



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1GBN  
Title : HUMAN ORNITHINE AMINOTRANSFERASE COMPLEXED WITH THE  
NEUROTOXIN GABACULINE  
Authors : Shah, S.A.; Shen, B.W.; Brunger, A.T.  
Deposited on : 1997-05-29  
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

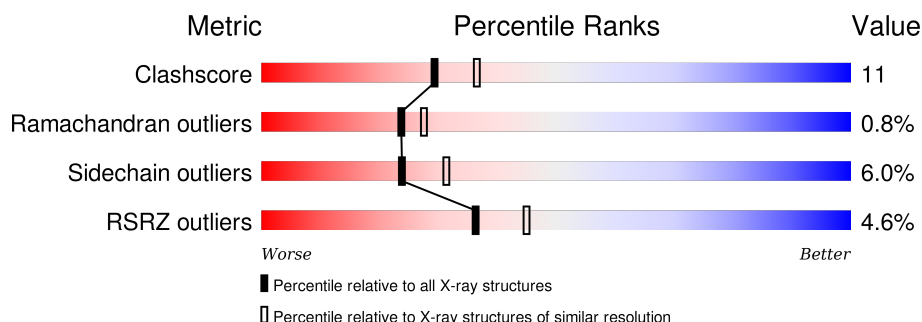
# 1 Overall quality at a glance

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	402	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	402	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	402	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>

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	GBC	B	440	X	-	-	-
3	GBC	C	440	X	-	-	-

## 2 Entry composition [i](#)

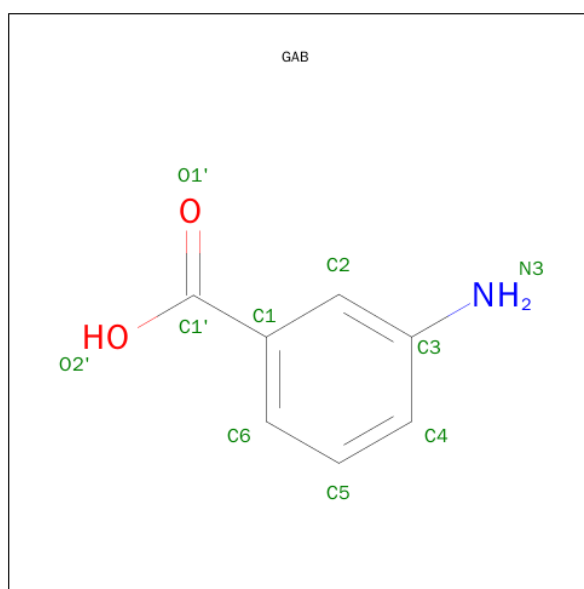
There are 4 unique types of molecules in this entry. The entry contains 11888 atoms, of which 2034 are hydrogens and 0 are deuteriums.

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 ORNITHINE AMINOTRANSFERASE.

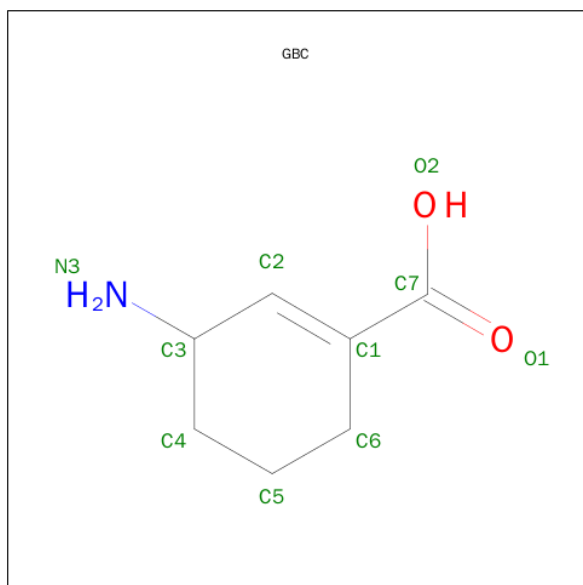
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	402	Total	C	H	N	O	S	27	0	0
			3828	2023	678	531	584	12			
1	B	402	Total	C	H	N	O	S	24	0	0
			3828	2023	678	531	584	12			
1	C	402	Total	C	H	N	O	S	11	0	0
			3828	2023	678	531	584	12			

- Molecule 2 is 3-AMINO BENZOIC ACID (three-letter code: GAB, PLP) (formula:  $C_7H_7NO_2$ ,  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			25	15	2	7	1		

- Molecule 3 is GABACULINE (three-letter code: GBC, PLP) (formula:  $C_7H_{11}NO_2$ ,  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	2	Total	C	N	O	P	0	0
			25	15	2	7	1		
3	C	2	Total	C	N	O	P	0	0
			25	15	2	7	1		

