Worldwide PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:04 AM GMT

PDB ID	:	3KQA
Title	:	MurA dead-end complex with terreic acid
Authors	:	Schonbrunn, E.
Deposited on	:	2009-11-17
Resolution	:	2.25 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

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 2.25 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		2.6%
RSRZ outliers		1.6%

Worse ▮ *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
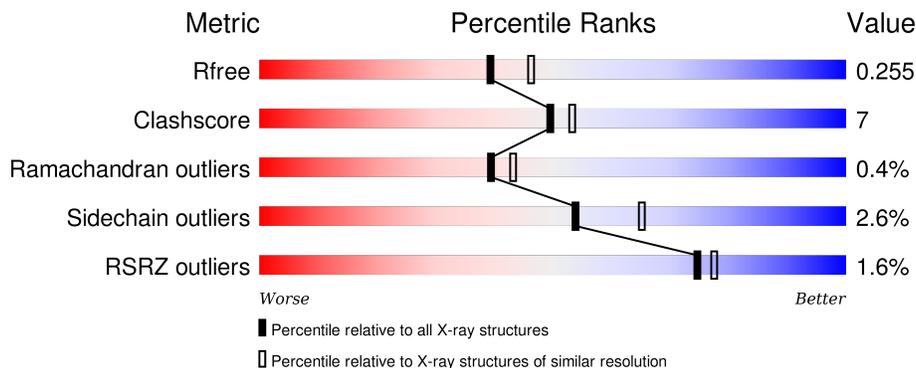
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	419	% 87% 13%
1	B	419	% 85% 14%
1	C	419	2% 84% 16% •
1	D	419	3% 79% 20% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13150 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total 3143	C 1976	N 554	O 599	S 14	0	0	0
1	B	419	Total 3143	C 1976	N 554	O 599	S 14	0	0	0
1	C	419	Total 3143	C 1976	N 554	O 599	S 14	0	0	0
1	D	419	Total 3143	C 1976	N 554	O 599	S 14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038

- Molecule 2 is (5S)-2,5-DIHYDROXY-3-METHYLCYCLOHEX-2-ENE-1,4-DIONE (three-letter code: TR9) (formula: $C_7H_8O_4$).
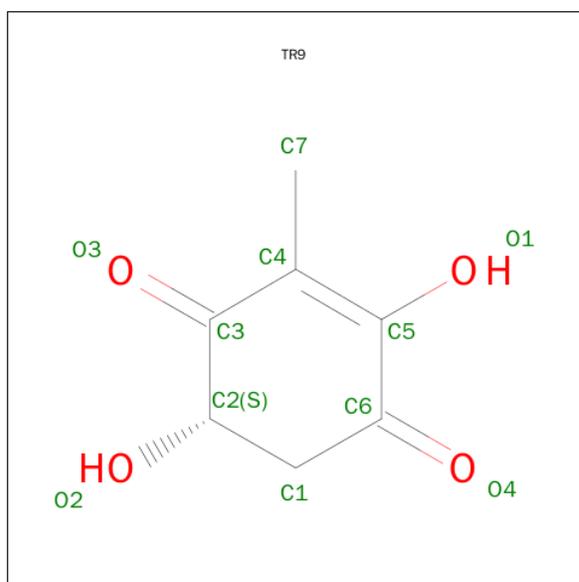
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 11	C 7	O 4	0	0
2	B	1	Total 11	C 7	O 4	0	0
2	C	1	Total 11	C 7	O 4	0	0
2	D	1	Total 11	C 7	O 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Ca 4	0	0
3	A	2	Total 2	Ca 2	0	0
3	D	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total 146	O 146	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	177	Total 177	O 177	0	0
4	C	125	Total 125	O 125	0	0
4	D	76	Total 76	O 76	0	0

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 errors 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: UDP-N-acetylglucosamine 1-carboxyvinyltransferase
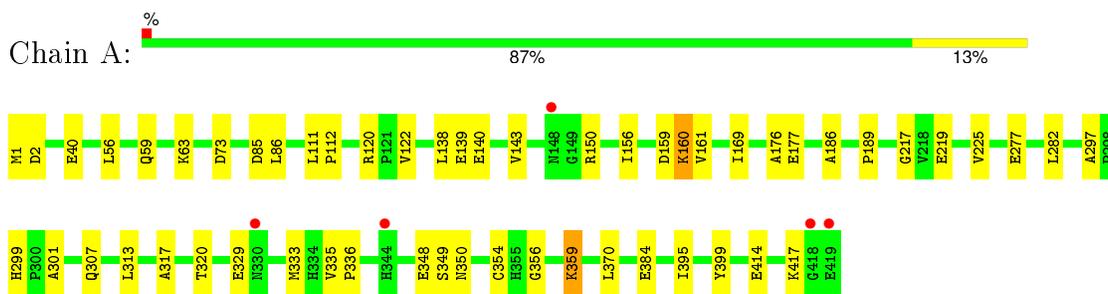
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

