



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:07 pm GMT

PDB ID : 4KY0
Title : Crystal structure of a substrate-free glutamate transporter homologue from *Thermococcus kodakarensis*
Authors : Guskov, A.; Jensen, S.; Rempel, S.; Hanelt, I.; Slotboom, D.J.
Deposited on : 2013-05-28
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

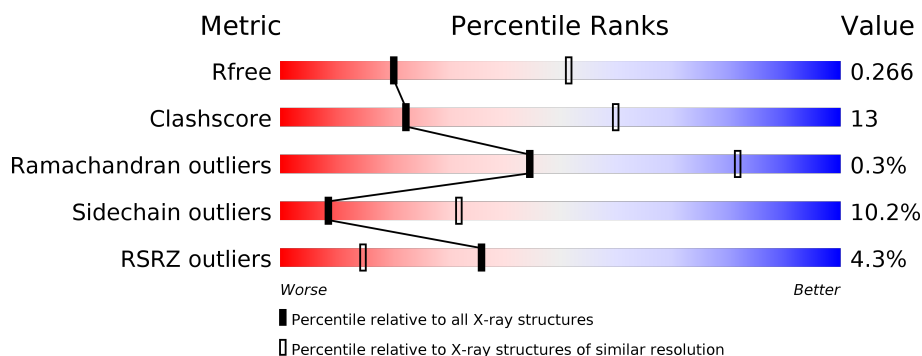
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 ≥ 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	431	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>5%</div> <div></div> </div> </div>
1	B	431	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div></div> </div> </div>
1	C	431	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>27%</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
2	PG4	B	501	-	-	-	X
2	PG4	C	502	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9360 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.

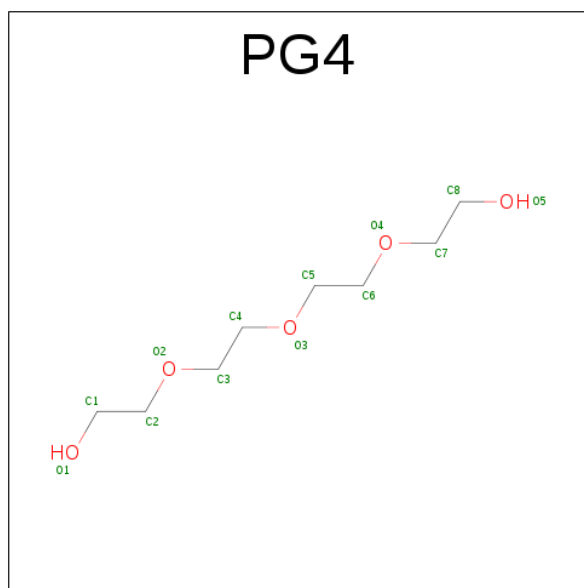
- Molecule 1 is a protein called Proton/glutamate symporter, SDF family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3097	2047	497	537	16			
1	B	413	Total	C	N	O	S	0	0	0
			3073	2031	493	533	16			
1	C	422	Total	C	N	O	S	0	0	0
			3138	2070	506	546	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	EXPRESSION TAG	UNP Q5JID0
B	431	HIS	-	EXPRESSION TAG	UNP Q5JID0
C	431	HIS	-	EXPRESSION TAG	UNP Q5JID0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).

