WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 05:13 pm GMT

PDB ID	:	4AH3
Title	:	Crystal structure of the holo omega-transaminase from Chromobacterium vi-olaceum
Authors	:	Sayer, C.; Isupov, M.N.; Littlechild, J.A.
Deposited on	:	2012-02-03
Resolution	:	1.57 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 1.57 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.
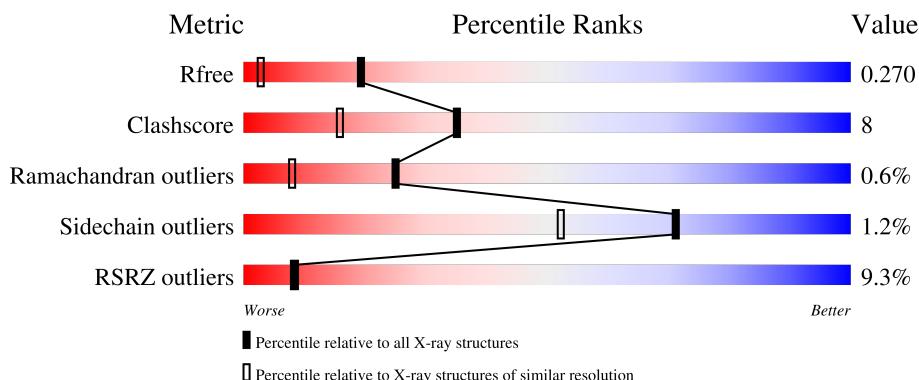
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 <=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	459	
1	B	459	
1	C	459	
1	D	459	
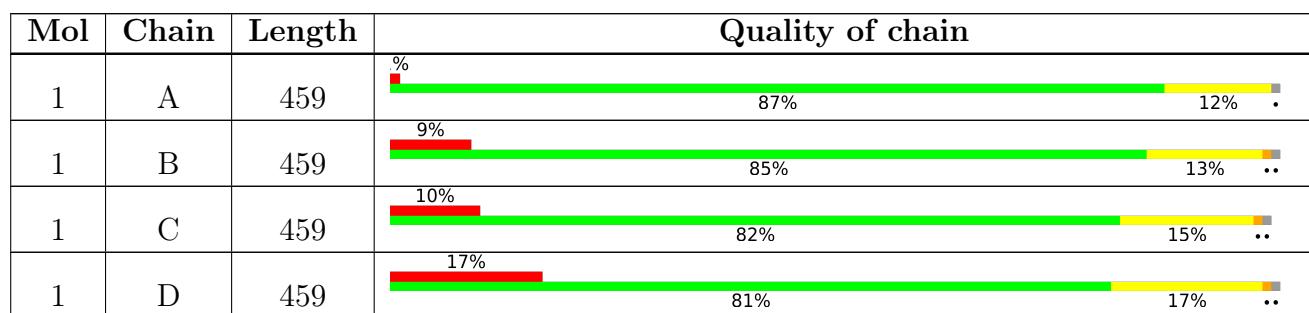
2　Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16845 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 OMEGA-TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total 3785	C 2431	N 655	O 678	S 21	0	36	0
1	B	455	Total 3755	C 2406	N 654	O 673	S 22	0	33	0
1	C	455	Total 3706	C 2374	N 645	O 664	S 23	0	23	0
1	D	454	Total 3674	C 2347	N 641	O 663	S 23	0	20	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
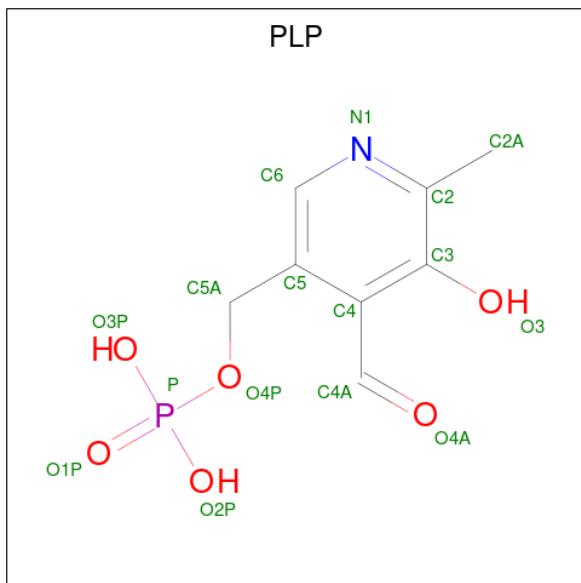
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	722	Total	O	0	0
			722	722		
3	B	560	Total	O	0	0
			560	560		
3	C	346	Total	O	0	0
			346	346		
3	D	237	Total	O	0	0
			237	237		

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: OMEGA-TRANSAMINASE
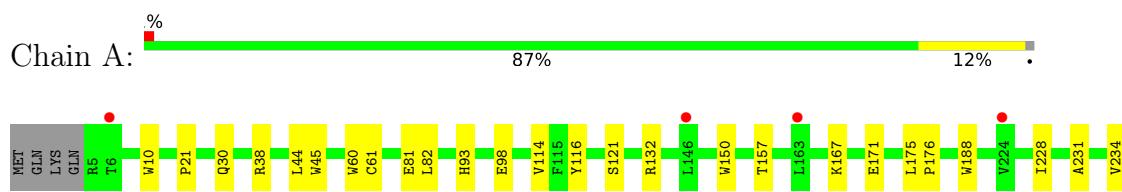
• Molecule 1: OMEGA-TRANSAMINASE

• Molecule 1: OMEGA-TRANSAMINASE

• Molecule 1: OMEGA-TRANSAMINASE

17%

Chain D:

81% 17%
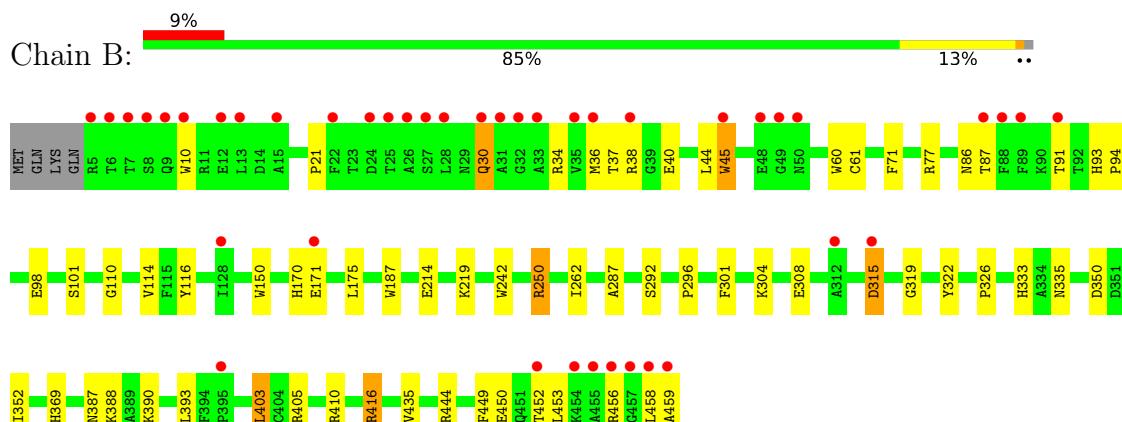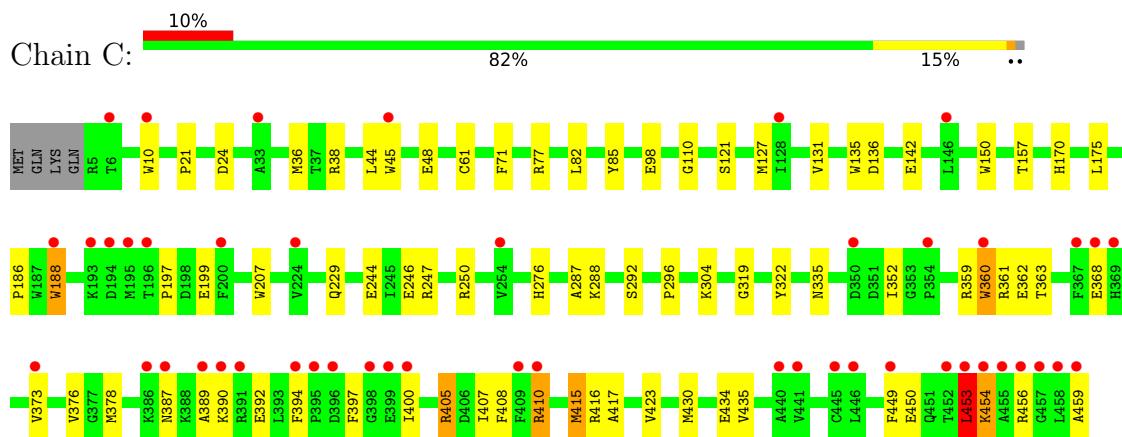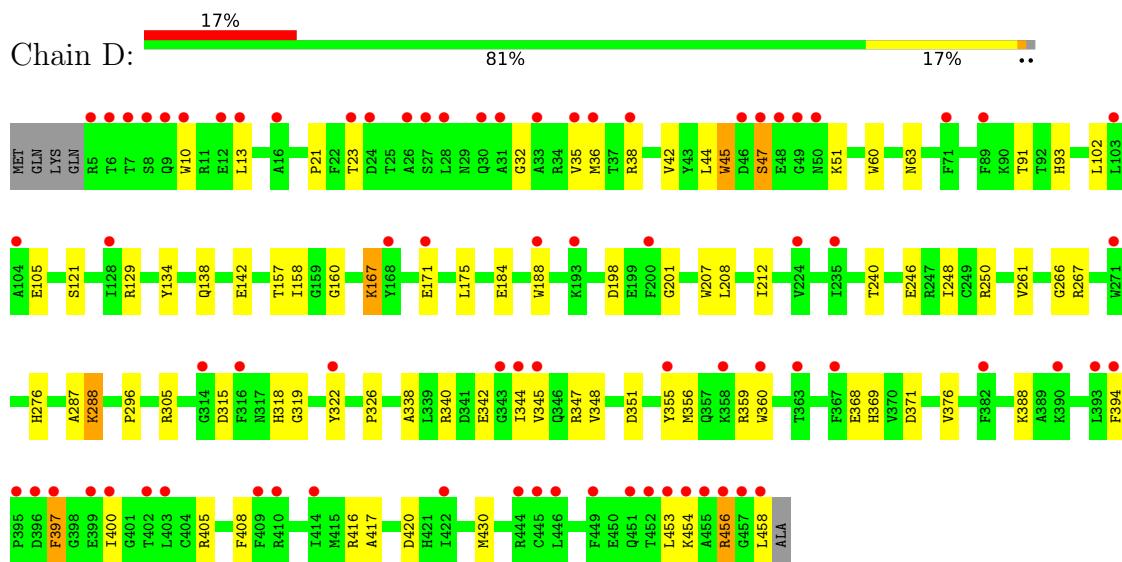
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.89Å 62.23Å 119.61Å 75.14° 81.73° 76.17°	Depositor
Resolution (Å)	115.19 – 1.57 26.65 – 1.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (115.19-1.57) 94.4 (26.65-1.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.222 , 0.273 0.220 , 0.270	Depositor DCC
R_{free} test set	11001 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16845	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.79	6/3989 (0.2%)	0.85	2/5391 (0.0%)
1	B	0.68	4/3948 (0.1%)	0.74	0/5332
1	C	0.65	8/3871 (0.2%)	0.70	0/5236
1	D	0.58	4/3825 (0.1%)	0.64	0/5173
All	All	0.68	22/15633 (0.1%)	0.74	2/21132 (0.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	TRP	CD2-CE2	6.33	1.49	1.41
1	A	242	TRP	CD2-CE2	6.03	1.48	1.41
1	C	135	TRP	CD2-CE2	5.71	1.48	1.41
1	A	271	TRP	CD2-CE2	5.60	1.48	1.41
1	B	242	TRP	CD2-CE2	5.54	1.48	1.41
1	C	360	TRP	CD2-CE2	5.44	1.47	1.41
1	B	150	TRP	CD2-CE2	5.43	1.47	1.41
