



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:37 PM UTC

PDB ID : 6DND / pdb\_00006dnd  
Title : Crystal structure of wild-type (WT) human Glutamate oxaloacetate transaminase 1 (GOT1)  
Authors : Assar, Z.; Holt, M.C.; Stein, A.J.; Lairson, L.; Lyssiotis, C.A.  
Deposited on : 2018-06-06  
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](mailto: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>.

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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

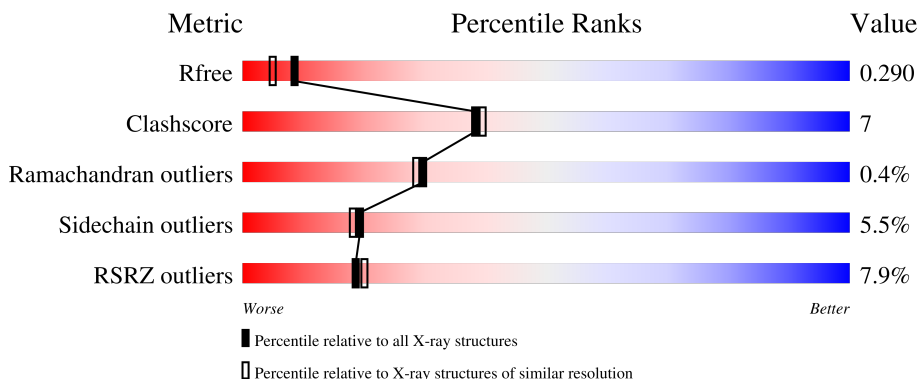
# 1 Overall quality at a glance

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  $\geq 3$ , 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	411	
1	B	411	

## 2 Entry composition [i](#)

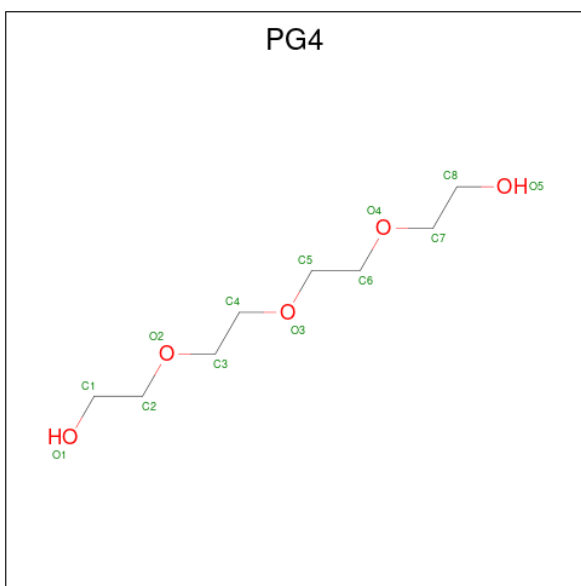
There are 4 unique types of molecules in this entry. The entry contains 6628 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	Total 3237	C 2070	N 562	O 596	S 9	0	4	0
1	B	410	Total 3244	C 2070	N 564	O 601	S 9	0	1	0

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 7	C 4	O 3	0	0
2	B	1	Total 7	C 4	O 3	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	8	1	6	1	0	0
3	B	1	16	8	1	6	1	0	0

