



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:54 PM UTC

PDB ID : 2COG / pdb_00002cog
Title : Crystal structure of oxidized human cytosolic branched-chain aminotransferase complexed with 4-methylvalerate
Authors : Goto, M.
Deposited on : 2005-05-17
Resolution : 2.10 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

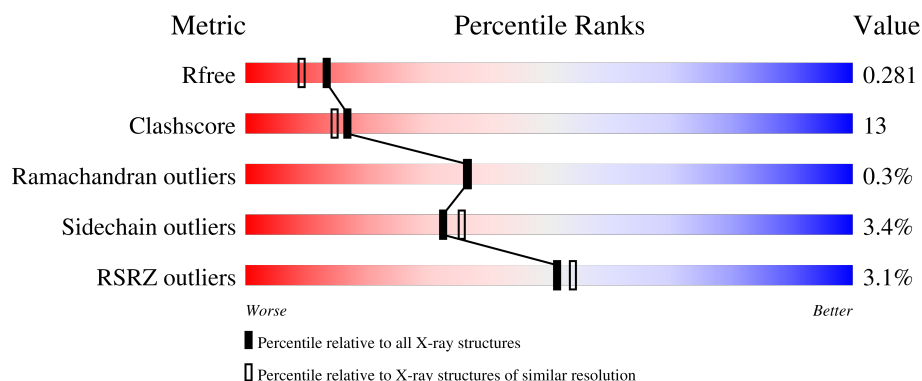
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	3% 66% 25% • 7%
1	B	386	2% 70% 21% • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6040 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.

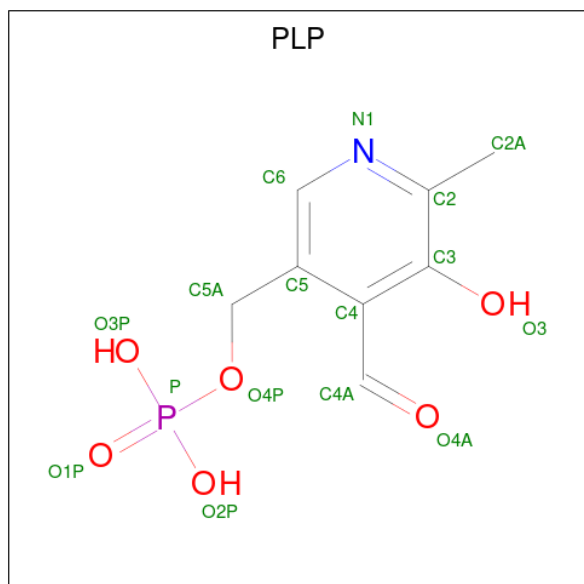
- Molecule 1 is a protein called branched chain aminotransferase 1, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2809	1811	462	521	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).



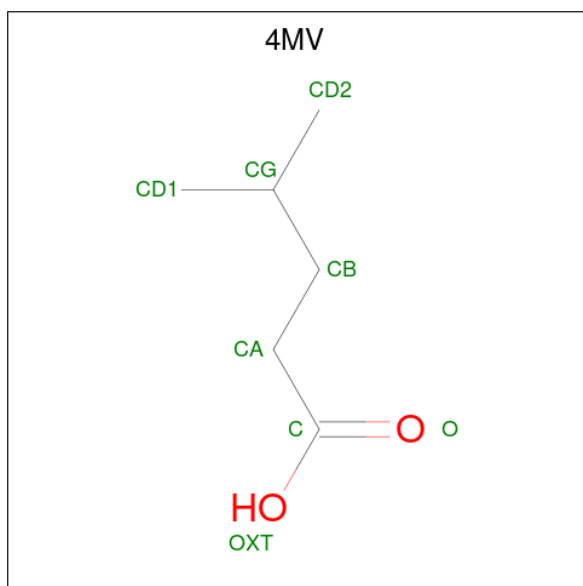
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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 4-METHYL VALERIC ACID (CCD ID: 4MV) (formula: C₆H₁₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	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		