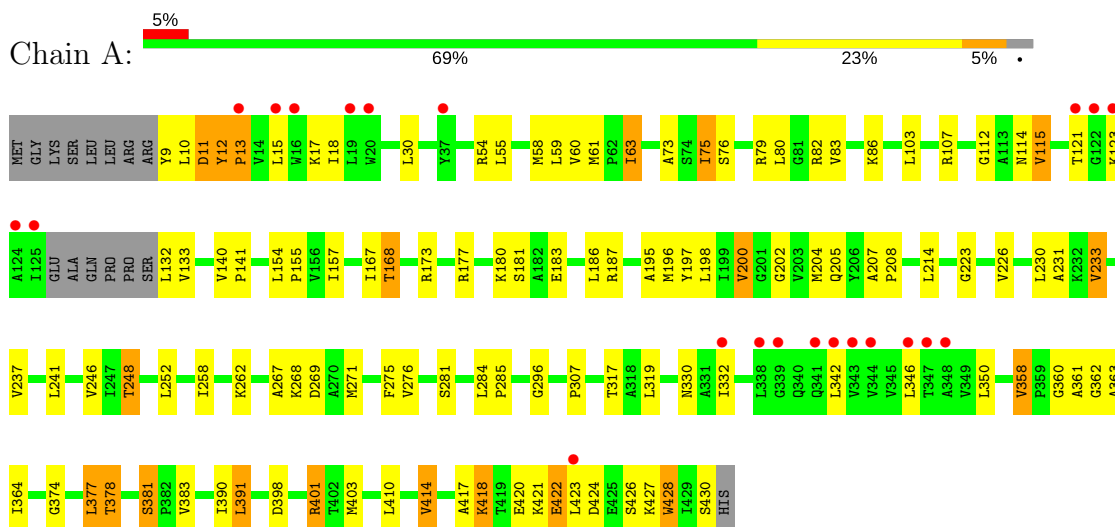


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		

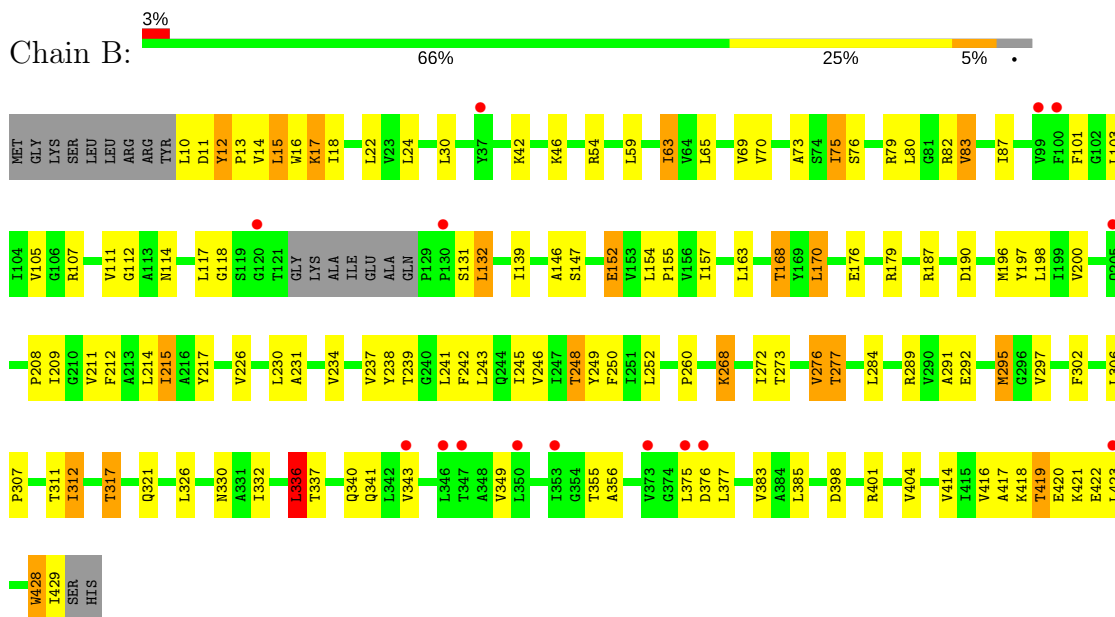
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

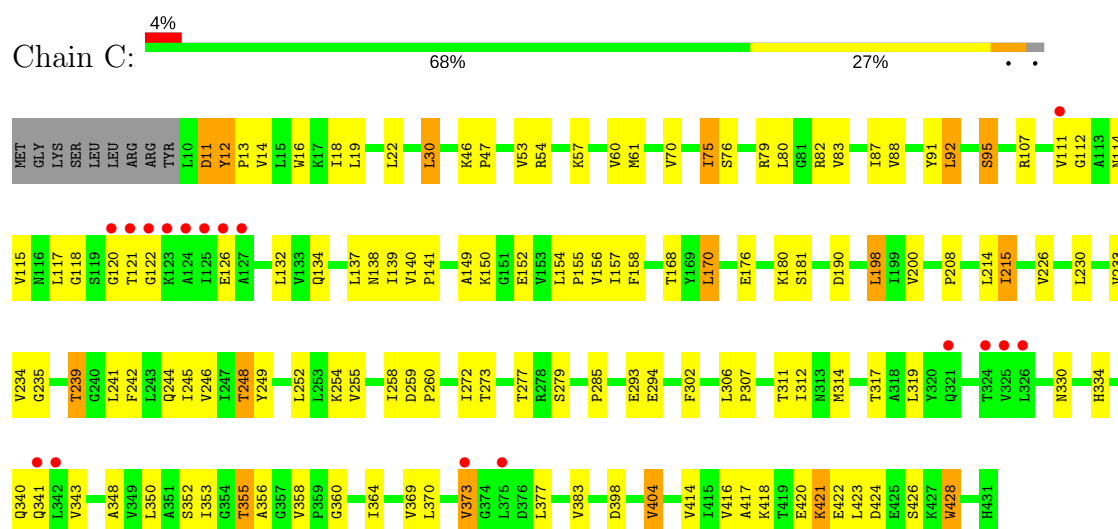
- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.57Å 117.57Å 309.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 3.00 48.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-3.00) 99.8 (48.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.212 , 0.266 0.209 , 0.266	Depositor DCC
R_{free} test set	2525 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	115.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9360	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: PG4

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	0.47	0/3153	0.70	1/4290 (0.0%)
1	B	0.45	0/3130	0.71	2/4261 (0.0%)
1	C	0.49	0/3197	0.70	0/4353
All	All	0.47	0/9480	0.70	3/12904 (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	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	154	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	132	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	LYS	Peptide
1	A	422	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	126	GLU	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	3097	0	3301	86	0
1	B	3073	0	3275	96	0
1	C	3138	0	3338	85	0
2	A	13	0	18	3	0
2	B	13	0	18	0	0
2	C	26	0	36	4	0
All	All	9360	0	9986	254	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 13.

