



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:06 PM EDT

PDB ID : 4KY0 / pdb_00004ky0
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

<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

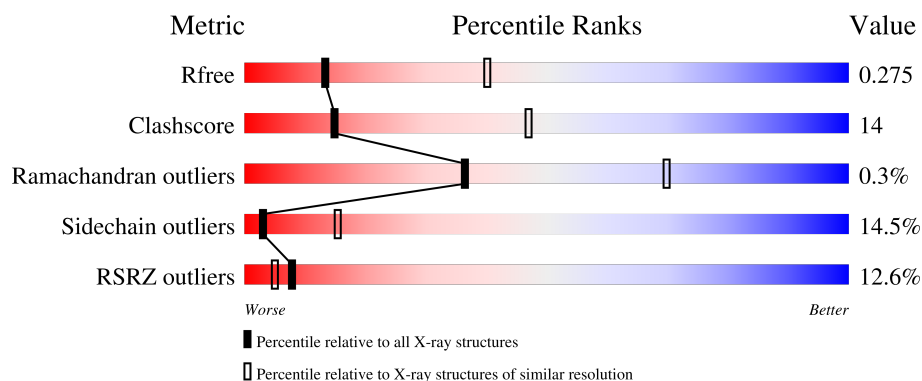
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	431	14% 65% 26% 6% .
1	B	431	11% 63% 25% 7% .
1	C	431	12% 64% 28% 5% .

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.

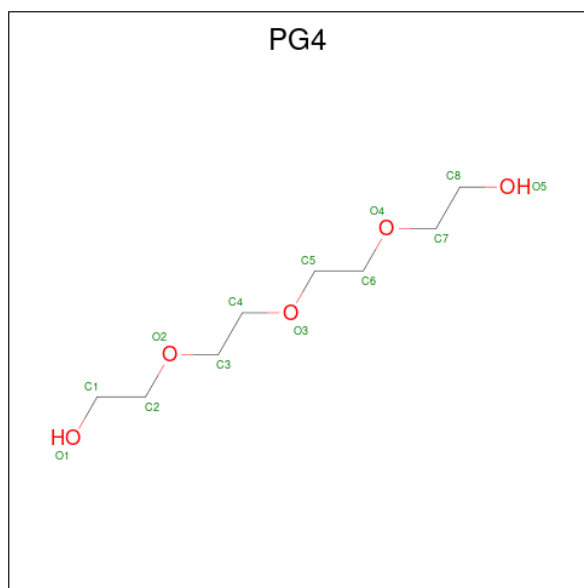
- Molecule 1 is a protein called Proton/glutamate symporter, SDF family.

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 (CCD ID: PG4) (formula: C₈H₁₈O₅).

