Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 06:42 pm GMT

PDB ID	:	2BTY
Title	:	Acetylglutamate kinase from Thermotoga maritima complexed with its inhibitor arginine
Authors	:	Gil-Ortiz, F.; Fernandez-Murga, M.L.; Fita, I.; Rubio, V.
Deposited on	:	2005-06-08
Resolution	:	2.75 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 (i) 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 (i)) were used in the production of this report:

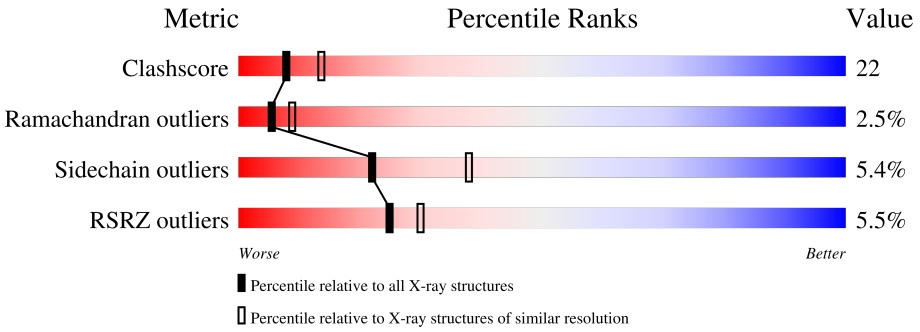
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	282	5%, 66%, 30%, • •
1	B	282	2%, 65%, 32%, • •
1	C	282	9%, 53%, 44%, •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NLG	A	1284	-	X	-	-
3	NLG	B	1284	-	X	-	X
3	NLG	C	1284	-	-	-	X

2 Entry composition (i)

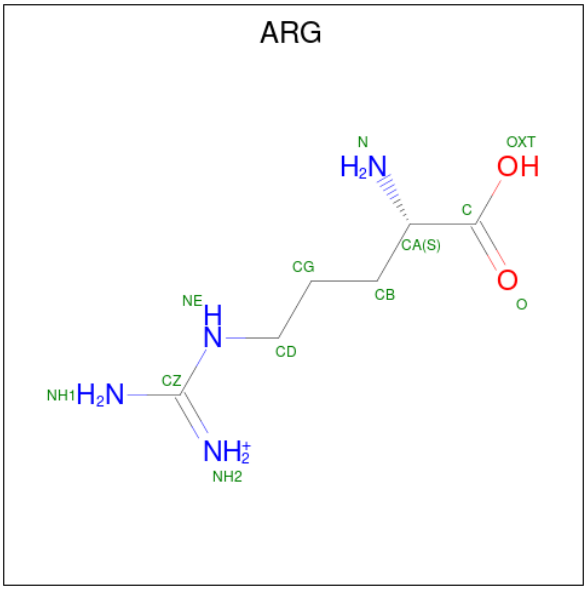
There are 5 unique types of molecules in this entry. The entry contains 6503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLGLUTAMATE KINASE.

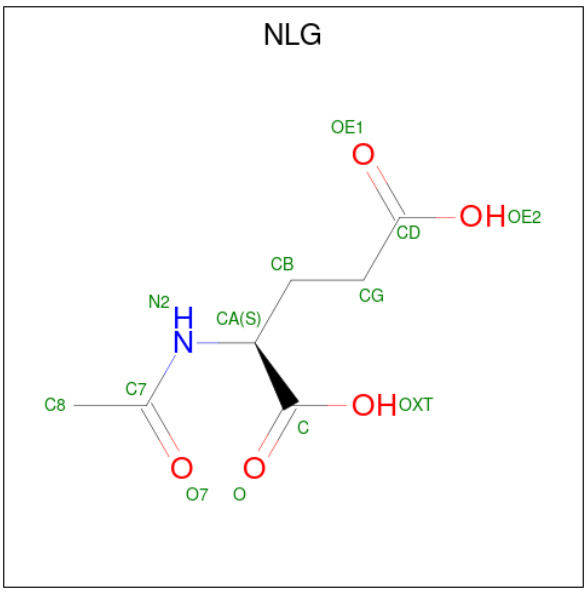
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2127	1360	357	398	12	8	0	0
1	B	282	2127	1360	357	398	12	0	0	0
1	C	282	2127	1360	357	398	12	74	0	0

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	6	4	2	0	0
2	B	1	12	6	4	2	0	0
2	C	1	12	6	4	2	0	0

- Molecule 3 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	7	1	5	0	0
			Total	C	N	O		
3	B	1	13	7	1	5	0	0
			Total	C	N	O		
3	C	1	13	7	1	5	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0

- Molecule 5 is water.

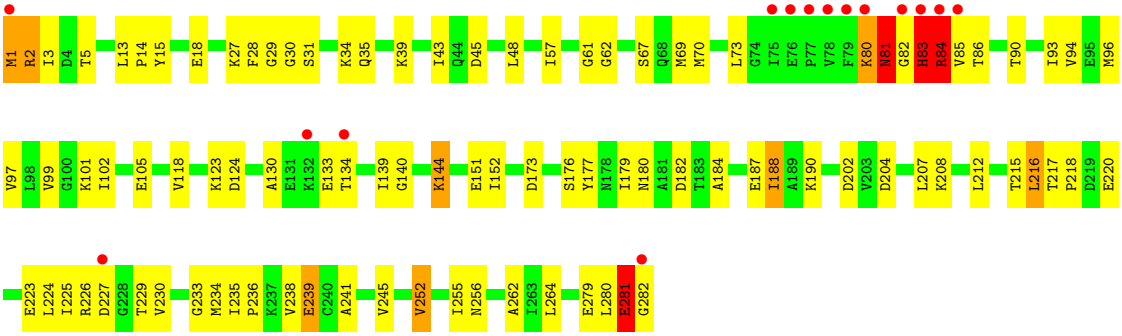
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	15	15	15	0	0
			Total	O		
5	B	15	15	15	0	0
			Total	O		
5	C	16	16	16	0	0

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.