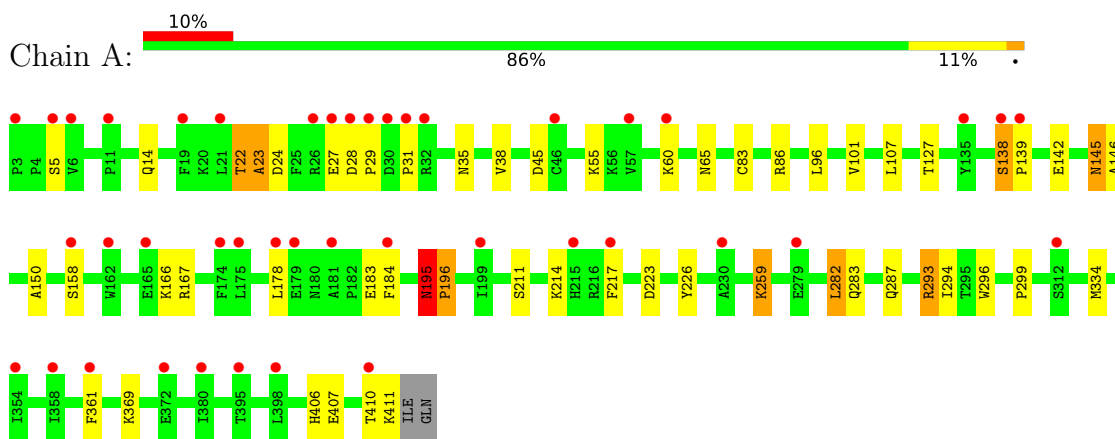
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	35	35	35	0	0
4	B	66	66	66	0	0

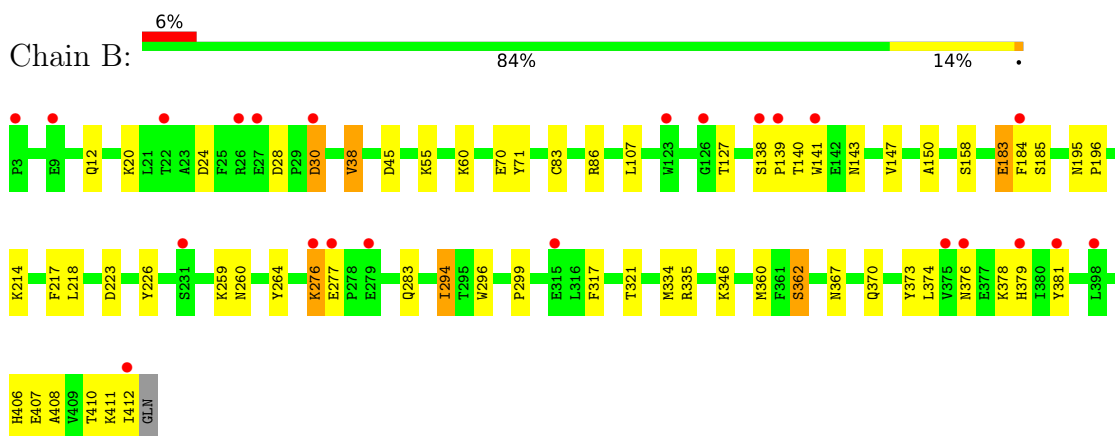
### 3 Residue-property plots [i](#)

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: Aspartate aminotransferase, cytoplasmic



- Molecule 1: Aspartate aminotransferase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.04Å 96.86Å 97.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.85 – 2.10 68.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.85-2.10) 99.9 (68.85-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.208 , 0.269 0.231 , 0.290	Depositor DCC
$R_{free}$ test set	2570 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PG4, 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	0.92	1/3332 (0.0%)	0.95	4/4533 (0.1%)
1	B	0.99	2/3328 (0.1%)	0.98	3/4525 (0.1%)
All	All	0.96	3/6660 (0.0%)	0.96	7/9058 (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	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	PRO	CA-C	5.19	1.56	1.52
1	B	299	PRO	CA-C	5.16	1.56	1.52
1	B	260	ASN	C-O	-5.14	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	6.70	119.60	111.82
1	A	195	ASN	C-N-CD	-6.66	105.96	120.60
1	B	376	ASN	N-CA-C	6.44	118.30	111.28
1	A	45	ASP	N-CA-C	6.12	120.36	113.02
1	A	23	ALA	N-CA-C	-5.73	104.96	111.14
1	B	45	ASP	N-CA-C	5.37	118.95	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	31	PRO	N-CA-C	5.05	120.17	113.86

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ASN	Peptide
1	B	195	ASN	Peptide

