1:C:334:VAL:HG23	2.02	0.40
2:B:501:GGL:OE2	2:D:502:GGL:HB3	2.21	0.40
1:A:103:ASP:O	1:A:295:LYS:HE3	2.20	0.40
1:C:349:LEU:HD21	1:C:416:ILE:HD13	2.03	0.40
1:D:56:CYS:O	1:D:283:CYS:HA	2.21	0.40
1:D:315:HIS:HE1	1:D:317:LEU:HB3	1.86	0.40
1:D:95:MET:HE1	1:D:326:VAL:HB	2.02	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	445/449 (99%)	425 (96%)	19 (4%)	1 (0%)	47	64
1	B	444/449 (99%)	424 (96%)	19 (4%)	1 (0%)	47	64
1	C	444/449 (99%)	423 (95%)	20 (4%)	1 (0%)	47	64
1	D	444/449 (99%)	421 (95%)	22 (5%)	1 (0%)	47	64
All	All	1777/1796 (99%)	1693 (95%)	80 (4%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	ASP
1	A	101	ASP
1	D	101	ASP
1	C	101	ASP

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	366/375 (98%)	361 (99%)	5 (1%)	67	80
1	B	364/375 (97%)	357 (98%)	7 (2%)	57	74
1	C	362/375 (96%)	359 (99%)	3 (1%)	81	89
1	D	360/375 (96%)	356 (99%)	4 (1%)	73	85
All	All	1452/1500 (97%)	1433 (99%)	19 (1%)	69	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	11	SER
1	B	14	SER
1	B	94	LYS
1	B	261	LYS
1	B	310	LEU
1	B	397	MET
1	A	1	MET
1	A	188	ASP
1	A	310	LEU
1	A	339	LYS
1	A	387	HIS
1	C	46	ARG
1	C	144	SER
1	C	310	LEU
1	D	14	SER
1	D	18	MET
1	D	310	LEU
1	D	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GGL	A	501	-	2,9,9	0.50	0	2,11,11	1.00	0
3	PLP	B	503	-	16,16,16	1.84	3 (18%)	20,23,23	1.43	2 (10%)
2	GGL	C	502	-	2,9,9	0.36	0	2,11,11	1.28	0
2	GGL	D	502	-	2,9,9	0.24	0	2,11,11	0.86	0
2	GGL	B	502	-	2,9,9	0.10	0	2,11,11	0.83	0
2	GGL	D	501	-	2,9,9	0.48	0	2,11,11	1.51	0
3	PLP	C	504	-	16,16,16	1.88	4 (25%)	20,23,23	1.31	2 (10%)
2	GGL	B	501	-	2,9,9	1.01	0	2,11,11	4.06	2 (100%)
2	GGL	C	503	-	2,9,9	0.40	0	2,11,11	1.08	0
2	GGL	C	501	-	2,9,9	0.48	0	2,11,11	1.23	0
3	PLP	D	503	-	16,16,16	1.87	5 (31%)	20,23,23	1.38	2 (10%)
3	PLP	A	502	-	16,16,16	1.87	3 (18%)	20,23,23	1.42	3 (15%)