All (254) 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:75:ILE:HD11	1:A:80:LEU:HD13	1.54	0.89
1:B:421:LYS:HA	1:B:423:LEU:HG	1.57	0.84
1:C:107:ARG:NH1	1:C:341:GLN:OE1	2.13	0.81
1:C:30:LEU:HD11	2:C:501:PG4:H32	1.61	0.80
1:A:181:SER:HA	1:B:187:ARG:HG2	1.63	0.80
1:C:241:LEU:HD23	1:C:319:LEU:HD23	1.64	0.80
1:A:421:LYS:HA	1:A:423:LEU:HG	1.66	0.78
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.65	0.77
1:B:112:GLY:HA3	1:B:330:ASN:HB2	1.64	0.77
1:A:140:VAL:O	1:B:54:ARG:NH1	2.19	0.75
1:B:15:LEU:HD13	1:B:16:TRP:H	1.52	0.74
1:B:418:LYS:HA	1:B:422:GLU:HB2	1.71	0.73
1:C:421:LYS:HA	1:C:423:LEU:HG	1.69	0.73
1:A:114:ASN:HB3	1:A:115:VAL:HG22	1.71	0.73
1:C:112:GLY:HA3	1:C:330:ASN:HB2	1.72	0.71
1:C:121:THR:HG22	1:C:122:GLY:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD23	1:C:272:ILE:HD11	1.72	0.70
1:C:134:GLN:NE2	1:C:138:ASN:OD1	2.22	0.70
1:B:79:ARG:HH22	1:B:421:LYS:HE3	1.58	0.69
1:B:63:ILE:HG12	1:B:196:MET:HB3	1.75	0.69
1:A:54:ARG:NH1	1:C:140:VAL:O	2.25	0.69
1:A:79:ARG:HD2	1:A:420:GLU:HG2	1.75	0.68
1:A:79:ARG:HH22	1:A:421:LYS:HE3	1.59	0.68
1:A:422:GLU:HB3	1:A:423:LEU:HA	1.76	0.68
1:C:112:GLY:HA3	1:C:330:ASN:CB	2.23	0.68
1:A:378:THR:O	1:A:381:SER:HB3	1.96	0.66
1:A:79:ARG:HH12	1:A:421:LYS:HG2	1.60	0.66
1:B:200:VAL:HG13	1:B:289:ARG:HD2	1.77	0.66
1:C:22:LEU:HD12	1:C:215:ILE:HG12	1.76	0.66
1:A:82:ARG:NE	1:A:420:GLU:OE2	2.28	0.65
1:B:139:ILE:HG12	1:B:154:LEU:HD23	1.76	0.65
1:B:336:LEU:HD22	1:B:341:GLN:HA	1.79	0.65
1:C:277:THR:HG22	1:C:279:SER:H	1.62	0.64
1:C:79:ARG:HH12	1:C:421:LYS:HG2	1.62	0.64
1:B:75:ILE:HG13	1:B:76:SER:H	1.63	0.64
1:A:275:PHE:HB2	1:A:403:MET:HG3	1.80	0.63
1:B:42:LYS:HB2	1:B:217:TYR:HE1	1.61	0.63
1:A:177:ARG:NH1	1:B:190:ASP:OD2	2.32	0.63
1:C:18:ILE:HA	1:C:208:PRO:HB3	1.81	0.62
1:C:248:THR:O	1:C:252:LEU:HB2	1.99	0.62
1:A:157:ILE:HD11	1:A:307:PRO:HB2	1.82	0.61
1:B:336:LEU:HD13	1:B:341:GLN:HB2	1.82	0.61
1:B:152:GLU:HG2	1:B:155:PRO:HG2	1.83	0.60
1:B:79:ARG:HH12	1:B:421:LYS:HG2	1.66	0.60
1:B:22:LEU:HD22	1:B:272:ILE:HG23	1.84	0.60
1:C:198:LEU:HD22	2:C:502:PG4:H71	1.83	0.60
1:A:11:ASP:OD1	1:A:11:ASP:N	2.30	0.59
1:B:10:LEU:HD12	1:B:12:TYR:H	1.67	0.59
1:B:10:LEU:HD12	1:B:11:ASP:HA	1.84	0.59
1:C:311:THR:HG22	1:C:356:ALA:HB2	1.85	0.59
1:B:75:ILE:HG13	1:B:76:SER:N	2.19	0.58
1:A:248:THR:O	1:A:252:LEU:HB2	2.05	0.57
1:C:91:TYR:O	1:C:95:SER:HB2	2.04	0.57
1:A:82:ARG:HD2	2:A:501:PG4:H81	1.86	0.57
1:A:424:ASP:OD1	1:A:426:SER:OG	2.13	0.57
1:C:75:ILE:HG13	1:C:76:SER:H	1.69	0.57
