



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:18 pm GMT

PDB ID : 4P3J  
Title : Apo inward-facing state of the glutamate transporter homologue GltPh in alkali-free conditions  
Authors : Verdon, G.; Boudker, O.  
Deposited on : 2014-03-08  
Resolution : 3.50 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

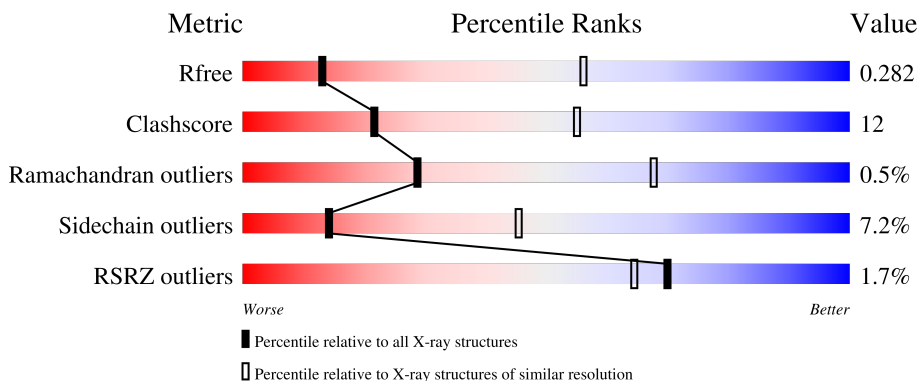
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	422	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>71%</div> <div>22%</div> <div>• •</div> </div>
1	C	422	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9091 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 GltPh.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3036	1996	490	532	18			
1	B	408	Total	C	N	O	S	0	0	0
			3015	1983	487	527	18			
1	C	411	Total	C	N	O	S	0	0	0
			3037	1997	490	532	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	55	CYS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	364	CYS	ALA	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421	PRO	-	expression tag	UNP O59010
A	422	ARG	-	expression tag	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	55	CYS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	364	CYS	ALA	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
B	421	PRO	-	expression tag	UNP O59010
B	422	ARG	-	expression tag	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	55	CYS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	364	CYS	ALA	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010
C	421	PRO	-	expression tag	UNP O59010
C	422	ARG	-	expression tag	UNP O59010

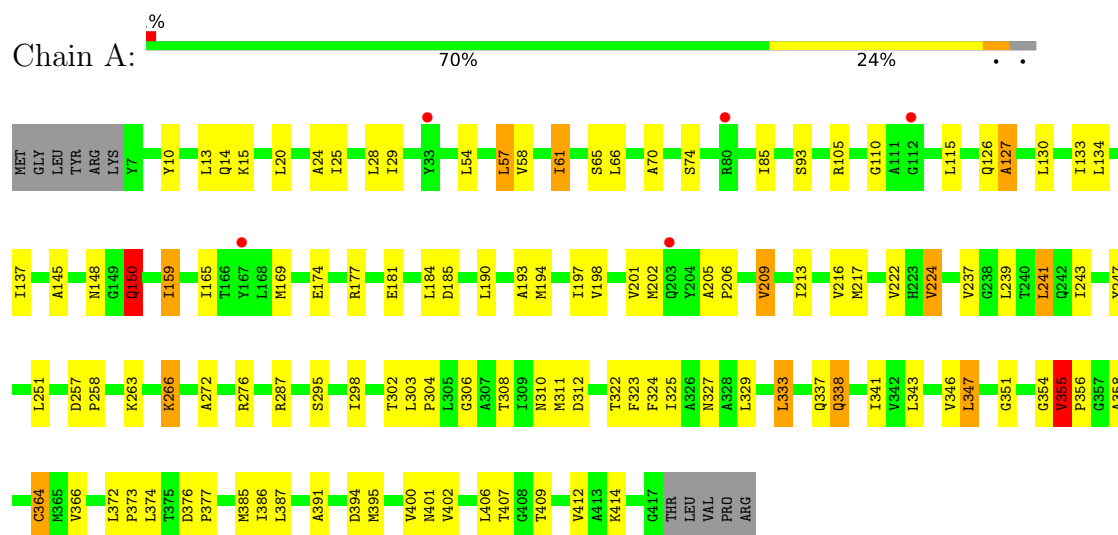
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Hg 1 1	0	0
2	B	1	Total Hg 1 1	0	0
2	C	1	Total Hg 1 1	0	0

