



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 2NWW / pdb_00002nww
Title : Crystal structure of GltPh in complex with TBOA
Authors : Gouaux, E.; Boudker, O.; Ryan, R.; Yernool, D.; Shimamoto, K.
Deposited on : 2006-11-16
Resolution : 3.20 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

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>.

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

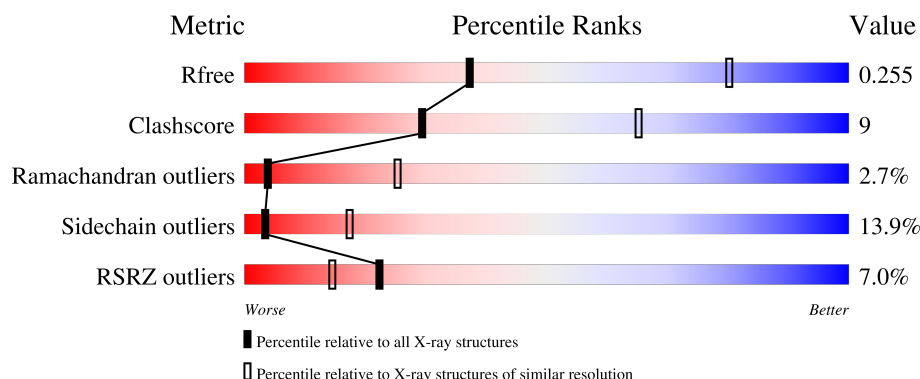
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 63%27%6%
1	B	422	5% 72%21%
1	C	422	11% 70%23%

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
2	TB1	A	423	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8772 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			
1	B	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			
1	C	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			

There are 36 discrepancies between the modelled and reference sequences:

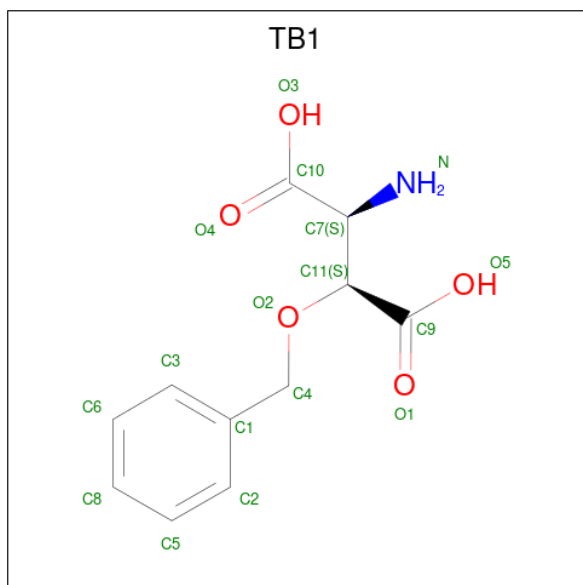
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	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	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	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	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

- Molecule 2 is (3S)-3-(BENZYLOXY)-L-ASPARTIC ACID (CCD ID: TB1) (formula: $C_{11}H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	11	1	5		
2	B	1	Total	C	N	O	0	0
			17	11	1	5		
2	C	1	Total	C	N	O	0	0
			17	11	1	5		