1:A:268:LYS:NZ	1:A:269:ASP:OD1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HG13	1:A:76:SER:N	2.21	0.56
1:A:112:GLY:HA3	1:A:330:ASN:CB	2.37	0.55
1:B:197:TYR:HA	1:B:200:VAL:HG12	1.87	0.55
1:A:79:ARG:NH1	1:A:420:GLU:HB3	2.21	0.55
1:C:61:MET:CE	1:C:156:VAL:HG21	2.36	0.55
1:A:86:LYS:HD2	2:A:501:PG4:H41	1.89	0.55
1:C:139:ILE:HG12	1:C:154:LEU:HD23	1.86	0.55
1:A:63:ILE:HG12	1:A:196:MET:HB3	1.87	0.55
1:B:248:THR:O	1:B:252:LEU:HB2	2.06	0.55
1:A:187:ARG:HG2	1:C:181:SER:HA	1.89	0.55
1:A:417:ALA:HB1	1:A:422:GLU:HA	1.89	0.55
1:B:226:VAL:O	1:B:231:ALA:HB2	2.07	0.55
1:C:428:TRP:N	1:C:428:TRP:CD1	2.74	0.55
1:A:183:GLU:O	1:A:187:ARG:HB2	2.06	0.54
1:B:422:GLU:HB3	1:B:423:LEU:HA	1.88	0.54
1:B:75:ILE:HD11	1:B:80:LEU:HD13	1.88	0.54
1:A:75:ILE:HG13	1:A:76:SER:H	1.72	0.54
1:A:418:LYS:HA	1:A:422:GLU:HB2	1.90	0.54
1:B:237:VAL:HG13	1:B:238:TYR:HD1	1.72	0.54
1:B:428:TRP:CD1	1:B:428:TRP:N	2.75	0.54
1:A:258:ILE:HD13	1:A:414:VAL:HG23	1.89	0.54
1:A:202:GLY:O	1:A:205:GLN:HB2	2.07	0.54
1:C:75:ILE:HG13	1:C:76:SER:N	2.23	0.54
1:C:114:ASN:HB2	1:C:115:VAL:HB	1.91	0.53
1:B:14:VAL:H	1:B:17:LYS:HZ3	1.55	0.53
1:A:410:LEU:O	1:A:414:VAL:HG13	2.08	0.52
1:B:326:LEU:HD23	1:B:336:LEU:HD11	1.91	0.52
1:B:197:TYR:HH	1:B:302:PHE:HE1	1.58	0.52
1:A:180:LYS:HZ3	1:B:187:ARG:NH1	2.08	0.52
1:B:70:VAL:HG21	1:B:190:ASP:HA	1.92	0.52
1:B:273:THR:O	1:B:277:THR:HB	2.09	0.52
1:B:18:ILE:HA	1:B:208:PRO:HB3	1.92	0.52
1:B:22:LEU:HD12	1:B:215:ILE:HG12	1.91	0.51
1:A:112:GLY:HA3	1:A:330:ASN:HB3	1.93	0.51
1:B:242:PHE:O	1:B:246:VAL:HB	2.09	0.51
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.91	0.51
1:B:14:VAL:O	1:B:17:LYS:HD2	2.10	0.51
1:C:311:THR:HA	1:C:356:ALA:HA	1.91	0.51
1:C:273:THR:O	1:C:277:THR:HB	2.10	0.51
1:C:141:PRO:HB3	1:C:155:PRO:HB3	1.92	0.51
1:B:209:ILE:O	1:B:212:PHE:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ALA:O	1:B:168:THR:OG1	2.28	0.50
1:C:79:ARG:HH22	1:C:421:LYS:HE2	1.77	0.50
1:A:360:GLY:O	1:A:364:ILE:HG12	2.11	0.50
1:C:70:VAL:HG21	1:C:190:ASP:HA	1.93	0.50
1:C:245:ILE:HA	1:C:249:TYR:CD2	2.47	0.50
1:A:204:MET:HA	1:A:207:ALA:HB2	1.94	0.50
1:C:348:ALA:O	1:C:352:SER:OG	2.24	0.49
1:A:167:ILE:HG21	1:A:186:LEU:HB2	1.94	0.49
1:A:422:GLU:CB	1:A:423:LEU:HA	2.42	0.49
1:A:428:TRP:CD1	1:A:428:TRP:N	2.80	0.49
1:B:42:LYS:HB2	1:B:217:TYR:CE1	2.45	0.49
1:C:11:ASP:HB3	1:C:12:TYR:HB3	1.94	0.49
1:C:258:ILE:HD13	1:C:414:VAL:HG12	1.94	0.49
1:B:103:LEU:O	1:B:107:ARG:HG2	2.13	0.49
1:A:60:VAL:HG22	1:A:285:PRO:HD3	1.93	0.49
1:B:16:TRP:CD1	1:B:268:LYS:HE3	2.47	0.49
1:A:237:VAL:O	1:A:241:LEU:HG	2.13	0.49
1:B:42:LYS:O	1:B:46:LYS:HB3	2.12	0.49