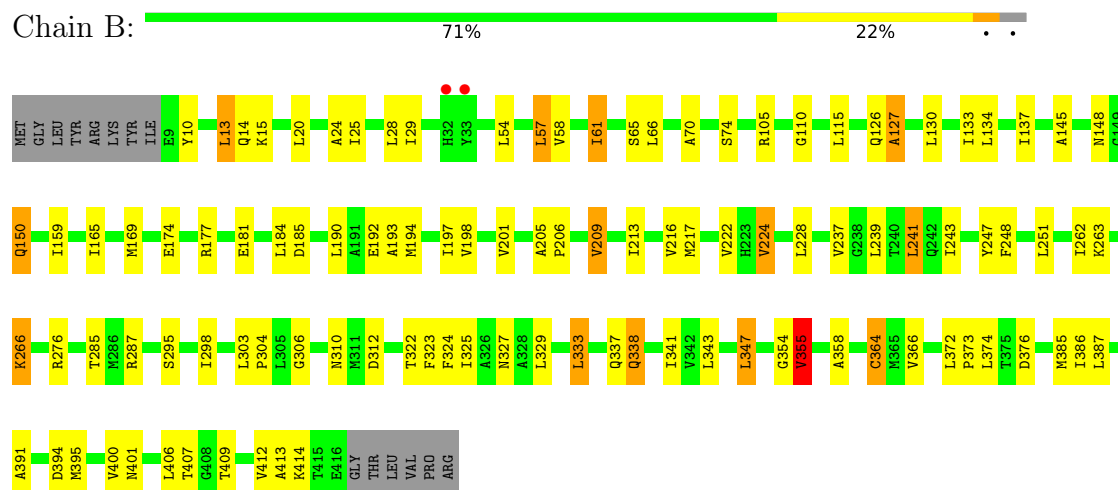
### 3 Residue-property plots

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: GltPh

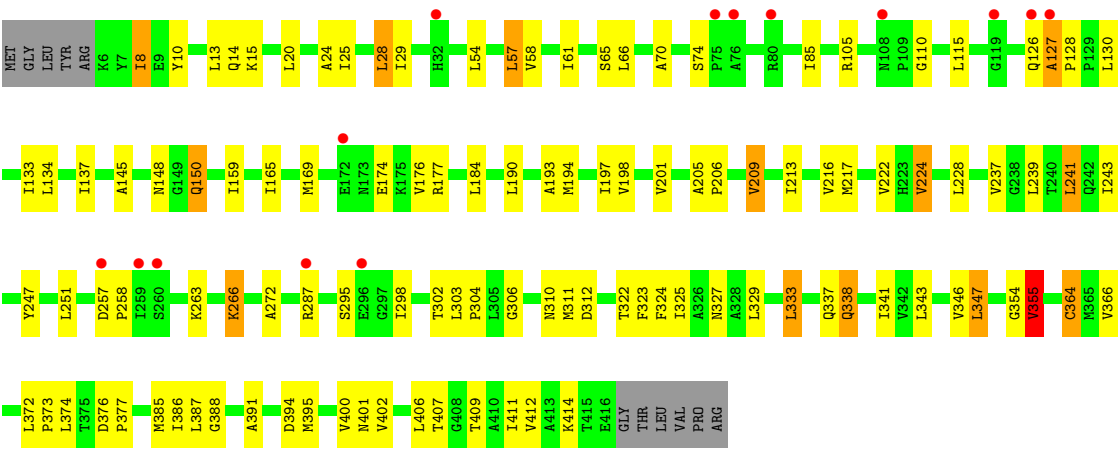


#### • Molecule 1: GltPh



#### • Molecule 1: GltPh





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.95Å 196.84Å 207.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50 14.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-3.50) 95.7 (14.99-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.263 , 0.278 0.263 , 0.282	Depositor DCC
$R_{free}$ test set	1335 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	134.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.30	0/3095	0.55	2/4223 (0.0%)
1	B	0.30	0/3074	0.54	1/4195 (0.0%)
1	C	0.30	0/3096	0.59	1/4225 (0.0%)
All	All	0.30	0/9265	0.56	4/12643 (0.0%)

