



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1OHW  
Title : 4-AMINO BUTYRATE-AMINOTRANSFERASE INACTIVATED BY  
GAMMA-VINYL GABA  
Authors : Storici, P.; Schirmer, T.  
Deposited on : 2003-06-03  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

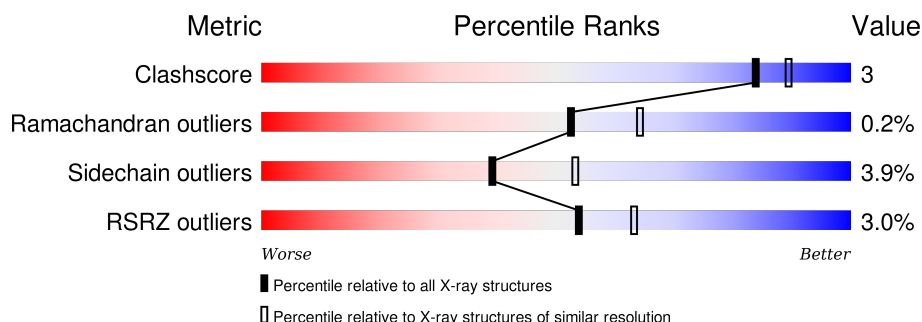
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	472	
1	B	472	
1	C	472	
1	D	472	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	VIG	A	700	-	-	-	X

## 2 Entry composition [i](#)

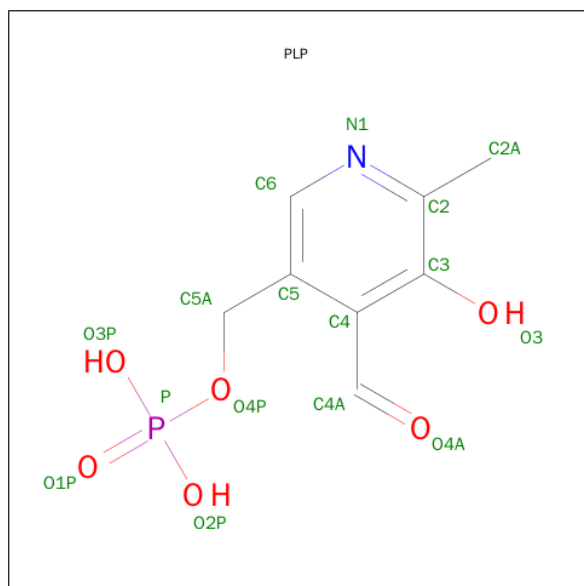
There are 5 unique types of molecules in this entry. The entry contains 15223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-AMINOBUTYRATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3600	2296	623	658	23			
1	B	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			
1	C	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			
1	D	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



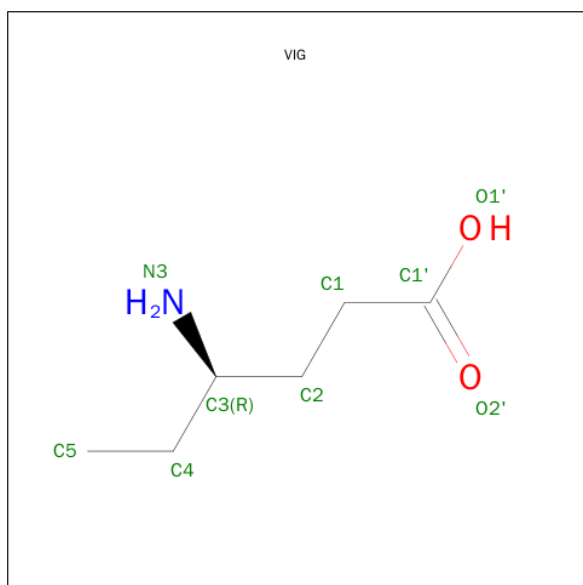
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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 4-AMINO HEXANOIC ACID (three-letter code: VIG) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		