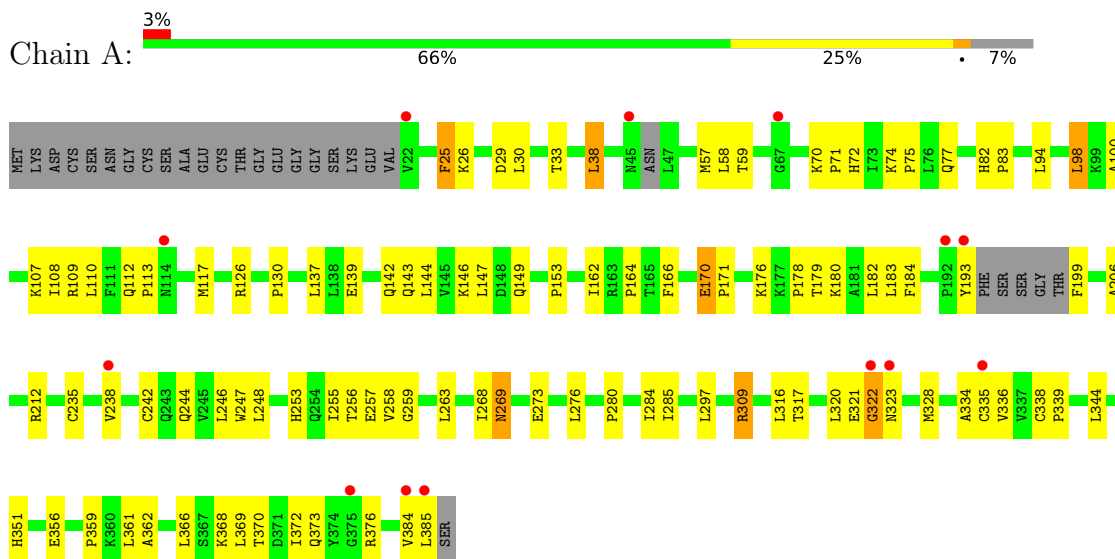
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total	O	0	0
			148	148		
5	B	203	Total	O	0	0
			203	203		

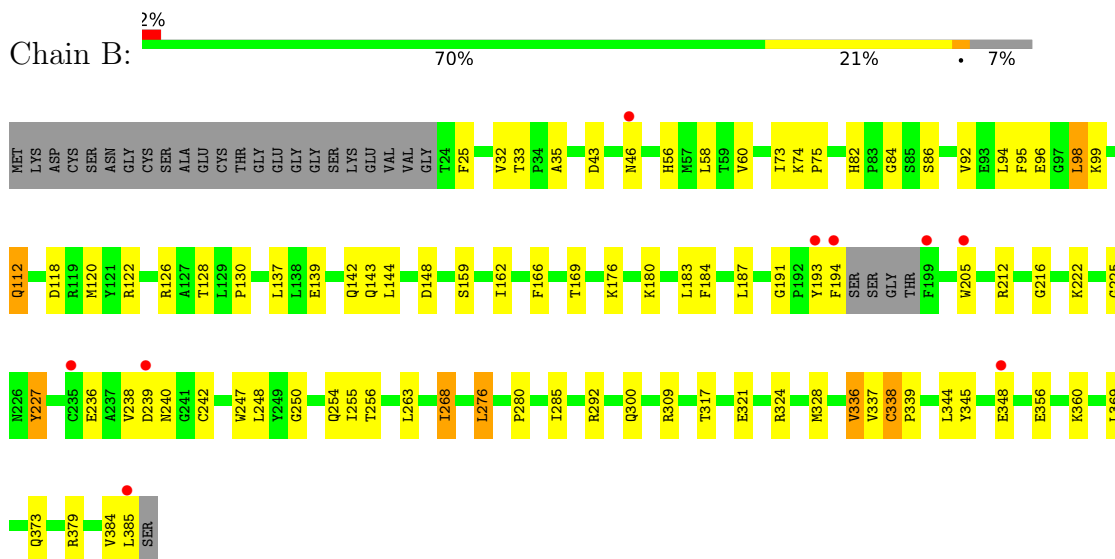
3 Residue-property plots [i](#)

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: branched chain aminotransferase 1, cytosolic



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.82Å 106.90Å 110.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.93-2.10) 95.5 (19.93-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.294 0.218 , 0.281	Depositor DCC
R_{free} test set	4509 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6040	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: MG, 4MV, 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	0.37	0/2880	0.90	4/3920 (0.1%)
1	B	0.40	0/2906	0.91	6/3953 (0.2%)
All	All	0.39	0/5786	0.90	10/7873 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	25	PHE	N-CA-C	-6.45	102.21	110.53
1	B	268	ILE	N-CA-C	-6.20	98.93	107.99
1	B	32	VAL	N-CA-C	5.98	116.73	107.99
1	B	276	LEU	N-CA-C	-5.86	98.97	108.52
1	B	73	ILE	N-CA-C	-5.65	98.30	107.28
1	A	33	THR	CA-C-N	5.49	125.50	119.90
1	A	33	THR	C-N-CA	5.49	125.50	119.90
1	B	216	GLY	N-CA-C	-5.39	107.89	115.32
1	B	250	GLY	N-CA-C	5.36	121.19	112.61
1	A	268	ILE	N-CA-C	-5.10	99.82	107.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	227	TYR	Sidechain

