



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 2COJ / pdb_00002coj
Title : Crystal structure of reduced human cytosolic branched-chain aminotransferase complexed with gabapentin
Authors : Goto, M.
Deposited on : 2005-05-17
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

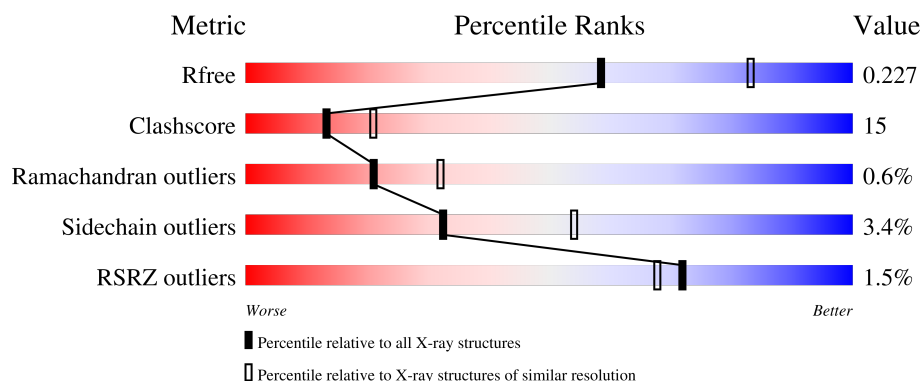
1 Overall quality at a glance

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	386	0% 63% 27% • 7%
1	B	386	2% 68% 23% • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5856 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.

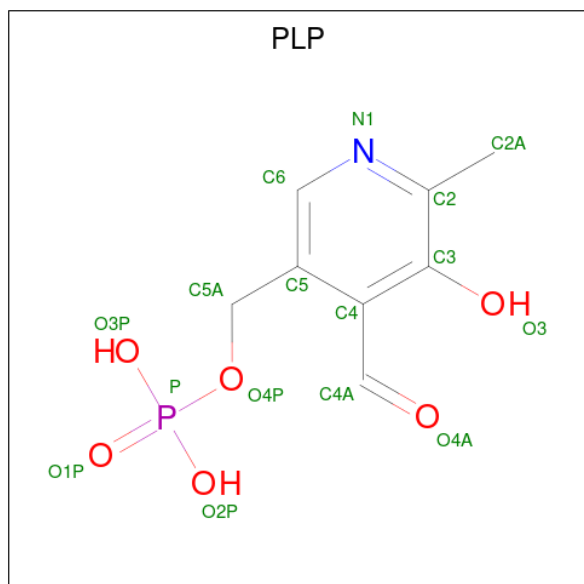
- Molecule 1 is a protein called branched chain aminotransferase 1, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2820	1820	463	522	15			
1	B	358	Total	C	N	O	S	0	0	0
			2833	1826	469	523	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	ARG	SER	engineered mutation	UNP P54687
B	379	ARG	SER	engineered mutation	UNP P54687

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



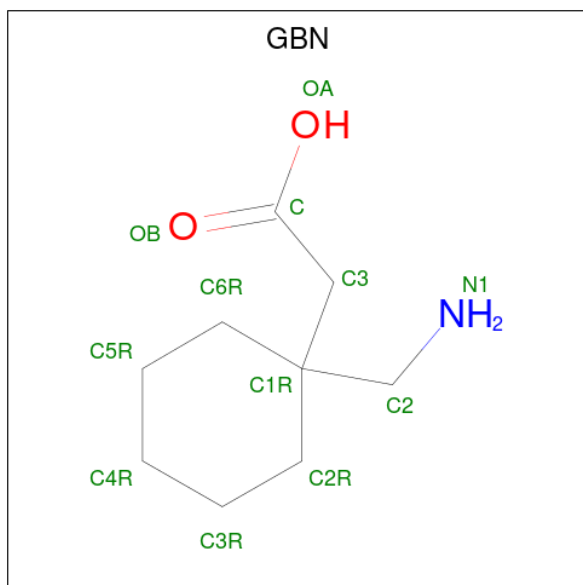
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is [1-(AMINOMETHYL)CYCLOHEXYL]ACETIC ACID (CCD ID: GBN) (formula: C₉H₁₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	79	Total	O	0	0
			79	79		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.87Å 106.63Å 109.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.44 – 2.40 42.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.2 (42.44-2.40) 92.1 (42.44-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.15 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.272 0.221 , 0.227	Depositor DCC
R_{free} test set	2882 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5856	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, MG, GBN