1:B:11:ASP:HB2	1:B:13:PRO:HD2	1.95	0.48
1:B:241:LEU:HD22	1:B:404:VAL:HB	1.93	0.48
1:B:82:ARG:HD2	1:B:420:GLU:OE2	2.13	0.48
1:C:422:GLU:HB3	1:C:423:LEU:HA	1.95	0.48
1:B:79:ARG:HD2	1:B:420:GLU:HG2	1.96	0.48
1:C:360:GLY:O	1:C:364:ILE:HG12	2.13	0.48
1:C:88:VAL:O	1:C:92:LEU:HD22	2.13	0.48
1:C:198:LEU:HD21	2:C:502:PG4:H61	1.94	0.48
1:B:291:ALA:HB2	1:B:306:LEU:HD11	1.96	0.48
1:A:141:PRO:HB3	1:A:155:PRO:HB3	1.96	0.48
1:B:417:ALA:HB1	1:B:422:GLU:HA	1.95	0.48
1:A:180:LYS:HD2	1:B:187:ARG:HD2	1.96	0.48
1:C:120:GLY:HA2	1:C:334:HIS:HD2	1.78	0.47
1:A:73:ALA:O	1:A:168:THR:OG1	2.29	0.47
1:B:101:PHE:O	1:B:105:VAL:HG22	2.14	0.47
1:B:295:MET:HG2	1:B:414:VAL:HG21	1.96	0.47
1:C:61:MET:HE1	1:C:156:VAL:HG21	1.96	0.47
1:B:13:PRO:HA	1:B:17:LYS:NZ	2.30	0.47
1:B:284:LEU:HD21	1:B:307:PRO:HA	1.96	0.47
1:C:112:GLY:HA3	1:C:330:ASN:HB3	1.94	0.47
1:C:370:LEU:O	1:C:373:VAL:HG12	2.15	0.47
1:A:281:SER:O	1:A:284:LEU:HB2	2.14	0.47
1:A:358:VAL:HG13	1:A:361:ALA:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLN:O	1:B:343:VAL:HG12	2.15	0.46
1:C:95:SER:OG	1:C:314:MET:HB2	2.15	0.46
1:A:103:LEU:O	1:A:107:ARG:HG2	2.14	0.46
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.69	0.46
1:A:11:ASP:CG	1:A:12:TYR:HA	2.36	0.46
1:A:79:ARG:HH11	1:A:420:GLU:HB3	1.80	0.46
1:B:337:THR:OG1	1:B:340:GLN:HG2	2.16	0.46
1:C:252:LEU:HA	1:C:252:LEU:HD12	1.80	0.46
1:C:352:SER:O	1:C:355:THR:HG23	2.15	0.46
1:B:226:VAL:HG13	1:B:234:VAL:HG21	1.98	0.46
1:A:195:ALA:HA	1:C:170:LEU:HD21	1.96	0.45
1:B:131:SER:OG	1:B:132:LEU:N	2.49	0.45
1:B:401:ARG:O	1:B:404:VAL:HG12	2.16	0.45
1:C:340:GLN:O	1:C:343:VAL:HG12	2.16	0.45
1:B:212:PHE:O	1:B:215:ILE:HD12	2.17	0.45
1:B:170:LEU:HD13	1:C:198:LEU:HD12	1.97	0.45
1:B:117:LEU:HD22	1:B:118:GLY:H	1.82	0.45
1:C:242:PHE:CE1	1:C:246:VAL:HG21	2.52	0.45
1:A:252:LEU:HA	1:A:252:LEU:HD12	1.87	0.45
1:B:176:GLU:HG2	1:B:179:ARG:NH2	2.32	0.45
1:A:363:ALA:HB1	1:A:391:LEU:HD12	1.99	0.45
1:C:424:ASP:OD1	1:C:426:SER:OG	2.27	0.45
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.80	0.45
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.80	0.44
1:C:79:ARG:O	1:C:83:VAL:HG23	2.17	0.44
1:C:150:LYS:HB2	1:C:152:GLU:HG3	1.98	0.44
1:A:226:VAL:O	1:A:231:ALA:HB2	2.17	0.44
1:C:244:GLN:HA	1:C:248:THR:HG23	1.99	0.44
1:B:75:ILE:HD11	1:B:80:LEU:CD1	2.46	0.44
1:A:86:LYS:CD	2:A:501:PG4:H41	2.46	0.44
1:A:59:LEU:O	1:A:63:ILE:HB	2.18	0.44
1:A:197:TYR:HA	1:A:200:VAL:HG13	1.99	0.44
1:A:267:ALA:O	1:A:271:MET:HG3	2.18	0.44
1:B:292:GLU:HB2	1:B:302:PHE:CZ	2.53	0.44