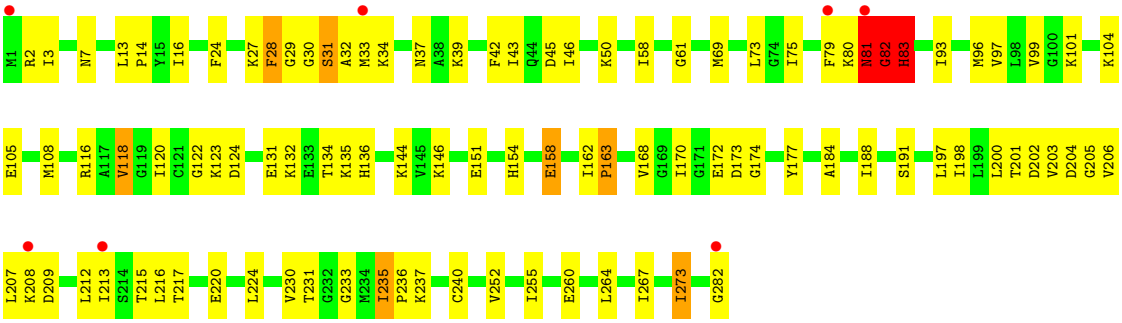
- Molecule 1: ACETYLGLUTAMATE KINASE

Chain A:



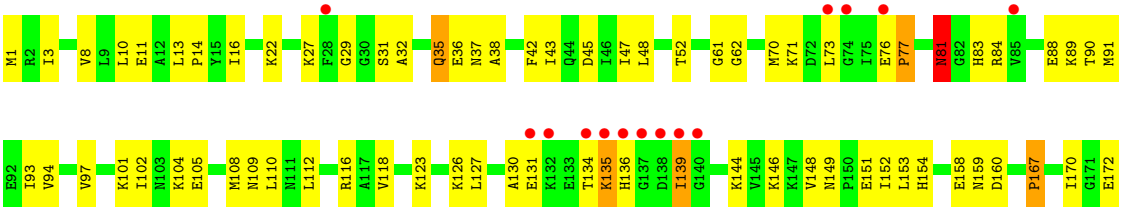
- Molecule 1: ACETYLGLUTAMATE KINASE

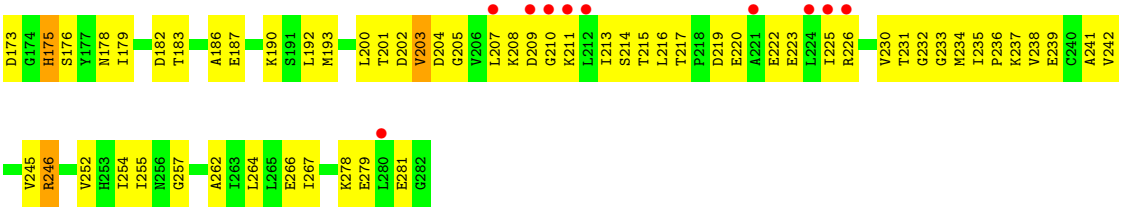
Chain B:



- Molecule 1: ACETYLGLUTAMATE KINASE

Chain C:




D173 G174 H175 S176 Y177 N178 I179 D182 T183 A186 E187 K190 S191 L192 M193 L200 T201 D202 V203 D204 G205 V206 L207 K208 D209 G210 K211 L212 I213 S214 T215 L216 T217 P218 D219 E220 A221 E222 E223 L224 I225 R226 V230 T231 G232 G233 M234 I235 P236 K237 V238 E239 C240 A241 V242
V245 R246 V252 H253 I254 I255 N256 G257 A262 I263 L264 L265 E266 I267 K278 E279 L280 E281 G282

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.00Å 207.71Å 118.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.75 40.60 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.95-2.75) 98.7 (40.60-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.273 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6503	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	1/2155 (0.0%)	0.76	3/2900 (0.1%)
1	B	0.56	1/2155 (0.0%)	0.83	9/2900 (0.3%)
1	C	0.43	0/2155	0.75	2/2900 (0.1%)
All	All	0.50	2/6465 (0.0%)	0.78	14/8700 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	GLY	C-OXT	12.79	1.47	1.23
1	A	282	GLY	C-OXT	10.18	1.42	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	ASN	CA-C-N	-8.54	99.12	116.20
1	B	81	ASN	C-N-CA	7.76	138.60	122.30
1	B	80	LYS	C-N-CA	7.43	140.27	121.70
1	B	82	GLY	N-CA-C	-7.20	95.09	113.10
1	C	81	ASN	CA-C-N	-7.14	101.93	116.20
1	A	80	LYS	C-N-CA	6.14	137.05	121.70
1	B	81	ASN	N-CA-C	6.00	127.20	111.00
1	B	83	HIS	CB-CA-C	-5.89	98.61	110.40
1	A	81	ASN	C-N-CA	5.36	133.55	122.30
1	B	81	ASN	O-C-N	5.20	132.04	123.20
1	A	281	GLU	CA-C-N	-5.14	105.93	116.20
1	C	81	ASN	C-N-CA	5.04	132.87	122.30
1	B	163	PRO	CA-N-CD	-5.03	104.46	111.50
1	B	81	ASN	CA-CB-CG	-5.02	102.36	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2127	0	2235	91	0
1	B	2127	0	2235	97	0
1	C	2127	0	2235	116	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
2	C	12	0	12	2	0
3	A	13	0	9	5	0
3	B	13	0	9	4	0
3	C	13	0	9	4	0
4	A	1	0	0	0	0
5	A	15	0	0	0	0
5	B	15	0	0	2	0
5	C	16	0	0	3	0
All	All	6503	0	6768	282	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 22.