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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	VAL	CG1-CB-CG2	-18.32	81.59	110.90
1	B	355	VAL	CG1-CB-CG2	-9.19	96.20	110.90
1	A	355	VAL	CG1-CB-CG2	-9.11	96.33	110.90
1	A	150	GLN	CA-CB-CG	5.89	126.36	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	GLN	Peptide



## 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	3036	0	3201	72	0
1	B	3015	0	3180	78	0
1	C	3037	0	3200	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
All	All	9091	0	9581	223	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 12.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:ND2	1:B:401:ASN:HA	1.85	0.91
1:A:145:ALA:HA	1:A:150:GLN:HG2	1.53	0.87
1:A:150:GLN:HE21	1:A:150:GLN:HA	1.43	0.83
1:C:364:CYS:SG	2:C:501:HG:HG	2.00	0.79
1:A:126:GLN:HB2	1:A:127:ALA:HB2	1.67	0.76
1:B:126:GLN:HB2	1:B:127:ALA:HB2	1.67	0.74
1:B:61:ILE:O	1:B:65:SER:HB2	1.87	0.73
1:A:61:ILE:O	1:A:65:SER:HB2	1.89	0.73
1:C:57:LEU:HD13	1:C:198:VAL:HG22	1.71	0.72
1:B:145:ALA:HA	1:B:150:GLN:CG	2.20	0.72
1:B:57:LEU:O	1:B:61:ILE:HG12	1.89	0.71
1:A:85:ILE:HD13	1:A:302:THR:HB	1.73	0.71
1:A:57:LEU:O	1:A:61:ILE:HG12	1.91	0.70
1:C:57:LEU:O	1:C:61:ILE:HG12	1.92	0.70
1:C:145:ALA:HA	1:C:150:GLN:CG	2.22	0.69
1:C:61:ILE:O	1:C:65:SER:HB2	1.92	0.69
1:B:57:LEU:HD13	1:B:198:VAL:HG22	1.76	0.68
1:A:57:LEU:HD13	1:A:198:VAL:HG22	1.75	0.67
1:A:354:GLY:HA2	1:A:355:VAL:O	1.94	0.67
1:C:150:GLN:HE21	1:C:150:GLN:HA	1.59	0.66
1:C:354:GLY:HA2	1:C:355:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLY:HA2	1:B:355:VAL:O	1.96	0.65
1:C:61:ILE:HG23	1:C:194:MET:HB3	1.79	0.65
1:A:61:ILE:HG23	1:A:194:MET:HB3	1.79	0.64
1:B:150:GLN:HE21	1:B:150:GLN:HA	1.61	0.64
1:A:311:MET:HB3	1:A:346:VAL:HG13	1.81	0.63
1:B:310:ASN:HD22	1:B:401:ASN:HA	1.63	0.63
1:B:355:VAL:CG1	1:B:358:ALA:HB2	2.27	0.63
1:B:58:VAL:HG21	1:B:364:CYS:SG	2.38	0.63
1:A:311:MET:HB3	1:A:346:VAL:CG1	2.29	0.63
1:A:355:VAL:CG1	1:A:358:ALA:HB2	2.29	0.63
1:B:61:ILE:HG23	1:B:194:MET:HB3	1.80	0.63
1:C:145:ALA:HA	1:C:150:GLN:HG2	1.81	0.62
1:B:145:ALA:HA	1:B:150:GLN:HG2	1.82	0.61
1:C:85:ILE:HD13	1:C:302:THR:HB	1.80	0.60
1:B:248:PHE:HZ	1:B:262:ILE:HG13	1.67	0.60
1:B:145:ALA:HA	1:B:150:GLN:HG3	1.83	0.59
1:C:130:LEU:HA	1:C:133:ILE:HG22	1.84	0.58
1:B:263:LYS:HA	1:B:266:LYS:HD2	1.85	0.58
1:A:130:LEU:HA	1:A:133:ILE:HG22	1.86	0.57
1:B:310:ASN:HD21	1:B:401:ASN:HA	1.67	0.57
1:A:150:GLN:HE21	1:A:150:GLN:CA	2.15	0.57
1:A:194:MET:O	1:A:198:VAL:HG23	2.05	0.57
1:A:372:LEU:HD12	1:A:372:LEU:H	1.71	0.56
1:B:24:ALA:O	1:B:28:LEU:HB2	2.05	0.56
1:C:10:TYR:HB3	1:C:15:LYS:HE3	1.87	0.56
1:C:263:LYS:HA	1:C:266:LYS:HD2	1.86	0.56
1:C:194:MET:O	1:C:198:VAL:HG23	2.05	0.56