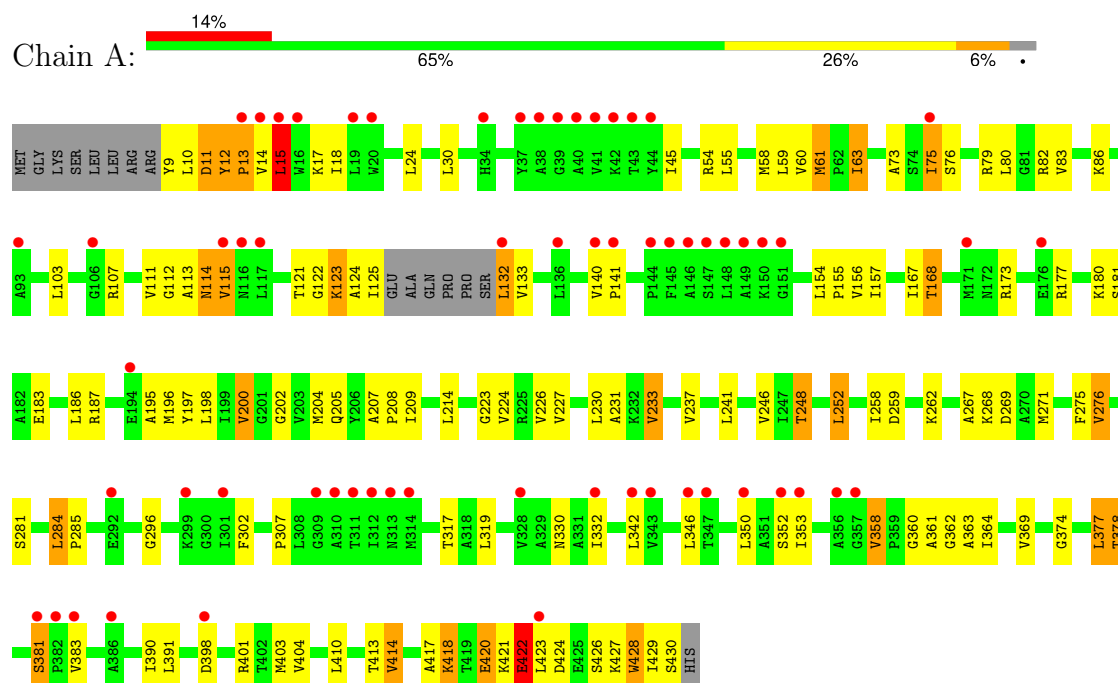


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 8	O 5	0	0
2	B	1	Total 13	C 8	O 5	0	0
2	C	1	Total 13	C 8	O 5	0	0
2	C	1	Total 13	C 8	O 5	0	0

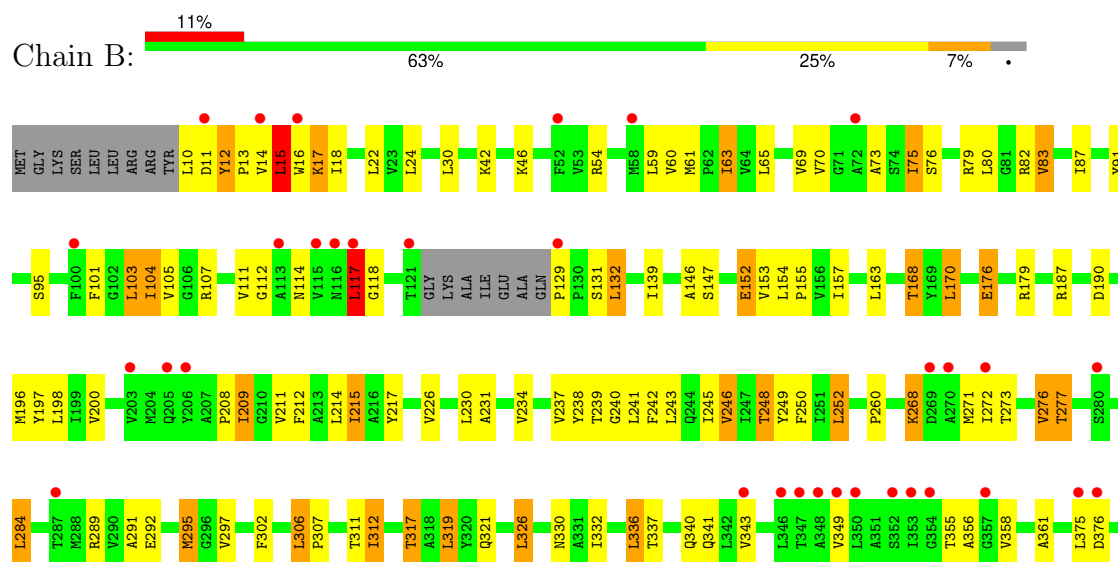
3 Residue-property plots

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: Proton/glutamate symporter, SDF family