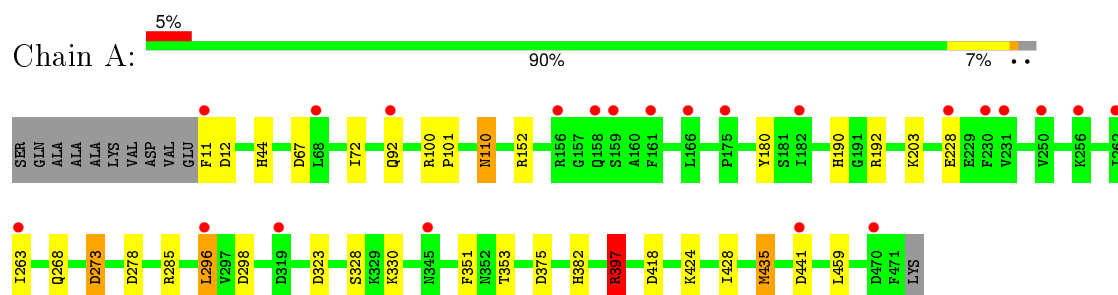
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	167	Total	O	0	0
			167	167		
5	C	177	Total	O	0	0
			177	177		
5	D	200	Total	O	0	0
			200	200		

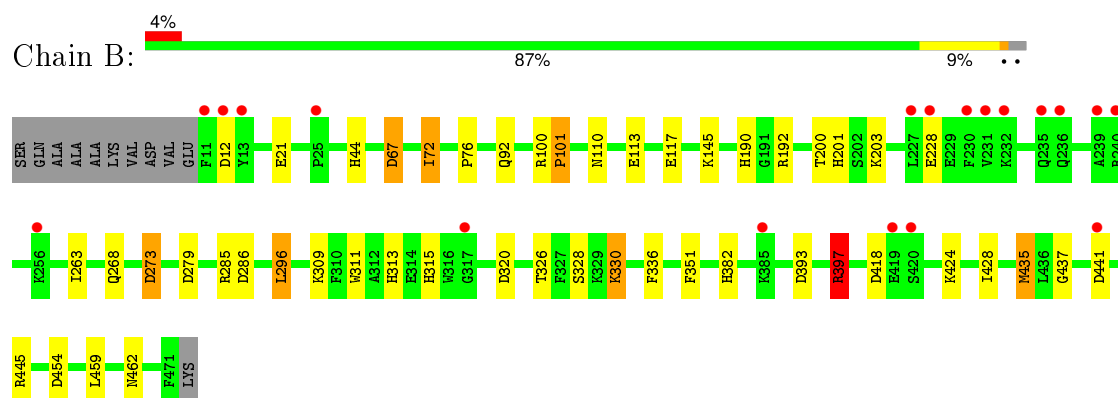
### 3 Residue-property plots

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

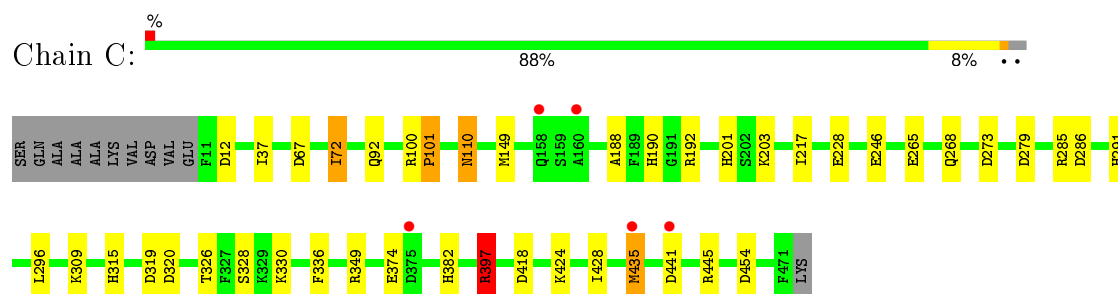
- Molecule 1: 4-AMINOBTYRATE AMINOTRANSFERASE