All (282) 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:C:208:LYS:HB2	1:C:213:ILE:HD11	1.24	1.08
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.20	1.05
1:C:208:LYS:CB	1:C:213:ILE:HD11	1.87	1.05
1:C:136:HIS:HB2	1:C:139:ILE:HD11	1.40	1.03
1:A:223:GLU:OE1	1:A:226:ARG:HD3	1.59	1.01
1:B:13:LEU:HA	1:B:16:ILE:HD12	1.43	0.98
1:B:231:THR:CA	1:B:235:ILE:HD11	1.92	0.98
1:B:82:GLY:HA3	1:B:136:HIS:HD2	1.28	0.96
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.33	0.93
1:B:46:ILE:HD12	1:B:58:ILE:HD11	1.52	0.92
1:A:225:ILE:HD13	1:A:235:ILE:HG23	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:THR:HA	1:B:235:ILE:HD11	1.53	0.89
1:B:30:GLY:N	3:B:1284:NLG:OE1	2.06	0.88
1:A:84:ARG:HG3	1:A:84:ARG:NH1	1.87	0.86
1:A:30:GLY:N	3:A:1284:NLG:OE1	2.09	0.85
1:B:61:GLY:HA3	3:B:1284:NLG:HBC1	1.57	0.85
1:B:235:ILE:HB	1:B:236:PRO:HD3	1.60	0.84
1:B:230:VAL:HG12	1:B:235:ILE:HD12	1.57	0.83
1:A:233:GLY:O	1:A:236:PRO:HD2	1.80	0.80
1:B:101:LYS:O	1:B:105:GLU:HG3	1.81	0.79
1:B:206:VAL:HG12	1:B:213:ILE:HD12	1.65	0.78
1:A:61:GLY:HA3	3:A:1284:NLG:HBC1	1.65	0.77
1:A:96:MET:HG2	1:B:96:MET:HG2	1.66	0.77
1:A:48:LEU:HD11	1:C:10:LEU:HD23	1.65	0.76
1:A:101:LYS:O	1:A:105:GLU:HG3	1.86	0.75
1:C:43:ILE:HD13	1:C:109:ASN:HB3	1.67	0.75
1:C:183:THR:O	1:C:187:GLU:HG2	1.87	0.75
1:B:207:LEU:C	1:B:209:ASP:H	1.91	0.73
1:B:154:HIS:O	1:B:158:GLU:HB2	1.88	0.73
1:C:42:PHE:CE1	1:C:200:LEU:HD11	2.23	0.73
1:A:13:LEU:CD1	1:C:48:LEU:HB3	2.18	0.73
1:C:207:LEU:HD22	1:C:210:GLY:O	1.89	0.73
1:C:172:GLU:CD	1:C:172:GLU:H	1.91	0.73
1:A:90:THR:O	1:A:94:VAL:HG23	1.89	0.72
1:B:231:THR:N	1:B:235:ILE:HD11	2.04	0.72
1:A:48:LEU:HD13	1:C:13:LEU:HD12	1.70	0.72
1:C:61:GLY:HA3	3:C:1284:NLG:HBC1	1.71	0.72
1:A:280:LEU:O	1:A:281:GLU:HB3	1.89	0.72
1:B:208:LYS:HG3	1:B:208:LYS:O	1.88	0.72
1:A:123:LYS:HE3	1:A:176:SER:HB3	1.71	0.72
1:C:214:SER:HB2	5:C:2014:HOH:O	1.89	0.71
1:A:39:LYS:O	1:A:43:ILE:HD13	1.91	0.71
1:C:136:HIS:HB2	1:C:139:ILE:CD1	2.20	0.71
1:C:136:HIS:O	1:C:139:ILE:HG12	1.92	0.70
1:A:226:ARG:HG2	1:A:226:ARG:NH1	2.03	0.70
1:B:81:ASN:HA	1:B:83:HIS:H	1.56	0.69
1:C:42:PHE:HE1	1:C:200:LEU:HD11	1.57	0.69
1:C:208:LYS:HB2	1:C:213:ILE:CD1	2.14	0.69
1:B:230:VAL:HG12	1:B:235:ILE:CD1	2.23	0.69
1:B:82:GLY:HA3	1:B:136:HIS:CD2	2.20	0.69
1:C:235:ILE:HB	1:C:236:PRO:HD3	1.74	0.68
1:A:13:LEU:HD13	1:C:48:LEU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG12	1:B:7:ASN:ND2	2.08	0.68
1:B:31:SER:HB2	1:B:202:ASP:OD2	1.94	0.67
1:C:173:ASP:OD2	1:C:175:HIS:HB2	1.94	0.67
1:B:73:LEU:O	1:B:75:ILE:HG13	1.94	0.67
1:C:91:MET:HE3	1:C:94:VAL:HB	1.76	0.67
1:C:45:ASP:OD1	1:C:264:LEU:HB2	1.96	0.66
1:B:135:LYS:HG3	1:B:136:HIS:ND1	2.10	0.66
1:B:46:ILE:CD1	1:B:58:ILE:HD11	2.24	0.66
1:C:242:VAL:HG12	1:C:246:ARG:HD2	1.78	0.65
1:C:183:THR:HG23	5:C:2012:HOH:O	1.96	0.65
1:B:50:LYS:HD2	1:B:162:ILE:HD11	1.77	0.65
1:A:207:LEU:HD23	1:A:212:LEU:HA	1.79	0.65
1:C:238:VAL:O	1:C:242:VAL:HG23	1.96	0.65
1:A:235:ILE:HB	1:A:236:PRO:HD3	1.77	0.64
1:C:27:LYS:HG2	1:C:182:ASP:OD2	1.96	0.64
1:A:93:ILE:O	1:A:97:VAL:HG23	1.98	0.63
1:C:213:ILE:HG21	1:C:216:LEU:HD21	1.81	0.63
1:C:116:ARG:HH11	1:C:160:ASP:HB3	1.63	0.63
1:C:135:LYS:HG3	1:C:136:HIS:ND1	2.13	0.63