## 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	3237	0	3147	45	0
1	B	3244	0	3179	49	0
2	A	7	0	8	0	0
2	B	7	0	9	0	0
3	A	16	0	7	3	0
3	B	16	0	7	4	0
4	A	35	0	0	2	0
4	B	66	0	0	2	0
All	All	6628	0	6357	89	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 7.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:B:30:ASP:CG	1:B:379:HIS:CD2	1.97	1.41
1:A:293:ARG:HD3	4:A:631:HOH:O	1.24	1.29
1:B:30:ASP:OD2	1:B:379:HIS:CD2	1.94	1.19
1:A:22:THR:HG22	1:A:35:ASN:HD21	1.04	1.15
1:B:259:LYS:HE2	3:B:502:PLP:O4A	1.46	1.13
1:B:138:SER:HB3	1:B:139:PRO:HD3	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:CG	1:B:379:HIS:HD2	1.43	1.05
1:B:138:SER:HB3	1:B:139:PRO:CD	1.87	1.05
1:A:138:SER:HB3	1:A:139:PRO:HD3	1.39	1.04
1:A:138:SER:HB3	1:A:139:PRO:CD	1.88	1.03
1:B:30:ASP:OD2	1:B:379:HIS:CG	2.17	0.97
1:B:28:ASP:OD2	1:B:381:TYR:OH	1.81	0.95
1:A:22:THR:HG22	1:A:35:ASN:ND2	1.85	0.91
1:A:293:ARG:HH21	1:A:293:ARG:HG3	1.34	0.90
1:B:259:LYS:CE	3:B:502:PLP:O4A	2.27	0.82
1:B:30:ASP:OD2	1:B:379:HIS:CB	2.28	0.81
1:B:30:ASP:CB	1:B:379:HIS:CD2	2.65	0.80
1:B:138:SER:CB	1:B:139:PRO:HD3	2.11	0.79
1:B:408:ALA:O	1:B:411:LYS:O	2.04	0.76
1:A:22:THR:CG2	1:A:35:ASN:HD21	1.94	0.74
1:B:30:ASP:OD1	1:B:379:HIS:HD2	1.70	0.74
1:A:28:ASP:OD2	1:A:29:PRO:HD2	1.90	0.72
1:B:30:ASP:OD2	1:B:379:HIS:HB2	1.89	0.72
1:A:406:HIS:O	1:A:410:THR:HG23	1.90	0.70
1:A:195:ASN:HD22	1:A:196:PRO:CA	2.04	0.70
1:B:184:PHE:HA	1:B:217:PHE:O	1.94	0.65
1:B:259:LYS:HD2	1:B:264:TYR:HE1	1.61	0.64
1:A:138:SER:CB	1:A:139:PRO:HD3	2.22	0.64
1:A:195:ASN:HD22	1:A:196:PRO:HA	1.64	0.62
1:B:259:LYS:HD2	1:B:264:TYR:CE1	2.36	0.61
1:B:183:GLU:HG2	1:B:217:PHE:HD2	1.65	0.60
1:A:293:ARG:HG3	1:A:293:ARG:NH2	2.08	0.60
1:A:195:ASN:HD22	1:A:195:ASN:C	2.11	0.59
1:A:166:LYS:O	1:A:166:LYS:HG2	2.03	0.58
1:A:145[A]:ASN:C	1:A:145[A]:ASN:ND2	2.63	0.56
1:A:294:ILE:HD13	1:B:150:ALA:CB	2.38	0.54
1:B:407:GLU:O	1:B:411:LYS:HG3	2.08	0.54
1:B:373:TYR:HB2	1:B:412:ILE:CD1	2.38	0.54
1:B:30:ASP:OD1	1:B:379:HIS:CD2	2.52	0.52
1:A:145[A]:ASN:C	1:A:145[A]:ASN:HD22	2.17	0.52
1:A:259:LYS:HZ3	3:A:502:PLP:C4A	2.23	0.52
1:A:407:GLU:O	1:A:411:LYS:HG3	2.10	0.52
1:B:317:PHE:O	1:B:321:THR:HG23	2.10	0.51
1:A:259:LYS:NZ	3:A:502:PLP:C4A	2.74	0.51