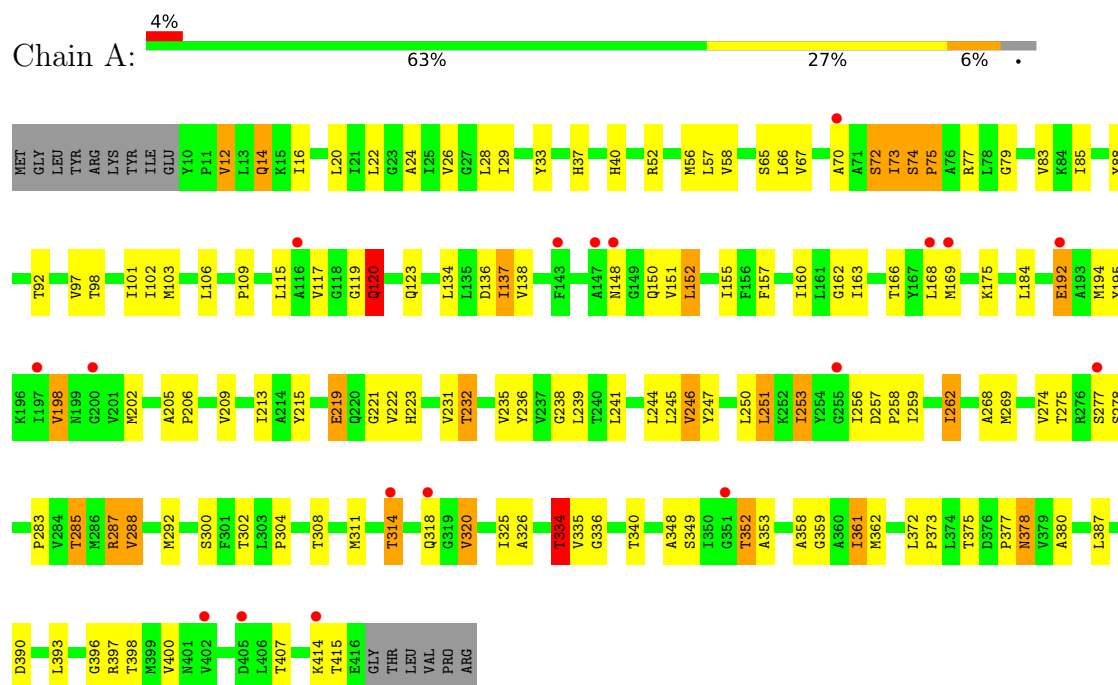
- Molecule 3 is water.

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

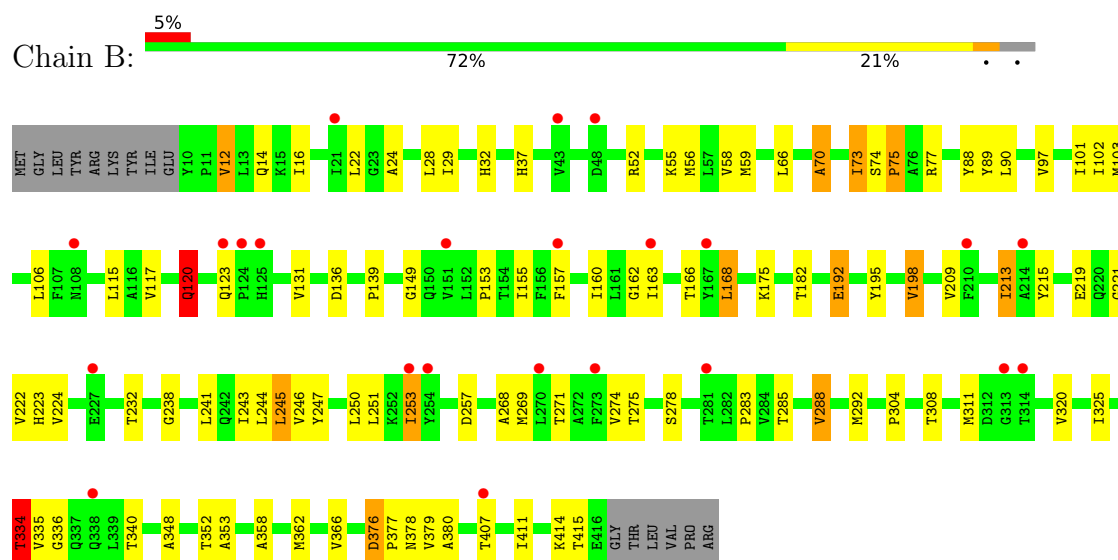
3 Residue-property plots [i](#)

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.