1	C	45	TRP	CD2-CE2	5.40	1.47	1.41
1	D	10	TRP	CD2-CE2	5.36	1.47	1.41
1	A	188	TRP	CD2-CE2	5.31	1.47	1.41
1	A	60	TRP	CD2-CE2	5.29	1.47	1.41
1	A	10	TRP	CD2-CE2	5.27	1.47	1.41
1	B	10	TRP	CD2-CE2	5.26	1.47	1.41
1	B	45	TRP	CD2-CE2	5.21	1.47	1.41
1	C	10	TRP	CD2-CE2	5.19	1.47	1.41
1	D	45	TRP	CD2-CE2	5.17	1.47	1.41
1	D	188	TRP	CD2-CE2	5.16	1.47	1.41
1	D	60	TRP	CD2-CE2	5.16	1.47	1.41
1	C	207	TRP	CD2-CE2	5.14	1.47	1.41
1	C	188[A]	TRP	CD2-CE2	5.04	1.47	1.41
1	C	188[B]	TRP	CD2-CE2	5.04	1.47	1.41
1	C	150	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	371	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	132	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	3785	0	3785	51	0
1	B	3755	0	3758	77	0
1	C	3706	0	3667	58	0
1	D	3674	0	3623	74	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	7	0	0
2	D	15	0	6	0	0
3	A	722	0	0	22	0
3	B	560	0	0	29	0
3	C	346	0	0	12	0
3	D	237	0	0	8	0
All	All	16845	0	14858	244	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 (244) 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:45[B]:TRP:CH2	3:A:2109:HOH:O	1.74	1.27
1:A:280[B]:GLN:HG3	3:A:2534:HOH:O	1.08	1.25
1:B:410[B]:ARG:NH2	3:B:2530:HOH:O	1.71	1.24
1:B:77[B]:ARG:NH1	3:B:2123:HOH:O	1.59	1.23
1:B:350[B]:ASP:OD2	3:B:2458:HOH:O	1.57	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247[B]:ARG:NH2	3:C:2239:HOH:O	1.66	1.21
1:A:250[B]:ARG:NH2	3:A:2491:HOH:O	1.69	1.19
1:B:34[B]:ARG:NH1	3:B:2035:HOH:O	1.61	1.18
1:B:38[A]:ARG:NH2	3:B:2041:HOH:O	1.74	1.17
1:B:38[B]:ARG:NE	3:B:2038:HOH:O	1.83	1.12
1:C:136[B]:ASP:OD2	3:C:2163:HOH:O	1.66	1.12
1:A:30[B]:GLN:OE1	3:A:2082:HOH:O	1.69	1.11
1:A:81[A]:GLU:OE2	3:A:2221:HOH:O	1.70	1.10
1:B:38[B]:ARG:CG	1:B:38[B]:ARG:HH11	1.67	1.05
1:A:228[B]:ILE:HD11	1:A:277:PHE:CZ	1.93	1.04
1:B:38[B]:ARG:HH11	1:B:38[B]:ARG:HG3	1.21	1.04
1:B:38[B]:ARG:CD	3:B:2038:HOH:O	2.06	1.02
1:A:38[B]:ARG:NH1	3:A:2096:HOH:O	1.92	1.01
1:B:388[A]:LYS:NZ	3:B:2483:HOH:O	1.92	1.01
1:D:198[A]:ASP:OD2	3:D:2142:HOH:O	1.82	0.98
1:A:250[B]:ARG:CZ	3:A:2491:HOH:O	2.03	0.98
1:B:214[B]:GLU:OE2	3:B:2330:HOH:O	1.83	0.96
1:B:38[B]:ARG:HD2	3:B:2038:HOH:O	1.61	0.95
1:B:36[B]:MET:HE2	1:B:44:LEU:HD22	1.46	0.95
1:C:110:GLY:HA2	1:C:304[B]:LYS:HE3	1.47	0.94
1:C:405:ARG:NH1	3:C:2333:HOH:O	2.00	0.94
1:D:38[A]:ARG:HD2	3:D:2024:HOH:O	1.68	0.93
1:B:87[B]:THR:HG21	3:B:2143:HOH:O	1.68	0.93
1:A:228[B]:ILE:HD11	1:A:277:PHE:HZ	1.35	0.90
1:A:45[B]:TRP:CZ3	3:A:2109:HOH:O	2.05	0.90
1:B:36[B]:MET:CE	1:B:44:LEU:HD22	2.01	0.89
1:C:304[B]:LYS:NZ	3:C:2147:HOH:O	1.79	0.88
1:B:410[B]:ARG:CZ	3:B:2530:HOH:O	2.15	0.87
1:B:101[B]:SER:OG	3:B:2157:HOH:O	1.92	0.87