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	0.40	0/2892	0.92	5/3936 (0.1%)
1	B	0.42	0/2906	0.95	13/3953 (0.3%)
All	All	0.41	0/5798	0.94	18/7889 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	TRP	N-CA-C	6.25	116.48	108.24
1	B	352	ILE	CA-C-N	6.20	127.58	119.84
1	B	352	ILE	C-N-CA	6.20	127.58	119.84
1	B	315	ASP	N-CA-C	-5.95	104.87	111.36
1	B	216	GLY	N-CA-C	-5.82	107.28	115.32
1	B	99	LYS	N-CA-C	5.72	118.89	109.85
1	B	268	ILE	N-CA-C	-5.67	99.71	107.99
1	B	276	LEU	N-CA-C	-5.63	99.23	108.41
1	B	376	ARG	N-CA-C	-5.58	106.55	113.19
1	B	43	ASP	CA-C-N	5.52	125.35	119.28
1	B	43	ASP	C-N-CA	5.52	125.35	119.28
1	A	263	LEU	N-CA-C	5.29	117.87	109.24
1	B	41	LYS	CA-C-N	5.24	125.24	120.21
1	B	41	LYS	C-N-CA	5.24	125.24	120.21
1	A	130	PRO	N-CA-C	5.23	119.30	111.14
1	B	45	ASN	N-CA-C	5.17	117.82	111.82
1	A	274	GLU	N-CA-C	-5.16	102.65	110.28
1	A	227	TYR	N-CA-C	5.07	119.46	113.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2820	0	2771	97	0
1	B	2833	0	2801	72	0
2	A	15	0	6	2	0
2	B	15	0	7	0	0
3	A	12	0	16	1	0
3	B	12	0	16	0	0
4	B	1	0	0	0	0
5	A	69	0	0	2	0
5	B	79	0	0	4	0
All	All	5856	0	5617	167	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 15.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG13	1:A:285:ILE:HD12	1.58	0.86
1:B:98:LEU:HD22	1:B:162:ILE:HB	1.58	0.86
1:A:142:GLN:HE21	1:A:385:LEU:HD11	1.42	0.84
1:B:351:HIS:HE1	1:B:356:GLU:OE1	1.61	0.83
1:B:246:LEU:HD11	1:B:255:ILE:HG23	1.59	0.83
1:A:222:LYS:HG2	1:A:286:LEU:HD11	1.66	0.74
1:A:369:LEU:O	1:A:373:GLN:HG3	1.87	0.74
1:B:351:HIS:CE1	1:B:356:GLU:OE1	2.46	0.68
1:B:356:GLU:HG3	5:B:484:HOH:O	1.93	0.68
1:B:33:THR:O	1:B:75:PRO:HD3	1.94	0.67
1:B:40:GLU:H	1:B:40:GLU:CD	2.01	0.67
1:A:29:ASP:O	1:A:31:ILE:HD12	1.96	0.66
1:B:35:ALA:H	1:B:56:HIS:HE1	1.44	0.65
1:A:112:GLN:N	1:A:113:PRO:HD3	2.11	0.65
1:A:351:HIS:HE1	1:A:356:GLU:OE1	1.80	0.65
1:A:108:ILE:CD1	1:A:149:GLN:HB2	2.28	0.64
1:B:221:CYS:CB	1:B:223:MET:HE3	2.27	0.64
1:A:170:GLU:HG3	1:A:178:PRO:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:CG	1:A:286:LEU:HD11	2.31	0.60
1:B:143:GLN:NE2	1:B:143:GLN:HA	2.15	0.60
1:A:215:LYS:HD3	1:A:249:TYR:OH	2.02	0.59
1:B:205:TRP:CZ3	1:B:236:GLU:OE2	2.56	0.59