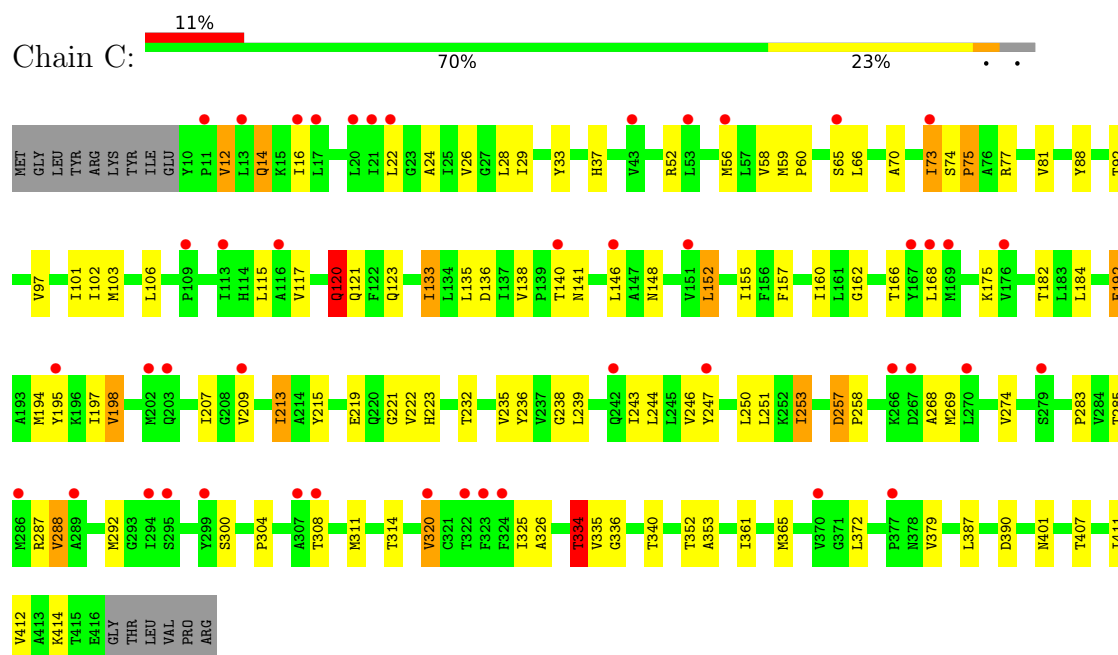
- Molecule 1: 425aa long hypothetical proton glutamate symport protein



- Molecule 1: 425aa long hypothetical proton glutamate symport protein



- Molecule 1: 425aa long hypothetical proton glutamate symport protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.25Å 115.25Å 322.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.20 99.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	74.8 (100.00-3.20) 75.2 (99.81-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.241 , 0.260 0.237 , 0.255	Depositor DCC
R_{free} test set	1516 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	135.0	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 217.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8772	wwPDB-VP
Average B, all atoms (Å ²)	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TB1

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	0.59	0/2961	1.00	4/4052 (0.1%)
1	B	0.53	0/2961	0.95	6/4052 (0.1%)
1	C	0.51	0/2961	0.95	6/4052 (0.1%)
All	All	0.54	0/8883	0.97	16/12156 (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	B	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	N-CA-C	8.24	118.83	108.45
1	A	14	GLN	N-CA-C	-8.18	104.17	114.56
1	B	175	LYS	N-CA-C	-7.63	104.50	113.88
1	C	14	GLN	N-CA-C	-7.05	104.55	113.72
1	A	67	VAL	N-CA-C	-7.02	103.93	110.53
1	C	175	LYS	N-CA-C	-6.59	105.77	113.88
1	B	257	ASP	CA-C-N	5.66	125.33	119.05
1	B	257	ASP	C-N-CA	5.66	125.33	119.05
1	A	175	LYS	N-CA-C	-5.60	106.12	113.12
1	C	257	ASP	CA-C-N	5.58	124.77	118.97
1	C	257	ASP	C-N-CA	5.58	124.77	118.97
1	B	120	GLN	N-CA-C	5.42	115.19	108.19
1	C	120	GLN	N-CA-C	5.25	114.96	108.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ILE	N-CA-C	-5.16	107.72	111.90
1	B	376	ASP	CA-C-N	5.11	124.77	119.56
1	B	376	ASP	C-N-CA	5.11	124.77	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ALA	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	2906	0	2955	71	0
1	B	2906	0	2955	41	0
1	C	2906	0	2955	56	0
2	A	17	0	11	2	0
2	B	17	0	11	1	0
2	C	17	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8772	0	8898	151	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 9.