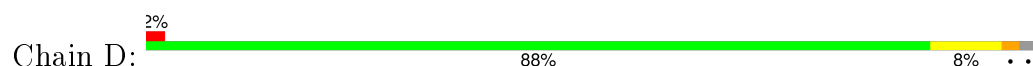
- Molecule 1: 4-AMINOBTYRATE AMINOTRANSFERASE

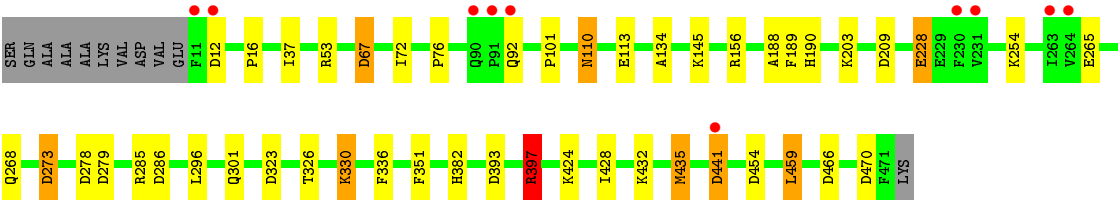


- Molecule 1: 4-AMINOBTYRATE AMINOTRANSFERASE



- Molecule 1: 4-AMINOBTYRATE AMINOTRANSFERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.66Å 226.71Å 71.37Å 90.00° 108.77° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (30.00-2.30) 95.9 (29.77-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.188 , 0.215 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.8	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 88722 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: VIG, FES, 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	0.45	0/3688	0.73	7/4988 (0.1%)
1	B	0.44	0/3689	0.71	10/4990 (0.2%)
1	C	0.47	0/3689	0.74	8/4990 (0.2%)
1	D	0.48	0/3689	0.75	13/4990 (0.3%)
All	All	0.46	0/14755	0.73	38/19958 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	ASP	CB-CG-OD2	7.30	124.88	118.30
1	C	319	ASP	CB-CG-OD2	7.08	124.67	118.30
1	C	320	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	12	ASP	CB-CG-OD2	6.53	124.17	118.30
1	C	12	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	397	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	12	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	397	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	278	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	323	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	397	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	466	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	397	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	286	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	418	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	286	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	320	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	375	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	67	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	441	ASP	CB-CG-OD2	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	418	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	418	ASP	CB-CG-OD2	5.38	123.15	118.30
1	C	279	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	298	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	278	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	279	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	286	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	445	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	D	454	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	323	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	445	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	393	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	12	ASP	CB-CG-OD2	5.07	122.87	118.30
1	B	67	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	273	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	393	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	279	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3600	0	3501	22	0
1	B	3601	0	3503	28	0
1	C	3601	0	3503	25	1
1	D	3601	0	3503	18	2
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	9	0	9	0	0
3	B	9	0	9	3	0
3	C	9	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	9	2	0
4	A	4	0	0	0	0
4	C	4	0	0	1	0
5	A	172	0	0	1	0
5	B	167	0	0	8	0
5	C	177	0	0	0	0
5	D	200	0	0	2	0
All	All	15223	0	14074	87	2

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 3.