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M1 F4 R11 E15 A25 I28 L29 F30 L33 E36 I41 L56 Q59 K63 D73 N76 V77 D85 L86 V87 F104 Q108 V109 S110 I111 P112 G113 G114 C115 A119 I126 F127 E130 K131 I136 E140 K144

N148 G149 R150 V157 M170 T174 L175 A176 E183 N184 P189 Q208 I215 E216 G217 V218 E219 R220 L221 L229 R232 L239 A243 I244 S245 V250 P256 L259 G276 E277 D278 W279 I280 S281 L282 D283 M284 A297 P298 H299 Q307 N314

L315 I323 T324 E325 F328 E329 N330 V335 P336 E337 L338 I339 R340 E348 T351 K359 G362 A363 Q364 L378 E384 T387 I392 I402 E403 K417 G418 E419
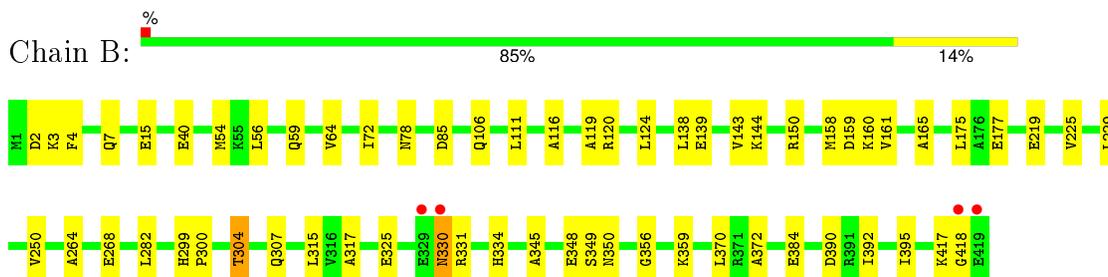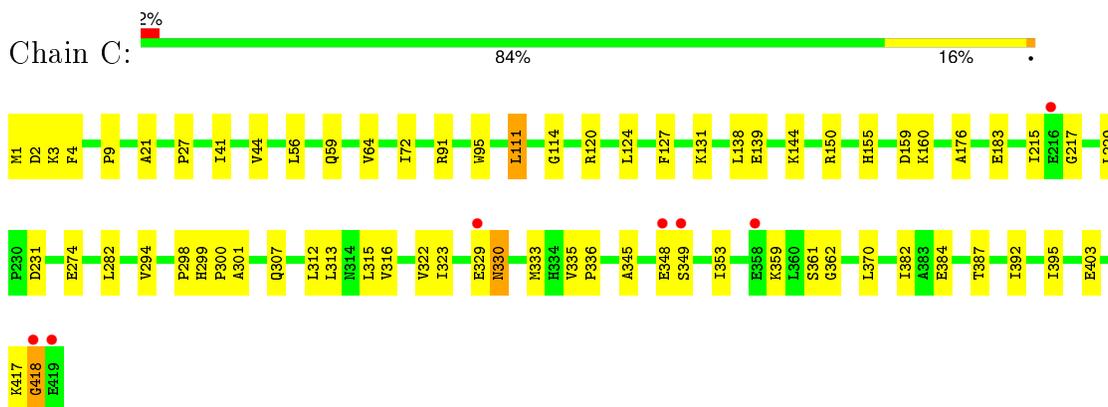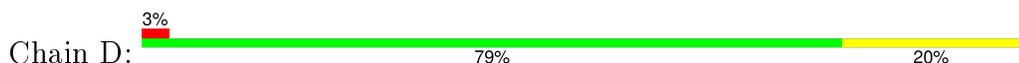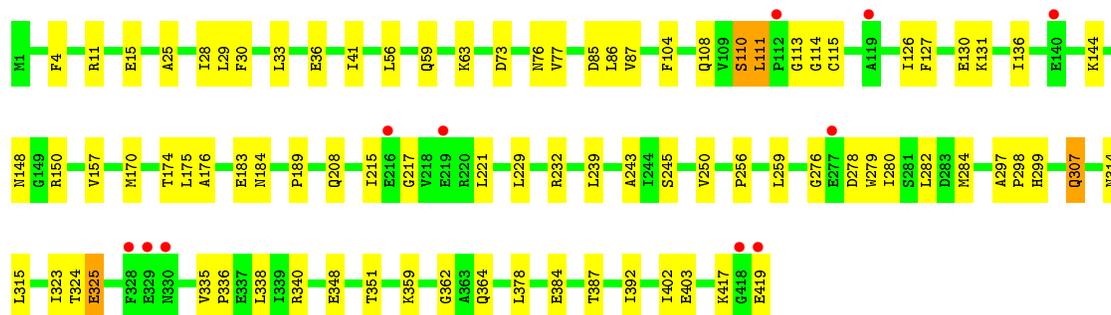
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.27Å 115.27Å 277.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.25 14.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.25) 99.8 (14.98-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.44 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.254 0.196 , 0.255	Depositor DCC
R_{free} test set	1063 reflections (1.20%)	DCC
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|>=0.45$, $<L^2>=0.28$	Xtriage
Outliers	0 of 88863 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13150	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.81 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2803e-03.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TR9, CA, IAS