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	GGL	A	501	-	-	1/3/9/9	-
3	PLP	B	503	-	-	2/8/8/8	0/1/1/1
2	GGL	C	502	-	-	1/3/9/9	-
2	GGL	D	502	-	-	1/3/9/9	-
2	GGL	B	502	-	-	3/3/9/9	-
2	GGL	D	501	-	-	0/3/9/9	-
3	PLP	C	504	-	-	2/8/8/8	0/1/1/1
2	GGL	B	501	-	-	1/3/9/9	-
2	GGL	C	503	-	-	0/3/9/9	-
2	GGL	C	501	-	-	0/3/9/9	-
3	PLP	D	503	-	-	2/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	502	-	-	3/8/8/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	PLP	C4-C4A	4.19	1.56	1.46
3	C	504	PLP	C4-C4A	4.01	1.55	1.46
3	A	502	PLP	C4-C4A	3.98	1.55	1.46
3	A	502	PLP	P-O3P	3.94	1.70	1.54
3	D	503	PLP	P-O2P	3.71	1.69	1.54
3	D	503	PLP	C4-C4A	3.67	1.54	1.46
3	C	504	PLP	P-O2P	3.62	1.68	1.54
3	B	503	PLP	P-O3P	3.60	1.68	1.54
3	C	504	PLP	C5A-C5	2.51	1.57	1.50
3	B	503	PLP	C5A-C5	2.50	1.57	1.50
3	D	503	PLP	C5A-C5	2.42	1.57	1.50
3	D	503	PLP	P-O3P	-2.27	1.46	1.54
3	A	502	PLP	C5A-C5	2.26	1.57	1.50
3	D	503	PLP	C4-C3	-2.15	1.37	1.40
3	C	504	PLP	C3-C2	2.05	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GGL	CB-CG-CD	-4.15	104.68	113.59
2	B	501	GGL	CG-CB-CA	3.98	123.12	113.84
3	D	503	PLP	O4A-C4A-C4	-3.00	118.37	124.91
3	B	503	PLP	C5-C6-N1	-2.73	119.28	123.82
3	A	502	PLP	C5-C6-N1	-2.60	119.49	123.82
3	C	504	PLP	C5-C6-N1	-2.54	119.59	123.82
3	A	502	PLP	O4A-C4A-C4	-2.47	119.54	124.91
3	D	503	PLP	C5-C6-N1	-2.43	119.77	123.82
3	C	504	PLP	O4A-C4A-C4	-2.24	120.03	124.91
3	A	502	PLP	O4P-C5A-C5	-2.22	105.12	109.35
3	B	503	PLP	O4A-C4A-C4	-2.08	120.39	124.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502	GGL	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
2	D	502	GGL	CA-CB-CG-CD
2	B	502	GGL	N-CA-CB-CG
2	B	502	GGL	C-CA-CB-CG
3	A	502	PLP	C3-C4-C4A-O4A
3	B	503	PLP	C3-C4-C4A-O4A
3	C	504	PLP	C3-C4-C4A-O4A
3	D	503	PLP	C3-C4-C4A-O4A
3	D	503	PLP	C5-C4-C4A-O4A
3	A	502	PLP	C5A-O4P-P-O1P
2	B	502	GGL	CA-CB-CG-CD
3	C	504	PLP	C5-C4-C4A-O4A
3	A	502	PLP	C5-C4-C4A-O4A
2	B	501	GGL	N-CA-CB-CG
2	A	501	GGL	CA-CB-CG-CD
3	B	503	PLP	C5-C4-C4A-O4A

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GGL	1	0
2	C	502	GGL	2	0
2	D	502	GGL	5	0
2	B	502	GGL	5	0
2	D	501	GGL	1	0
2	B	501	GGL	6	0
2	C	503	GGL	6	0
2	C	501	GGL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	447/449 (99%)	-0.64	1 (0%) 95 96	18, 27, 39, 57	0
1	B	446/449 (99%)	-0.60	0 100 100	19, 29, 42, 64	0
1	C	446/449 (99%)	-0.46	0 100 100	24, 34, 47, 62	0
1	D	446/449 (99%)	-0.56	1 (0%) 95 96	19, 31, 46, 78	0
All	All	1785/1796 (99%)	-0.56	2 (0%) 95 96	18, 30, 45, 78	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.2
1	A	378	GLU	2.1

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. 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(\AA^2)	Q<0.9
2	GGL	C	502	10/10	0.65	0.42	39,48,65,65	17
2	GGL	C	503	10/10	0.73	0.38	29,43,57,57	17
2	GGL	D	502	10/10	0.78	0.35	30,37,49,49	17
2	GGL	B	502	10/10	0.79	0.36	26,33,40,40	17
2	GGL	D	501	10/10	0.82	0.29	27,33,44,44	17
2	GGL	A	501	10/10	0.85	0.30	27,31,39,39	17
2	GGL	C	501	10/10	0.85	0.29	23,33,42,44	17
2	GGL	B	501	10/10	0.86	0.26	25,35,48,48	17
3	PLP	C	504	16/16	0.97	0.14	27,32,38,45	0
3	PLP	A	502	16/16	0.97	0.14	26,33,38,41	0
3	PLP	D	503	16/16	0.98	0.12	29,35,41,46	0
3	PLP	B	503	16/16	0.98	0.14	23,29,34,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.