All (87) 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:190:HIS:CE1	1:A:263:ILE:HG12	1.86	1.10
1:A:190:HIS:HE1	1:A:263:ILE:HG12	1.23	0.96
1:C:309:LYS:HG2	1:C:315:HIS:CE1	2.08	0.89
1:B:454:ASP:HB3	5:B:2154:HOH:O	1.75	0.87
1:B:382:HIS:CD2	5:B:2154:HOH:O	2.27	0.86
1:A:190:HIS:CE1	1:A:263:ILE:CG1	2.64	0.81
1:C:309:LYS:CG	1:C:315:HIS:CE1	2.68	0.77
1:D:228:GLU:HG3	5:D:2103:HOH:O	1.87	0.74
1:B:382:HIS:HD2	5:B:2154:HOH:O	1.65	0.68
1:B:382:HIS:CE1	5:B:2134:HOH:O	2.47	0.66
1:A:190:HIS:CE1	1:A:263:ILE:CD1	2.81	0.63
1:B:424:LYS:O	1:B:428:ILE:HG12	2.00	0.61
1:B:397:ARG:HG2	1:B:397:ARG:HH11	1.65	0.61
1:B:190:HIS:CE1	1:B:263:ILE:HG12	2.35	0.61
1:C:424:LYS:O	1:C:428:ILE:HG12	2.02	0.59
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.67	0.59
1:D:113:GLU:CB	5:D:2055:HOH:O	2.50	0.59
1:B:454:ASP:CB	5:B:2154:HOH:O	2.43	0.58
1:C:397:ARG:HH11	1:C:397:ARG:HG2	1.67	0.58
1:B:309:LYS:HG2	1:B:315:HIS:CE1	2.39	0.58
1:D:397:ARG:HH11	1:D:397:ARG:HG2	1.69	0.57
1:A:190:HIS:ND1	1:A:263:ILE:CD1	2.67	0.57
1:A:152:ARG:HD2	1:A:180:TYR:CE1	2.41	0.55
1:C:72:ILE:HG21	3:C:700:VIG:H4C2	1.89	0.54
1:D:424:LYS:O	1:D:428:ILE:HG12	2.07	0.54
1:C:309:LYS:HG3	1:C:315:HIS:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:O	1:A:428:ILE:HG12	2.09	0.53
1:B:72:ILE:HG21	3:B:700:VIG:H4C2	1.91	0.53
1:B:382:HIS:HE1	5:B:2134:HOH:O	1.86	0.52
1:C:382:HIS:NE2	1:C:454:ASP:OD2	2.43	0.50
1:B:67:ASP:HA	1:B:435:MET:HB2	1.94	0.49
1:C:246:GLU:HG3	1:C:291:HIS:NE2	2.28	0.49
1:D:67:ASP:HA	1:D:435:MET:HB2	1.94	0.49
1:C:192:ARG:HB3	1:D:145:LYS:NZ	2.28	0.48
1:C:192:ARG:NE	3:C:700:VIG:O1'	2.43	0.48
1:C:67:ASP:HA	1:C:435:MET:HB2	1.96	0.47
1:D:190:HIS:HE1	1:D:265:GLU:HG3	1.77	0.47
1:A:152:ARG:HD2	1:A:180:TYR:HE1	1.79	0.47
1:D:16:PRO:HD3	1:D:459:LEU:HD21	1.95	0.47
1:A:268:GLN:O	1:A:273:ASP:HA	2.15	0.47
1:A:67:ASP:HA	1:A:435:MET:HB2	1.96	0.47
1:B:437:GLY:N	5:B:2149:HOH:O	2.47	0.46
1:B:462:ASN:HB3	5:B:2156:HOH:O	2.16	0.46
1:B:311:TRP:HB2	1:B:313:HIS:CE1	2.51	0.45