1:A:294:ILE:HD13	1:B:150:ALA:HB1	1.93	0.51
1:A:226:TYR:CZ	1:A:361[B]:PHE:HE2	2.29	0.50
1:B:406:HIS:O	1:B:410:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:HB2	1:B:294:ILE:HD12	1.94	0.50
1:A:138:SER:CB	1:A:139:PRO:CD	2.65	0.50
1:A:334:MET:HA	1:A:334:MET:HE2	1.94	0.49
1:B:38:VAL:HG13	4:B:662:HOH:O	2.13	0.49
1:A:107:LEU:HD11	1:B:107:LEU:HD11	1.95	0.48
1:B:378:LYS:HE2	1:B:407:GLU:OE1	2.13	0.48
1:B:60:LYS:HD2	4:B:633:HOH:O	2.14	0.48
1:B:30:ASP:OD2	1:B:379:HIS:HD2	1.56	0.47
1:A:145[A]:ASN:HD22	1:A:146:ALA:N	2.13	0.47
1:B:83:CYS:SG	1:B:86:ARG:NH2	2.85	0.47
1:B:335:ARG:HH12	1:B:362:SER:HB2	1.80	0.47
1:B:30:ASP:HB2	1:B:379:HIS:CD2	2.50	0.47
1:A:138:SER:HB3	1:A:139:PRO:HD2	1.85	0.46
1:A:195:ASN:C	1:A:195:ASN:ND2	2.72	0.46
1:B:185:SER:HB2	1:B:218:LEU:HD22	1.97	0.46
1:B:373:TYR:HB2	1:B:412:ILE:HD12	1.97	0.46
1:A:293:ARG:CD	4:A:631:HOH:O	2.08	0.45
1:A:83:CYS:SG	1:A:86:ARG:NH1	2.88	0.45
1:B:226:TYR:OH	3:B:502:PLP:O3	2.27	0.45
1:A:28:ASP:HA	1:A:29:PRO:HD3	1.75	0.44
1:B:276:LYS:HB3	1:B:276:LYS:HE3	1.36	0.44
1:B:138:SER:CB	1:B:139:PRO:CD	2.62	0.44
1:A:107:LEU:HD23	1:A:296:TRP:CE2	2.53	0.43
1:A:184:PHE:HA	1:A:217:PHE:O	2.18	0.43
1:B:140:THR:HG23	1:B:141:TRP:O	2.18	0.43
1:B:223:ASP:OD2	3:B:502:PLP:N1	2.51	0.43
1:A:223:ASP:OD2	3:A:502:PLP:N1	2.52	0.43
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.76	0.43
1:A:96:LEU:HD23	1:A:101:VAL:HG21	2.01	0.42
1:B:107:LEU:HD23	1:B:296:TRP:CE2	2.53	0.42
1:B:334:MET:HE2	1:B:334:MET:HA	2.01	0.42
1:A:226:TYR:CZ	1:A:361[B]:PHE:CE2	3.08	0.41
1:A:293:ARG:NH2	1:A:293:ARG:CG	2.73	0.41
1:B:143:ASN:O	1:B:147:VAL:HG23	2.21	0.41
1:A:226:TYR:OH	1:A:361[B]:PHE:HE2	2.04	0.41
1:A:5:SER:HB2	1:B:276:LYS:HB2	2.03	0.40
1:A:23:ALA:O	1:A:24:ASP:C	2.63	0.40
1:A:195:ASN:HD22	1:A:196:PRO:N	2.19	0.40
1:B:367:ASN:H	1:B:370:GLN:NE2	2.18	0.40
1:B:20:LYS:HE3	1:B:24:ASP:OD1	2.20	0.40
1:A:217:PHE:CD1	1:A:217:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:O	1:B:71:TYR:C	2.65	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	411/411 (100%)	393 (96%)	16 (4%)	2 (0%)	24	22
1	B	409/411 (100%)	395 (97%)	13 (3%)	1 (0%)	43	44
All	All	820/822 (100%)	788 (96%)	29 (4%)	3 (0%)	30	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	PRO
1	B	196	PRO
1	A	138	SER