1:C:278:LYS:HE2	1:C:279:GLU:O	1.99	0.63
1:B:37:ASN:HB3	1:B:260:GLU:OE2	1.98	0.63
1:B:235:ILE:CD1	1:B:235:ILE:N	2.62	0.63
1:A:73:LEU:HD13	1:B:73:LEU:HD13	1.81	0.62
1:B:203:VAL:HG12	1:B:204:ASP:N	2.14	0.62
1:B:207:LEU:HD23	1:B:212:LEU:HA	1.80	0.62
1:B:151:GLU:OE1	1:B:151:GLU:N	2.27	0.62
1:C:71:LYS:HE3	1:C:77:PRO:CD	2.30	0.62
1:B:42:PHE:CE1	1:B:200:LEU:HD11	2.35	0.61
1:A:233:GLY:C	1:A:236:PRO:HD2	2.21	0.61
1:A:133:GLU:HA	1:A:144:LYS:HG2	1.83	0.61
1:B:13:LEU:HD23	1:B:16:ILE:CD1	2.31	0.61
1:B:134:THR:HG22	1:B:134:THR:O	1.99	0.61
1:B:208:LYS:HB2	1:B:213:ILE:HD11	1.82	0.60
1:C:186:ALA:O	1:C:190:LYS:HG3	2.01	0.60
1:B:201:THR:HG22	1:B:237:LYS:HE3	1.83	0.59
1:C:61:GLY:HA3	3:C:1284:NLG:CB	2.32	0.59
1:A:217:THR:OG1	1:A:220:GLU:HG3	2.02	0.59
1:B:132:LYS:HD2	1:B:177:TYR:HE2	1.67	0.59
1:C:254:ILE:N	1:C:254:ILE:HD12	2.18	0.58
1:C:231:THR:HG22	1:C:232:GLY:N	2.17	0.58
1:C:233:GLY:O	1:C:236:PRO:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD23	1:A:93:ILE:HD13	1.85	0.58
1:A:96:MET:HG2	1:B:96:MET:CG	2.32	0.58
1:B:231:THR:CA	1:B:235:ILE:CD1	2.78	0.58
1:A:235:ILE:O	1:A:239:GLU:HB2	2.04	0.57
1:C:255:ILE:HD12	1:C:262:ALA:HB1	1.86	0.57
1:C:217:THR:OG1	1:C:220:GLU:HG3	2.04	0.57
1:C:234:MET:O	1:C:238:VAL:HG23	2.04	0.57
1:C:27:LYS:HE2	1:C:29:GLY:HA2	1.87	0.57
1:C:11:GLU:O	1:C:14:PRO:HD2	2.05	0.57
1:C:215:THR:HG22	1:C:216:LEU:N	2.19	0.57
1:A:13:LEU:HD12	1:C:48:LEU:HB3	1.87	0.56
1:A:223:GLU:O	1:A:227:ASP:HB2	2.04	0.56
1:A:134:THR:HG22	1:A:134:THR:O	2.03	0.56
1:B:197:LEU:HB3	1:B:252:VAL:HG22	1.88	0.56
1:C:62:GLY:H	3:C:1284:NLG:HBC1	1.70	0.56
1:A:48:LEU:HD11	1:C:10:LEU:CD2	2.33	0.56
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.02	0.56
1:C:241:ALA:O	1:C:245:VAL:HG23	2.06	0.55
1:C:90:THR:O	1:C:94:VAL:HG23	2.07	0.55
1:C:230:VAL:HG13	1:C:234:MET:HG3	1.88	0.55
1:A:13:LEU:HB2	1:C:48:LEU:HD22	1.89	0.54
1:C:35:GLN:O	1:C:37:ASN:N	2.39	0.54
1:A:67:SER:O	1:A:70:MET:HB2	2.08	0.54
1:C:123:LYS:HE3	1:C:176:SER:OG	2.06	0.54
1:A:99:VAL:HG11	1:B:104:LYS:HE3	1.88	0.54
1:A:241:ALA:CB	1:A:252:VAL:HG21	2.37	0.54
1:C:242:VAL:O	1:C:246:ARG:HG3	2.07	0.54
1:C:32:ALA:HB2	1:C:257:GLY:O	2.08	0.54
1:C:108:MET:O	1:C:112:LEU:HG	2.07	0.54
1:B:172:GLU:C	1:B:174:GLY:H	2.09	0.54
1:C:71:LYS:HE3	1:C:77:PRO:HD3	1.89	0.54
1:B:235:ILE:HD12	1:B:235:ILE:N	2.22	0.53
1:A:204:ASP:HA	1:A:256:ASN:HB2	1.89	0.53
1:B:42:PHE:HE1	1:B:200:LEU:HD11	1.72	0.53
1:A:73:LEU:HD23	1:A:93:ILE:CD1	2.38	0.53
1:B:30:GLY:N	3:B:1284:NLG:CD	2.72	0.53
1:B:230:VAL:C	1:B:235:ILE:HD11	2.29	0.53
1:C:123:LYS:HG2	1:C:170:ILE:HB	1.91	0.52
1:C:223:GLU:HA	1:C:226:ARG:HD2	1.91	0.52
1:B:45:ASP:OD1	1:B:264:LEU:HB2	2.10	0.52
1:C:131:GLU:OE2	1:C:146:LYS:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:O	1:B:33:MET:N	2.43	0.52
1:C:223:GLU:OE1	1:C:226:ARG:HD2	2.10	0.52
1:C:154:HIS:O	1:C:158:GLU:HG3	2.10	0.52
1:A:234:MET:O	1:A:238:VAL:HG23	2.09	0.52
1:A:280:LEU:O	1:A:281:GLU:CB	2.53	0.51
1:C:71:LYS:HE3	1:C:77:PRO:CG	2.39	0.51
1:C:136:HIS:CB	1:C:139:ILE:HD11	2.27	0.51
1:A:31:SER:HB2	1:A:202:ASP:CG	2.31	0.51
1:A:180:ASN:OD1	1:A:182:ASP:HB2	2.10	0.51
1:B:24:PHE:HE1	1:B:267:ILE:HD13	1.76	0.51
1:B:61:GLY:HA3	3:B:1284:NLG:CB	2.37	0.51