1:A:61:ILE:O	1:A:65:SER:CB	2.54	0.56
1:B:61:ILE:O	1:B:65:SER:CB	2.53	0.56
1:B:130:LEU:HA	1:B:133:ILE:HG22	1.88	0.56
1:A:24:ALA:O	1:A:28:LEU:HB2	2.06	0.55
1:B:322:THR:HG21	1:B:341:ILE:HG21	1.88	0.55
1:C:311:MET:HB3	1:C:346:VAL:HG13	1.87	0.55
1:B:324:PHE:HD2	1:B:386:ILE:HD11	1.72	0.55
1:A:263:LYS:HA	1:A:266:LYS:HD2	1.86	0.55
1:C:372:LEU:H	1:C:372:LEU:HD12	1.71	0.55
1:C:145:ALA:HA	1:C:150:GLN:HG3	1.88	0.55
1:B:194:MET:O	1:B:198:VAL:HG23	2.07	0.55
1:B:372:LEU:HD12	1:B:372:LEU:H	1.72	0.55
1:C:24:ALA:O	1:C:28:LEU:HB2	2.07	0.54
1:C:311:MET:HB3	1:C:346:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:HG2	1:B:395:MET:HA	1.90	0.54
1:A:10:TYR:HB3	1:A:15:LYS:HE3	1.90	0.53
1:B:13:LEU:HD11	1:B:276:ARG:HG3	1.90	0.53
1:C:324:PHE:HD2	1:C:386:ILE:HD11	1.73	0.53
1:C:306:GLY:O	1:C:310:ASN:HB2	2.09	0.53
1:C:322:THR:HG21	1:C:341:ILE:HG21	1.91	0.53
1:B:10:TYR:HB3	1:B:15:LYS:HE3	1.90	0.53
1:A:322:THR:HG21	1:A:341:ILE:HG21	1.90	0.53
1:A:355:VAL:HG11	1:A:358:ALA:HB2	1.91	0.53
1:C:409:THR:HA	1:C:412:VAL:HG12	1.91	0.53
1:B:306:GLY:O	1:B:310:ASN:HB2	2.10	0.52
1:B:323:PHE:O	1:B:327:ASN:HB2	2.10	0.52
1:B:355:VAL:HG12	1:B:358:ALA:HB2	1.91	0.52
1:C:61:ILE:O	1:C:65:SER:CB	2.57	0.52
1:B:355:VAL:HG11	1:B:358:ALA:HB2	1.90	0.52
1:A:409:THR:HA	1:A:412:VAL:HG12	1.90	0.52
1:B:295:SER:HB3	1:B:298:ILE:HD12	1.92	0.52
1:A:306:GLY:O	1:A:310:ASN:HB2	2.09	0.52
1:A:20:LEU:HD12	1:A:213:ILE:HG12	1.93	0.51
1:A:28:LEU:HD21	1:A:222:VAL:HG13	1.92	0.51
1:C:239:LEU:HG	1:C:400:VAL:CG2	2.41	0.51
1:B:20:LEU:HD12	1:B:213:ILE:HG12	1.93	0.51
1:A:58:VAL:HG21	1:A:364:CYS:SG	2.51	0.50
1:B:28:LEU:HD21	1:B:222:VAL:HG13	1.93	0.50
1:C:169:MET:HA	1:C:177:ARG:HG3	1.92	0.50
1:C:54:LEU:HD23	1:C:387:LEU:HD11	1.93	0.50
1:A:324:PHE:HD2	1:A:386:ILE:HD11	1.75	0.50
1:A:323:PHE:O	1:A:327:ASN:HB2	2.11	0.50
1:C:20:LEU:HD12	1:C:213:ILE:HG12	1.93	0.50
1:B:239:LEU:HG	1:B:400:VAL:CG2	2.42	0.50
1:B:409:THR:HA	1:B:412:VAL:HG12	1.92	0.49
1:C:295:SER:HB3	1:C:298:ILE:HD12	1.94	0.49
1:A:295:SER:HB3	1:A:298:ILE:HD12	1.94	0.49
1:A:54:LEU:HD23	1:A:387:LEU:HD11	1.94	0.49
1:A:308:THR:HB	1:A:351:GLY:HA2	1.95	0.49
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.47	0.49
1:B:169:MET:HA	1:B:177:ARG:HG3	1.94	0.49
1:A:169:MET:HA	1:A:177:ARG:HG3	1.95	0.49
1:C:323:PHE:O	1:C:327:ASN:HB2	2.12	0.49
1:A:355:VAL:HG12	1:A:358:ALA:HB2	1.93	0.48
1:C:25:ILE:O	1:C:29:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD23	1:B:387:LEU:HD11	1.95	0.48
1:C:205:ALA:N	1:C:206:PRO:HD2	2.29	0.48
1:B:197:ILE:O	1:B:201:VAL:HG23	2.13	0.48
1:C:28:LEU:HD21	1:C:222:VAL:HG13	1.94	0.48
1:C:324:PHE:HZ	1:C:385:MET:HE2	1.78	0.48
1:B:70:ALA:O	1:B:74:SER:HB2	2.13	0.48