### 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	343/350 (98%)	318 (93%)	25 (7%)	13	10
1	B	348/350 (99%)	333 (96%)	15 (4%)	26	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	691/700 (99%)	651 (94%)	40 (6%)	19	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	THR
1	A	27	GLU
1	A	38	VAL
1	A	55	LYS
1	A	60	LYS
1	A	65	ASN
1	A	127	THR
1	A	142	GLU
1	A	145[A]	ASN
1	A	145[B]	ASN
1	A	158	SER
1	A	167	ARG
1	A	178	LEU
1	A	183	GLU
1	A	195	ASN
1	A	211	SER
1	A	214	LYS
1	A	259	LYS
1	A	282	LEU
1	A	283	GLN
1	A	287[A]	GLN
1	A	287[B]	GLN
1	A	293	ARG
1	A	369	LYS
1	B	12	GLN
1	B	30	ASP
1	B	38	VAL
1	B	55	LYS
1	B	127	THR
1	B	158	SER
1	B	183	GLU
1	B	214	LYS
1	B	276	LYS
1	B	277	GLU
1	B	283	GLN
1	B	294	ILE

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Mol	Chain	Res	Type
1	B	346	LYS
1	B	362	SER
1	B	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	14	GLN
1	A	128	ASN
1	A	195	ASN
1	A	227	GLN
1	B	12	GLN
1	B	190	HIS
1	B	215	HIS
1	B	283	GLN
1	B	352	ASN
1	B	370	GLN
1	B	376	ASN
1	B	379	HIS
1	B	406	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](#)

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$
3	PLP	A	502	-	16,16,16	2.74	3 (18%)	20,23,23	2.17	7 (35%)
2	PG4	B	501	-	6,6,12	0.67	0	5,5,11	0.87	0
2	PG4	A	501	-	6,6,12	0.61	0	5,5,11	0.67	0
3	PLP	B	502	-	16,16,16	2.73	6 (37%)	20,23,23	2.01	6 (30%)