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	2809	0	2760	78	0
1	B	2833	0	2799	66	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
3	A	8	0	11	0	0
3	B	8	0	11	0	0
4	B	1	0	0	0	0
5	A	148	0	0	4	0
5	B	203	0	0	5	0
All	All	6040	0	5595	144	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 13.

All (144) 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:B:336:VAL:HG13	1:B:337:VAL:HG23	1.48	0.93
1:A:109:ARG:HG2	1:A:384:VAL:HG22	1.48	0.93
1:B:35:ALA:H	1:B:56:HIS:HE1	1.24	0.83
1:A:142:GLN:HE21	1:A:385:LEU:HD12	1.46	0.80
1:A:142:GLN:NE2	1:A:385:LEU:HD12	1.98	0.78
1:A:170:GLU:HG2	1:A:179:THR:H	1.49	0.77
1:B:384:VAL:HG12	1:B:385:LEU:HG	1.65	0.77
1:B:126:ARG:HG3	5:B:465:HOH:O	1.84	0.76
1:B:300:GLN:NE2	1:B:379:ARG:HH22	1.84	0.76
1:A:284:ILE:HG13	1:A:285:ILE:HD12	1.69	0.73
1:A:269:ASN:ND2	1:A:273:GLU:H	1.87	0.73
1:B:345:TYR:O	1:B:348:GLU:HG2	1.90	0.71
1:B:98:LEU:CD2	1:B:162:ILE:HD12	2.21	0.70
1:B:98:LEU:HD22	1:B:162:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:O	1:A:373:GLN:HG3	1.94	0.67
1:A:370:THR:HG22	1:A:376:ARG:HH22	1.58	0.67
1:B:317:THR:O	1:B:321:GLU:HG3	1.95	0.66
1:A:351:HIS:HE1	1:A:356:GLU:OE1	1.77	0.66
1:A:110:LEU:HB3	1:A:113:PRO:HG3	1.77	0.66
1:A:246:LEU:HD11	1:A:255:ILE:HG23	1.76	0.66
1:A:255:ILE:CG2	1:A:263:LEU:HD13	2.26	0.65
1:B:74:LYS:HB2	1:B:75:PRO:HD2	1.78	0.64
1:A:108:ILE:CD1	1:A:149:GLN:HB2	2.26	0.64
1:A:74:LYS:HE3	1:A:77:GLN:HE21	1.64	0.63
1:A:170:GLU:HG3	1:A:178:PRO:HA	1.80	0.62
1:B:56:HIS:HD2	1:B:148:ASP:OD2	1.81	0.62
1:B:236:GLU:HA	1:B:239:ASP:OD1	2.00	0.62
1:A:139:GLU:O	1:A:143:GLN:HG2	2.00	0.61
1:A:170:GLU:OE1	1:A:171:PRO:HD2	2.01	0.61
1:A:284:ILE:HG13	1:A:285:ILE:CD1	2.32	0.60
1:B:263:LEU:C	1:B:263:LEU:HD23	2.26	0.59
1:A:170:GLU:CG	1:A:179:THR:H	2.15	0.59
1:A:269:ASN:HD21	1:A:273:GLU:H	1.49	0.58
1:A:258:VAL:HG23	1:A:263:LEU:HB2	1.86	0.57
1:A:182:LEU:C	1:A:182:LEU:HD13	2.31	0.56
1:A:317:THR:O	1:A:321:GLU:HG2	2.06	0.56
1:A:193:TYR:HB2	1:A:334:ALA:HB1	1.88	0.56
1:A:269:ASN:C	1:A:269:ASN:HD22	2.12	0.56
1:A:58:LEU:HD12	1:A:72:HIS:O	2.05	0.56
1:A:320:LEU:C	1:A:322:GLY:H	2.14	0.55
1:A:112:GLN:N	1:A:113:PRO:HD3	2.22	0.55
1:A:235:CYS:O	1:A:238:VAL:HG22	2.07	0.55
1:B:336:VAL:HG22	1:B:369:LEU:HD13	1.88	0.54
1:B:256:THR:HB	1:B:285:ILE:HD11	1.89	0.54