1:C:110:GLY:HA3	1:C:327:ASN:HB3	1.96	0.48
1:C:333:LEU:HD13	1:C:337:GLN:HB2	1.95	0.48
1:A:333:LEU:HD13	1:A:337:GLN:HB2	1.95	0.48
1:C:134:LEU:O	1:C:137:ILE:HG12	2.14	0.48
1:A:239:LEU:HG	1:A:400:VAL:CG2	2.43	0.48
1:A:237:VAL:O	1:A:241:LEU:HB2	2.14	0.47
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.49	0.47
1:B:333:LEU:HD13	1:B:337:GLN:HB2	1.95	0.47
1:A:193:ALA:O	1:A:197:ILE:HG13	2.15	0.47
1:A:324:PHE:HZ	1:A:385:MET:HE2	1.79	0.47
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.48	0.47
1:C:197:ILE:O	1:C:201:VAL:HG23	2.14	0.47
1:A:110:GLY:HA3	1:A:327:ASN:HB3	1.96	0.47
1:C:70:ALA:O	1:C:74:SER:HB2	2.15	0.47
1:B:193:ALA:O	1:B:197:ILE:HG13	2.15	0.47
1:A:25:ILE:O	1:A:29:ILE:HG12	2.15	0.46
1:A:197:ILE:O	1:A:201:VAL:HG23	2.15	0.46
1:C:237:VAL:O	1:C:241:LEU:HB2	2.14	0.46
1:B:134:LEU:O	1:B:137:ILE:HG12	2.15	0.46
1:C:216:VAL:HG11	1:C:385:MET:HG2	1.97	0.46
1:B:237:VAL:O	1:B:241:LEU:HB2	2.15	0.46
1:A:303:LEU:N	1:A:304:PRO:HD2	2.31	0.46
1:B:310:ASN:ND2	1:B:312:ASP:OD2	2.49	0.46
1:C:303:LEU:N	1:C:304:PRO:HD2	2.31	0.46
1:C:343:LEU:O	1:C:347:LEU:HB2	2.16	0.46
1:A:165:ILE:HG21	1:A:184:LEU:HB2	1.98	0.46
1:B:373:PRO:HG2	1:B:376:ASP:HB2	1.98	0.46
1:C:165:ILE:HG21	1:C:184:LEU:HB2	1.98	0.46
1:C:341:ILE:HG23	1:C:366:VAL:HG21	1.98	0.45
1:A:70:ALA:O	1:A:74:SER:HB2	2.16	0.45
1:B:110:GLY:HA3	1:B:327:ASN:HB3	1.97	0.45
1:B:205:ALA:N	1:B:206:PRO:HD2	2.31	0.45
1:B:239:LEU:HG	1:B:400:VAL:HG23	1.98	0.45
1:B:285:THR:HG22	1:B:406:LEU:HD21	1.99	0.45
1:C:127:ALA:HA	1:C:128:PRO:HD3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:OG	1:A:311:MET:HB2	2.17	0.45
1:B:216:VAL:HG11	1:B:385:MET:HG2	1.97	0.45
1:A:391:ALA:O	1:A:395:MET:HG3	2.17	0.45
1:B:341:ILE:HG23	1:B:366:VAL:HG21	1.99	0.45
1:A:134:LEU:O	1:A:137:ILE:HG12	2.17	0.45
1:A:310:ASN:ND2	1:A:312:ASP:OD2	2.50	0.45
1:B:25:ILE:O	1:B:29:ILE:HG12	2.16	0.45
1:B:192:GLU:HG2	1:C:176:VAL:HG13	1.98	0.45
1:B:303:LEU:N	1:B:304:PRO:HD2	2.31	0.45
1:B:310:ASN:ND2	1:B:401:ASN:CA	2.70	0.45
1:C:239:LEU:HG	1:C:400:VAL:HG23	1.99	0.45
1:A:66:LEU:HD22	1:A:159:ILE:HD11	1.99	0.45
1:A:343:LEU:O	1:A:347:LEU:HB2	2.17	0.45
1:B:217:MET:SD	1:B:224:VAL:HG23	2.57	0.45
1:C:58:VAL:HG21	1:C:364:CYS:SG	2.56	0.44
1:A:205:ALA:N	1:A:206:PRO:HD2	2.32	0.44
1:A:190:LEU:O	1:A:194:MET:HG2	2.17	0.44
1:C:213:ILE:H	1:C:213:ILE:HG13	1.67	0.44
1:A:341:ILE:HG23	1:A:366:VAL:HG21	1.99	0.44
1:C:66:LEU:HD22	1:C:159:ILE:HD11	2.00	0.44
1:B:150:GLN:HE21	1:B:150:GLN:CA	2.30	0.44
1:B:190:LEU:O	1:B:194:MET:HG2	2.18	0.44
1:B:310:ASN:HD22	1:B:401:ASN:CG	2.22	0.44
1:A:216:VAL:HG11	1:A:385:MET:HG2	2.00	0.44
1:B:165:ILE:HG21	1:B:184:LEU:HB2	1.98	0.44
1:C:54:LEU:CD2	1:C:387:LEU:HD11	2.48	0.44