1:C:130:ALA:HB2	1:C:179:ILE:HD11	1.92	0.51
1:A:27:LYS:HD2	1:A:28:PHE:N	2.26	0.51
1:A:45:ASP:OD1	1:A:264:LEU:HB2	2.09	0.51
1:A:62:GLY:HA2	1:A:102:ILE:HD13	1.93	0.51
1:A:80:LYS:HG3	1:A:85:VAL:HG21	1.92	0.51
1:C:217:THR:HG23	1:C:220:GLU:OE1	2.10	0.51
1:A:130:ALA:HB2	1:A:179:ILE:HD11	1.92	0.51
1:A:124:ASP:HB3	1:B:118:VAL:HB	1.93	0.51
1:B:231:THR:C	1:B:235:ILE:CD1	2.79	0.51
1:B:203:VAL:CG1	1:B:204:ASP:N	2.74	0.50
1:B:217:THR:OG1	1:B:220:GLU:HG3	2.12	0.50
1:C:89:LYS:O	1:C:93:ILE:HD13	2.11	0.50
1:C:149:ASN:HB3	1:C:151:GLU:OE1	2.11	0.50
1:B:231:THR:HA	1:B:235:ILE:CD1	2.34	0.50
1:B:122:GLY:HA3	1:B:168:VAL:O	2.12	0.50
1:B:215:THR:HG22	1:B:216:LEU:N	2.25	0.50
1:A:187:GLU:OE2	1:A:190:LYS:NZ	2.37	0.50
1:B:120:ILE:HB	1:B:124:ASP:OD2	2.12	0.49
1:B:203:VAL:HG12	1:B:205:GLY:H	1.78	0.49
1:A:184:ALA:O	1:A:188:ILE:HG23	2.12	0.49
1:C:231:THR:CG2	1:C:232:GLY:N	2.76	0.49
1:A:69:MET:O	1:A:73:LEU:HB2	2.13	0.48
1:A:223:GLU:O	1:A:223:GLU:HG3	2.12	0.48
1:B:45:ASP:OD2	5:B:2003:HOH:O	2.19	0.48
1:C:22:LYS:HE3	5:C:2004:HOH:O	2.12	0.48
1:C:101:LYS:O	1:C:105:GLU:HG3	2.13	0.48
1:C:43:ILE:O	1:C:47:ILE:HG12	2.12	0.48
1:B:34:LYS:HD2	1:B:34:LYS:HA	1.64	0.48
1:B:116:ARG:HG2	5:B:2005:HOH:O	2.14	0.47
1:B:123:LYS:HG2	1:B:170:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:OE1	1:B:144:LYS:HE3	2.14	0.47
1:C:172:GLU:CD	1:C:172:GLU:N	2.66	0.47
1:C:203:VAL:O	1:C:205:GLY:N	2.46	0.47
1:A:241:ALA:HB1	1:A:252:VAL:HG21	1.96	0.47
1:A:255:ILE:HD12	1:A:262:ALA:HB1	1.96	0.47
1:B:207:LEU:C	1:B:209:ASP:N	2.65	0.47
1:A:48:LEU:HB3	1:C:13:LEU:CD1	2.45	0.47
1:C:215:THR:CG2	1:C:216:LEU:N	2.77	0.47
1:B:220:GLU:O	1:B:224:LEU:HG	2.15	0.47
1:B:201:THR:HG22	1:B:237:LYS:CE	2.45	0.47
1:B:134:THR:O	1:B:134:THR:CG2	2.63	0.47
1:C:245:VAL:HG22	1:C:252:VAL:HG23	1.96	0.47
1:A:13:LEU:CB	1:C:48:LEU:HD22	2.44	0.46
1:A:215:THR:HG22	1:A:216:LEU:N	2.31	0.46
1:B:230:VAL:CG1	1:B:235:ILE:HD12	2.37	0.46
1:C:267:ILE:HA	2:C:1283:ARG:N	2.30	0.46
1:C:88:GLU:OE1	1:C:88:GLU:HA	2.15	0.46
1:C:238:VAL:O	1:C:241:ALA:HB3	2.16	0.46
1:C:127:LEU:O	1:C:148:VAL:HA	2.16	0.46
1:A:48:LEU:HB3	1:C:13:LEU:HD13	1.97	0.46
1:A:151:GLU:H	1:A:151:GLU:CD	2.19	0.46
1:B:172:GLU:C	1:B:174:GLY:N	2.69	0.46
1:C:94:VAL:HG11	1:C:178:ASN:OD1	2.16	0.46
1:B:31:SER:C	1:B:33:MET:H	2.19	0.46
1:B:237:LYS:O	1:B:240:CYS:HB3	2.15	0.46
1:B:131:GLU:HG3	1:B:144:LYS:HE3	1.98	0.46
1:A:3:ILE:H	1:A:3:ILE:HG13	1.60	0.45
1:A:241:ALA:O	1:A:245:VAL:HG23	2.16	0.45
1:C:62:GLY:N	3:C:1284:NLG:HBC1	2.30	0.45
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.82	0.45
1:C:233:GLY:C	1:C:236:PRO:HD2	2.37	0.45
1:A:61:GLY:HA3	3:A:1284:NLG:CB	2.42	0.45
1:B:82:GLY:O	1:B:83:HIS:CG	2.68	0.45
1:C:201:THR:HG22	1:C:237:LYS:HD3	1.98	0.45
1:A:29:GLY:C	3:A:1284:NLG:OE1	2.55	0.45
1:A:34:LYS:HB3	1:A:35:GLN:OE1	2.16	0.45
1:A:13:LEU:HD12	1:C:48:LEU:HD13	1.98	0.45
1:A:152:ILE:HD13	1:B:118:VAL:HG11	1.99	0.45
1:C:208:LYS:HB3	1:C:213:ILE:HD11	1.86	0.45
1:A:13:LEU:HB2	1:A:14:PRO:HD3	1.98	0.45
1:B:93:ILE:O	1:B:97:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:THR:HG22	1:C:144:LYS:NZ	2.32	0.45
1:A:27:LYS:HD2	1:A:27:LYS:C	2.37	0.45
1:B:27:LYS:HE2	1:B:29:GLY:HA2	1.99	0.45
1:C:225:ILE:HD11	1:C:238:VAL:HG11	1.98	0.45