All (151) 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:155:ILE:HD11	1:A:304:PRO:HB2	1.61	0.83
1:A:157:PHE:HD1	1:C:56:MET:HE2	1.43	0.82
1:A:209:VAL:HG22	1:A:274:VAL:HG21	1.63	0.80
1:A:74:SER:HB2	1:A:75:PRO:HD3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.74	0.68
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.76	0.68
1:B:192:GLU:HB3	1:C:168:LEU:HD21	1.78	0.66
1:A:318:GLN:HE22	1:A:362:MET:HE2	1.61	0.65
1:C:387:LEU:HA	1:C:390:ASP:HB2	1.78	0.65
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.79	0.65
1:A:134:LEU:O	1:A:137:ILE:HG13	1.98	0.63
1:B:251:LEU:HD13	1:B:407:THR:HG23	1.81	0.63
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.13	0.63
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.82	0.62
1:C:311:MET:HB3	1:C:314:THR:HB	1.82	0.62
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.83	0.60
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.83	0.60
1:A:311:MET:HB3	1:A:314:THR:HB	1.83	0.59
1:B:209:VAL:HG22	1:B:274:VAL:HG21	1.85	0.59
1:A:195:TYR:O	1:A:198:VAL:HG12	2.03	0.59
1:B:358:ALA:HB3	2:B:423:TB1:H5	1.84	0.59
1:B:195:TYR:O	1:B:198:VAL:HG12	2.03	0.58
1:B:103:MET:HE3	1:B:238:GLY:HA2	1.85	0.56
1:C:215:TYR:CE1	1:C:219:GLU:HG3	2.39	0.56
1:A:120:GLN:HB2	1:A:380:ALA:HB1	1.88	0.56
1:C:103:MET:HE3	1:C:238:GLY:HA2	1.88	0.55
1:A:334:THR:O	1:A:336:GLY:N	2.40	0.55
1:A:268:ALA:HB1	1:A:285:THR:HG23	1.88	0.55
1:C:59:MET:HE2	1:C:146:LEU:HA	1.88	0.55
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.87	0.55
1:B:55:LYS:HB3	1:C:140:THR:HG23	1.89	0.54
1:A:215:TYR:CE1	1:A:219:GLU:HG3	2.43	0.54
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.21	0.54
1:B:74:SER:HB2	1:B:75:PRO:HD3	1.89	0.53
1:C:221:GLY:C	1:C:223:HIS:H	2.16	0.53
1:A:314:THR:HA	1:A:397:ARG:HD2	1.90	0.53
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.91	0.53
1:A:85:ILE:HG21	1:A:302:THR:HG22	1.91	0.52
1:A:232:THR:HA	1:A:393:LEU:HD21	1.92	0.52
1:B:334:THR:O	1:B:336:GLY:N	2.43	0.52
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.91	0.52
1:B:247:TYR:O	1:B:251:LEU:HB2	2.09	0.51
1:B:73:ILE:HB	1:B:77:ARG:HG2	1.92	0.51
1:C:209:VAL:HG22	1:C:274:VAL:HG21	1.93	0.51
1:C:195:TYR:O	1:C:198:VAL:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:TYR:CE1	1:B:219:GLU:HG3	2.46	0.51
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.93	0.51
1:A:325:ILE:HG22	1:A:372:LEU:HD13	1.93	0.51
1:A:157:PHE:CD1	1:C:56:MET:HE2	2.34	0.51