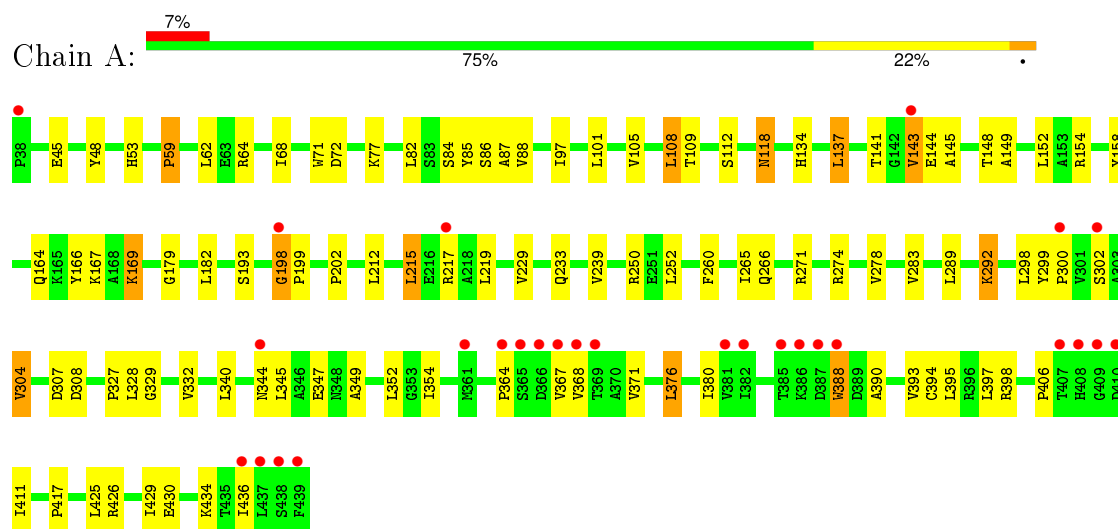
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	116	Total	O	0	0
			116	116		
4	C	119	Total	O	0	0
			119	119		

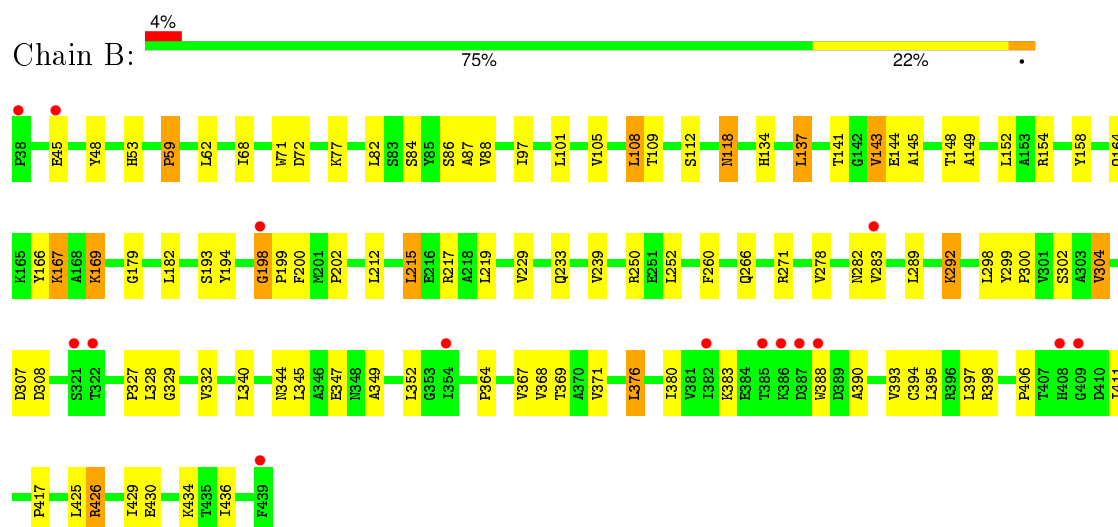
### 3 Residue-property plots

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.

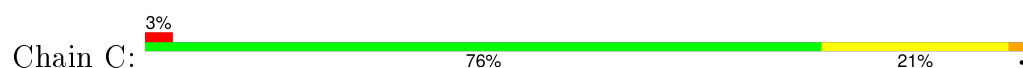
#### • Molecule 1: ORNITHINE AMINOTRANSFERASE