1:C:61:ILE:HG23	1:C:194:MET:CB	2.46	0.44
1:A:406:LEU:HA	1:A:409:THR:HG22	2.00	0.43
1:A:202:MET:HE2	1:A:276:ARG:HH12	1.82	0.43
1:B:13:LEU:HG	1:B:276:ARG:NE	2.34	0.43
1:A:239:LEU:HG	1:A:400:VAL:HG23	1.99	0.43
1:B:324:PHE:HZ	1:B:385:MET:HE2	1.83	0.43
1:B:343:LEU:O	1:B:347:LEU:HB2	2.17	0.43
1:C:406:LEU:HA	1:C:409:THR:HG22	2.00	0.43
1:A:373:PRO:HG2	1:A:376:ASP:HB2	2.00	0.43
1:B:298:ILE:HG21	1:B:413:ALA:HB2	2.01	0.43
1:C:193:ALA:O	1:C:197:ILE:HG13	2.18	0.43
1:B:251:LEU:HG	1:B:407:THR:HG23	1.99	0.43
1:C:310:ASN:ND2	1:C:312:ASP:OD2	2.52	0.43
1:B:66:LEU:HD22	1:B:159:ILE:HD11	2.00	0.42
1:C:272:ALA:HB2	1:C:402:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASP:HA	1:C:377:PRO:HD3	1.86	0.42
1:B:391:ALA:O	1:B:395:MET:HG3	2.19	0.42
1:C:373:PRO:HG2	1:C:376:ASP:HB2	2.01	0.42
1:B:105:ARG:HH21	1:B:338:GLN:HG3	1.84	0.42
1:A:105:ARG:HH21	1:A:338:GLN:HG3	1.85	0.42
1:C:391:ALA:O	1:C:395:MET:HG3	2.19	0.42
1:C:310:ASN:ND2	1:C:401:ASN:HA	2.34	0.42
1:A:209:VAL:O	1:A:213:ILE:HG13	2.19	0.42
1:A:217:MET:SD	1:A:224:VAL:HG23	2.60	0.42
1:C:8:ILE:C	1:C:10:TYR:H	2.22	0.42
1:C:217:MET:SD	1:C:224:VAL:HG23	2.60	0.42
1:A:272:ALA:HB2	1:A:402:VAL:HG21	2.01	0.42
1:B:228:LEU:HD21	1:B:385:MET:HB3	2.01	0.42
1:C:10:TYR:HD2	1:C:15:LYS:HG3	1.85	0.42
1:B:209:VAL:O	1:B:213:ILE:HG13	2.20	0.42
1:A:376:ASP:HA	1:A:377:PRO:HD3	1.86	0.41
1:B:54:LEU:CD2	1:B:387:LEU:HD11	2.50	0.41
1:C:190:LEU:O	1:C:194:MET:HG2	2.20	0.41
1:A:61:ILE:HG23	1:A:194:MET:CB	2.47	0.41
1:A:181:GLU:O	1:A:185:ASP:HB2	2.20	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.92	0.41
1:C:228:LEU:HD21	1:C:385:MET:HB3	2.02	0.41
1:A:251:LEU:HG	1:A:407:THR:HG23	2.03	0.41
1:A:15:LYS:HB3	1:A:206:PRO:HB3	2.03	0.41
1:B:61:ILE:HG23	1:B:194:MET:CB	2.48	0.41
1:C:251:LEU:HA	1:C:411:ILE:HD11	2.03	0.41
1:B:126:GLN:CB	1:B:127:ALA:HB2	2.45	0.41
1:B:181:GLU:O	1:B:185:ASP:HB2	2.21	0.41
1:C:209:VAL:O	1:C:213:ILE:HG13	2.21	0.41
1:C:251:LEU:HG	1:C:407:THR:HG23	2.01	0.41
1:B:248:PHE:HZ	1:B:262:ILE:CG1	2.34	0.40
1:C:15:LYS:HB3	1:C:206:PRO:HB3	2.03	0.40
1:A:310:ASN:ND2	1:A:401:ASN:HA	2.36	0.40
1:A:198:VAL:CG1	1:A:356:PRO:HG2	2.51	0.40
1:B:406:LEU:HA	1:B:409:THR:HG22	2.03	0.40
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.92	0.40
1:C:105:ARG:HH21	1:C:338:GLN:HG3	1.86	0.40
1:C:209:VAL:CG2	1:C:388:GLY:HA2	2.51	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	409/422 (97%)	387 (95%)	20 (5%)	2 (0%)	29	68
1	B	406/422 (96%)	387 (95%)	17 (4%)	2 (0%)	29	68
1	C	409/422 (97%)	386 (94%)	21 (5%)	2 (0%)	29	68
All	All	1224/1266 (97%)	1160 (95%)	58 (5%)	6 (0%)	29	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ALA
1	B	127	ALA
1	C	127	ALA
1	C	355	VAL
1	A	355	VAL
1	B	355	VAL