1:B:235:ILE:CB	1:B:236:PRO:HD3	2.36	0.44
1:C:116:ARG:NH1	1:C:159:ASN:O	2.50	0.44
1:A:134:THR:O	1:A:134:THR:CG2	2.66	0.44
1:B:97:VAL:O	1:B:101:LYS:HB3	2.17	0.44
1:B:79:PHE:HB3	1:B:81:ASN:HD22	1.82	0.44
1:C:35:GLN:O	1:C:38:ALA:N	2.45	0.44
1:C:126:LYS:O	1:C:149:ASN:ND2	2.37	0.44
1:A:85:VAL:HG22	1:A:139:ILE:HA	1.99	0.44
1:A:226:ARG:NH1	1:A:226:ARG:CG	2.74	0.44
1:A:230:VAL:HG13	1:A:234:MET:HG3	1.99	0.44
1:A:82:GLY:O	1:A:83:HIS:CB	2.66	0.44
1:A:99:VAL:CG1	1:B:104:LYS:HE3	2.47	0.44
1:A:176:SER:C	1:A:177:TYR:HD1	2.20	0.44
1:A:218:PRO:HG2	1:A:279:GLU:OE1	2.17	0.43
1:B:13:LEU:HD23	1:B:16:ILE:HD12	1.99	0.43
1:C:235:ILE:HG22	1:C:239:GLU:OE1	2.17	0.43
1:A:48:LEU:HD22	1:C:13:LEU:CB	2.48	0.43
1:C:93:ILE:O	1:C:97:VAL:HG23	2.18	0.43
1:C:76:GLU:CD	1:C:76:GLU:H	2.21	0.43
1:C:146:LYS:O	1:C:146:LYS:HG2	2.18	0.43
1:A:5:THR:HA	1:C:8:VAL:HG21	2.00	0.43
1:A:208:LYS:HG3	1:A:229:THR:HG21	2.01	0.43
1:B:73:LEU:HD23	1:B:93:ILE:CD1	2.49	0.43
1:C:43:ILE:HG23	1:C:110:LEU:HD23	2.00	0.43
1:B:39:LYS:O	1:B:43:ILE:HG12	2.18	0.43
1:C:13:LEU:HB2	1:C:14:PRO:HD3	1.99	0.43
1:C:255:ILE:HD12	1:C:262:ALA:CB	2.47	0.43
1:B:82:GLY:O	1:B:83:HIS:CB	2.66	0.43
1:B:198:ILE:HD11	1:B:267:ILE:HD11	2.00	0.43
1:B:231:THR:C	1:B:235:ILE:HD13	2.39	0.43
1:C:222:GLU:O	1:C:226:ARG:HG3	2.19	0.43
1:A:1:MET:O	1:A:2:ARG:C	2.57	0.43
1:B:24:PHE:CE1	1:B:267:ILE:HD13	2.53	0.43
1:C:208:LYS:N	1:C:211:LYS:O	2.50	0.42
1:A:86:THR:O	1:A:140:GLY:HA3	2.19	0.42
1:A:204:ASP:N	1:A:256:ASN:HD22	2.16	0.42
1:C:209:ASP:O	1:C:211:LYS:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HD12	1:A:43:ILE:N	2.34	0.42
1:B:184:ALA:O	1:B:188:ILE:HG13	2.20	0.42
1:B:233:GLY:O	1:B:236:PRO:HD2	2.19	0.42
1:A:13:LEU:HD22	1:C:52:THR:CG2	2.50	0.42
1:C:192:LEU:O	1:C:193:MET:HB2	2.19	0.42
1:A:62:GLY:N	3:A:1284:NLG:HGC2	2.35	0.42
1:C:13:LEU:O	1:C:16:ILE:HB	2.20	0.42
1:C:109:ASN:HD22	1:C:109:ASN:HA	1.67	0.42
1:A:15:TYR:CE2	2:A:1283:ARG:HA	2.55	0.41
1:B:215:THR:CG2	1:B:216:LEU:N	2.83	0.41
1:C:167:PRO:O	1:C:179:ILE:HB	2.20	0.41
1:B:69:MET:O	1:B:73:LEU:HB2	2.19	0.41
1:B:273:ILE:HD12	1:B:273:ILE:C	2.40	0.41
1:A:99:VAL:HG12	1:B:99:VAL:HG12	2.03	0.41
1:A:224:LEU:HB3	1:A:230:VAL:HG23	2.02	0.41
1:B:231:THR:C	1:B:235:ILE:HD11	2.35	0.41
1:C:254:ILE:HD12	1:C:254:ILE:H	1.86	0.41
1:B:131:GLU:OE2	1:B:146:LYS:HD2	2.20	0.41
1:C:73:LEU:HD12	1:C:73:LEU:HA	1.92	0.41
1:C:266:GLU:O	2:C:1283:ARG:N	2.54	0.41
1:A:223:GLU:OE1	1:A:223:GLU:HA	2.21	0.41
1:C:152:ILE:HG23	1:C:153:LEU:N	2.36	0.41
1:C:201:THR:CG2	1:C:237:LYS:HD3	2.51	0.41
1:C:102:ILE:HD13	1:C:105:GLU:OE2	2.22	0.40
1:B:28:PHE:HD1	1:B:28:PHE:HA	1.75	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	280/282 (99%)	258 (92%)	18 (6%)	4 (1%)	11 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	280/282 (99%)	256 (91%)	18 (6%)	6 (2%)	7 12
1	C	280/282 (99%)	241 (86%)	28 (10%)	11 (4%)	3 4
All	All	840/846 (99%)	755 (90%)	64 (8%)	21 (2%)	5 9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	83	HIS
1	B	32	ALA
1	B	83	HIS
1	C	36	GLU
1	C	81	ASN
1	C	83	HIS
1	C	281	GLU
1	A	2	ARG
1	A	84	ARG
1	B	2	ARG
1	B	31	SER
1	C	204	ASP
1	C	135	LYS
1	B	82	GLY
1	C	31	SER
1	C	70	MET
1	B	273	ILE
1	C	77	PRO
1	C	167	PRO
1	C	203	VAL