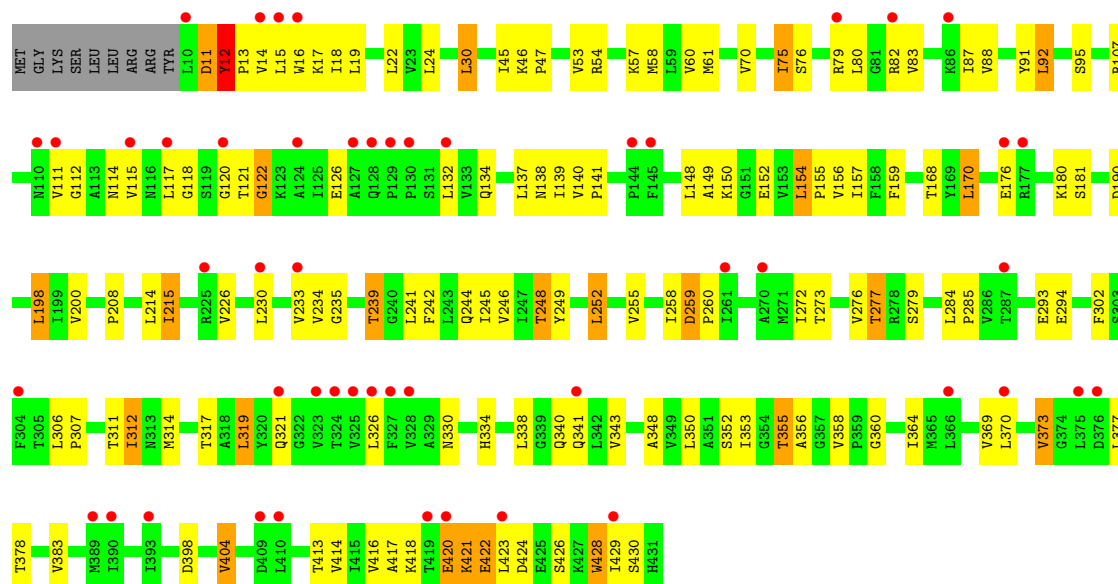


• Molecule 1: Proton/glutamate symporter, SDF family





- 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 48.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-3.00) 99.8 (48.00-3.00)	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 0.222 , 0.275	Depositor DCC
R_{free} test set	2526 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	115.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 52.0	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	0.91	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	0.65	0/3153	1.06	10/4290 (0.2%)
1	B	0.63	0/3130	1.06	11/4261 (0.3%)
1	C	0.69	0/3197	1.07	10/4353 (0.2%)
All	All	0.66	0/9480	1.06	31/12904 (0.2%)

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 (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	GLU	N-CA-C	-9.50	100.88	111.14
1	B	422	GLU	N-CA-C	-9.32	101.08	111.14
1	C	422	GLU	N-CA-C	-8.91	101.52	111.14
1	C	12	TYR	CA-C-N	7.49	126.76	118.97
1	C	12	TYR	C-N-CA	7.49	126.76	118.97
1	A	15	LEU	N-CA-C	7.18	121.99	113.23
1	C	17	LYS	N-CA-C	6.96	119.89	111.82
1	B	129	PRO	CA-C-N	6.95	126.87	119.85
1	B	129	PRO	C-N-CA	6.95	126.87	119.85
1	A	353	ILE	N-CA-C	6.79	116.94	110.42
1	A	124	ALA	N-CA-C	6.63	118.41	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	LEU	N-CA-C	6.26	119.70	109.24
1	B	15	LEU	N-CA-C	6.21	118.90	109.95
1	A	259	ASP	CA-C-N	6.08	125.97	119.28
1	A	259	ASP	C-N-CA	6.08	125.97	119.28
1	A	113	ALA	N-CA-C	6.01	118.33	111.11
1	B	361	ALA	N-CA-C	5.83	117.63	111.28
1	C	378	THR	CA-C-N	5.72	125.65	119.76
1	C	378	THR	C-N-CA	5.72	125.65	119.76
1	B	306	LEU	CA-C-N	-5.59	113.26	119.19
1	B	306	LEU	C-N-CA	-5.59	113.26	119.19
1	B	104	ILE	N-CA-C	5.55	115.75	110.53
1	C	259	ASP	CA-C-N	5.49	125.31	119.28
1	C	259	ASP	C-N-CA	5.49	125.31	119.28
1	A	352	SER	N-CA-C	5.48	119.97	113.28
1	B	379	PRO	CA-C-O	-5.25	115.36	121.34
1	C	122	GLY	N-CA-C	-5.17	100.93	113.18
1	C	430	SER	N-CA-C	5.12	119.57	112.45
1	B	60	VAL	N-CA-C	5.11	115.33	110.42
1	A	114	ASN	CA-C-N	5.07	130.83	121.70
1	A	114	ASN	C-N-CA	5.07	130.83	121.70

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
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	92	0
1	B	3073	0	3275	101	0
1	C	3138	0	3338	89	0
2	A	13	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	18	0	0
2	C	26	0	36	4	0
All	All	9360	0	9986	267	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 14.