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	0.55	0/3179	0.71	1/4305 (0.0%)
1	B	0.57	0/3179	0.74	0/4305
1	C	0.53	0/3179	0.71	0/4305
1	D	0.45	0/3179	0.67	0/4305
All	All	0.53	0/12716	0.71	1/17220 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	VAL	N-CA-C	-5.01	97.46	111.00

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	3143	0	3215	43	0
1	B	3143	0	3215	38	0
1	C	3143	0	3215	48	0
1	D	3143	0	3215	53	0
2	A	11	0	5	3	0
2	B	11	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	11	0	6	0	0
2	D	11	0	5	1	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	146	0	0	2	0
4	B	177	0	0	2	0
4	C	125	0	0	3	0
4	D	76	0	0	0	0
All	All	13150	0	12881	180	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 7.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASN:HD22	1:B:330:ASN:H	1.13	0.89
1:C:111:LEU:HD13	1:C:114:GLY:HA3	1.56	0.86
1:C:359:LYS:HD3	1:C:384:GLU:HB2	1.57	0.85
1:A:277:GLU:HG2	1:C:274:GLU:OE1	1.80	0.81
1:B:150:ARG:HD2	1:B:177:GLU:HG3	1.64	0.79
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.68	0.76
1:D:15:GLU:HG2	1:D:250:VAL:HB	1.68	0.75
1:B:138:LEU:HD22	2:B:500:TR9:H2	1.69	0.74
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.71	0.72
1:B:150:ARG:HD2	1:B:177:GLU:CG	2.19	0.72
1:A:138:LEU:HD22	2:A:500:TR9:H2	1.70	0.72
1:B:330:ASN:N	1:B:330:ASN:HD22	1.84	0.70
1:A:40:GLU:HB3	1:A:225:VAL:HG22	1.73	0.70
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.73	0.69
1:C:127:PHE:O	1:C:131:LYS:HG2	1.93	0.69
1:B:304:THR:HG22	1:B:325:GLU:OE2	1.93	0.68
1:B:219:GLU:HG3	4:B:494:HOH:O	1.94	0.68
1:A:150:ARG:NH2	1:A:219:GLU:HA	2.09	0.67
1:A:120:ARG:HD2	4:A:446:HOH:O	1.93	0.66
1:D:63:LYS:HE3	1:D:76:ASN:HD22	1.59	0.65
1:C:329:GLU:O	1:C:330:ASN:HB3	1.96	0.65
1:B:330:ASN:H	1:B:330:ASN:ND2	1.89	0.65
1:B:116:ALA:HB3	1:B:120:ARG:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD21	1:C:345:ALA:HB2	1.79	0.64
1:A:176:ALA:O	1:A:217:GLY:HA3	1.98	0.64
1:B:124:LEU:HB3	1:B:165:ALA:HB2	1.79	0.63
1:B:317:ALA:O	1:B:356:GLY:HA3	1.99	0.63
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.81	0.62
1:B:304:THR:HB	1:B:331:ARG:NH1	2.15	0.62
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.15	0.61
1:B:161:VAL:HG23	4:B:536:HOH:O	2.00	0.61
1:C:150:ARG:HH11	1:C:150:ARG:HG2	1.66	0.60