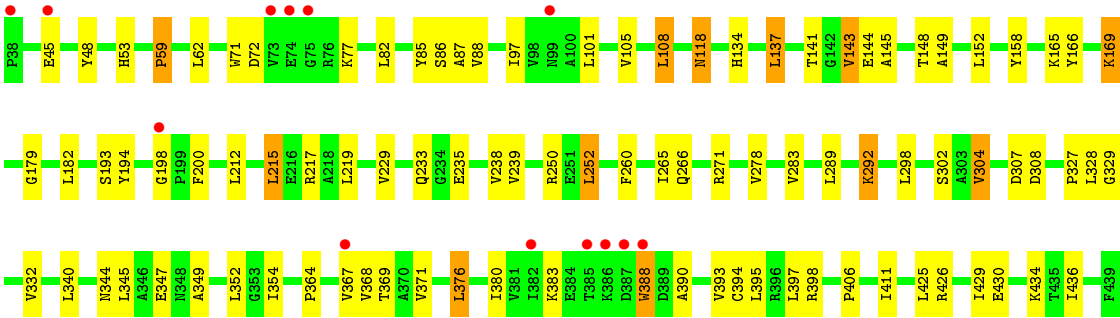


#### • Molecule 1: ORNITHINE AMINOTRANSFERASE



#### • Molecule 1: ORNITHINE AMINOTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.01Å 115.01Å 185.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 43.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.9 (50.00-2.30) 87.0 (43.89-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.38 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.209 , 0.235 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.0	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55195 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/3223	0.64	0/4375
1	B	0.38	1/3223 (0.0%)	0.64	0/4375
1	C	0.37	0/3223	0.63	0/4375
All	All	0.37	1/9669 (0.0%)	0.64	0/13125

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	LYS	CE-NZ	5.16	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3150	678	3156	87	0
1	B	3150	678	3156	84	0
1	C	3150	678	3156	68	0
2	A	25	0	12	0	0
3	B	25	0	15	0	0
3	C	25	0	13	2	0
4	A	94	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	116	0	0	4	0
4	C	119	0	0	1	0
All	All	9854	2034	9508	214	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 11.