1:B:238:VAL:C	1:B:240:ASN:H	2.14	0.54
1:A:269:ASN:HD21	1:A:273:GLU:HG3	1.73	0.54
1:B:94:LEU:HD12	1:B:94:LEU:C	2.32	0.53
1:B:169:THR:OG1	1:B:180:LYS:HG2	2.08	0.53
1:B:82:HIS:ND1	1:B:84:GLY:N	2.49	0.53
1:B:33:THR:O	1:B:75:PRO:HD3	2.08	0.53
1:B:205:TRP:CH2	1:B:236:GLU:OE2	2.62	0.53
1:B:242:CYS:SG	1:B:344:LEU:HD22	2.48	0.53
1:B:144:LEU:HG	1:B:187:LEU:HD11	1.92	0.52
1:A:212:ARG:HB2	1:A:247:TRP:CE3	2.45	0.51
1:A:25:PHE:HB2	1:A:71:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:A:372:ILE:HG13	2.10	0.51
1:B:292:ARG:O	1:B:292:ARG:HD3	2.10	0.51
1:B:98:LEU:HD23	5:B:569:HOH:O	2.10	0.51
1:A:130:PRO:HG2	1:A:166:PHE:HZ	1.76	0.51
1:A:94:LEU:C	1:A:94:LEU:HD12	2.36	0.50
1:A:370:THR:HG22	1:A:376:ARG:NH2	2.27	0.50
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.26	0.50
1:A:57:MET:HE2	1:A:59:THR:CG2	2.42	0.50
1:B:35:ALA:N	1:B:56:HIS:HE1	2.03	0.49
1:A:74:LYS:HB2	1:A:75:PRO:CD	2.43	0.49
1:B:112:GLN:HE21	1:B:112:GLN:HA	1.78	0.49
1:B:86:SER:HB2	1:B:92:VAL:HG21	1.95	0.49
1:A:212:ARG:HB2	1:A:247:TRP:CD2	2.48	0.49
1:A:269:ASN:ND2	1:A:269:ASN:C	2.68	0.48
1:A:98:LEU:N	1:A:98:LEU:HD23	2.29	0.48
1:A:142:GLN:HB3	1:A:385:LEU:HD12	1.96	0.48
1:A:38:LEU:HB3	5:A:449:HOH:O	2.13	0.48
1:A:253:HIS:HA	5:A:554:HOH:O	2.12	0.48
1:A:182:LEU:HD12	1:A:184:PHE:HD2	1.79	0.48
1:A:199:PHE:CE1	1:A:366:LEU:HD22	2.49	0.48
1:B:35:ALA:H	1:B:56:HIS:CE1	2.16	0.48
1:A:206:ALA:HB1	1:A:248:LEU:HD11	1.96	0.48
1:A:26:LYS:HE3	1:A:29:ASP:OD2	2.14	0.47
1:A:142:GLN:HB3	1:A:385:LEU:CD1	2.45	0.47
1:B:280:PRO:HD3	1:B:309:ARG:C	2.39	0.47
1:A:244:GLN:OE1	1:A:259:GLY:HA3	2.15	0.47
1:A:255:ILE:HG22	1:A:263:LEU:HD13	1.95	0.46
1:B:25:PHE:CD2	1:B:60:VAL:HG11	2.50	0.46
1:A:242:CYS:SG	1:A:344:LEU:HD22	2.56	0.46
1:B:118:ASP:O	1:B:122:ARG:HG3	2.15	0.46
1:A:70:LYS:O	1:A:72:HIS:HD2	1.99	0.46
1:A:117:MET:HA	1:A:117:MET:HE2	1.97	0.46
1:B:205:TRP:HH2	1:B:236:GLU:OE2	1.99	0.45
1:B:212:ARG:HB2	1:B:247:TRP:CD2	2.51	0.45
1:B:143:GLN:NE2	1:B:143:GLN:HA	2.31	0.45
1:B:193:TYR:HD2	1:B:194:PHE:CE1	2.34	0.45
1:A:297:LEU:HD13	1:A:368:LYS:HG2	1.97	0.45
1:B:99:LYS:HD3	1:B:159:SER:OG	2.17	0.45
1:B:43:ASP:HB3	1:B:46:ASN:OD1	2.16	0.45
1:B:336:VAL:CG2	1:B:369:LEU:HD13	2.47	0.45
1:A:100:ALA:HA	1:A:109:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HB2	1:A:109:ARG:NH1	2.33	0.44