1:B:325:ILE:HG21	1:B:379:VAL:HG13	1.92	0.51
1:B:120:GLN:HB2	1:B:380:ALA:HB1	1.93	0.50
1:C:24:ALA:O	1:C:28:LEU:HB2	2.11	0.50
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.93	0.50
1:C:334:THR:O	1:C:336:GLY:N	2.44	0.50
1:A:138:VAL:O	1:C:52:ARG:NH2	2.32	0.50
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.77	0.49
1:C:268:ALA:HB1	1:C:285:THR:HG22	1.94	0.49
1:A:148:ASN:O	1:A:150:GLN:HG2	2.13	0.49
1:A:247:TYR:O	1:A:251:LEU:HB2	2.12	0.49
1:A:259:ILE:H	1:A:259:ILE:HD12	1.77	0.49
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.28	0.49
1:C:236:TYR:HA	1:C:239:LEU:HD12	1.93	0.49
1:A:359:GLY:H	2:A:423:TB1:H5	1.78	0.48
1:B:24:ALA:O	1:B:28:LEU:HB2	2.12	0.48
1:A:109:PRO:HB3	1:A:231:VAL:HG22	1.96	0.48
1:C:97:VAL:O	1:C:101:ILE:HG12	2.11	0.48
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.95	0.48
1:A:348:ALA:O	1:A:352:THR:HB	2.13	0.48
1:A:202:MET:HG3	1:A:287:ARG:HH12	1.79	0.48
1:B:271:THR:O	1:B:275:THR:OG1	2.28	0.48
1:C:215:TYR:CZ	1:C:219:GLU:HG3	2.49	0.48
1:A:65:SER:O	1:A:300:SER:CB	2.62	0.47
1:A:152:LEU:HD13	1:A:308:THR:HG21	1.95	0.47
1:A:221:GLY:C	1:A:223:HIS:H	2.22	0.47
1:B:12:VAL:C	1:B:14:GLN:H	2.21	0.47
1:A:73:ILE:HB	1:A:77:ARG:HG2	1.96	0.47
1:C:251:LEU:HD13	1:C:407:THR:HG23	1.96	0.47
1:A:236:TYR:CE1	1:A:396:GLY:HA3	2.49	0.47
1:A:275:THR:HG22	1:A:277:SER:HB3	1.96	0.47
1:C:325:ILE:HG21	1:C:379:VAL:HG13	1.97	0.47
1:C:401:ASN:ND2	2:C:423:TB1:O4	2.31	0.47
1:A:12:VAL:C	1:A:14:GLN:H	2.22	0.46
1:A:387:LEU:HA	1:A:390:ASP:HB2	1.96	0.46
1:A:103:MET:HE3	1:A:238:GLY:HA2	1.97	0.46
1:B:268:ALA:HB1	1:B:285:THR:HG22	1.97	0.46
1:A:358:ALA:HA	1:A:361:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:H	1:C:141:ASN:HD22	1.62	0.46
1:C:247:TYR:O	1:C:251:LEU:HB2	2.15	0.46
1:A:209:VAL:HG13	1:A:274:VAL:HG11	1.98	0.46
1:B:243:ILE:HG22	1:B:244:LEU:HD23	1.99	0.45
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.51	0.45
1:B:288:VAL:O	1:B:292:MET:HB2	2.16	0.45
1:A:348:ALA:HB1	1:A:362:MET:HG2	1.99	0.45
1:C:243:ILE:HA	1:C:247:TYR:CD1	2.52	0.45
1:A:56:MET:CE	1:B:157:PHE:HD1	2.30	0.45
1:A:79:GLY:O	1:A:83:VAL:HG23	2.17	0.45
1:C:73:ILE:HB	1:C:77:ARG:HG2	1.98	0.45
1:A:168:LEU:HD21	1:C:192:GLU:HB3	1.98	0.45
1:A:117:VAL:HG13	1:A:377:PRO:O	2.16	0.45
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.86	0.45
1:A:262:ILE:HD13	1:A:262:ILE:HA	1.74	0.45
1:B:221:GLY:C	1:B:223:HIS:H	2.25	0.45
1:A:97:VAL:O	1:A:101:ILE:HG12	2.17	0.45
1:C:288:VAL:O	1:C:292:MET:HB2	2.17	0.44