All (214) 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:367:VAL:HG13	1:A:388:TRP:HH2	1.35	0.92
1:C:367:VAL:HG13	1:C:388:TRP:HH2	1.37	0.89
1:C:233:GLN:HB2	1:C:239:VAL:HG22	1.59	0.85
1:B:233:GLN:HB2	1:B:239:VAL:HG22	1.59	0.85
1:A:367:VAL:HG13	1:A:388:TRP:CH2	2.13	0.84
1:A:233:GLN:HB2	1:A:239:VAL:HG22	1.58	0.82
1:C:367:VAL:HG13	1:C:388:TRP:CH2	2.14	0.81
1:C:137:LEU:HB3	1:C:304:VAL:HG13	1.66	0.77
1:A:137:LEU:HB3	1:A:304:VAL:HG13	1.66	0.77
1:B:137:LEU:HB3	1:B:304:VAL:HG13	1.65	0.77
1:B:143:VAL:HG13	1:B:179:GLY:HA3	1.68	0.75
1:A:158:TYR:OH	1:B:198:GLY:HA2	1.86	0.74
1:B:194:TYR:CE2	1:C:217:ARG:NH1	2.55	0.74
1:A:143:VAL:HG13	1:A:179:GLY:HA3	1.70	0.73
1:A:101:LEU:HD23	1:B:105:VAL:HG11	1.71	0.72
1:A:105:VAL:HG11	1:B:101:LEU:HD23	1.70	0.72
1:A:278:VAL:HG22	1:A:283:VAL:HB	1.71	0.71
1:C:143:VAL:HG13	1:C:179:GLY:HA3	1.72	0.71
1:C:278:VAL:HG22	1:C:283:VAL:HB	1.71	0.70
1:A:198:GLY:HA2	1:B:158:TYR:OH	1.91	0.70
1:B:278:VAL:HG22	1:B:283:VAL:HB	1.72	0.70
1:B:233:GLN:HB2	1:B:239:VAL:CG2	2.24	0.68
1:A:367:VAL:HG12	1:A:368:VAL:HG23	1.77	0.66
1:A:233:GLN:HB2	1:A:239:VAL:CG2	2.25	0.66
1:A:158:TYR:OH	1:A:166:TYR:HA	1.96	0.66
1:B:158:TYR:OH	1:B:166:TYR:HA	1.96	0.66
1:C:158:TYR:OH	1:C:166:TYR:HA	1.96	0.66
1:B:367:VAL:HG12	1:B:368:VAL:HG23	1.79	0.65
1:C:367:VAL:HG12	1:C:368:VAL:HG23	1.79	0.65
1:C:233:GLN:HB2	1:C:239:VAL:CG2	2.25	0.64
1:A:278:VAL:CG2	1:A:283:VAL:HB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:VAL:CG2	1:C:283:VAL:HB	2.28	0.63
1:A:217:ARG:NH1	4:A:454:HOH:O	2.30	0.63
1:C:349:ALA:HA	1:C:376:LEU:CD2	2.29	0.63
1:A:154:ARG:HG2	1:B:198:GLY:HA3	1.79	0.63
1:A:349:ALA:HA	1:A:376:LEU:CD2	2.29	0.62
1:B:349:ALA:HA	1:B:376:LEU:CD2	2.28	0.62
1:A:198:GLY:HA3	1:B:154:ARG:HG2	1.80	0.61
1:B:101:LEU:O	1:B:105:VAL:HG13	2.01	0.61
1:B:278:VAL:CG2	1:B:283:VAL:HB	2.30	0.61
1:B:217:ARG:HD3	4:B:482:HOH:O	2.00	0.61
1:A:250:ARG:O	1:A:250:ARG:HD3	2.01	0.60
1:C:250:ARG:HD3	1:C:250:ARG:O	2.02	0.59
1:A:101:LEU:O	1:A:105:VAL:HG13	2.03	0.58
1:B:250:ARG:O	1:B:250:ARG:HD3	2.02	0.58
1:A:158:TYR:HH	1:B:198:GLY:HA2	1.69	0.58
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.86	0.58
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.86	0.58
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.86	0.57
1:C:48:TYR:O	1:C:53:HIS:HE1	1.87	0.57
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.86	0.57
1:B:367:VAL:HG11	1:B:436:ILE:CG2	2.35	0.57
1:C:101:LEU:O	1:C:105:VAL:HG13	2.04	0.57
1:B:62:LEU:HA	1:B:72:ASP:HA	1.87	0.57
1:B:48:TYR:O	1:B:53:HIS:HE1	1.88	0.56
1:A:199:PRO:HB2	1:B:202:PRO:HG2	1.87	0.56
1:A:48:TYR:O	1:A:53:HIS:HE1	1.87	0.56
1:C:367:VAL:HG11	1:C:436:ILE:CG2	2.35	0.56
1:A:367:VAL:HG11	1:A:436:ILE:CG2	2.35	0.56
1:A:101:LEU:CD2	1:B:105:VAL:HG11	2.35	0.55
1:A:105:VAL:HG11	1:B:101:LEU:CD2	2.37	0.55
1:B:101:LEU:HD12	1:B:328:LEU:HD11	1.89	0.55
1:A:202:PRO:HG2	1:B:199:PRO:HB2	1.89	0.55
1:C:367:VAL:CG1	1:C:388:TRP:HH2	2.14	0.54
1:A:217:ARG:HD2	4:A:454:HOH:O	2.07	0.54
1:C:145:ALA:HB2	1:C:302:SER:OG	2.08	0.54
1:A:367:VAL:HG22	1:A:388:TRP:CH2	2.43	0.53
1:A:367:VAL:CG1	1:A:388:TRP:HH2	2.13	0.53
1:A:145:ALA:HB2	1:A:302:SER:OG	2.09	0.53
1:C:62:LEU:HA	1:C:72:ASP:HA	1.90	0.53
1:C:367:VAL:HG22	1:C:388:TRP:CH2	2.44	0.52
1:A:367:VAL:HG11	1:A:436:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:HIS:HB2	1:B:307:ASP:HA	1.91	0.52