All (267) 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:58:MET:HE2	1:C:159:PHE:HD1	1.49	0.76
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
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:A:54:ARG:NH1	1:C:140:VAL:O	2.25	0.69
1:B:63:ILE:HG12	1:B:196:MET:HB3	1.75	0.69
1:A:79:ARG:HD2	1:A:420:GLU:HG2	1.75	0.68
1:A:61:MET:HE3	1:A:156:VAL:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:LYS:HZ3	1:B:187:ARG:NH1	2.04	0.56
1:A:75:ILE:HG13	1:A:76:SER:N	2.21	0.56
1:A:268:LYS:NZ	1:A:269:ASP:OD1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:ILE:HD11	1:B:80:LEU:HD13	1.88	0.54
1:B:422:GLU:HB3	1:B:423:LEU:HA	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:61:MET:HE1	1:C:156:VAL:HG21	1.90	0.53
1:C:114:ASN:HB2	1:C:115:VAL:HB	1.91	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: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:428:TRP:CD1	1:B:428:TRP:H	2.28	0.52
1:B:18:ILE:HA	1:B:208:PRO:HB3	1.92	0.52
1:A:268:LYS:HA	1:A:271:MET:HE2	1.92	0.51
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:A:58:MET:HE2	1:C:159:PHE:CD1	2.39	0.51
1:C:273:THR:O	1:C:277:THR:HB	2.10	0.51
1:A:11:ASP:CG	1:A:12:TYR:HA	2.36	0.51
1:C:141:PRO:HB3	1:C:155:PRO:HB3	1.92	0.51
1:B:73:ALA:O	1:B:168:THR:OG1	2.28	0.50
1:B:209:ILE:O	1:B:212:PHE:HB3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:H	1:B:17:LYS:HZ3	1.60	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:82:ARG:HD2	1:B:420:GLU:OE2	2.13	0.48
1:B:241:LEU:HD22	1:B:404:VAL:HB	1.93	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:88:VAL:O	1:C:92:LEU:HD22	2.13	0.48
1:C:360:GLY:O	1:C:364:ILE:HG12	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:B:268:LYS:HA	1:B:271:MET:HE2	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: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
1:C:424:ASP:OD1	1:C:426:SER:OG	2.27	0.47
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: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:HD12	1:C:252:LEU:HA	1.80	0.46
1:C:352:SER:O	1:C:355:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:LEU:HD13	1:C:198:LEU:HD12	1.97	0.45
1:B:212:PHE:O	1:B:215:ILE:HD12	2.17	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:HD12	1:A:252:LEU:HA	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:A:214:LEU:HD23	1:A:214:LEU:HA	1.80	0.45
1:A:410:LEU:HD23	1:A:410:LEU:HA	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:B:14:VAL:H	1:B:17:LYS:NZ	2.15	0.44
1:B:240:GLY:C	1:B:319:LEU:HD21	2.42	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:HD12	1:C:87:ILE:HA	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:61:MET:HE1	1:B:153:VAL:HG22	2.01	0.43
1:A:112:GLY:HA3	1:A:330:ASN:HB2	2.01	0.42
1:A:346:LEU:HD13	1:A:346:LEU:HA	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:HB3	1:A:268:LYS:HE3	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:HA	1:A:377:LEU:HD12	1.57	0.42
1:B:239:THR:O	1:B:243:LEU:HB2	2.20	0.42
1:C:83:VAL:HG13	1:C:416:VAL:HG11	2.02	0.42
1:C:241:LEU:HD22	1:C:404:VAL:HB	2.00	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:HD23	1:C:214:LEU:HA	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:C:45:ILE:C	1:C:47:PRO:HD2	2.45	0.41
1:B:75:ILE:CG1	1:B:76:SER:H	2.32	0.41
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.86	0.41
1:B:250:PHE:CD1	1:B:260:PRO:HB3	2.55	0.41
1:A:230:LEU:HA	1:A:233:VAL:HG13	2.01	0.41
1:B:91:TYR:O	1:B:95:SER:OG	2.30	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:HA	1:C:137:LEU:HD23	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:LEU:CB	1:A:276:VAL:HG13	2.50	0.41
1:A:226:VAL:O	1:A:226:VAL:HG12	2.20	0.41
1:B:230:LEU:HD23	1:B:230:LEU:HA	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:HA	1:B:312:ILE:HD12	1.86	0.41
1:C:58:MET:HE2	1:C:58:MET:HB3	1.90	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:15:LEU:HA	1:A:17:LYS:HE2	2.03	0.40
1:A:180:LYS:HZ3	1:B:187:ARG:HH11	1.67	0.40
1:A:18:ILE:HA	1:A:208:PRO:HB3	2.03	0.40
1:A:122:GLY:HA3	1:A:123:LYS:C	2.45	0.40
1:A:302:PHE:CD1	1:A:302:PHE:C	2.98	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:HB3	1:A:421:LYS:HE2	1.84	0.40
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.84	0.40
1:B:245:ILE:HA	1:B:249:TYR:CD2	2.57	0.40
1:C:61:MET:HE3	1:C:148:LEU:HD23	2.02	0.40
1:C:180:LYS:HE2	1:C:180:LYS:HB3	1.80	0.40
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.86	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	412/431 (96%)	392 (95%)	18 (4%)	2 (0%)	24	60
1	B	409/431 (95%)	391 (96%)	17 (4%)	1 (0%)	43	76
1	C	420/431 (97%)	400 (95%)	19 (4%)	1 (0%)	43	76
All	All	1241/1293 (96%)	1183 (95%)	54 (4%)	4 (0%)	36	70