### 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	319/330 (97%)	296 (93%)	23 (7%)	14	45
1	B	317/330 (96%)	295 (93%)	22 (7%)	15	47
1	C	319/330 (97%)	295 (92%)	24 (8%)	13	43
All	All	955/990 (96%)	886 (93%)	69 (7%)	14	45

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	GLN
1	A	57	LEU
1	A	61	ILE
1	A	115	LEU
1	A	148	ASN
1	A	150	GLN
1	A	159	ILE
1	A	174	GLU
1	A	209	VAL
1	A	224	VAL
1	A	241	LEU
1	A	266	LYS
1	A	287	ARG
1	A	325	ILE
1	A	329	LEU
1	A	333	LEU
1	A	338	GLN
1	A	347	LEU
1	A	364	CYS
1	A	374	LEU
1	A	394	ASP
1	A	414	LYS
1	B	13	LEU
1	B	14	GLN
1	B	57	LEU
1	B	61	ILE
1	B	115	LEU
1	B	148	ASN
1	B	150	GLN
1	B	174	GLU
1	B	209	VAL
1	B	224	VAL
1	B	241	LEU
1	B	266	LYS
1	B	287	ARG
1	B	325	ILE
1	B	329	LEU
1	B	333	LEU
1	B	338	GLN
1	B	347	LEU
1	B	364	CYS