1:B:367:VAL:HG11	1:B:436:ILE:HG23	1.90	0.52
1:A:62:LEU:HA	1:A:72:ASP:HA	1.90	0.52
1:A:158:TYR:HE2	1:B:198:GLY:H	1.56	0.52
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.92	0.52
1:A:198:GLY:HA2	1:B:158:TYR:HH	1.73	0.52
1:C:393:VAL:O	1:C:397:LEU:HB2	2.09	0.52
1:B:145:ALA:HB2	1:B:302:SER:OG	2.10	0.52
1:A:137:LEU:HG	1:A:148:THR:HG21	1.92	0.51
1:C:367:VAL:HG11	1:C:436:ILE:HG23	1.90	0.51
1:C:340:LEU:HD23	1:C:345:LEU:HD12	1.92	0.51
1:A:112:SER:HB3	1:B:84:SER:HA	1.92	0.51
1:B:340:LEU:HD23	1:B:345:LEU:HD12	1.93	0.51
1:B:194:TYR:CD2	1:C:217:ARG:NH1	2.79	0.51
1:A:364:PRO:HG2	1:A:367:VAL:HB	1.92	0.51
1:C:137:LEU:HG	1:C:148:THR:HG21	1.93	0.50
1:A:134:HIS:HB2	1:A:307:ASP:HA	1.92	0.50
1:B:250:ARG:HD2	4:B:514:HOH:O	2.12	0.50
1:C:134:HIS:HB2	1:C:307:ASP:HA	1.91	0.50
1:A:300:PRO:HD3	1:B:299:TYR:CZ	2.46	0.50
1:C:87:ALA:HA	1:C:292:LYS:HB3	1.94	0.50
1:C:430:GLU:O	1:C:434:LYS:HG2	2.12	0.49
1:B:393:VAL:O	1:B:397:LEU:HB2	2.11	0.49
1:B:59:PRO:HG2	1:B:398:ARG:NH1	2.27	0.49
1:A:59:PRO:HG2	1:A:398:ARG:NH1	2.26	0.49
1:B:364:PRO:HG2	1:B:367:VAL:HB	1.95	0.49
1:A:393:VAL:O	1:A:397:LEU:HB2	2.13	0.49
1:A:87:ALA:HA	1:A:292:LYS:HB3	1.94	0.49
1:B:137:LEU:HG	1:B:148:THR:HG21	1.95	0.48
1:C:364:PRO:HG2	1:C:367:VAL:HB	1.94	0.48
1:B:134:HIS:CD2	1:B:308:ASP:H	2.31	0.48
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.95	0.47
1:C:134:HIS:CD2	1:C:308:ASP:H	2.31	0.47
1:C:59:PRO:HG2	1:C:398:ARG:NH1	2.28	0.47
1:A:198:GLY:H	1:B:158:TYR:HE2	1.62	0.47
1:A:154:ARG:HG2	1:B:198:GLY:CA	2.43	0.47
1:B:87:ALA:HA	1:B:292:LYS:HB3	1.96	0.47
1:A:198:GLY:CA	1:B:154:ARG:HG2	2.45	0.47
1:C:134:HIS:HD2	1:C:308:ASP:H	1.61	0.47
1:A:352:LEU:HB3	1:A:425:LEU:HD22	1.97	0.47
1:B:344:ASN:O	1:B:347:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TYR:N	1:B:166:TYR:CD1	2.78	0.47
1:A:430:GLU:O	1:A:434:LYS:HG2	2.15	0.47
1:B:430:GLU:O	1:B:434:LYS:HG2	2.15	0.47
1:B:271:ARG:HH21	1:B:376:LEU:HB3	1.79	0.47
1:C:395:LEU:O	1:C:398:ARG:HB3	2.15	0.47
1:C:141:THR:OG1	1:C:144:GLU:HG3	2.15	0.47
1:A:425:LEU:O	1:A:429:ILE:HG13	2.15	0.46
1:A:134:HIS:CD2	1:A:308:ASP:H	2.33	0.46
1:A:64:ARG:HD2	4:A:533:HOH:O	2.15	0.46
1:C:425:LEU:O	1:C:429:ILE:HG13	2.15	0.46
1:A:265:ILE:O	1:A:292:LYS:HD2	2.15	0.46
1:B:194:TYR:CZ	1:C:217:ARG:NH1	2.82	0.46
1:A:390:ALA:HB1	1:A:406:PRO:HB3	1.98	0.46
1:C:271:ARG:HH21	1:C:376:LEU:HB3	1.81	0.46
1:B:134:HIS:HD2	1:B:308:ASP:H	1.62	0.46
1:A:299:TYR:CZ	1:B:300:PRO:HD3	2.51	0.46
1:A:271:ARG:HH21	1:A:376:LEU:HB3	1.81	0.46
1:A:71:TRP:CZ2	1:A:77:LYS:HE2	2.51	0.46
1:A:169:LYS:HB3	1:A:169:LYS:NZ	2.31	0.46
1:A:344:ASN:O	1:A:347:GLU:HG2	2.16	0.45
1:C:166:TYR:N	1:C:166:TYR:CD1	2.81	0.45
1:A:134:HIS:HD2	1:A:308:ASP:H	1.64	0.45
1:A:84:SER:HA	1:B:112:SER:HB3	1.97	0.45
1:B:390:ALA:HB1	1:B:406:PRO:HB3	1.97	0.45
1:B:352:LEU:HB3	1:B:425:LEU:HD22	1.97	0.45
1:B:169:LYS:HB3	1:B:169:LYS:NZ	2.31	0.45
1:C:194:TYR:HB2	1:C:200:PHE:CE1	2.52	0.45
1:C:352:LEU:HB3	1:C:425:LEU:HD22	1.98	0.45
1:A:395:LEU:O	1:A:398:ARG:HB3	2.16	0.45
1:A:329:GLY:O	1:A:332:VAL:HG22	2.16	0.45
1:C:265:ILE:O	1:C:292:LYS:HD2	2.16	0.45
1:A:109:THR:HG21	1:B:298:LEU:HG	1.99	0.45
1:B:118:ASN:HD22	1:B:118:ASN:H	1.65	0.45
1:C:165:LYS:HG2	4:C:502:HOH:O	2.17	0.45
1:A:298:LEU:HG	1:B:109:THR:HG21	1.98	0.45