1:A:85:ILE:HG12	1:A:302:THR:HB	1.98	0.44
1:B:88:TYR:HD2	1:B:89:TYR:CD2	2.35	0.44
1:C:251:LEU:HD23	1:C:258:PRO:HA	1.99	0.44
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.99	0.44
1:C:326:ALA:HB2	1:C:372:LEU:HD11	1.99	0.44
1:A:57:LEU:HD22	1:A:194:MET:HE3	1.99	0.44
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.98	0.44
1:C:74:SER:HB2	1:C:75:PRO:HD3	2.00	0.44
1:C:365:MET:HE2	1:C:365:MET:HB3	1.82	0.44
1:C:194:MET:HA	1:C:197:ILE:HD12	2.00	0.43
1:A:398:THR:HG23	2:A:423:TB1:C10	2.48	0.43
1:A:251:LEU:HD23	1:A:258:PRO:HA	2.01	0.43
1:B:213:ILE:H	1:B:213:ILE:HG13	1.64	0.43
1:C:12:VAL:C	1:C:14:GLN:H	2.27	0.43
1:A:24:ALA:O	1:A:28:LEU:HB2	2.19	0.43
1:B:376:ASP:HA	1:B:377:PRO:HD3	1.81	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.81	0.43
1:A:251:LEU:HD13	1:A:407:THR:HG23	2.00	0.43
1:A:103:MET:HE1	1:A:241:LEU:HD22	2.00	0.43
1:A:137:ILE:HG23	1:A:152:LEU:HB3	2.01	0.43
1:A:378:ASN:HD22	1:A:378:ASN:HA	1.54	0.42
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.87	0.42
1:A:40:HIS:HB2	1:A:215:TYR:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:O	1:B:101:ILE:HG12	2.19	0.42
1:B:59:MET:HG3	1:C:141:ASN:ND2	2.34	0.42
1:C:81:VAL:HG13	1:C:412:VAL:HG11	2.02	0.42
1:B:52:ARG:HG3	1:C:135:LEU:HD22	2.02	0.42
1:A:241:LEU:O	1:A:245:LEU:HB2	2.20	0.42
1:A:205:ALA:N	1:A:206:PRO:HD2	2.36	0.41
1:B:241:LEU:O	1:B:245:LEU:HB2	2.21	0.41
1:C:198:VAL:HG13	1:C:287:ARG:HD2	2.03	0.41
1:C:207:ILE:HD13	1:C:207:ILE:HA	1.87	0.41
1:A:246:VAL:O	1:A:250:LEU:HB2	2.21	0.41
1:A:288:VAL:O	1:A:292:MET:HB2	2.21	0.41
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.93	0.41
1:C:213:ILE:H	1:C:213:ILE:HG13	1.71	0.41
1:A:192:GLU:HB3	1:B:168:LEU:HD21	2.02	0.41
1:A:373:PRO:C	1:A:375:THR:H	2.28	0.41
1:B:52:ARG:NH2	1:C:138:VAL:O	2.47	0.41
1:C:60:PRO:HB2	1:C:194:MET:HG3	2.03	0.41
1:C:120:GLN:HB2	1:C:121:GLN:H	1.66	0.41
1:C:65:SER:O	1:C:300:SER:CB	2.69	0.40
1:A:326:ALA:HB2	1:A:372:LEU:HD11	2.02	0.40
1:B:348:ALA:HB1	1:B:362:MET:HG2	2.03	0.40
1:C:235:VAL:HG22	1:C:320:VAL:HG11	2.03	0.40
1:A:157:PHE:HE1	1:C:194:MET:HE1	1.86	0.40
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.56	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	405/422 (96%)	363 (90%)	29 (7%)	13 (3%)	3 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	405/422 (96%)	368 (91%)	27 (7%)	10 (2%)	4	27
1	C	405/422 (96%)	364 (90%)	31 (8%)	10 (2%)	4	27
All	All	1215/1266 (96%)	1095 (90%)	87 (7%)	33 (3%)	4	25