5.3.2 Protein sidechains (i)

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	229/229 (100%)	215 (94%)	14 (6%)	18 33
1	B	229/229 (100%)	217 (95%)	12 (5%)	23 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	229/229 (100%)	218 (95%)	11 (5%)	25 44
All	All	687/687 (100%)	650 (95%)	37 (5%)	22 38

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	GLU
1	A	57	ILE
1	A	81	ASN
1	A	83	HIS
1	A	84	ARG
1	A	118	VAL
1	A	144	LYS
1	A	173	ASP
1	A	188	ILE
1	A	216	LEU
1	A	239	GLU
1	A	252	VAL
1	A	281	GLU
1	B	14	PRO
1	B	28	PHE
1	B	81	ASN
1	B	83	HIS
1	B	108	MET
1	B	118	VAL
1	B	158	GLU
1	B	163	PRO
1	B	173	ASP
1	B	191	SER
1	B	235	ILE
1	B	255	ILE
1	C	1	MET
1	C	3	ILE
1	C	35	GLN
1	C	81	ASN
1	C	84	ARG
1	C	118	VAL
1	C	139	ILE
1	C	175	HIS
1	C	202	ASP
1	C	219	ASP

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Mol	Chain	Res	Type
1	C	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	B	7	ASN
1	B	81	ASN
1	B	109	ASN
1	B	136	HIS
1	C	7	ASN
1	C	37	ASN
1	C	109	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NLG	C	1284	-	12,12,12	3.48	4 (33%)	15,15,15	4.29	10 (66%)
2	ARG	A	1283	-	10,11,11	0.79	1 (10%)	11,13,13	0.63	0
3	NLG	B	1284	-	12,12,12	4.77	8 (66%)	15,15,15	3.59	8 (53%)
2	ARG	C	1283	-	10,11,11	0.79	0	11,13,13	0.47	0
3	NLG	A	1284	-	12,12,12	4.77	8 (66%)	15,15,15	3.59	8 (53%)
2	ARG	B	1283	-	10,11,11	0.93	1 (10%)	11,13,13	0.60	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
3	NLG	C	1284	-	-	0/13/13/13	-
2	ARG	A	1283	-	-	1/11/11/11	-
3	NLG	B	1284	-	-	2/13/13/13	-
2	ARG	C	1283	-	-	1/11/11/11	-
3	NLG	A	1284	-	-	3/13/13/13	-
2	ARG	B	1283	-	-	0/11/11/11	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1284	NLG	C8-C7	-11.48	1.26	1.50
3	A	1284	NLG	C8-C7	-11.47	1.26	1.50
3	C	1284	NLG	C8-C7	-9.42	1.31	1.50
3	A	1284	NLG	CA-C	-6.97	1.34	1.52
3	B	1284	NLG	CA-C	-6.94	1.34	1.52
3	A	1284	NLG	C7-N2	-6.53	1.12	1.34
3	B	1284	NLG	C7-N2	-6.52	1.12	1.34
3	C	1284	NLG	C7-N2	-5.76	1.14	1.34
3	B	1284	NLG	O7-C7	3.85	1.32	1.23
3	A	1284	NLG	O7-C7	3.84	1.31	1.23
3	A	1284	NLG	CA-N2	3.77	1.53	1.45
3	B	1284	NLG	CA-N2	3.74	1.53	1.45
3	A	1284	NLG	OXT-C	2.92	1.40	1.30
3	B	1284	NLG	OXT-C	2.91	1.40	1.30
3	C	1284	NLG	OXT-C	2.57	1.39	1.30
3	B	1284	NLG	O-C	2.27	1.29	1.22
3	A	1284	NLG	O-C	2.26	1.29	1.22
3	C	1284	NLG	CB-CG	2.25	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1283	ARG	OXT-C	-2.14	1.23	1.30
3	A	1284	NLG	CB-CG	2.11	1.59	1.52
3	B	1284	NLG	CB-CG	2.10	1.59	1.52
2	B	1283	ARG	OXT-C	-2.04	1.23	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1284	NLG	OXT-C-O	-10.20	100.93	124.09
3	A	1284	NLG	OXT-C-O	-9.51	102.51	124.09
3	B	1284	NLG	OXT-C-O	-9.50	102.51	124.09
3	C	1284	NLG	CA-N2-C7	8.78	147.57	121.48
3	A	1284	NLG	CA-N2-C7	6.05	139.45	121.48
3	B	1284	NLG	CA-N2-C7	6.04	139.44	121.48