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%)	275 (85%)	50 (15%)	2	13
1	B	324/338 (96%)	279 (86%)	45 (14%)	3	17
1	C	330/338 (98%)	283 (86%)	47 (14%)	3	16
All	All	979/1014 (96%)	837 (86%)	142 (14%)	3	15

All (142) 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	14	VAL
1	A	15	LEU

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Mol	Chain	Res	Type
1	A	24	LEU
1	A	30	LEU
1	A	45	ILE
1	A	61	MET
1	A	63	ILE
1	A	83	VAL
1	A	111	VAL
1	A	115	VAL
1	A	125	ILE
1	A	132	LEU
1	A	154	LEU
1	A	168	THR
1	A	173	ARG
1	A	198	LEU
1	A	200	VAL
1	A	209	ILE
1	A	224	VAL
1	A	227	VAL
1	A	233	VAL
1	A	246	VAL
1	A	248	THR
1	A	252	LEU
1	A	262	LYS
1	A	276	VAL
1	A	284	LEU
1	A	317	THR
1	A	319	LEU
1	A	332	ILE
1	A	350	LEU
1	A	358	VAL
1	A	369	VAL
1	A	377	LEU
1	A	378	THR
1	A	381	SER
1	A	383	VAL
1	A	398	ASP
1	A	404	VAL
1	A	413	THR
1	A	414	VAL
1	A	418	LYS
1	A	420	GLU
1	A	428	TRP

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Mol	Chain	Res	Type
1	A	429	ILE
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	103	LEU
1	B	104	ILE
1	B	111	VAL
1	B	114	ASN
1	B	117	LEU
1	B	132	LEU
1	B	147	SER
1	B	152	GLU
1	B	168	THR
1	B	170	LEU
1	B	176	GLU
1	B	198	LEU
1	B	209	ILE
1	B	215	ILE
1	B	246	VAL
1	B	248	THR
1	B	252	LEU
1	B	268	LYS
1	B	276	VAL
1	B	277	THR
1	B	284	LEU
1	B	295	MET
1	B	312	ILE
1	B	317	THR
1	B	319	LEU
1	B	321	GLN
1	B	326	LEU
1	B	336	LEU
1	B	355	THR
1	B	358	VAL
1	B	375	LEU
1	B	376	ASP
1	B	385	LEU

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Mol	Chain	Res	Type
1	B	398	ASP
1	B	419	THR
1	B	423	LEU
1	B	428	TRP
1	B	429	ILE
1	C	11	ASP
1	C	12	TYR
1	C	14	VAL
1	C	15	LEU
1	C	16	TRP
1	C	24	LEU
1	C	30	LEU
1	C	54	ARG
1	C	57	LYS
1	C	92	LEU
1	C	111	VAL
1	C	132	LEU
1	C	154	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
1	C	248	THR
1	C	252	LEU
1	C	276	VAL
1	C	277	THR
1	C	284	LEU
1	C	293	GLU
1	C	312	ILE
1	C	317	THR
1	C	319	LEU
1	C	321	GLN
1	C	326	LEU
1	C	338	LEU
1	C	350	LEU
1	C	355	THR
1	C	358	VAL
1	C	369	VAL