1:B:21:PRO:HB3	1:D:319:GLY:HA3	1.60	0.84
1:A:167:LYS:O	1:A:171[B]:GLU:HG2	1.77	0.84
1:A:250[B]:ARG:NE	3:A:2491:HOH:O	2.09	0.82
1:B:38[B]:ARG:HG3	1:B:38[B]:ARG:NH1	1.90	0.82
1:C:36[B]:MET:HE2	1:C:44:LEU:HD13	1.62	0.82
1:B:110:GLY:HA2	1:B:304[A]:LYS:HE3	1.62	0.81
1:A:171[B]:GLU:OE2	3:A:2403:HOH:O	1.97	0.81
1:D:208[A]:LEU:HD22	1:D:248:ILE:HG21	1.63	0.80
1:D:36[B]:MET:HE2	1:D:36[B]:MET:HA	1.64	0.79
1:A:81[B]:GLU:HG3	3:A:2203:HOH:O	1.83	0.79
1:D:208[A]:LEU:HD22	1:D:248:ILE:CG2	2.11	0.79
1:D:208[A]:LEU:HD21	1:D:212:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36[B]:MET:HE2	1:B:44:LEU:CD2	2.14	0.78
1:A:228[B]:ILE:CD1	1:A:277:PHE:CZ	2.67	0.77
1:A:81[A]:GLU:CD	3:A:2221:HOH:O	2.15	0.77
1:A:451:GLN:NE2	3:A:2714:HOH:O	2.19	0.75
1:C:48:GLU:OE1	1:C:48:GLU:HA	1.86	0.75
1:D:371:ASP:OD2	1:D:388[B]:LYS:HG3	1.87	0.74
1:A:98[A]:GLU:OE1	3:A:2250:HOH:O	2.03	0.74
1:D:368:GLU:O	1:D:388[A]:LYS:HD2	1.88	0.74
1:B:214[B]:GLU:CD	3:B:2330:HOH:O	2.20	0.73
1:B:34[B]:ARG:HG2	1:D:91:THR:HG22	1.70	0.72
1:B:36[B]:MET:HE2	1:B:44:LEU:HB3	1.72	0.71
1:B:40:GLU:HG2	3:B:2012:HOH:O	1.90	0.70
1:D:208[A]:LEU:CD2	1:D:212:ILE:CD1	2.70	0.69
1:A:228[B]:ILE:HD11	1:A:277:PHE:CE2	2.27	0.69
1:B:319:GLY:HA3	1:D:21:PRO:HB3	1.76	0.68
1:A:45[B]:TRP:HH2	3:A:2109:HOH:O	1.33	0.68
3:B:2142:HOH:O	1:D:23[A]:THR:HG21	1.94	0.68
1:A:228[B]:ILE:CD1	1:A:277:PHE:CE2	2.77	0.67
1:B:308[B]:GLU:OE2	3:B:2420:HOH:O	0.67	0.66
1:B:387:ASN:HD22	1:B:390:LYS:H	1.43	0.66
1:D:38[A]:ARG:CD	3:D:2024:HOH:O	2.35	0.66
1:B:315[A]:ASP:OD2	3:B:2427:HOH:O	0.65	0.65
1:B:38[B]:ARG:HH11	1:B:38[B]:ARG:HG2	1.59	0.65
1:B:87[B]:THR:HG23	1:D:21:PRO:HD2	1.78	0.65
1:D:208[A]:LEU:CD2	1:D:212:ILE:HD11	2.26	0.65
1:B:36[B]:MET:CE	1:B:44:LEU:CD2	2.75	0.65
1:B:34[B]:ARG:CG	1:D:91:THR:HG22	2.26	0.64
1:B:60:TRP:HE1	1:B:416[B]:ARG:HH21	1.45	0.64
1:A:280[B]:GLN:CG	3:A:2534:HOH:O	1.89	0.64
1:B:77[B]:ARG:CZ	3:B:2123:HOH:O	2.19	0.63
1:C:142[B]:GLU:OE1	3:C:2174:HOH:O	0.63	0.63
1:B:30:GLN:HE21	1:B:30:GLN:HA	1.64	0.62
1:B:304[A]:LYS:HE2	3:B:2413:HOH:O	1.99	0.61
1:D:356[B]:MET:CE	1:D:360:TRP:HE3	2.12	0.61
1:A:319:GLY:HA3	1:C:21:PRO:HB3	1.83	0.61
1:C:387:ASN:HB3	1:C:392:GLU:HB3	1.82	0.61
1:D:35:VAL:HB	1:D:47[A]:SER:HB2	1.82	0.60
1:D:246:GLU:O	1:D:250[A]:ARG:HG2	2.01	0.60
1:B:416[B]:ARG:NH1	3:B:2351:HOH:O	2.18	0.60
1:A:315[B]:ASP:OD1	1:C:24:ASP:HB2	2.01	0.60
1:D:208[A]:LEU:HD23	1:D:212:ILE:CD1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36[B]:MET:SD	1:B:37:THR:N	2.75	0.59
1:B:452:THR:O	1:B:456:ARG:HG2	2.03	0.59
1:C:415[A]:MET:HG3	1:C:423:VAL:O	2.03	0.59