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Mol	Chain	Res	Type
1	B	374	LEU
1	B	394	ASP
1	B	414	LYS
1	C	8	ILE
1	C	13	LEU
1	C	14	GLN
1	C	28	LEU
1	C	57	LEU
1	C	115	LEU
1	C	148	ASN
1	C	150	GLN
1	C	174	GLU
1	C	209	VAL
1	C	224	VAL
1	C	241	LEU
1	C	266	LYS
1	C	287	ARG
1	C	325	ILE
1	C	329	LEU
1	C	333	LEU
1	C	338	GLN
1	C	347	LEU
1	C	355	VAL
1	C	364	CYS
1	C	374	LEU
1	C	394	ASP
1	C	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	310	ASN
1	B	150	GLN
1	B	310	ASN
1	C	150	GLN
1	C	310	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	411/422 (97%)	-0.48	5 (1%) 79 73	86, 138, 184, 208	0
1	B	408/422 (96%)	-0.46	2 (0%) 91 88	91, 134, 183, 233	0
1	C	411/422 (97%)	-0.41	14 (3%) 45 40	92, 149, 217, 285	0
All	All	1230/1266 (97%)	-0.45	21 (1%) 70 64	86, 139, 198, 285	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	ALA	4.8
1	A	112	GLY	3.5
1	B	33	TYR	3.4
1	C	257	ASP	3.2
1	A	80	ARG	3.1
1	C	108	ASN	2.9
1	C	75	PRO	2.9
1	C	260	SER	2.7
1	A	33	TYR	2.6
1	B	32	HIS	2.6
1	C	127	ALA	2.6
1	C	259	ILE	2.5
1	C	32	HIS	2.3
1	C	126	GLN	2.3
1	C	80	ARG	2.2
1	C	296	GLU	2.2
1	C	287	ARG	2.2
1	C	119	GLY	2.1
1	C	172	GLU	2.1
1	A	167	TYR	2.0
1	A	203	GLN	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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	HG	B	501	1/1	0.88	0.09	202,202,202,202	1
2	HG	A	501	1/1	0.92	0.07	213,213,213,213	1
2	HG	C	501	1/1	0.96	0.05	226,226,226,226	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.