1:B:317:THR:HG22	1:B:349:VAL:HG22	1.99	0.44
1:C:418:LYS:HA	1:C:422:GLU:HB2	2.00	0.44
1:B:87:ILE:HD12	1:B:87:ILE:HA	1.87	0.43
1:C:87:ILE:HA	1:C:87:ILE:HD12	1.76	0.43
1:A:362:GLY:N	1:A:401:ARG:HH12	2.15	0.43
1:A:13:PRO:HA	1:A:17:LYS:NZ	2.33	0.43
1:A:342:LEU:HG	1:A:346:LEU:HD23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:HG22	1:C:285:PRO:HD3	2.00	0.43
1:A:296:GLY:HA3	1:A:427:LYS:HG3	2.01	0.43
1:B:326:LEU:HB2	1:B:341:GLN:NE2	2.33	0.43
1:B:146:ALA:HB2	1:C:149:ALA:O	2.18	0.43
1:C:82:ARG:HD2	1:C:420:GLU:OE2	2.19	0.43
1:A:132:LEU:HB3	1:A:133:VAL:H	1.58	0.43
1:B:14:VAL:H	1:B:17:LYS:NZ	2.15	0.43
1:C:75:ILE:HD11	1:C:80:LEU:HD13	1.99	0.43
1:C:226:VAL:HB	2:C:501:PG4:H22	2.00	0.43
1:C:226:VAL:HG13	1:C:234:VAL:HG21	2.01	0.43
1:A:54:ARG:HD3	1:C:137:LEU:O	2.19	0.43
1:A:112:GLY:HA3	1:A:330:ASN:HB2	2.01	0.42
1:A:346:LEU:HA	1:A:346:LEU:HD13	1.87	0.42
1:A:422:GLU:HB3	1:A:423:LEU:CA	2.48	0.42
1:B:428:TRP:H	1:B:428:TRP:HD1	1.67	0.42
1:A:268:LYS:HE3	1:A:268:LYS:HB3	1.86	0.42
1:C:46:LYS:N	1:C:47:PRO:HD2	2.34	0.42
1:B:311:THR:HA	1:B:356:ALA:HA	2.00	0.42
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.71	0.42
1:C:252:LEU:O	1:C:255:VAL:HG12	2.19	0.42
1:A:121:THR:HB	1:A:374:GLY:O	2.19	0.42
1:B:79:ARG:O	1:B:83:VAL:HG13	2.20	0.42
1:C:312:ILE:HD12	1:C:353:ILE:HG23	2.00	0.42
1:A:377:LEU:HD12	1:A:377:LEU:HA	1.57	0.42
1:B:239:THR:O	1:B:243:LEU:HB2	2.20	0.42
1:C:241:LEU:HD22	1:C:404:VAL:HB	2.00	0.42
1:C:83:VAL:HG13	1:C:416:VAL:HG11	2.02	0.42
1:B:336:LEU:HA	1:B:340:GLN:OE1	2.20	0.42
1:C:117:LEU:HD23	1:C:118:GLY:N	2.34	0.42
1:A:75:ILE:CG1	1:A:76:SER:H	2.33	0.42
1:B:10:LEU:CG	1:B:11:ASP:HA	2.50	0.42
1:B:211:VAL:HA	1:B:276:VAL:HG11	2.02	0.42
1:C:214:LEU:HA	1:C:214:LEU:HD23	1.72	0.42
1:C:235:GLY:O	1:C:239:THR:HG23	2.20	0.42
1:C:294:GLU:OE2	1:C:294:GLU:HA	2.20	0.42
1:A:187:ARG:CZ	1:C:180:LYS:HD2	2.49	0.42
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.90	0.42
1:B:416:VAL:O	1:B:419:THR:OG1	2.35	0.42
1:C:11:ASP:HB3	1:C:12:TYR:CB	2.49	0.42
1:B:332:ILE:HD13	1:B:383:VAL:HG22	2.01	0.41
1:B:103:LEU:HA	1:B:103:LEU:HD12	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PHE:CD1	1:B:260:PRO:HB3	2.55	0.41
1:B:75:ILE:CG1	1:B:76:SER:H	2.32	0.41
1:A:230:LEU:HA	1:A:233:VAL:HG13	2.01	0.41
1:C:259:ASP:HA	1:C:260:PRO:HD3	1.84	0.41
1:B:297:VAL:HA	1:B:422:GLU:O	2.20	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.88	0.41
1:C:302:PHE:O	1:C:306:LEU:HB2	2.21	0.41
1:B:15:LEU:HD13	1:B:16:TRP:N	2.29	0.41
1:A:223:GLY:O	1:A:226:VAL:HG23	2.21	0.41
1:B:59:LEU:O	1:B:63:ILE:HB	2.21	0.41