1:A:166:TYR:CD1	1:A:166:TYR:N	2.80	0.45
1:B:425:LEU:O	1:B:429:ILE:HG13	2.16	0.45
1:B:406:PRO:HA	1:B:411:ILE:O	2.17	0.45
1:C:344:ASN:O	1:C:347:GLU:HG2	2.16	0.45
1:C:71:TRP:CZ2	1:C:77:LYS:HE2	2.52	0.44
1:C:329:GLY:O	1:C:332:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH1	4:A:453:HOH:O	2.50	0.44
1:B:395:LEU:O	1:B:398:ARG:HB3	2.16	0.44
1:C:169:LYS:HB3	1:C:169:LYS:NZ	2.32	0.44
1:B:71:TRP:CZ2	1:B:77:LYS:HE2	2.52	0.44
1:C:390:ALA:HB1	1:C:406:PRO:HB3	1.99	0.44
1:C:369:THR:HG23	1:C:383:LYS:HB2	1.99	0.44
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.99	0.44
1:B:215:LEU:HD22	1:B:219:LEU:HG	2.00	0.44
1:B:141:THR:OG1	1:B:144:GLU:HG3	2.18	0.44
1:B:371:VAL:HG22	1:B:380:ILE:HG22	1.98	0.44
1:B:369:THR:HG23	1:B:383:LYS:HB2	2.00	0.44
1:B:108:LEU:HD13	1:B:327:PRO:HG2	2.00	0.44
1:B:154:ARG:NH1	4:B:539:HOH:O	2.46	0.44
1:B:329:GLY:O	1:B:332:VAL:HG22	2.17	0.44
1:A:406:PRO:HA	1:A:411:ILE:O	2.18	0.43
1:A:154:ARG:NH1	4:A:519:HOH:O	2.43	0.43
1:B:97:ILE:HG22	1:B:298:LEU:HD22	2.00	0.43
1:C:118:ASN:H	1:C:118:ASN:HD22	1.65	0.43
1:A:141:THR:OG1	1:A:144:GLU:HG3	2.17	0.43
1:C:406:PRO:HA	1:C:411:ILE:O	2.19	0.43
1:C:86:SER:HB3	1:C:266:GLN:HG3	2.01	0.43
1:A:86:SER:HB3	1:A:266:GLN:HG3	2.00	0.43
1:A:371:VAL:HG22	1:A:380:ILE:HG22	2.01	0.43
1:A:250:ARG:C	1:A:250:ARG:HD3	2.37	0.42
1:B:164:GLN:NE2	1:B:167:LYS:HD2	2.34	0.42
1:B:86:SER:HB3	1:B:266:GLN:HG3	2.01	0.42
1:A:344:ASN:HB3	1:A:347:GLU:CG	2.49	0.42
1:C:215:LEU:HD22	1:C:219:LEU:HG	2.00	0.42
1:A:164:GLN:NE2	1:A:167:LYS:HD2	2.34	0.42
1:C:108:LEU:HD13	1:C:327:PRO:HG2	2.00	0.42
1:B:344:ASN:HB3	1:B:347:GLU:CG	2.49	0.42
1:A:118:ASN:HD22	1:A:118:ASN:H	1.66	0.42
1:C:250:ARG:HD3	1:C:250:ARG:C	2.39	0.42
1:B:88:VAL:O	1:B:88:VAL:HG23	2.20	0.42
1:C:252:LEU:HA	1:C:252:LEU:HD12	1.94	0.42
1:B:376:LEU:HD13	1:B:376:LEU:HA	1.90	0.42
1:A:97:ILE:HG22	1:A:298:LEU:HD22	2.01	0.42
1:C:238:VAL:O	1:C:238:VAL:HG12	2.20	0.42
1:C:371:VAL:HG22	1:C:380:ILE:HG22	2.00	0.42
1:A:215:LEU:HD22	1:A:219:LEU:HG	2.00	0.42
1:C:101:LEU:HD12	1:C:328:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:CYS:SG	1:B:406:PRO:HD3	2.60	0.41
1:C:344:ASN:HB3	1:C:347:GLU:CG	2.50	0.41
1:C:85:TYR:CE2	3:C:440:GBC:H62	2.56	0.41
1:A:68:ILE:HG22	1:A:417:PRO:HB2	2.02	0.41
1:B:426:ARG:HG3	4:B:551:HOH:O	2.21	0.41
1:C:367:VAL:HG22	1:C:388:TRP:HH2	1.86	0.41
1:A:394:CYS:SG	1:A:406:PRO:HD3	2.60	0.41
1:C:235:GLU:CG	3:C:440:GBC:H42	2.51	0.41
1:C:394:CYS:SG	1:C:406:PRO:HD3	2.61	0.41
1:B:68:ILE:HG22	1:B:417:PRO:HB2	2.03	0.41
1:B:250:ARG:HB2	1:B:283:VAL:CG1	2.51	0.41
1:A:88:VAL:HG23	1:A:88:VAL:O	2.21	0.41
1:B:194:TYR:HB2	1:B:200:PHE:CE1	2.57	0.40
1:A:250:ARG:HB2	1:A:283:VAL:CG1	2.51	0.40
1:A:376:LEU:HD13	1:A:376:LEU:HA	1.91	0.40
1:C:85:TYR:O	1:C:86:SER:HB3	2.21	0.40
1:A:85:TYR:O	1:A:86:SER:HB3	2.20	0.40
1:C:88:VAL:O	1:C:88:VAL:HG23	2.21	0.40
1:A:108:LEU:HD13	1:A:327:PRO:HG2	2.02	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	400/402 (100%)	377 (94%)	20 (5%)	3 (1%)	24	27
1	B	400/402 (100%)	377 (94%)	20 (5%)	3 (1%)	24	27
1	C	400/402 (100%)	377 (94%)	20 (5%)	3 (1%)	24	27
All	All	1200/1206 (100%)	1131 (94%)	60 (5%)	9 (1%)	24	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	GLY
1	A	292	LYS
1	B	198	GLY
1	B	292	LYS
1	C	198	GLY
1	C	292	LYS
1	B	59	PRO
1	A	59	PRO
1	C	59	PRO