1:A:11:PHE:N	5:A:2001:HOH:O	2.48	0.45
1:C:201:HIS:CE1	1:C:217:ILE:HG12	2.51	0.45
1:C:72:ILE:CG2	3:C:700:VIG:H4C2	2.46	0.45
1:C:190:HIS:HE1	1:C:265:GLU:HG3	1.80	0.45
1:D:188:ALA:HB1	1:D:190:HIS:NE2	2.31	0.45
1:C:100:ARG:HA	1:C:101:PRO:HD3	1.87	0.45
1:B:200:THR:O	1:B:201:HIS:ND1	2.50	0.44
4:C:800:FES:S2	1:D:134:ALA:HB3	2.57	0.44
1:C:268:GLN:O	1:C:273:ASP:HA	2.18	0.44
1:A:100:ARG:HA	1:A:101:PRO:HD3	1.84	0.44
1:A:353:THR:OG1	3:B:700:VIG:H3	2.17	0.44
1:B:326:THR:HG22	1:B:336:PHE:HB3	2.00	0.44
1:C:149:MET:HG2	1:C:349:ARG:NH2	2.33	0.44
1:B:76:PRO:HB3	1:B:330:LYS:HG3	2.01	0.43
1:B:311:TRP:CB	1:B:313:HIS:CE1	3.01	0.43
1:A:110:ASN:HD22	1:A:110:ASN:C	2.22	0.43
1:A:110:ASN:ND2	1:A:110:ASN:C	2.71	0.43
1:B:268:GLN:O	1:B:273:ASP:HA	2.18	0.43
1:D:189:PHE:CE1	3:D:700:VIG:H2C1	2.54	0.43
1:C:192:ARG:HB3	1:D:145:LYS:HZ3	1.84	0.43
1:B:309:LYS:CG	1:B:315:HIS:CE1	3.02	0.42
1:C:201:HIS:CE1	1:C:217:ILE:CD1	3.02	0.42
1:C:192:ARG:HD2	1:D:351:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ALA:HB1	1:C:190:HIS:NE2	2.33	0.42
1:B:72:ILE:CG2	3:B:700:VIG:H4C2	2.48	0.42
1:D:326:THR:HG22	1:D:336:PHE:HB3	2.01	0.42
1:D:268:GLN:O	1:D:273:ASP:HA	2.19	0.42
1:C:201:HIS:CE1	1:C:217:ILE:HD13	2.54	0.42
1:B:100:ARG:HA	1:B:101:PRO:HD3	1.85	0.42
1:A:190:HIS:ND1	1:A:263:ILE:HD13	2.35	0.42
1:C:110:ASN:C	1:C:110:ASN:HD22	2.24	0.42
1:D:301:GLN:NE2	3:D:700:VIG:H5C3	2.35	0.41
1:D:110:ASN:C	1:D:110:ASN:HD22	2.24	0.41
1:A:192:ARG:HB3	1:B:145:LYS:NZ	2.35	0.41
1:B:113:GLU:O	1:B:117:GLU:HG3	2.21	0.41
1:A:190:HIS:ND1	1:A:263:ILE:HD11	2.35	0.41
1:C:110:ASN:C	1:C:110:ASN:ND2	2.74	0.41
1:D:76:PRO:HB3	1:D:330:LYS:HG3	2.02	0.40
1:A:351:PHE:O	1:B:192:ARG:HD2	2.20	0.40
1:B:263:ILE:HD12	1:B:296:LEU:HD13	2.03	0.40
1:C:326:THR:HG22	1:C:336:PHE:HB3	2.03	0.40
1:A:192:ARG:HD2	1:B:351:PHE:O	2.22	0.40
1:A:263:ILE:HD12	1:A:296:LEU:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ARG:O	1:D:432:LYS:NZ[1_455]	1.75	0.45
1:C:374:GLU:OE1	1:D:254:LYS:NZ[1_554]	2.10	0.10