1:D:36[B]:MET:SD	1:D:44:LEU:HD22	2.42	0.59
1:C:77[B]:ARG:NH2	3:C:2110:HOH:O	0.74	0.59
1:A:93:HIS:CE1	1:A:326:PRO:HG3	2.38	0.58
1:C:188[B]:TRP:CZ2	1:C:197:PRO:HD3	2.39	0.58
1:B:36[B]:MET:HE2	1:B:44:LEU:CB	2.34	0.58
1:C:61:CYS:O	1:C:292:SER:HA	2.05	0.57
1:C:36[B]:MET:CE	1:C:44:LEU:HD13	2.34	0.57
1:D:208[A]:LEU:HD23	1:D:212:ILE:HD12	1.86	0.57
1:D:208[A]:LEU:CD2	1:D:212:ILE:HD12	2.33	0.57
1:A:351[B]:ASP:OD1	1:A:432:ARG:NH2	2.39	0.56
1:C:352[B]:ILE:HD11	1:C:435:VAL:HG21	1.88	0.56
1:A:416[A]:ARG:HD2	3:A:2673:HOH:O	2.05	0.56
1:B:38[B]:ARG:CG	1:B:38[B]:ARG:NH1	2.40	0.56
1:B:94:PRO:O	1:B:98[A]:GLU:HG2	2.06	0.56
1:B:315[B]:ASP:HB3	3:B:2427:HOH:O	2.05	0.56
1:C:276:HIS:CE1	1:C:376:VAL:HG21	2.41	0.56
1:D:38[A]:ARG:NE	3:D:2024:HOH:O	2.38	0.56
1:B:86:ASN:O	1:B:91[B]:THR:HG23	2.05	0.56
1:B:98[B]:GLU:HG2	1:B:333:HIS:CD2	2.41	0.55
1:A:175:LEU:HB3	1:A:176:PRO:HA	1.89	0.55
1:D:36[B]:MET:HA	1:D:36[B]:MET:CE	2.34	0.55
1:C:360:TRP:HH2	1:C:415[B]:MET:CE	2.19	0.55
1:A:304:LYS:HE3	3:A:2542:HOH:O	2.06	0.54
1:C:199:GLU:HA	3:C:2231:HOH:O	2.07	0.54
1:D:344:ILE:O	1:D:348:VAL:HG23	2.06	0.54
1:D:21:PRO:O	1:D:23[A]:THR:HG23	2.07	0.54
1:B:458:LEU:O	1:B:459:ALA:OXT	2.25	0.54
1:D:261:VAL:HG12	1:D:288:LYS:HD2	1.89	0.54
1:B:304[A]:LYS:CE	3:B:2413:HOH:O	2.54	0.53
1:B:93:HIS:CE1	1:B:326:PRO:HG3	2.43	0.53
1:D:356[B]:MET:CE	1:D:360:TRP:CE3	2.91	0.53
1:A:228[B]:ILE:HD13	1:A:277:PHE:CE2	2.44	0.53
1:B:116:TYR:HD2	3:B:2190:HOH:O	1.91	0.53
1:D:201:GLY:HA3	1:D:240[A]:THR:HG23	1.91	0.52
1:D:208[A]:LEU:HD22	1:D:248:ILE:HG22	1.87	0.52
1:C:450:GLU:HA	1:C:453:LEU:HD13	1.92	0.51
1:B:250[B]:ARG:HG2	3:B:2366:HOH:O	2.11	0.51
1:B:36[B]:MET:HE1	1:B:45:TRP:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:O	1:D:105:GLU:HG2	2.10	0.51
1:D:167:LYS:O	1:D:171:GLU:HG2	2.11	0.51
1:C:361:ARG:HA	1:C:373:VAL:HG11	1.93	0.51
1:C:244:GLU:CD	1:C:247[A]:ARG:HH21	2.15	0.50
1:D:160:GLY:HA3	3:D:2082:HOH:O	2.11	0.50
1:B:449:PHE:CE2	1:B:453:LEU:HD12	2.47	0.50
1:D:405:ARG:HA	1:D:408:PHE:HD2	1.76	0.50
1:B:170:HIS:HA	1:B:175:LEU:HB2	1.93	0.50
1:A:21:PRO:HB3	1:C:319:GLY:HA3	1.93	0.50
1:B:369:HIS:HD2	1:B:450:GLU:OE1	1.95	0.50
1:A:121:SER:HA	3:A:2310:HOH:O	2.12	0.49
1:A:410[B]:ARG:NH2	1:A:448:GLU:OE2	2.37	0.49
1:A:61:CYS:O	1:A:292:SER:HA	2.13	0.49
1:B:87[B]:THR:HG23	1:D:21:PRO:CD	2.42	0.49
1:A:322:TYR:CD2	1:C:296:PRO:HA	2.48	0.49
1:C:48:GLU:OE1	1:C:48:GLU:CA	2.60	0.49
1:C:405:ARG:HD2	3:C:2332:HOH:O	2.13	0.49
1:D:36[B]:MET:HE1	1:D:44:LEU:HB3	1.95	0.49
1:C:170:HIS:HA	1:C:175:LEU:HB2	1.95	0.49
1:D:397:PHE:CE1	1:D:420:ASP:HB2	2.48	0.49
1:B:304[A]:LYS:NZ	3:B:2413:HOH:O	2.42	0.48