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Mol	Chain	Res	Type
1	C	373	VAL
1	C	377	LEU
1	C	383	VAL
1	C	398	ASP
1	C	404	VAL
1	C	413	THR
1	C	420	GLU
1	C	421	LYS
1	C	428	TRP
1	C	429	ILE

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	116	ASN
1	A	172	ASN
1	B	116	ASN
1	C	172	ASN
1	C	321	GLN
1	C	431	HIS

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 oligosaccharides 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	C	501	-	12,12,12	0.75	0	11,11,11	0.32	0
2	PG4	B	501	-	12,12,12	0.76	0	11,11,11	0.35	0
2	PG4	C	502	-	12,12,12	0.80	0	11,11,11	0.36	0
2	PG4	A	501	-	12,12,12	0.80	0	11,11,11	0.40	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	C	501	-	-	6/10/10/10	-
2	PG4	B	501	-	-	2/10/10/10	-
2	PG4	C	502	-	-	6/10/10/10	-
2	PG4	A	501	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502	PG4	C3-C4-O3-C5
2	C	501	PG4	O2-C3-C4-O3
2	C	502	PG4	O2-C3-C4-O3
2	B	501	PG4	O3-C5-C6-O4
2	C	501	PG4	O3-C5-C6-O4
2	C	502	PG4	C1-C2-O2-C3
2	C	502	PG4	C8-C7-O4-C6
2	C	502	PG4	O4-C7-C8-O5
2	A	501	PG4	O2-C3-C4-O3
2	A	501	PG4	C5-C6-O4-C7
2	A	501	PG4	C1-C2-O2-C3
2	C	501	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
2	C	502	PG4	C6-C5-O3-C4
2	A	501	PG4	C4-C3-O2-C2
2	C	501	PG4	C8-C7-O4-C6
2	A	501	PG4	C3-C4-O3-C5
2	C	501	PG4	C5-C6-O4-C7
2	C	501	PG4	O1-C1-C2-O2
2	B	501	PG4	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PG4	2	0
2	C	502	PG4	2	0
2	A	501	PG4	3	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%)	0.49	62 (14%) 5 3	56, 95, 153, 237	0
1	B	413/431 (95%)	0.32	46 (11%) 10 6	61, 97, 141, 219	0
1	C	422/431 (97%)	0.36	50 (11%) 9 5	57, 85, 151, 222	0
All	All	1251/1293 (96%)	0.39	158 (12%) 8 5	56, 92, 148, 237	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	GLN	8.6
1	A	346	LEU	6.8
1	A	44	TYR	6.5
1	A	382	PRO	6.2
1	B	423	LEU	6.1
1	A	312	ILE	5.9
1	B	424	ASP	5.9
1	C	82	ARG	5.7
1	A	314	MET	5.6
1	A	16	TRP	5.5
1	A	117	LEU	5.4
1	A	357	GLY	5.4
1	B	353	ILE	5.4
1	A	332	ILE	5.3
1	C	324	THR	5.2
1	C	325	VAL	5.0
1	C	117	LEU	5.0
1	B	100	PHE	4.9
1	C	423	LEU	4.9
1	C	145	PHE	4.7
1	B	350	LEU	4.7
1	B	346	LEU	4.6
1	C	375	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	4.6
1	A	40	ALA	4.5
1	A	311	THR	4.4
1	A	116	ASN	4.3
1	B	422	GLU	4.3
1	C	115	VAL	4.2
1	B	121	THR	4.2
1	C	327	PHE	4.1
1	C	328	VAL	4.1
1	A	43	THR	4.1
1	C	326	LEU	4.1
1	B	116	ASN	4.0
1	A	194	GLU	3.9
1	B	115	VAL	3.9
1	B	425	GLU	3.8
1	B	347	THR	3.8
1	A	356	ALA	3.8
1	C	130	PRO	3.8