## 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	459/472 (97%)	439 (96%)	19 (4%)	1 (0%)	52	64
1	B	459/472 (97%)	441 (96%)	17 (4%)	1 (0%)	52	64
1	C	459/472 (97%)	439 (96%)	19 (4%)	1 (0%)	52	64
1	D	459/472 (97%)	440 (96%)	19 (4%)	0	100	100
All	All	1836/1888 (97%)	1759 (96%)	74 (4%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	B	328	SER
1	C	328	SER

### 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	383/408 (94%)	368 (96%)	15 (4%)	39	53
1	B	383/408 (94%)	368 (96%)	15 (4%)	39	53
1	C	383/408 (94%)	370 (97%)	13 (3%)	44	59
1	D	383/408 (94%)	366 (96%)	17 (4%)	35	46
All	All	1532/1632 (94%)	1472 (96%)	60 (4%)	39	53

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	72	ILE
1	A	92	GLN
1	A	110	ASN
1	A	203	LYS
1	A	228	GLU
1	A	273	ASP
1	A	285	ARG

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Mol	Chain	Res	Type
1	A	296	LEU
1	A	330	LYS
1	A	382	HIS
1	A	397	ARG
1	A	435	MET
1	A	441	ASP
1	A	459	LEU
1	B	21	GLU
1	B	44	HIS
1	B	72	ILE
1	B	92	GLN
1	B	101	PRO
1	B	110	ASN
1	B	203	LYS
1	B	228	GLU
1	B	285	ARG
1	B	296	LEU
1	B	330	LYS
1	B	397	ARG
1	B	435	MET
1	B	441	ASP
1	B	459	LEU
1	C	37	ILE
1	C	72	ILE
1	C	92	GLN
1	C	101	PRO
1	C	110	ASN
1	C	203	LYS
1	C	228	GLU
1	C	285	ARG
1	C	296	LEU
1	C	330	LYS
1	C	397	ARG
1	C	435	MET
1	C	441	ASP
1	D	37	ILE
1	D	53	ARG
1	D	72	ILE
1	D	92	GLN
1	D	101	PRO
1	D	110	ASN
1	D	203	LYS

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Mol	Chain	Res	Type
1	D	228	GLU
1	D	273	ASP
1	D	285	ARG
1	D	296	LEU
1	D	330	LYS
1	D	382	HIS
1	D	397	ARG
1	D	435	MET
1	D	441	ASP
1	D	459	LEU

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

Mol	Chain	Res	Type
1	A	55	ASN
1	A	110	ASN
1	A	313	HIS
1	A	338	HIS
1	B	55	ASN
1	B	110	ASN
1	B	315	HIS
1	B	382	HIS
1	C	110	ASN
1	C	315	HIS
1	C	338	HIS
1	D	92	GLN
1	D	110	ASN
1	D	455	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 carbohydrates in this entry.

## 5.6 Ligand geometry

10 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	600	3	15,15,16	0.82	0	21,22,23	1.28	4 (19%)
3	VIG	A	700	1,2	5,8,8	0.25	0	5,9,9	0.77	0
4	FES	A	800	1	0,4,4	0.00	-	0,4,4	0.00	-
2	PLP	B	600	3	15,15,16	0.77	0	21,22,23	1.01	1 (4%)
3	VIG	B	700	1,2	5,8,8	0.36	0	5,9,9	0.77	0
2	PLP	C	600	3	15,15,16	0.85	1 (6%)	21,22,23	1.08	2 (9%)
3	VIG	C	700	1,2	5,8,8	0.43	0	5,9,9	0.89	0
4	FES	C	800	1	0,4,4	0.00	-	0,4,4	0.00	-
2	PLP	D	600	3	15,15,16	0.79	0	21,22,23	1.11	1 (4%)
3	VIG	D	700	1,2	5,8,8	0.51	0	5,9,9	0.94	0

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	600	3	-	0/6/6/8	0/1/1/1
3	VIG	A	700	1,2	-	0/5/7/7	0/0/0/0
4	FES	A	800	1	-	0/0/4/4	0/1/1/1
2	PLP	B	600	3	-	0/6/6/8	0/1/1/1
3	VIG	B	700	1,2	-	0/5/7/7	0/0/0/0
2	PLP	C	600	3	-	0/6/6/8	0/1/1/1
3	VIG	C	700	1,2	-	0/5/7/7	0/0/0/0
4	FES	C	800	1	-	0/0/4/4	0/1/1/1
2	PLP	D	600	3	-	0/6/6/8	0/1/1/1
3	VIG	D	700	1,2	-	0/5/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	PLP	C6-N1	2.07	1.38	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	PLP	C4A-C4-C5	-3.26	117.49	120.88
2	C	600	PLP	C4A-C4-C5	-2.74	118.03	120.88
2	A	600	PLP	C4A-C4-C5	-2.24	118.55	120.88
2	A	600	PLP	C5-C6-N1	-2.19	120.05	123.86
2	B	600	PLP	C4A-C4-C5	-2.16	118.63	120.88
2	C	600	PLP	C5-C6-N1	-2.13	120.17	123.86
2	A	600	PLP	O4P-C5A-C5	2.39	112.95	108.99
2	A	600	PLP	C6-C5-C4	2.57	120.33	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	VIG	3	0
3	C	700	VIG	3	0
4	C	800	FES	1	0
3	D	700	VIG	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 ⓘ