1:B:183:LEU:HD12	1:B:184:PHE:N	2.33	0.44
1:A:146:LYS:HD2	1:A:385:LEU:HD22	2.00	0.43
1:B:95:PHE:O	1:B:222:LYS:HB3	2.19	0.43
1:B:300:GLN:HE22	1:B:379:ARG:HH22	1.58	0.43
1:B:263:LEU:HD11	1:B:328:MET:HE3	2.00	0.43
1:B:292:ARG:HD2	5:B:613:HOH:O	2.18	0.43
5:A:461:HOH:O	1:B:225:GLY:HA3	2.18	0.43
1:B:96:GLU:HG3	1:B:120:MET:HB2	2.00	0.43
1:B:369:LEU:O	1:B:373:GLN:HG3	2.18	0.43
1:B:227:TYR:CD1	1:B:227:TYR:N	2.87	0.43
1:A:126:ARG:NH1	5:A:527:HOH:O	2.51	0.43
1:B:128:THR:HA	5:B:519:HOH:O	2.18	0.43
1:A:182:LEU:CD1	1:A:184:PHE:HD2	2.32	0.43
1:A:256:THR:OG1	1:A:257:GLU:N	2.52	0.42
1:B:222:LYS:NZ	2:B:410:PLP:O3	2.50	0.42
1:A:335:CYS:C	1:A:336:VAL:HG23	2.44	0.42
1:A:359:PRO:HB2	1:A:362:ALA:HB3	2.02	0.42
1:B:384:VAL:CG1	1:B:385:LEU:HG	2.44	0.42
1:B:94:LEU:HG	1:B:166:PHE:HB3	2.01	0.42
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.71	0.42
1:A:280:PRO:HD3	1:A:309:ARG:C	2.45	0.42
1:A:316:LEU:CD2	1:A:328:MET:HE1	2.50	0.42
1:B:248:LEU:HA	1:B:254:GLN:O	2.19	0.42
1:A:320:LEU:C	1:A:322:GLY:N	2.78	0.42
1:A:257:GLU:OE1	2:A:410:PLP:N1	2.54	0.41
1:B:255:ILE:O	1:B:255:ILE:HG13	2.20	0.41
1:A:108:ILE:HD13	1:A:149:GLN:HB2	1.99	0.41
1:A:57:MET:HE2	1:A:59:THR:HG22	2.01	0.41
1:B:344:LEU:N	1:B:344:LEU:HD12	2.36	0.41
1:A:98:LEU:HD23	1:A:98:LEU:H	1.85	0.41
1:B:139:GLU:OE2	1:B:143:GLN:HG2	2.21	0.41
1:B:142:GLN:HE21	1:B:142:GLN:HB3	1.61	0.41
1:B:58:LEU:C	1:B:58:LEU:HD13	2.46	0.41
1:B:191:GLY:HA3	5:B:627:HOH:O	2.21	0.41
1:A:30:LEU:HD23	1:A:71:PRO:HG2	2.03	0.41
1:A:193:TYR:CG	1:A:334:ALA:HB1	2.56	0.41
1:B:336:VAL:HG22	1:B:369:LEU:CD1	2.50	0.41
1:A:82:HIS:HA	1:A:83:PRO:HD3	1.96	0.40
1:B:238:VAL:C	1:B:240:ASN:N	2.77	0.40
1:B:256:THR:HB	1:B:285:ILE:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:O	1:A:164:PRO:HD3	2.21	0.40
1:B:268:ILE:O	1:B:324:ARG:NH1	2.51	0.40
1:B:338:CYS:HA	1:B:339:PRO:HD2	1.92	0.40
1:A:182:LEU:HD11	1:A:184:PHE:HB3	2.02	0.40
1:A:199:PHE:CG	1:A:339:PRO:HG2	2.56	0.40
1:A:323:ASN:N	1:A:323:ASN:HD22	2.19	0.40
1:B:130:PRO:HG2	1:B:166:PHE:HZ	1.86	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	352/386 (91%)	333 (95%)	17 (5%)	2 (1%)	21	18
1	B	354/386 (92%)	333 (94%)	21 (6%)	0	100	100
All	All	706/772 (92%)	666 (94%)	38 (5%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	PRO
1	A	322	GLY