1:A:38:LEU:N	1:A:38:LEU:HD22	2.18	0.59
1:A:170:GLU:HG2	1:A:179:THR:H	1.67	0.59
1:B:126:ARG:HG2	1:B:223:MET:HE1	1.84	0.58
1:A:58:LEU:HD12	1:A:72:HIS:O	2.04	0.58
1:B:263:LEU:C	1:B:263:LEU:HD13	2.29	0.58
1:A:138:LEU:O	1:A:142:GLN:HG2	2.02	0.57
1:A:102:ARG:HH11	1:A:106:ASN:ND2	2.02	0.57
1:A:269:ASN:ND2	1:A:273:GLU:H	2.02	0.57
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.69	0.57
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.19	0.57
1:A:309:ARG:HD2	1:A:311:LEU:HD21	1.86	0.57
1:A:110:LEU:HB3	1:A:113:PRO:HG3	1.86	0.57
1:A:269:ASN:C	1:A:269:ASN:HD22	2.11	0.56
1:A:142:GLN:NE2	1:A:385:LEU:HD21	2.21	0.56
1:A:284:ILE:HG13	1:A:285:ILE:CD1	2.33	0.56
1:B:205:TRP:CZ3	1:B:207:ASN:HB2	2.40	0.56
1:A:51:THR:HG22	1:A:52:VAL:HG23	1.88	0.55
1:A:263:LEU:HD23	1:A:263:LEU:C	2.31	0.55
1:A:142:GLN:NE2	1:A:385:LEU:HD11	2.17	0.54
1:A:48:VAL:O	1:A:51:THR:HB	2.08	0.54
1:B:143:GLN:HA	1:B:143:GLN:HE21	1.71	0.53
1:B:221:CYS:SG	1:B:223:MET:HE3	2.49	0.53
1:B:258:VAL:CG2	1:B:263:LEU:HD23	2.38	0.53
1:B:35:ALA:H	1:B:56:HIS:CE1	2.26	0.53
1:B:98:LEU:CD2	1:B:162:ILE:HB	2.36	0.53
1:A:120:MET:HE1	1:A:183:LEU:HD21	1.91	0.53
1:A:111:PHE:C	1:A:113:PRO:HD3	2.35	0.52
1:A:199:PHE:CE1	1:A:366:LEU:HD22	2.45	0.52
1:A:262:ASN:O	1:A:330:GLY:HA2	2.11	0.51
1:A:269:ASN:HD21	1:A:273:GLU:H	1.58	0.51
1:A:182:LEU:C	1:A:182:LEU:HD13	2.35	0.51
1:B:108:ILE:HB	1:B:385:LEU:HD23	1.91	0.51
1:A:384:VAL:HG12	1:A:385:LEU:N	2.25	0.51
1:B:335:CYS:O	1:B:336:VAL:HB	2.10	0.51
1:B:56:HIS:HD2	1:B:148:ASP:OD2	1.93	0.50
1:B:300:GLN:HE22	1:B:379:ARG:HH12	1.58	0.50
1:B:227:TYR:N	1:B:227:TYR:CD1	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:SER:H	1:B:243:GLN:NE2	2.10	0.50
1:A:170:GLU:CG	1:A:178:PRO:HA	2.42	0.50
1:B:138:LEU:O	1:B:142:GLN:HG3	2.11	0.49
1:A:170:GLU:OE2	1:A:176:LYS:HE3	2.12	0.49
1:B:243:GLN:O	1:B:244:GLN:HG2	2.12	0.49
1:B:327:GLU:OE1	1:B:359:PRO:HB2	2.10	0.49
1:A:102:ARG:HH11	1:A:106:ASN:HD21	1.61	0.49
1:A:234:GLN:O	1:A:237:ALA:HB3	2.12	0.49
1:B:170:GLU:HG2	1:B:176:LYS:HE2	1.95	0.49
1:B:218:THR:HG23	1:B:226:ASN:OD1	2.12	0.48
1:A:357:ASN:O	1:A:359:PRO:HA	2.14	0.48
1:B:103:GLY:HA3	1:B:109:ARG:HH12	1.77	0.48