### 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, 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	461/472 (97%)	0.10	22 (4%) 34 43	9, 14, 15, 23	0
1	B	461/472 (97%)	0.20	19 (4%) 41 50	9, 13, 15, 24	0
1	C	461/472 (97%)	0.01	5 (1%) 82 86	9, 14, 15, 21	0
1	D	461/472 (97%)	-0.12	10 (2%) 65 73	10, 14, 15, 26	0
All	All	1844/1888 (97%)	0.05	56 (3%) 54 63	9, 14, 15, 26	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	5.2
1	B	231	VAL	4.9
1	C	158	GLN	4.3
1	A	158	GLN	3.9
1	B	12	ASP	3.8
1	A	161	PHE	3.7
1	B	441	ASP	3.5
1	A	296	LEU	3.4
1	C	441	ASP	3.3
1	B	230	PHE	3.3
1	A	263	ILE	3.2
1	B	13	TYR	3.1
1	A	256	LYS	3.1
1	A	11	PHE	3.1
1	B	232	LYS	3.1
1	A	345	ASN	3.0
1	D	11	PHE	3.0
1	A	441	ASP	2.9
1	A	159	SER	2.9
1	B	419	GLU	2.8
1	B	420	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	160	ALA	2.7
1	A	250	VAL	2.7
1	B	235	GLN	2.7
1	D	92	GLN	2.7
1	D	231	VAL	2.6
1	B	228	GLU	2.6
1	A	319	ASP	2.5
1	B	227	LEU	2.5
1	D	91	PRO	2.5
1	A	228	GLU	2.5
1	B	240	ARG	2.4
1	B	385	LYS	2.4
1	A	230	PHE	2.3
1	B	256	LYS	2.3
1	C	375	ASP	2.3
1	A	156	ARG	2.3
1	D	264	VAL	2.2
1	A	92	GLN	2.2
1	B	239	ALA	2.2
1	A	182	ILE	2.2
1	D	90	GLN	2.2
1	B	317	GLY	2.2
1	D	263	ILE	2.2
1	A	262	ILE	2.1
1	D	441	ASP	2.1
1	B	25	PRO	2.1
1	A	68	LEU	2.1
1	D	230	PHE	2.1
1	A	175	PRO	2.1
1	A	231	VAL	2.0
1	D	12	ASP	2.0
1	A	166	LEU	2.0
1	B	236	GLN	2.0
1	A	470	ASP	2.0
1	C	435	MET	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	VIG	A	700	9/9	0.92	0.17	2.60	29,29,34,35	0
3	VIG	D	700	9/9	0.90	0.16	1.85	25,26,29,31	0
3	VIG	B	700	9/9	0.92	0.14	0.65	27,27,32,32	0
2	PLP	A	600	15/16	0.96	0.14	0.41	19,21,25,28	0
2	PLP	B	600	15/16	0.95	0.14	0.40	18,22,25,27	0
3	VIG	C	700	9/9	0.94	0.14	0.08	23,23,26,27	0
2	PLP	C	600	15/16	0.97	0.11	-0.48	13,18,20,22	0
2	PLP	D	600	15/16	0.98	0.10	-0.55	19,21,24,25	0
4	FES	C	800	4/4	0.99	0.04	-3.16	20,21,21,22	0
4	FES	A	800	4/4	0.99	0.04	-3.19	18,21,21,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.