5.3.2 Protein sidechains [i](#)

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	305/334 (91%)	292 (96%)	13 (4%)	26	27
1	B	310/334 (93%)	302 (97%)	8 (3%)	40	46
All	All	615/668 (92%)	594 (97%)	21 (3%)	32	35

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

Mol	Chain	Res	Type
1	A	38	LEU
1	A	98	LEU
1	A	137	LEU
1	A	144	LEU
1	A	147	LEU
1	A	170	GLU
1	A	176	LYS
1	A	183	LEU
1	A	269	ASN
1	A	276	LEU
1	A	309	ARG
1	A	338	CYS
1	A	361	LEU
1	B	98	LEU
1	B	112	GLN
1	B	137	LEU
1	B	176	LYS
1	B	276	LEU
1	B	336	VAL
1	B	338	CYS
1	B	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	112	GLN
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

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Mol	Chain	Res	Type
1	A	373	GLN
1	B	56	HIS
1	B	78	ASN
1	B	106	ASN
1	B	112	GLN
1	B	142	GLN
1	B	143	GLN
1	B	200	ASN
1	B	262	ASN
1	B	300	GLN
1	B	323	ASN
1	B	351	HIS

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 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	4MV	A	420	-	7,7,7	0.82	0	8,8,8	0.77	0
3	4MV	B	420	-	7,7,7	0.90	0	8,8,8	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	B	410	1	15,15,16	1.12	1 (6%)	21,22,23	1.44	5 (23%)
2	PLP	A	410	1	15,15,16	1.56	2 (13%)	21,22,23	2.10	5 (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	4MV	A	420	-	-	2/5/5/5	-
3	4MV	B	420	-	-	2/5/5/5	-
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PLP	C3-C2	-3.36	1.37	1.41
2	A	410	PLP	C2A-C2	3.23	1.55	1.50
2	B	410	PLP	C2A-C2	2.61	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PLP	O4P-C5A-C5	5.83	120.28	109.36
2	A	410	PLP	O2P-P-O4P	-4.71	94.38	106.67
2	B	410	PLP	O4P-C5A-C5	3.27	115.48	109.36
2	A	410	PLP	C4A-C4-C5	2.90	123.93	120.94
2	B	410	PLP	C4A-C4-C5	2.26	123.27	120.94
2	B	410	PLP	C5A-C5-C6	-2.19	115.79	119.36
2	A	410	PLP	O3P-P-O1P	2.12	119.11	110.83
2	B	410	PLP	O3P-P-O1P	2.09	118.97	110.83
2	A	410	PLP	C4A-C4-C3	-2.05	117.10	120.52
2	B	410	PLP	O2P-P-O4P	-2.05	101.32	106.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	420	4MV	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	B	420	4MV	O-C-CA-CB
3	A	420	4MV	OXT-C-CA-CB
3	A	420	4MV	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	PLP	1	0
2	A	410	PLP	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

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	358/386 (92%)	0.48	13 (3%) 46 48	14, 27, 45, 61	0
1	B	358/386 (92%)	0.13	9 (2%) 58 61	12, 21, 39, 55	0
All	All	716/772 (92%)	0.30	22 (3%) 51 54	12, 24, 41, 61	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	LEU	4.7
1	A	192	PRO	4.1
1	A	384	VAL	4.1
1	B	46	ASN	3.9
1	B	235	CYS	3.8
1	A	22	VAL	3.6
1	B	385	LEU	3.5
1	A	45	ASN	3.4
1	A	323	ASN	3.0
1	A	238	VAL	2.8
1	B	193	TYR	2.8
1	B	239	ASP	2.8
1	B	199	PHE	2.7
1	A	193	TYR	2.6
1	B	205	TRP	2.5
1	B	194	PHE	2.3
1	A	114	ASN	2.2
1	A	322	GLY	2.2
1	A	67	GLY	2.1
1	A	375	GLY	2.1
1	B	348	GLU	2.0
1	A	335	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	MG	B	430	1/1	0.57	0.29	38,38,38,38	0
3	4MV	A	420	8/8	0.76	0.16	39,41,44,45	0
3	4MV	B	420	8/8	0.81	0.13	28,31,37,37	0
2	PLP	B	410	15/16	0.96	0.07	12,16,19,21	0
2	PLP	A	410	15/16	0.96	0.07	17,22,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.