1:D:121:SER:HB3	1:D:157:THR:HG23	1.95	0.48
1:D:42:VAL:HG11	1:D:430:MET:HG3	1.94	0.48
1:D:356[B]:MET:HE1	1:D:360:TRP:CE3	2.49	0.48
1:C:246:GLU:O	1:C:250[A]:ARG:HG2	2.13	0.47
1:A:416[A]:ARG:HB3	1:A:423:VAL:CG2	2.44	0.47
1:B:296:PRO:HA	1:D:322:TYR:CD2	2.50	0.47
1:D:416:ARG:HG3	1:D:417:ALA:N	2.30	0.47
1:C:98[B]:GLU:OE1	3:C:2131:HOH:O	2.20	0.47
1:D:93:HIS:CE1	1:D:326:PRO:HG3	2.49	0.47
1:B:403[A]:LEU:HD12	3:B:2523:HOH:O	2.14	0.47
1:D:32:GLY:HA2	3:D:2003:HOH:O	2.15	0.47
1:C:352[B]:ILE:HD12	1:C:378:MET:SD	2.55	0.47
1:D:355:TYR:CE1	1:D:359:ARG:HG3	2.50	0.46
1:B:250[B]:ARG:HD3	3:B:2372:HOH:O	2.14	0.46
1:B:322:TYR:CD2	1:D:296:PRO:HA	2.49	0.46
1:C:186:PRO:HD2	1:C:229:GLN:OE1	2.15	0.46
1:D:134:TYR:O	1:D:138:GLN:HG2	2.15	0.46
1:D:416:ARG:HD2	3:D:2225:HOH:O	2.16	0.46
1:D:276:HIS:CE1	1:D:376:VAL:HG21	2.50	0.46
1:D:453:LEU:HD23	1:D:458:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HG2	1:A:366:ARG:HH11	1.81	0.46
1:B:61:CYS:O	1:B:292:SER:HA	2.16	0.46
1:B:352[B]:ILE:HD11	1:B:435:VAL:HG21	1.98	0.46
1:A:82:LEU:HB2	1:C:38:ARG:HA	1.99	0.46
1:D:63:ASN:OD1	1:D:267:ARG:NH2	2.49	0.45
1:B:36[B]:MET:HE3	1:B:44:LEU:HD22	1.93	0.45
1:D:338:ALA:O	1:D:342:GLU:HB2	2.16	0.45
1:C:453:LEU:HB3	1:C:459:ALA:HB2	1.97	0.45
1:A:234:VAL:HG12	1:A:234:VAL:O	2.16	0.45
1:C:188[B]:TRP:CD1	1:C:197:PRO:HA	2.51	0.45
1:C:389:ALA:N	3:C:2327:HOH:O	2.25	0.45
1:C:453:LEU:O	1:C:454:LYS:C	2.55	0.45
1:D:347:ARG:HG3	1:D:351:ASP:HB3	1.98	0.45
1:D:356[B]:MET:HE1	1:D:360:TRP:HE3	1.80	0.45
1:D:454:LYS:C	1:D:456[B]:ARG:H	2.21	0.45
1:A:121:SER:HB3	1:A:157:THR:HG23	1.99	0.44
1:A:416[A]:ARG:CD	3:A:2673:HOH:O	2.50	0.44
1:D:134:TYR:OH	1:D:305:ARG:NE	2.48	0.44
1:C:121:SER:HB3	1:C:157:THR:HG23	1.98	0.44
1:D:394:PHE:CG	1:D:400:ILE:HG13	2.52	0.44
1:C:407:ILE:HG12	1:C:410:ARG:HH12	1.83	0.44
1:C:359:ARG:NH1	1:C:362[B]:GLU:OE2	2.51	0.44
1:B:187:TRP:CH2	1:B:393:LEU:HD11	2.52	0.44
1:D:454:LYS:C	1:D:456[A]:ARG:H	2.21	0.44
1:D:45:TRP:CZ2	1:D:51:LYS:HG3	2.53	0.44
1:D:184:GLU:HB3	1:D:207:TRP:CE3	2.52	0.44
1:C:127:MET:O	1:C:131:VAL:HG23	2.17	0.43
1:B:37:THR:OG1	1:B:38[B]:ARG:CD	2.66	0.43
1:D:388[B]:LYS:HE3	3:D:2215:HOH:O	2.17	0.43
1:C:368:GLU:HB2	3:C:2321:HOH:O	2.18	0.43
1:C:352[B]:ILE:HD11	1:C:435:VAL:CG2	2.48	0.43
1:B:60:TRP:CD2	1:B:262:ILE:HD13	2.54	0.43
1:C:450:GLU:HA	1:C:453:LEU:CD1	2.49	0.42
1:D:456[A]:ARG:HE	1:D:458:LEU:CD1	2.32	0.42
1:C:363:THR:HG23	3:C:2318:HOH:O	2.19	0.42
1:C:244:GLU:OE2	1:C:247[A]:ARG:NH2	2.38	0.42
1:C:416[B]:ARG:HG3	1:C:417:ALA:N	2.32	0.42
1:D:142:GLU:H	1:D:142:GLU:CD	2.22	0.42
1:A:358:LYS:O	1:A:362[A]:GLU:HG3	2.20	0.42
1:D:129:ARG:HD3	1:D:318:HIS:ND1	2.33	0.42