### 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	336/336 (100%)	316 (94%)	20 (6%)	24	31
1	B	336/336 (100%)	316 (94%)	20 (6%)	24	31
1	C	336/336 (100%)	316 (94%)	20 (6%)	24	31
All	All	1008/1008 (100%)	948 (94%)	60 (6%)	24	31

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

Mol	Chain	Res	Type
1	A	45	GLU
1	A	82	LEU
1	A	108	LEU
1	A	118	ASN
1	A	137	LEU
1	A	143	VAL
1	A	152	LEU
1	A	169	LYS
1	A	182	LEU
1	A	193	SER
1	A	212	LEU
1	A	215	LEU
1	A	229	VAL
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	260	PHE
1	A	304	VAL
1	A	354	ILE
1	A	376	LEU
1	A	388	TRP
1	A	426	ARG
1	B	45	GLU
1	B	82	LEU
1	B	108	LEU
1	B	118	ASN
1	B	137	LEU
1	B	143	VAL
1	B	152	LEU
1	B	169	LYS
1	B	182	LEU
1	B	193	SER
1	B	212	LEU
1	B	215	LEU
1	B	229	VAL
1	B	252	LEU
1	B	260	PHE
1	B	282	ASN
1	B	304	VAL
1	B	376	LEU
1	B	388	TRP
1	B	426	ARG
1	C	45	GLU
1	C	82	LEU
1	C	108	LEU
1	C	118	ASN
1	C	137	LEU
1	C	143	VAL
1	C	152	LEU
1	C	169	LYS
1	C	182	LEU
1	C	193	SER
1	C	212	LEU
1	C	215	LEU
1	C	229	VAL
1	C	252	LEU
1	C	260	PHE
1	C	304	VAL

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Mol	Chain	Res	Type
1	C	354	ILE
1	C	376	LEU
1	C	388	TRP
1	C	426	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	118	ASN
1	A	132	ASN
1	A	134	HIS
1	A	164	GLN
1	A	176	ASN
1	A	266	GLN
1	A	319	HIS
1	A	400	ASN
1	A	408	HIS
1	B	53	HIS
1	B	118	ASN
1	B	132	ASN
1	B	134	HIS
1	B	164	GLN
1	B	176	ASN
1	B	266	GLN
1	B	282	ASN
1	B	319	HIS
1	B	400	ASN
1	B	408	HIS
1	C	53	HIS
1	C	118	ASN
1	C	132	ASN
1	C	134	HIS
1	C	164	GLN
1	C	176	ASN
1	C	319	HIS
1	C	400	ASN
1	C	408	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 ⓘ

6 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	GAB	A	440	2	7,10,10	1.19	1 (14%)	9,13,13	0.74	0
2	PLP	A	441	2	15,15,16	2.08	3 (20%)	21,22,23	1.48	4 (19%)
3	GBC	B	440	3	8,10,10	4.22	6 (75%)	3,13,13	2.82	3 (100%)
3	PLP	B	441	3	15,15,16	1.80	3 (20%)	21,22,23	1.36	4 (19%)
3	GBC	C	440	3	8,10,10	4.39	6 (75%)	3,13,13	2.80	3 (100%)
3	PLP	C	441	3	15,15,16	2.23	4 (26%)	21,22,23	1.38	4 (19%)