1	A	342	LEU	3.8
1	A	115	VAL	3.7
1	B	343	VAL	3.6
1	C	111	VAL	3.6
1	B	11	ASP	3.6
1	A	144	PRO	3.6
1	B	375	LEU	3.6
1	A	145	PHE	3.5
1	A	42	LYS	3.5
1	B	389	MET	3.5
1	A	310	ALA	3.5
1	B	385	LEU	3.4
1	C	376	ASP	3.4
1	A	343	VAL	3.4
1	A	132	LEU	3.4
1	C	287	THR	3.4
1	A	383	VAL	3.3
1	B	352	SER	3.3
1	B	206	TYR	3.3
1	A	15	LEU	3.3
1	A	37	TYR	3.3
1	A	148	LEU	3.3
1	C	10	LEU	3.2
1	C	233	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLU	3.1
1	C	110	ASN	3.1
1	C	129	PRO	3.1
1	C	127	ALA	3.1
1	A	313	ASN	3.1
1	C	393	ILE	3.1
1	A	147	SER	3.1
1	B	383	VAL	3.1
1	C	14	VAL	3.1
1	C	230	LEU	3.0
1	C	323	VAL	3.0
1	B	376	ASP	3.0
1	C	389	MET	3.0
1	B	418	LYS	2.9
1	C	270	ALA	2.9
1	B	270	ALA	2.9
1	A	39	GLY	2.9
1	C	304	PHE	2.9
1	A	20	TRP	2.9
1	B	280	SER	2.8
1	A	93	ALA	2.8
1	C	420	GLU	2.8
1	C	261	ILE	2.8
1	C	176	GLU	2.8
1	A	309	GLY	2.8
1	B	413	THR	2.8
1	C	321	GLN	2.8
1	A	41	VAL	2.7
1	A	136	LEU	2.7
1	A	353	ILE	2.7
1	B	427	LYS	2.7
1	B	357	GLY	2.7
1	A	347	THR	2.7
1	C	120	GLY	2.6
1	B	428	TRP	2.6
1	A	301	ILE	2.6
1	B	287	THR	2.6
1	B	354	GLY	2.6
1	C	132	LEU	2.5
1	B	14	VAL	2.5
1	A	34	HIS	2.5
1	B	203	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	75	ILE	2.5
1	A	423	LEU	2.5
1	A	151	GLY	2.5
1	B	349	VAL	2.5
1	A	352	SER	2.4
1	A	141	PRO	2.4
1	A	149	ALA	2.4
1	C	16	TRP	2.4
1	A	328	VAL	2.4
1	A	350	LEU	2.4
1	A	381	SER	2.4
1	C	409	ASP	2.4
1	C	225	ARG	2.4
1	A	13	PRO	2.4
1	A	140	VAL	2.4
1	C	79	ARG	2.3
1	B	113	ALA	2.3
1	C	429	ILE	2.3
1	B	52	PHE	2.3
1	C	15	LEU	2.3
1	B	129	PRO	2.3
1	B	426	SER	2.3
1	C	390	ILE	2.3
1	C	419	THR	2.3
1	B	58	MET	2.3
1	C	366	LEU	2.3
1	C	341	GLN	2.3
1	A	150	LYS	2.3
1	A	299	LYS	2.3
1	C	86	LYS	2.3
1	A	398	ASP	2.2
1	B	272	ILE	2.2
1	B	269	ASP	2.2
1	B	409	ASP	2.2
1	A	38	ALA	2.2
1	A	386	ALA	2.2
1	C	144	PRO	2.2
1	C	128	GLN	2.1
1	C	410	LEU	2.1
1	A	292	GLU	2.1
1	A	106	GLY	2.1
1	B	348	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	VAL	2.1
1	B	117	LEU	2.1
1	A	146	ALA	2.1
1	B	16	TRP	2.0
1	B	72	ALA	2.0
1	C	124	ALA	2.0
1	C	177	ARG	2.0
1	C	370	LEU	2.0
1	A	171	MET	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 oligosaccharides 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, 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(Å ²)	Q<0.9
2	PG4	C	501	13/13	0.76	0.32	87,127,149,150	0
2	PG4	B	501	13/13	0.79	0.22	88,111,139,140	0
2	PG4	A	501	13/13	0.80	0.23	81,106,137,142	0
2	PG4	C	502	13/13	0.83	0.28	89,127,143,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.