1:C:75:ILE:CG1	1:C:76:SER:H	2.33	0.41
1:A:226:VAL:HG12	1:A:226:VAL:O	2.20	0.41
1:A:214:LEU:CB	1:A:276:VAL:HG13	2.50	0.41
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.89	0.41
1:B:17:LYS:HB2	1:B:208:PRO:HG3	2.02	0.41
1:A:55:LEU:O	1:A:58:MET:HB3	2.20	0.41
1:B:312:ILE:HD12	1:B:312:ILE:HA	1.86	0.41
1:C:417:ALA:HB1	1:C:422:GLU:HA	2.03	0.41
1:B:65:LEU:O	1:B:69:VAL:HG23	2.21	0.41
1:A:58:MET:HE3	1:C:158:PHE:HD2	1.86	0.41
1:A:15:LEU:HA	1:A:17:LYS:HE2	2.03	0.40
1:A:18:ILE:HA	1:A:208:PRO:HB3	2.03	0.40
1:A:390:ILE:HD13	1:A:390:ILE:HA	1.89	0.40
1:C:53:VAL:HG23	1:C:214:LEU:HD11	2.02	0.40
1:A:15:LEU:HD11	1:A:205:GLN:OE1	2.21	0.40
1:B:239:THR:HG22	1:B:243:LEU:HD22	2.02	0.40
1:B:336:LEU:HD22	1:B:341:GLN:CA	2.50	0.40
1:C:139:ILE:HG12	1:C:154:LEU:CD2	2.52	0.40
1:A:421:LYS:HE2	1:A:421:LYS:HB3	1.84	0.40
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.84	0.40
1:B:245:ILE:HA	1:B:249:TYR:CD2	2.57	0.40
1:C:180:LYS:HB3	1:C:180:LYS:HE2	1.80	0.40
1:C:230:LEU:HA	1:C:230:LEU:HD23	1.86	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	412/431 (96%)	392 (95%)	18 (4%)	2 (0%)	32	74
1	B	409/431 (95%)	391 (96%)	17 (4%)	1 (0%)	51	86
1	C	420/431 (97%)	400 (95%)	19 (4%)	1 (0%)	51	86
All	All	1241/1293 (96%)	1183 (95%)	54 (4%)	4 (0%)	44	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	B	75	ILE
1	C	75	ILE
1	A	13	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	325/338 (96%)	292 (90%)	33 (10%)	8	32
1	B	324/338 (96%)	291 (90%)	33 (10%)	8	32
1	C	330/338 (98%)	296 (90%)	34 (10%)	8	31
All	All	979/1014 (96%)	879 (90%)	100 (10%)	8	32

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	10	LEU
1	A	11	ASP
1	A	12	TYR
1	A	30	LEU
1	A	61	MET
1	A	63	ILE
1	A	83	VAL
1	A	115	VAL
1	A	168	THR
1	A	173	ARG
1	A	198	LEU
1	A	200	VAL
1	A	233	VAL
1	A	246	VAL
1	A	248	THR
1	A	262	LYS
1	A	317	THR
1	A	319	LEU
1	A	332	ILE
1	A	350	LEU
1	A	358	VAL
1	A	377	LEU
1	A	378	THR
1	A	381	SER
1	A	383	VAL
1	A	391	LEU
1	A	398	ASP
1	A	401	ARG
1	A	414	VAL
1	A	418	LYS
1	A	428	TRP
1	A	430	SER
1	B	12	TYR
1	B	15	LEU
1	B	17	LYS
1	B	24	LEU
1	B	30	LEU
1	B	63	ILE
1	B	83	VAL
1	B	111	VAL
1	B	114	ASN
1	B	147	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	152	GLU
1	B	168	THR
1	B	170	LEU
1	B	198	LEU
1	B	215	ILE
1	B	248	THR
1	B	268	LYS
1	B	276	VAL
1	B	277	THR
1	B	295	MET
1	B	312	ILE
1	B	317	THR
1	B	321	GLN
1	B	336	LEU
1	B	355	THR
1	B	375	LEU
1	B	376	ASP
1	B	377	LEU
1	B	385	LEU
1	B	398	ASP
1	B	419	THR
1	B	428	TRP
1	B	429	ILE
1	C	11	ASP
1	C	12	TYR
1	C	14	VAL
1	C	16	TRP
1	C	30	LEU
1	C	54	ARG