1:A:102:ARG:HD3	1:A:106:ASN:ND2	2.28	0.48
1:A:103:GLY:C	1:A:105:ASP:H	2.21	0.48
1:A:110:LEU:HB3	1:A:113:PRO:CG	2.44	0.48
1:A:235:CYS:O	1:A:238:VAL:HG22	2.14	0.48
1:B:94:LEU:HD12	1:B:94:LEU:C	2.39	0.48
1:A:58:LEU:O	1:A:184:PHE:HA	2.14	0.48
1:B:98:LEU:CD2	1:B:162:ILE:HD12	2.44	0.48
1:B:58:LEU:C	1:B:58:LEU:HD13	2.39	0.47
1:B:310:TYR:O	1:B:311:LEU:HD23	2.13	0.47
1:A:238:VAL:HG23	1:A:239:ASP:N	2.29	0.47
1:A:94:LEU:C	1:A:94:LEU:HD12	2.39	0.47
1:A:320:LEU:HD11	1:A:352:ILE:HD13	1.97	0.47
1:A:155:SER:HB3	1:A:158:ALA:HB3	1.96	0.47
1:A:309:ARG:HD2	1:A:311:LEU:CD2	2.45	0.47
1:B:369:LEU:O	1:B:373:GLN:HG3	2.14	0.47
1:A:112:GLN:N	1:A:113:PRO:CD	2.77	0.47
1:A:335:CYS:O	1:A:337:VAL:N	2.46	0.47
1:B:155:SER:HB3	1:B:158:ALA:HB3	1.97	0.46
1:A:317:THR:O	1:A:321:GLU:HG2	2.16	0.46
1:B:313:MET:HE2	1:B:345:TYR:CG	2.51	0.46
1:B:103:GLY:HA3	1:B:109:ARG:NH1	2.31	0.46
1:A:255:ILE:HD12	1:A:263:LEU:HD11	1.98	0.45
1:B:130:PRO:HG2	1:B:166:PHE:HZ	1.81	0.45
1:A:22:VAL:O	1:A:22:VAL:HG13	2.17	0.45
1:A:98:LEU:N	1:A:98:LEU:HD23	2.32	0.45
1:B:360:LYS:HB3	1:B:360:LYS:HZ3	1.82	0.45
1:A:82:HIS:ND1	1:A:83:PRO:HD2	2.32	0.45
1:A:74:LYS:HB2	1:A:75:PRO:CD	2.47	0.45
1:A:320:LEU:HD11	1:A:352:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD11	1:A:149:GLN:HB2	1.98	0.45
1:B:203:SER:H	1:B:243:GLN:HE22	1.65	0.45
1:B:384:VAL:O	1:B:385:LEU:C	2.59	0.45
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.82	0.45
1:A:130:PRO:HG2	1:A:166:PHE:HZ	1.82	0.44
1:A:139:GLU:HA	1:A:142:GLN:HG3	2.00	0.44
1:A:255:ILE:O	1:A:255:ILE:HG13	2.16	0.44
1:B:58:LEU:HD13	1:B:59:THR:N	2.32	0.44
1:B:335:CYS:O	1:B:336:VAL:CB	2.64	0.44
1:B:248:LEU:HA	1:B:254:GLN:O	2.17	0.44
1:A:120:MET:CE	1:A:183:LEU:HD21	2.48	0.44
1:A:132:PHE:CE1	1:A:137:LEU:HD12	2.53	0.44
1:A:309:ARG:HB2	5:A:480:HOH:O	2.17	0.44
1:A:353:PRO:HA	1:A:356:GLU:OE1	2.17	0.44
1:B:34:PRO:HA	1:B:56:HIS:HE1	1.83	0.43
1:B:65:GLU:CD	1:B:65:GLU:H	2.25	0.43
1:B:263:LEU:HD22	1:B:264:PHE:N	2.33	0.43
1:A:188:SER:O	1:A:190:VAL:HG13	2.18	0.43
1:B:63:SER:O	1:B:67:GLY:N	2.52	0.43
1:A:227:TYR:N	1:A:227:TYR:CD1	2.86	0.43
1:A:84:GLY:O	1:A:85:SER:C	2.62	0.43
1:B:40:GLU:OE2	1:B:40:GLU:N	2.37	0.43
1:B:286:LEU:HA	1:B:287:PRO:HD3	1.84	0.43