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	THR
1	A	335	VAL
1	A	353	ALA
1	B	73	ILE
1	B	334	THR
1	B	335	VAL
1	B	353	ALA
1	C	12	VAL
1	C	335	VAL
1	A	12	VAL
1	A	73	ILE
1	A	222	VAL
1	B	12	VAL
1	B	66	LEU
1	C	73	ILE
1	C	334	THR
1	A	66	LEU
1	A	72	SER
1	A	115	LEU
1	B	75	PRO
1	B	115	LEU
1	B	222	VAL
1	C	66	LEU
1	C	115	LEU
1	C	222	VAL
1	C	353	ALA
1	A	75	PRO
1	A	123	GLN
1	B	123	GLN
1	C	75	PRO
1	C	123	GLN
1	A	74	SER
1	A	119	GLY

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	283/330 (86%)	237 (84%)	46 (16%)	2	12
1	B	283/330 (86%)	245 (87%)	38 (13%)	4	19
1	C	283/330 (86%)	249 (88%)	34 (12%)	5	23
All	All	849/990 (86%)	731 (86%)	118 (14%)	3	17

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	20	LEU
1	A	22	LEU
1	A	26	VAL
1	A	29	ILE
1	A	33	TYR
1	A	37	HIS
1	A	72	SER
1	A	98	THR
1	A	102	ILE
1	A	106	LEU
1	A	120	GLN
1	A	137	ILE
1	A	151	VAL
1	A	152	LEU
1	A	160	ILE
1	A	163	ILE
1	A	166	THR
1	A	169	MET
1	A	184	LEU
1	A	192	GLU
1	A	198	VAL
1	A	213	ILE
1	A	219	GLU
1	A	232	THR
1	A	244	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	246	VAL
1	A	251	LEU
1	A	253	ILE
1	A	256	ILE
1	A	262	ILE
1	A	269	MET
1	A	278	SER
1	A	285	THR
1	A	287	ARG
1	A	288	VAL
1	A	314	THR
1	A	320	VAL
1	A	334	THR
1	A	340	THR
1	A	349	SER
1	A	352	THR
1	A	361	ILE
1	A	378	ASN
1	A	414	LYS
1	A	415	THR
1	B	16	ILE
1	B	22	LEU
1	B	29	ILE
1	B	32	HIS
1	B	37	HIS
1	B	90	LEU
1	B	102	ILE
1	B	106	LEU
1	B	117	VAL
1	B	120	GLN
1	B	131	VAL
1	B	160	ILE
1	B	163	ILE
1	B	166	THR
1	B	168	LEU
1	B	182	THR
1	B	192	GLU
1	B	198	VAL
1	B	213	ILE
1	B	224	VAL
1	B	232	THR
1	B	245	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	VAL
1	B	253	ILE
1	B	269	MET
1	B	278	SER
1	B	288	VAL
1	B	308	THR
1	B	311	MET
1	B	320	VAL
1	B	334	THR
1	B	340	THR
1	B	352	THR
1	B	366	VAL
1	B	378	ASN
1	B	411	ILE
1	B	414	LYS
1	B	415	THR
1	C	16	ILE
1	C	22	LEU
1	C	26	VAL
1	C	29	ILE
1	C	33	TYR
1	C	37	HIS
1	C	102	ILE
1	C	106	LEU
1	C	117	VAL
1	C	120	GLN
1	C	133	ILE
1	C	148	ASN
1	C	152	LEU
1	C	160	ILE
1	C	166	THR
1	C	182	THR
1	C	184	LEU
1	C	192	GLU
1	C	198	VAL
1	C	213	ILE
1	C	232	THR
1	C	244	LEU
1	C	246	VAL
1	C	253	ILE
1	C	269	MET
1	C	288	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	308	THR
1	C	320	VAL
1	C	334	THR
1	C	340	THR
1	C	352	THR
1	C	361	ILE
1	C	411	ILE
1	C	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	148	ASN
1	A	173	ASN
1	A	310	ASN
1	A	318	GLN
1	A	378	ASN
1	B	120	GLN
1	B	123	GLN
1	B	173	ASN
1	B	368	HIS
1	B	378	ASN
1	C	120	GLN
1	C	188	ASN
1	C	203	GLN
1	C	310	ASN
1	C	378	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

3 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	TB1	C	423	-	16,17,17	1.55	2 (12%)	19,22,22	1.69	2 (10%)
2	TB1	A	423	-	16,17,17	1.71	3 (18%)	19,22,22	1.54	1 (5%)
2	TB1	B	423	-	16,17,17	1.58	2 (12%)	19,22,22	1.43	1 (5%)

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	TB1	C	423	-	-	10/17/17/17	0/1/1/1
2	TB1	A	423	-	-	10/17/17/17	0/1/1/1
2	TB1	B	423	-	-	11/17/17/17	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	423	TB1	C4-C1	-4.76	1.39	1.50
2	B	423	TB1	C4-C1	-4.47	1.40	1.50
2	A	423	TB1	C4-C1	-3.86	1.41	1.50
2	A	423	TB1	O2-C11	3.44	1.46	1.42
2	A	423	TB1	O1-C9	3.33	1.32	1.22
2	B	423	TB1	O2-C11	2.88	1.45	1.42
2	C	423	TB1	O2-C11	2.24	1.44	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	423	TB1	O2-C4-C1	5.70	122.98	109.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	423	TB1	O2-C4-C1	5.66	122.89	109.91
2	B	423	TB1	O2-C4-C1	5.30	122.08	109.91
2	C	423	TB1	O2-C11-C9	-3.73	106.68	112.26

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	423	TB1	C7-C11-O2-C4
2	A	423	TB1	O2-C11-C9-O5
2	A	423	TB1	O2-C11-C9-O1
2	A	423	TB1	O2-C11-C7-N
2	A	423	TB1	C9-C11-C7-C10
2	A	423	TB1	C9-C11-C7-N
2	B	423	TB1	C7-C11-O2-C4
2	B	423	TB1	O2-C11-C9-O5
2	B	423	TB1	O2-C11-C9-O1
2	B	423	TB1	O2-C11-C7-N
2	B	423	TB1	C9-C11-C7-C10
2	B	423	TB1	C9-C11-C7-N
2	C	423	TB1	C7-C11-O2-C4
2	C	423	TB1	O2-C11-C9-O5
2	C	423	TB1	O2-C11-C9-O1
2	C	423	TB1	C9-C11-C7-C10
2	C	423	TB1	O4-C10-C7-N
2	C	423	TB1	C1-C4-O2-C11
2	A	423	TB1	C9-C11-O2-C4
2	C	423	TB1	C9-C11-O2-C4
2	C	423	TB1	O2-C11-C7-N
2	B	423	TB1	O4-C10-C7-N
2	B	423	TB1	C9-C11-O2-C4
2	A	423	TB1	O2-C11-C7-C10
2	A	423	TB1	O3-C10-C7-N
2	B	423	TB1	O2-C11-C7-C10
2	C	423	TB1	O3-C10-C7-N
2	B	423	TB1	C1-C4-O2-C11
2	B	423	TB1	O3-C10-C7-N
2	A	423	TB1	O4-C10-C7-N
2	C	423	TB1	C9-C11-C7-N