1:A:114[B]:VAL:HG23	1:A:116:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:PHE:CZ	1:B:335:ASN:HA	2.54	0.42
1:D:208[A]:LEU:HD21	1:D:212:ILE:CD1	2.34	0.42
1:A:250[A]:ARG:NH2	3:A:2500:HOH:O	2.53	0.42
1:B:114[B]:VAL:HG12	1:B:301:PHE:CD2	2.55	0.42
1:A:44:LEU:HD11	1:C:85:TYR:CE1	2.55	0.41
1:A:296:PRO:HA	1:C:322:TYR:CD2	2.55	0.41
1:C:387:ASN:ND2	1:C:390:LYS:HE2	2.35	0.41
1:D:369:HIS:CD2	1:D:453:LEU:HD13	2.55	0.41
1:A:38[A]:ARG:HA	1:C:82:LEU:HB2	2.02	0.41
1:C:449:PHE:O	1:C:453:LEU:HD12	2.20	0.41
1:D:266:GLY:HA2	1:D:345:VAL:HG13	2.03	0.41
1:B:219[B]:LYS:HB3	1:B:219[B]:LYS:HE3	1.92	0.41
3:B:2157:HOH:O	1:D:13:LEU:HB3	2.21	0.41
1:A:251[B]:LYS:HE2	3:A:2459:HOH:O	2.21	0.41
1:C:407:ILE:HG22	1:C:408:PHE:N	2.36	0.40
1:C:71:PHE:CZ	1:C:335:ASN:HA	2.56	0.40
1:A:231:ALA:HA	1:A:416[B]:ARG:NH2	2.37	0.40
1:C:394:PHE:CG	1:C:400:ILE:HG13	2.57	0.40
1:C:430:MET:HG3	1:C:434:GLU:HB3	2.02	0.40
1:D:158:ILE:HG23	1:D:175:LEU:CD2	2.50	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	489/459 (106%)	472 (96%)	15 (3%)	2 (0%)	34	15
1	B	486/459 (106%)	470 (97%)	15 (3%)	1 (0%)	47	25
1	C	476/459 (104%)	448 (94%)	23 (5%)	5 (1%)	14	3
1	D	472/459 (103%)	445 (94%)	24 (5%)	3 (1%)	25	8
All	All	1923/1836 (105%)	1835 (95%)	77 (4%)	11 (1%)	25	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ALA
1	C	397	PHE
1	C	453	LEU
1	C	454	LYS
1	A	287	ALA
1	C	288	LYS
1	D	287	ALA
1	D	288	LYS
1	A	288	LYS
1	C	287	ALA
1	D	397	PHE

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	400/368 (109%)	398 (100%)	2 (0%)	88	80
1	B	397/368 (108%)	386 (97%)	11 (3%)	43	17
1	C	387/368 (105%)	381 (98%)	6 (2%)	62	39
1	D	384/368 (104%)	376 (98%)	8 (2%)	53	27
All	All	1568/1472 (106%)	1541 (98%)	27 (2%)	71	36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376[A]	VAL
1	A	376[B]	VAL
1	B	30	GLN
1	B	250[A]	ARG
1	B	250[B]	ARG
1	B	315[A]	ASP
1	B	315[B]	ASP
1	B	403[A]	LEU
1	B	403[B]	LEU

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Mol	Chain	Res	Type
1	B	405	ARG
1	B	416[A]	ARG
1	B	416[B]	ARG
1	B	444	ARG
1	C	405	ARG
1	C	410	ARG
1	C	415[A]	MET
1	C	415[B]	MET
1	C	453	LEU
1	C	456	ARG
1	D	47[A]	SER
1	D	47[B]	SER
1	D	167	LYS
1	D	315[A]	ASP
1	D	315[B]	ASP
1	D	340	ARG
1	D	456[A]	ARG
1	D	456[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	151	ASN
1	B	30	GLN
1	B	50	ASN
1	B	151	ASN
1	B	369	HIS
1	B	387	ASN
1	C	9	GLN
1	D	369	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	PLP	A	1288	1	15,15,16	2.93	3 (20%)	20,22,23	1.89	6 (30%)
2	PLP	C	1288	1	15,15,16	3.23	3 (20%)	20,22,23	2.38	4 (20%)
2	PLP	B	1288	1	15,15,16	2.97	3 (20%)	20,22,23	2.45	5 (25%)