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	PLP	A	502	-	-	3/8/8/8	0/1/1/1
2	PG4	B	501	-	-	3/4/4/10	-
2	PG4	A	501	-	-	2/4/4/10	-
3	PLP	B	502	-	-	4/8/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PLP	C3-C2	6.90	1.48	1.41
3	A	502	PLP	C4-C5	6.83	1.51	1.42
3	A	502	PLP	C3-C2	5.87	1.47	1.41
3	A	502	PLP	C4-C3	5.25	1.49	1.41
3	B	502	PLP	C4-C5	5.03	1.49	1.42
3	B	502	PLP	C4-C3	4.48	1.48	1.41
3	B	502	PLP	P-O3P	-2.80	1.44	1.54
3	B	502	PLP	P-O2P	-2.65	1.44	1.54
3	B	502	PLP	P-O1P	-2.27	1.43	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PLP	O4P-C5A-C5	5.40	119.48	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLP	C4-C3-C2	-4.95	117.36	120.14
3	A	502	PLP	O4P-C5A-C5	4.70	118.16	109.36
3	A	502	PLP	C6-N1-C2	3.55	125.63	119.20
3	B	502	PLP	C4-C3-C2	-3.25	118.31	120.14
3	B	502	PLP	C3-C4-C5	-3.01	115.86	118.28
3	B	502	PLP	O3P-P-O2P	2.67	117.80	107.80
3	A	502	PLP	C2A-C2-N1	2.40	122.17	117.64
3	B	502	PLP	O3P-P-O4P	-2.39	100.44	106.67
3	A	502	PLP	C5A-C5-C6	-2.31	115.60	119.36
3	B	502	PLP	C3-C4-C4A	2.29	122.99	119.84
3	A	502	PLP	C2A-C2-C3	-2.23	118.19	120.80
3	A	502	PLP	O2P-P-O1P	2.12	119.10	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PLP	C4-C5-C5A-O4P
3	A	502	PLP	C6-C5-C5A-O4P
3	B	502	PLP	C4-C5-C5A-O4P
3	B	502	PLP	C6-C5-C5A-O4P
3	B	502	PLP	C3-C4-C4A-O4A
2	B	501	PG4	O1-C1-C2-O2
2	A	501	PG4	O3-C5-C6-O4
2	B	501	PG4	C4-C3-O2-C2
2	B	501	PG4	C1-C2-O2-C3
3	B	502	PLP	C5-C4-C4A-O4A
3	A	502	PLP	C5A-O4P-P-O2P
2	A	501	PG4	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PLP	3	0
3	B	502	PLP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	409/411 (99%)	0.89	42 (10%) 12 12	30, 60, 82, 99	4 (0%)
1	B	410/411 (99%)	0.60	23 (5%) 30 32	27, 52, 74, 91	1 (0%)
All	All	819/822 (99%)	0.74	65 (7%) 18 20	27, 56, 81, 99	5 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ASP	4.8
1	B	138	SER	4.7
1	B	30	ASP	4.4
1	B	412	ILE	4.2
1	A	3	PRO	4.1
1	B	27	GLU	4.0
1	B	379	HIS	4.0
1	A	179	GLU	3.9
1	B	126	GLY	3.8
1	B	277	GLU	3.8
1	A	138	SER	3.7
1	A	181	ALA	3.7
1	B	315	GLU	3.6
1	A	28	ASP	3.5
1	A	27	GLU	3.5
1	A	26	ARG	3.5
1	A	139	PRO	3.4
1	A	184	PHE	3.3
1	A	217	PHE	3.3
1	A	174	PHE	3.2
1	B	3	PRO	3.2
1	B	184	PHE	3.2
1	B	9	GLU	3.1
1	B	26	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	3.0
1	A	135	TYR	3.0
1	B	376	ASN	2.9
1	A	60	LYS	2.9
1	A	6	VAL	2.9
1	A	32	ARG	2.9
1	A	46	CYS	2.8
1	A	199	ILE	2.8
1	A	19	PHE	2.6
1	A	361[A]	PHE	2.6
1	A	178	LEU	2.6
1	A	11	PRO	2.6
1	B	123	TRP	2.6
1	A	158	SER	2.6
1	B	375	VAL	2.5
1	B	279	GLU	2.4
1	A	21	LEU	2.4
1	A	215	HIS	2.4
1	A	29	PRO	2.4
1	B	141	TRP	2.4
1	B	381	TYR	2.3
1	A	410	THR	2.3
1	B	22	THR	2.3
1	A	279	GLU	2.3
1	A	380	ILE	2.3
1	B	231	SER	2.3
1	A	358	ILE	2.3
1	A	372	GLU	2.2
1	A	175	LEU	2.2
1	A	230	ALA	2.2
1	B	276	LYS	2.2
1	A	31	PRO	2.1
1	A	5	SER	2.1
1	A	312	SER	2.1
1	A	162	TRP	2.1
1	A	354	ILE	2.1
1	A	57	VAL	2.1
1	A	398	LEU	2.1
1	B	139	PRO	2.1
1	B	398	LEU	2.0
1	A	395	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PG4	B	501	7/13	0.78	0.15	51,59,74,83	0
2	PG4	A	501	7/13	0.84	0.14	67,70,74,76	0
3	PLP	A	502	16/16	0.95	0.13	39,73,97,105	10
3	PLP	B	502	16/16	0.96	0.09	37,62,71,71	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.