3	B	1284	NLG	OXT-C-CA	4.98	129.95	113.40
3	A	1284	NLG	OXT-C-CA	4.98	129.94	113.40
3	C	1284	NLG	OXT-C-CA	4.87	129.58	113.40
3	C	1284	NLG	C8-C7-N2	4.44	123.61	116.10
3	C	1284	NLG	OE2-CD-CG	-3.14	103.92	114.03
3	C	1284	NLG	OE1-CD-CG	3.04	132.84	123.08
3	C	1284	NLG	O7-C7-N2	-3.00	116.43	121.95
3	A	1284	NLG	OE1-CD-CG	2.70	131.77	123.08
3	B	1284	NLG	OE1-CD-CG	2.70	131.74	123.08
3	A	1284	NLG	OE2-CD-CG	-2.68	105.41	114.03
3	B	1284	NLG	OE2-CD-CG	-2.68	105.43	114.03
3	B	1284	NLG	O7-C7-N2	2.66	126.85	121.95
3	A	1284	NLG	O7-C7-N2	2.65	126.83	121.95
3	B	1284	NLG	C8-C7-N2	-2.54	111.80	116.10
3	A	1284	NLG	C8-C7-N2	-2.52	111.83	116.10
3	A	1284	NLG	CB-CA-N2	2.37	115.66	110.88
3	B	1284	NLG	CB-CA-N2	2.37	115.66	110.88
3	C	1284	NLG	CB-CG-CD	-2.28	106.44	112.51
3	C	1284	NLG	O-C-CA	2.20	129.48	122.26
3	C	1284	NLG	C-CA-N2	-2.04	105.71	110.55

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1284	NLG	C8-C7-N2-CA
3	A	1284	NLG	O7-C7-N2-CA
3	B	1284	NLG	C8-C7-N2-CA

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Mol	Chain	Res	Type	Atoms
3	B	1284	NLG	O7-C7-N2-CA
3	A	1284	NLG	CA-CB-CG-CD
2	A	1283	ARG	NE-CD-CG-CB
2	C	1283	ARG	CG-CD-NE-CZ

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1284	NLG	4	0
2	A	1283	ARG	1	0
3	B	1284	NLG	4	0
2	C	1283	ARG	2	0
3	A	1284	NLG	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	281/282 (99%)	0.09	15 (5%)	26	31	27, 46, 83, 101	0
1	B	282/282 (100%)	0.08	7 (2%)	57	66	28, 46, 78, 94	0
1	C	273/282 (96%)	0.50	24 (8%)	10	11	33, 62, 103, 110	0
All	All	836/846 (98%)	0.22	46 (5%)	25	30	27, 51, 95, 110	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	LYS	6.3
1	A	134	THR	5.0
1	C	139	ILE	4.8
1	C	85	VAL	4.6
1	A	79	PHE	4.3
1	C	138	ASP	3.9
1	C	225	ILE	3.7
1	C	209	ASP	3.6
1	C	74	GLY	3.6
1	C	280	LEU	3.6
1	A	77	PRO	3.3
1	C	73	LEU	3.2
1	A	78	VAL	3.2
1	B	33	MET	3.2
1	C	140	GLY	3.1
1	C	210	GLY	3.1
1	C	135	LYS	3.0
1	C	76	GLU	2.9
1	B	1	MET	2.8
1	C	212	LEU	2.8
1	B	282	GLY	2.7
1	C	131	GLU	2.7
1	A	1	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	82	GLY	2.6
1	C	221	ALA	2.6
1	C	207	LEU	2.6
1	C	28	PHE	2.6
1	A	85	VAL	2.6
1	B	208	LYS	2.5
1	A	76	GLU	2.5
1	A	83	HIS	2.5
1	B	213	ILE	2.5
1	C	136	HIS	2.4
1	C	226	ARG	2.4
1	A	282	GLY	2.4
1	C	211	LYS	2.4
1	C	224	LEU	2.4
1	A	75	ILE	2.4
1	A	84	ARG	2.3
1	B	81	ASN	2.2
1	C	137	GLY	2.2
1	B	79	PHE	2.2
1	A	132	LYS	2.1
1	C	134	THR	2.1
1	A	227	ASP	2.1
1	C	132	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NLG	C	1284	13/13	0.49	0.70	61,62,63,64	13
3	NLG	B	1284	13/13	0.60	0.46	68,69,70,71	13
3	NLG	A	1284	13/13	0.72	0.29	68,70,72,72	13
2	ARG	C	1283	12/12	0.87	0.18	51,57,62,62	0
4	K	A	1285	1/1	0.89	0.10	78,78,78,78	0
2	ARG	B	1283	12/12	0.95	0.20	41,43,46,46	0
2	ARG	A	1283	12/12	0.95	0.19	32,38,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.