2	PLP	D	1288	1	15,15,16	3.09	3 (20%)	20,22,23	1.84	5 (25%)

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	PLP	A	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1288	1	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1288	PLP	C5-C4	8.61	1.50	1.40
2	B	1288	PLP	C5-C4	8.32	1.49	1.40
2	D	1288	PLP	C5-C4	8.22	1.49	1.40
2	A	1288	PLP	C5-C4	8.10	1.49	1.40
2	C	1288	PLP	C3-C2	7.63	1.48	1.40
2	D	1288	PLP	C3-C2	7.31	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1288	PLP	C3-C2	6.60	1.47	1.40
2	A	1288	PLP	C3-C2	5.86	1.46	1.40
2	A	1288	PLP	C3-C4	4.14	1.48	1.40
2	C	1288	PLP	C3-C4	4.14	1.48	1.40
2	D	1288	PLP	C3-C4	3.56	1.47	1.40
2	B	1288	PLP	C3-C4	3.15	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1288	PLP	C4A-C4-C5	7.85	129.02	120.94
2	C	1288	PLP	C4A-C4-C5	7.65	128.82	120.94
2	D	1288	PLP	C4A-C4-C5	5.02	126.11	120.94
2	B	1288	PLP	C3-C4-C5	-4.65	113.72	118.74
2	C	1288	PLP	C3-C4-C5	-4.63	113.74	118.74
2	A	1288	PLP	C4A-C4-C5	4.59	125.66	120.94
2	B	1288	PLP	C6-C5-C4	3.38	120.82	118.16
2	A	1288	PLP	C3-C2-N1	-3.25	116.57	120.77
2	A	1288	PLP	C3-C4-C5	-3.23	115.25	118.74
2	D	1288	PLP	C3-C4-C5	-3.10	115.39	118.74
2	A	1288	PLP	C6-N1-C2	2.96	124.64	119.17
2	B	1288	PLP	C2A-C2-C3	-2.69	117.57	120.89
2	C	1288	PLP	C6-C5-C4	2.43	120.07	118.16
2	D	1288	PLP	C2A-C2-C3	-2.42	117.90	120.89
2	C	1288	PLP	O4P-C5A-C5	2.34	113.81	109.35
2	D	1288	PLP	C6-C5-C4	2.34	120.00	118.16
2	D	1288	PLP	C2A-C2-N1	2.28	122.13	117.67
2	A	1288	PLP	C5A-C5-C6	-2.18	115.78	119.37
2	A	1288	PLP	C2A-C2-N1	2.06	121.69	117.67
2	B	1288	PLP	C4A-C4-C3	-2.02	117.07	120.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	455/459 (99%)	0.02	4 (0%)	84	85	8, 15, 27, 42	0
1	B	455/459 (99%)	0.43	42 (9%)	9	8	10, 21, 45, 73	0
1	C	455/459 (99%)	0.78	47 (10%)	6	6	10, 27, 61, 109	0
1	D	454/459 (98%)	1.09	76 (16%)	1	1	19, 34, 63, 93	0
All	All	1819/1836 (99%)	0.58	169 (9%)	8	8	8, 24, 54, 109	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	ALA	9.9
1	C	455	ALA	8.4
1	C	458	LEU	8.1
1	D	457	GLY	7.6
1	D	455	ALA	7.4
1	D	456[A]	ARG	7.1
1	D	10	TRP	6.9
1	D	409	PHE	6.6
1	C	452	THR	6.0
1	C	456	ARG	5.9
1	B	459	ALA	5.7
1	D	449	PHE	5.4
1	C	395	PRO	5.3
1	D	6	THR	5.2
1	D	31	ALA	5.1
1	D	458	LEU	4.9
1	B	10	TRP	4.8
1	C	390	LYS	4.8
1	D	35	VAL	4.7
1	B	5	ARG	4.6
1	C	188[A]	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	394	PHE	4.6
1	D	403	LEU	4.6
1	C	194	ASP	4.5
1	B	455	ALA	4.5
1	D	188	TRP	4.5
1	B	7	THR	4.2
1	D	7	THR	4.2
1	B	27	SER	4.2
1	C	457	GLY	4.2
1	C	396	ASP	4.1
1	B	15	ALA	4.1
1	B	312	ALA	4.0
1	C	6	THR	3.9
1	B	28	LEU	3.9
1	B	30	GLN	3.9
1	D	9	GLN	3.9