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	423	TB1	1	0
2	A	423	TB1	2	0
2	B	423	TB1	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/422 (96%)	0.06	18 (4%) 39 24	162, 192, 224, 262	0
1	B	407/422 (96%)	0.31	23 (5%) 29 19	158, 202, 229, 263	0
1	C	407/422 (96%)	0.59	45 (11%) 10 7	163, 204, 237, 274	0
All	All	1221/1266 (96%)	0.32	86 (7%) 22 14	158, 199, 231, 274	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	LEU	7.2
1	C	167	TYR	6.8
1	C	267	ASP	5.5
1	C	16	ILE	5.3
1	C	324	PHE	5.2
1	C	286	MET	4.8
1	B	124	PRO	4.7
1	B	48	ASP	4.4
1	B	123	GLN	4.4
1	B	314	THR	4.4
1	A	169	MET	4.3
1	C	308	THR	4.3
1	C	17	LEU	4.0
1	B	163	ILE	3.9
1	B	210	PHE	3.9
1	C	140	THR	3.8
1	B	108	ASN	3.7
1	B	214	ALA	3.6
1	C	279	SER	3.5
1	B	167	TYR	3.4
1	B	227	GLU	3.4
1	A	405	ASP	3.4
1	C	322	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	295	SER	3.3
1	A	255	GLY	3.3
1	C	247	TYR	3.3
1	C	116	ALA	3.3
1	A	200	GLY	3.2
1	C	209	VAL	3.1
1	A	168	LEU	3.1
1	A	148	ASN	3.0
1	A	277	SER	3.0
1	C	202	MET	3.0
1	B	313	GLY	3.0
1	C	370	VAL	3.0
1	C	169	MET	3.0
1	C	289	ALA	3.0
1	C	377	PRO	2.8
1	B	338	GLN	2.8
1	C	299	TYR	2.8
1	C	65	SER	2.8
1	C	294	ILE	2.8
1	B	281	THR	2.8
1	C	13	LEU	2.7
1	B	151	VAL	2.7
1	B	407	THR	2.7
1	A	147	ALA	2.7
1	A	192	GLU	2.7
1	C	307	ALA	2.6
1	C	53	LEU	2.5
1	A	197	ILE	2.5
1	C	56	MET	2.5
1	A	318	GLN	2.5
1	A	314	THR	2.4
1	C	21	ILE	2.4
1	A	70	ALA	2.4
1	B	270	LEU	2.4
1	C	73	ILE	2.3
1	B	125	HIS	2.3
1	A	143	PHE	2.3
1	B	273	PHE	2.3
1	C	323	PHE	2.3
1	C	176	VAL	2.3
1	A	414	LYS	2.3
1	C	20	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	22	LEU	2.3
1	C	168	LEU	2.3
1	A	402	VAL	2.3
1	C	195	TYR	2.3
1	C	203	GLN	2.3
1	B	157	PHE	2.3
1	B	43	VAL	2.2
1	C	43	VAL	2.2
1	C	11	PRO	2.2
1	C	146	LEU	2.1
1	C	242	GLN	2.1
1	C	109	PRO	2.1
1	A	351	GLY	2.1
1	C	266	LYS	2.1
1	A	116	ALA	2.1
1	B	253	ILE	2.1
1	C	151	VAL	2.0
1	C	320	VAL	2.0
1	B	21	ILE	2.0
1	B	254	TYR	2.0
1	C	113	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TB1	A	423	17/17	0.77	0.55	179,185,198,198	0
2	TB1	C	423	17/17	0.82	0.22	203,208,210,211	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TB1	B	423	17/17	0.92	0.15	237,242,252,252	0

6.5 Other polymers [i](#)

There are no such residues in this entry.