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	GAB	A	440	2	-	0/0/4/4	0/1/1/1
2	PLP	A	441	2	-	0/6/6/8	0/1/1/1
3	GBC	B	440	3	1/1/3/4	0/0/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	B	441	3	-	0/6/6/8	0/1/1/1
3	GBC	C	440	3	1/1/3/4	0/0/14/14	0/1/1/1
3	PLP	C	441	3	-	0/6/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	440	GBC	C4-C3	-8.44	1.37	1.53
3	B	440	GBC	C4-C3	-7.61	1.39	1.53
3	C	441	PLP	C3-C2	-6.29	1.36	1.40
2	A	441	PLP	C3-C2	-5.52	1.37	1.40
3	C	440	GBC	C5-C4	-5.09	1.39	1.53
3	B	440	GBC	C5-C4	-5.01	1.39	1.53
3	B	440	GBC	C3-C2	-4.32	1.39	1.49
3	C	440	GBC	C3-C2	-4.29	1.39	1.49
3	B	441	PLP	C3-C2	-4.21	1.37	1.40
3	B	440	GBC	C5-C6	-4.04	1.38	1.52
3	C	440	GBC	C5-C6	-3.93	1.39	1.52
3	C	440	GBC	C6-C1	-2.95	1.39	1.49
3	B	440	GBC	C6-C1	-2.89	1.39	1.49
3	C	441	PLP	C2-N1	2.24	1.38	1.34
2	A	441	PLP	P-O2P	2.25	1.62	1.54
3	B	441	PLP	P-O2P	2.35	1.63	1.54
3	C	441	PLP	C4A-C4	2.54	1.56	1.51
2	A	440	GAB	C3-N3	3.07	1.49	1.38
3	C	441	PLP	P-O2P	3.14	1.66	1.54
3	B	441	PLP	C4A-C4	3.37	1.58	1.51
2	A	441	PLP	C4A-C4	3.58	1.59	1.51
3	C	440	GBC	C2-C1	3.78	1.40	1.34
3	B	440	GBC	C2-C1	3.89	1.40	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	441	PLP	O2P-P-O4P	-2.94	98.10	106.56
3	B	441	PLP	O2P-P-O4P	-2.47	99.45	106.56
3	C	441	PLP	C5-C6-N1	-2.14	120.15	123.86
3	C	441	PLP	C2A-C2-C3	-2.10	118.51	121.04
3	B	441	PLP	O2P-P-O1P	-2.09	103.85	110.58
2	A	441	PLP	O3P-P-O1P	2.39	118.27	110.58
3	C	441	PLP	C6-C5-C4	2.43	120.21	118.15
3	C	440	GBC	C4-C3-N3	2.47	119.02	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	441	PLP	C6-C5-C4	2.48	120.25	118.15
3	B	441	PLP	C6-C5-C4	2.54	120.30	118.15
3	B	440	GBC	C4-C3-N3	2.60	119.42	110.93
3	C	441	PLP	O3P-P-O1P	2.61	118.97	110.58
3	B	440	GBC	C4-C3-C2	2.75	119.76	108.65
3	C	440	GBC	C4-C3-C2	2.79	119.94	108.65
3	B	441	PLP	O3P-P-O1P	2.95	120.09	110.58
3	B	440	GBC	C4-C5-C6	3.10	120.09	111.31
3	C	440	GBC	C4-C5-C6	3.11	120.12	111.31
2	A	441	PLP	O4P-C5A-C5	3.31	114.47	108.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	440	GBC	C3
3	B	440	GBC	C3

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	440	GBC	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	402/402 (100%)	0.46	28 (6%)	19	27	7, 20, 40, 66	6 (1%)
1	B	402/402 (100%)	0.27	15 (3%)	45	54	7, 19, 38, 64	5 (1%)
1	C	402/402 (100%)	0.23	13 (3%)	51	60	8, 20, 39, 65	3 (0%)
All	All	1206/1206 (100%)	0.32	56 (4%)	36	45	7, 20, 39, 66	14 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	388	TRP	8.4
1	A	367	VAL	8.1
1	B	198	GLY	6.0
1	A	388	TRP	5.9
1	C	386	LYS	5.7
1	C	387	ASP	5.2
1	A	386	LYS	5.1
1	A	365	SER	5.0
1	B	387	ASP	4.9
1	A	364	PRO	4.9
1	A	409	GLY	4.9
1	A	368	VAL	4.8
1	C	385	THR	4.5
1	A	439	PHE	4.2
1	C	367	VAL	4.2
1	B	385	THR	4.1
1	B	38	PRO	4.1
1	C	198	GLY	4.0
1	A	198	GLY	4.0
1	A	407	THR	3.9
1	A	387	ASP	3.9
1	A	408	HIS	3.8
1	C	73	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	366	ASP	3.4
1	A	369	THR	3.2
1	A	436	ILE	3.2
1	C	38	PRO	3.2
1	A	410	ASP	3.2
1	C	382	ILE	3.1
1	A	217	ARG	3.1
1	B	408	HIS	2.9
1	A	385	THR	2.9
1	B	388	TRP	2.9
1	A	361	MET	2.9
1	A	38	PRO	2.8
1	B	386	LYS	2.8
1	B	283	VAL	2.7
1	C	99	ASN	2.7
1	B	409	GLY	2.7
1	A	143	VAL	2.7
1	C	75	GLY	2.6
1	A	300	PRO	2.5
1	B	382	ILE	2.4
1	A	438	SER	2.4
1	B	439	PHE	2.4
1	A	302	SER	2.4
1	C	74	GLU	2.3
1	C	45	GLU	2.3
1	A	381	VAL	2.2
1	B	321	SER	2.2
1	B	354	ILE	2.2
1	A	437	LEU	2.2
1	B	322	THR	2.2
1	A	382	ILE	2.1
1	A	344	ASN	2.1
1	B	45	GLU	2.1

## 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 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( $\text{\AA}^2$ )	Q<0.9
3	GBC	C	440	10/10	0.90	0.17	0.16	17,19,22,23	0
2	GAB	A	440	10/10	0.91	0.19	-0.19	24,25,28,28	0
3	PLP	C	441	15/16	0.96	0.16	-0.27	15,18,20,21	0
3	PLP	B	441	15/16	0.97	0.16	-0.62	12,13,17,17	0
2	PLP	A	441	15/16	0.97	0.17	-0.74	10,14,17,20	0
3	GBC	B	440	10/10	0.93	0.16	-0.78	16,17,27,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.