1	B	26	ALA	3.9
1	B	31	ALA	3.8
1	D	30	GLN	3.8
1	C	389	ALA	3.8
1	D	395	PRO	3.8
1	D	16	ALA	3.6
1	B	8[A]	SER	3.6
1	C	453	LEU	3.6
1	B	50	ASN	3.6
1	B	457	GLY	3.5
1	D	451[A]	GLN	3.5
1	D	128	ILE	3.5
1	B	89	PHE	3.5
1	D	452	THR	3.5
1	B	49	GLY	3.5
1	D	271	TRP	3.4
1	B	458	LEU	3.4
1	B	35	VAL	3.4
1	B	6	THR	3.4
1	B	33	ALA	3.3
1	D	453	LEU	3.3
1	D	390	LYS	3.3
1	D	50	ASN	3.2
1	B	13	LEU	3.2
1	C	196	THR	3.2
1	C	441	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	13	LEU	3.2
1	C	33	ALA	3.2
1	B	395	PRO	3.2
1	C	367	PHE	3.1
1	D	168	TYR	3.1
1	B	12	GLU	3.1
1	B	48	GLU	3.1
1	D	28	LEU	3.1
1	C	440	ALA	3.1
1	B	32	GLY	3.0
1	B	9[A]	GLN	3.0
1	C	224	VAL	3.0
1	D	12	GLU	3.0
1	D	343	GLY	2.9
1	C	449	PHE	2.9
1	D	344	ILE	2.9
1	D	36[A]	MET	2.9
1	D	454	LYS	2.9
1	D	104	ALA	2.9
1	C	200	PHE	2.8
1	D	367	PHE	2.8
1	B	128	ILE	2.8
1	D	5	ARG	2.8
1	B	91[A]	THR	2.8
1	D	396	ASP	2.8
1	D	27	SER	2.8
1	C	368	GLU	2.8
1	C	399	GLU	2.8
1	D	48	GLU	2.8
1	C	454	LYS	2.8
1	D	103	LEU	2.8
1	B	36[A]	MET	2.8
1	C	195	MET	2.8
1	C	369	HIS	2.8
1	D	23[A]	THR	2.7
1	C	45	TRP	2.7
1	D	400	ILE	2.7
1	D	414	ILE	2.7
1	C	10	TRP	2.7
1	C	373	VAL	2.7
1	D	399	GLU	2.6
1	D	355	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	89	PHE	2.6
1	D	445	CYS	2.6
1	D	444	ARG	2.6
1	C	360	TRP	2.6
1	D	360	TRP	2.6
1	B	456	ARG	2.6
1	D	26	ALA	2.5
1	D	171	GLU	2.5
1	B	315[A]	ASP	2.5
1	B	25	THR	2.5
1	B	22	PHE	2.5
1	D	71	PHE	2.5
1	C	386	LYS	2.5
1	C	400	ILE	2.5
1	D	46	ASP	2.5
1	C	350[A]	ASP	2.5
1	A	146	LEU	2.4
1	D	49	GLY	2.4
1	D	402	THR	2.4
1	D	200	PHE	2.4
1	D	224	VAL	2.4
1	D	8	SER	2.4
1	A	6	THR	2.4
1	B	454	LYS	2.4
1	C	446	LEU	2.4
1	D	33	ALA	2.3
1	D	345	VAL	2.3
1	D	422	ILE	2.3
1	D	363	THR	2.3
1	D	235	ILE	2.3
1	B	171	GLU	2.3
1	B	38[A]	ARG	2.3
1	D	24	ASP	2.3
1	C	410	ARG	2.3
1	C	128	ILE	2.3
1	D	446	LEU	2.2
1	B	452	THR	2.2
1	C	409	PHE	2.2
1	D	394	PHE	2.2
1	C	391	ARG	2.2
1	B	87[A]	THR	2.2
1	D	393	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	24	ASP	2.2
1	D	382	PHE	2.1
1	C	146	LEU	2.1
1	D	316	PHE	2.1
1	D	38[A]	ARG	2.1
1	A	163	LEU	2.1
1	C	193	LYS	2.1
1	D	322	TYR	2.1
1	D	314	GLY	2.1
1	B	45	TRP	2.1
1	C	445	CYS	2.1
1	D	358	LYS	2.1
1	A	224	VAL	2.1
1	C	254	VAL	2.1
1	C	354	PRO	2.1
1	C	387	ASN	2.1
1	B	88	PHE	2.1
1	D	47[A]	SER	2.0
1	D	410	ARG	2.0
1	D	397	PHE	2.0
1	C	398	GLY	2.0
1	D	193	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
2	PLP	D	1288	15/16	0.95	0.11	21,25,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	C	1288	15/16	0.96	0.07	17,18,27,34	0
2	PLP	A	1288	15/16	0.97	0.08	9,10,13,23	0
2	PLP	B	1288	15/16	0.97	0.07	14,20,24,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.