1:A:94:LEU:CD2	1:A:124:ALA:HA	2.49	0.43
1:B:375:GLY:C	1:B:377:GLU:H	2.26	0.43
1:B:126:ARG:HD2	5:B:508:HOH:O	2.18	0.43
1:A:335:CYS:C	1:A:336:VAL:HG23	2.44	0.43
1:B:352:ILE:C	1:B:354:THR:H	2.27	0.43
1:B:114:ASN:HB2	5:B:454:HOH:O	2.18	0.42
1:A:102:ARG:HD3	1:A:106:ASN:HD22	1.84	0.42
1:A:222:LYS:NZ	2:A:410:PLP:O3	2.44	0.42
1:B:202:VAL:HA	1:B:243:GLN:OE1	2.19	0.42
1:B:34:PRO:HA	1:B:56:HIS:CE1	2.55	0.42
1:B:98:LEU:HD13	1:B:98:LEU:N	2.34	0.42
1:A:227:TYR:OH	2:A:410:PLP:O3	2.31	0.42
1:A:254:GLN:NE2	5:A:429:HOH:O	2.51	0.42
1:A:183:LEU:HD13	1:A:184:PHE:N	2.34	0.42
1:A:214:TRP:CE3	1:B:214:TRP:HB2	2.55	0.42
1:A:335:CYS:C	1:A:337:VAL:N	2.78	0.42
1:A:384:VAL:HG12	1:A:385:LEU:H	1.84	0.42
1:B:109:ARG:HA	1:B:383:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HG2	1:B:166:PHE:CZ	2.55	0.42
1:A:269:ASN:ND2	1:A:271:ASP:H	2.18	0.41
1:A:95:PHE:CE1	1:A:222:LYS:HE3	2.54	0.41
1:A:316:LEU:HD21	1:A:328:MET:HE1	2.02	0.41
1:A:368:LYS:O	1:A:372:ILE:HG13	2.21	0.41
1:A:54:THR:OG1	1:A:187:LEU:HB2	2.21	0.41
1:A:260:THR:OG1	3:A:420:GBN:N1	2.54	0.41
1:B:222:LYS:HG3	1:B:286:LEU:HD11	2.02	0.41
1:A:38:LEU:N	1:A:38:LEU:CD2	2.82	0.41
1:A:85:SER:O	1:A:89:HIS:HD2	2.04	0.41
1:A:94:LEU:HG	1:A:166:PHE:HB3	2.01	0.41
1:A:321:GLU:O	1:A:321:GLU:HG3	2.21	0.41
1:B:292:ARG:HD2	5:B:506:HOH:O	2.19	0.41
1:B:43:ASP:HA	1:B:44:PRO:HD3	1.88	0.40
1:B:58:LEU:HD22	1:B:72:HIS:O	2.22	0.40
1:A:30:LEU:HD23	1:A:71:PRO:HG2	2.02	0.40
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.87	0.40
1:A:142:GLN:HB3	1:A:385:LEU:HD21	2.02	0.40
1:A:186:LEU:HD21	1:B:83:PRO:HB2	2.02	0.40
1:A:372:ILE:HD13	1:A:379:ARG:HD3	2.03	0.40
1:B:361:LEU:O	1:B:365:ILE:HG13	2.21	0.40
1:A:33:THR:HA	1:A:34:PRO:HD2	1.95	0.40
1:A:117:MET:HA	1:A:117:MET:HE2	2.03	0.40
1:B:108:ILE:HD13	1:B:152:VAL:HG21	2.03	0.40
1:B:379:ARG:C	1:B:381:TRP:H	2.30	0.40
1:B:264:PHE:CD2	1:B:276:LEU:HD11	2.57	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	353/386 (92%)	325 (92%)	27 (8%)	1 (0%)	36	50
1	B	354/386 (92%)	333 (94%)	18 (5%)	3 (1%)	16	25
All	All	707/772 (92%)	658 (93%)	45 (6%)	4 (1%)	21	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	ASP
1	A	322	GLY
1	B	353	PRO
1	B	336	VAL