1	C	57	LYS
1	C	92	LEU
1	C	95	SER
1	C	111	VAL
1	C	132	LEU
1	C	168	THR
1	C	170	LEU
1	C	176	GLU
1	C	198	LEU
1	C	200	VAL
1	C	215	ILE
1	C	233	VAL
1	C	239	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	248	THR
1	C	254	LYS
1	C	293	GLU
1	C	317	THR
1	C	350	LEU
1	C	355	THR
1	C	358	VAL
1	C	369	VAL
1	C	373	VAL
1	C	377	LEU
1	C	383	VAL
1	C	398	ASP
1	C	404	VAL
1	C	421	LYS
1	C	428	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PG4	A	501	-	12,12,12	0.79	0	11,11,11	0.40	0
2	PG4	B	501	-	12,12,12	0.75	0	11,11,11	0.35	0
2	PG4	C	501	-	12,12,12	0.75	0	11,11,11	0.32	0
2	PG4	C	502	-	12,12,12	0.80	0	11,11,11	0.36	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	PG4	A	501	-	-	0/10/10/10	0/0/0/0
2	PG4	B	501	-	-	0/10/10/10	0/0/0/0
2	PG4	C	501	-	-	0/10/10/10	0/0/0/0
2	PG4	C	502	-	-	0/10/10/10	0/0/0/0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PG4	3	0
2	C	501	PG4	2	0
2	C	502	PG4	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, 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	416/431 (96%)	-0.14	22 (5%)	27 11	56, 95, 153, 237	0
1	B	413/431 (95%)	-0.19	15 (3%)	43 18	61, 97, 141, 219	0
1	C	422/431 (97%)	-0.24	17 (4%)	39 16	57, 85, 151, 222	0
All	All	1251/1293 (96%)	-0.19	54 (4%)	36 15	56, 92, 148, 237	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	ALA	6.9
1	A	125	ILE	6.8
1	A	124	ALA	4.7
1	C	125	ILE	4.2
1	B	376	ASP	4.0
1	B	205	GLN	3.9
1	B	375	LEU	3.9
1	C	123	LYS	3.8
1	A	343	VAL	3.7
1	A	346	LEU	3.6
1	A	423	LEU	3.6
1	A	348	ALA	3.5
1	A	16	TRP	3.5
1	A	20	TRP	3.5
1	C	375	LEU	3.4
1	A	347	THR	3.4
1	C	341	GLN	3.4
1	B	423	LEU	3.3
1	A	342	LEU	3.3
1	B	346	LEU	3.2
1	C	127	ALA	3.1
1	A	338	LEU	3.0
1	A	332	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	13	PRO	3.0
1	C	325	VAL	3.0
1	C	126	GLU	2.8
1	C	121	THR	2.8
1	B	353	ILE	2.7
1	A	123	LYS	2.6
1	B	350	LEU	2.5
1	A	339	GLY	2.5
1	C	321	GLN	2.5
1	C	324	THR	2.5
1	A	15	LEU	2.5
1	C	122	GLY	2.5
1	B	100	PHE	2.4
1	C	120	GLY	2.4
1	B	120	GLY	2.4
1	B	347	THR	2.4
1	C	326	LEU	2.3
1	A	37	TYR	2.3
1	A	344	VAL	2.3
1	B	37	TYR	2.3
1	B	343	VAL	2.2
1	A	121	THR	2.2
1	B	373	VAL	2.2
1	A	122	GLY	2.1
1	A	19	LEU	2.1
1	B	99	VAL	2.1
1	C	342	LEU	2.1
1	A	341	GLN	2.1
1	C	111	VAL	2.1
1	C	373	VAL	2.0
1	B	130	PRO	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	PG4	C	502	13/13	0.31	1.00	8.86	89,127,143,145	0
2	PG4	B	501	13/13	0.64	0.84	5.13	88,111,139,140	0
2	PG4	C	501	13/13	0.72	0.30	1.92	87,127,149,150	0
2	PG4	A	501	13/13	0.77	0.21	1.65	81,106,137,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.