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	306/334 (92%)	294 (96%)	12 (4%)	28	48
1	B	310/334 (93%)	301 (97%)	9 (3%)	37	60
All	All	616/668 (92%)	595 (97%)	21 (3%)	32	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	112	GLN
1	A	137	LEU
1	A	142	GLN
1	A	144	LEU
1	A	147	LEU
1	A	170	GLU
1	A	269	ASN
1	A	276	LEU
1	A	309	ARG
1	A	361	LEU
1	A	378	GLU

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Mol	Chain	Res	Type
1	B	60	VAL
1	B	65	GLU
1	B	98	LEU
1	B	112	GLN
1	B	137	LEU
1	B	176	LYS
1	B	243	GLN
1	B	273	GLU
1	B	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	78	ASN
1	A	106	ASN
1	A	112	GLN
1	A	114	ASN
1	A	142	GLN
1	A	254	GLN
1	A	269	ASN
1	A	299	HIS
1	A	300	GLN
1	A	323	ASN
1	A	351	HIS
1	B	46	ASN
1	B	56	HIS
1	B	106	ASN
1	B	112	GLN
1	B	114	ASN
1	B	142	GLN
1	B	143	GLN
1	B	200	ASN
1	B	243	GLN
1	B	254	GLN
1	B	300	GLN
1	B	351	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GBN	A	420	-	11,12,12	2.10	3 (27%)	13,16,16	5.79	3 (23%)
2	PLP	B	410	1	15,15,16	1.48	3 (20%)	21,22,23	1.56	4 (19%)
2	PLP	A	410	1	15,15,16	1.56	3 (20%)	21,22,23	2.08	4 (19%)
3	GBN	B	420	-	11,12,12	2.04	3 (27%)	13,16,16	5.74	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GBN	A	420	-	-	0/8/18/18	0/1/1/1
2	PLP	B	410	1	-	0/6/6/8	0/1/1/1
2	PLP	A	410	1	-	0/6/6/8	0/1/1/1
3	GBN	B	420	-	-	0/8/18/18	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PLP	C2A-C2	4.08	1.56	1.50
3	B	420	GBN	C3-C	-3.80	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	420	GBN	C3-C	-3.71	1.39	1.50
3	A	420	GBN	C3-C1R	3.14	1.58	1.54
2	B	410	PLP	C2A-C2	3.11	1.55	1.50
3	B	420	GBN	C3-C1R	2.92	1.58	1.54
3	A	420	GBN	C2R-C3R	2.71	1.59	1.52
3	B	420	GBN	C2R-C3R	2.62	1.58	1.52
2	A	410	PLP	C3-C2	-2.15	1.38	1.41
2	B	410	PLP	P-O3P	-2.11	1.47	1.54
2	B	410	PLP	C5A-C5	2.08	1.56	1.50
2	A	410	PLP	C4A-C4	2.06	1.55	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	420	GBN	C2-C1R-C3	-19.73	87.79	110.49
3	B	420	GBN	C2-C1R-C3	-19.41	88.16	110.49
3	B	420	GBN	C1R-C3-C	5.39	128.97	115.99
2	A	410	PLP	O4P-C5A-C5	5.26	119.21	109.36
3	A	420	GBN	C1R-C3-C	5.06	128.17	115.99
2	A	410	PLP	O2P-P-O4P	-5.01	93.62	106.67
3	B	420	GBN	C3R-C2R-C1R	-3.81	107.34	113.62
2	B	410	PLP	O4P-C5A-C5	3.71	116.30	109.36
3	A	420	GBN	C3R-C2R-C1R	-3.58	107.72	113.62
2	A	410	PLP	C4A-C4-C5	3.12	124.16	120.94
2	B	410	PLP	O2P-P-O4P	-3.04	98.74	106.67
2	B	410	PLP	O3P-P-O1P	2.40	120.18	110.83
2	A	410	PLP	C5A-C5-C6	-2.20	115.77	119.36
2	B	410	PLP	C4A-C4-C5	2.13	123.14	120.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	420	GBN	1	0
2	A	410	PLP	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 [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	359/386 (93%)	0.00	5 (1%) 73 69	20, 33, 49, 63	0
1	B	358/386 (92%)	-0.07	6 (1%) 69 65	17, 29, 44, 62	0
All	All	717/772 (92%)	-0.03	11 (1%) 72 68	17, 31, 47, 63	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	VAL	4.2
1	B	385	LEU	3.8
1	B	193	TYR	3.4
1	A	45	ASN	3.3
1	B	375	GLY	3.0
1	B	192	PRO	2.7
1	A	385	LEU	2.6
1	A	194	PHE	2.5
1	A	321	GLU	2.3
1	B	205	TRP	2.2
1	B	104	VAL	2.2

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 oligosaccharides in this entry.

6.4 Ligands

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	MG	B	430	1/1	0.90	0.18	32,32,32,32	0
3	GBN	A	420	12/12	0.91	0.09	28,33,36,40	0
3	GBN	B	420	12/12	0.93	0.09	21,24,28,29	0
2	PLP	B	410	15/16	0.96	0.07	21,24,26,26	0
2	PLP	A	410	15/16	0.96	0.08	24,29,32,33	0

6.5 Other polymers

There are no such residues in this entry.