1:D:176:ALA:O	1:D:217:GLY:HA3	2.00	0.60
1:D:110:SER:O	1:D:111:LEU:HG	2.02	0.59
1:C:56:LEU:HD23	1:C:56:LEU:C	2.23	0.59
1:D:315:LEU:HD12	1:D:338:LEU:HD13	1.84	0.58
1:D:87:VAL:HG21	1:D:110:SER:O	2.04	0.58
1:A:2:ASP:OD1	1:A:417:LYS:HD3	2.04	0.58
1:D:157:VAL:HG22	1:D:183:GLU:HG3	1.84	0.58
1:D:63:LYS:HE3	1:D:76:ASN:ND2	2.18	0.57
1:D:4:PHE:CD1	1:D:392:ILE:HG21	2.39	0.57
1:D:189:PRO:HD3	1:D:299:HIS:CD2	2.39	0.57
1:B:359:LYS:HD3	1:B:384:GLU:HB2	1.87	0.56
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.41	0.56
1:B:330:ASN:N	1:B:330:ASN:ND2	2.49	0.55
1:D:157:VAL:HA	1:D:183:GLU:HB2	1.88	0.55
1:B:54:MET:HG2	1:B:64:VAL:HG11	1.89	0.55
1:A:348:GLU:O	1:A:349:SER:HB3	2.07	0.55
1:C:111:LEU:CD1	1:C:114:GLY:HA3	2.33	0.55
1:C:333:MET:HE3	1:C:333:MET:HA	1.88	0.55
1:D:150:ARG:HD2	1:D:175:LEU:O	2.07	0.55
1:D:127:PHE:O	1:D:131:LYS:HG2	2.07	0.54
1:B:2:ASP:OD1	1:B:417:LYS:HD3	2.07	0.54
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.89	0.54
1:D:113:GLY:O	1:D:115:CYS:N	2.40	0.54
1:A:313:LEU:C	1:A:313:LEU:HD23	2.28	0.54
1:D:282:LEU:C	1:D:282:LEU:HD23	2.28	0.53
1:D:108:GLN:OE1	1:D:144:LYS:HE2	2.08	0.53
1:C:139:GLU:HG3	1:C:144:LYS:HE3	1.89	0.53
1:A:189:PRO:HD3	1:A:299:HIS:CD2	2.44	0.52
1:C:329:GLU:O	1:C:330:ASN:CB	2.57	0.52
1:B:139:GLU:HG3	1:B:144:LYS:HE3	1.92	0.52
1:D:243:ALA:HA	1:D:284:MET:CG	2.40	0.51
1:B:64:VAL:HG13	1:B:72:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:HIS:HE1	1:C:183:GLU:OE2	1.94	0.51
1:D:362:GLY:HA2	1:D:387:THR:OG1	2.12	0.51
1:D:402:ILE:HG23	1:D:403:GLU:N	2.26	0.50
1:A:317:ALA:O	1:A:356:GLY:HA3	2.12	0.50
1:C:150:ARG:NH1	4:C:459:HOH:O	2.44	0.50
1:A:56:LEU:O	1:A:56:LEU:HD23	2.12	0.50
1:D:108:GLN:HG3	1:D:144:LYS:HG2	1.92	0.49
1:D:28:ILE:HG22	1:D:41:ILE:HD13	1.93	0.49
1:D:115:CYS:HA	2:D:500:TR9:H2	1.94	0.49
1:A:160:LYS:NZ	1:A:160:LYS:HB2	2.28	0.49
1:B:282:LEU:HD23	1:B:282:LEU:C	2.33	0.49
1:A:333:MET:HG3	4:A:515:HOH:O	2.12	0.49
1:A:370:LEU:CD1	1:A:395:ILE:HA	2.43	0.48
1:D:359:LYS:HD3	1:D:384:GLU:HB2	1.95	0.48
1:A:150:ARG:HD2	1:A:177:GLU:HB2	1.94	0.48
1:D:77:VAL:HB	1:D:104:PHE:CZ	2.49	0.48
1:D:232:ARG:HB2	1:D:259:LEU:HD21	1.96	0.48
1:B:40:GLU:HB3	1:B:225:VAL:HG22	1.95	0.48
1:D:59:GLN:HG2	1:D:86:LEU:HD12	1.95	0.48
1:B:264:ALA:O	1:B:268:GLU:HG3	2.13	0.48
1:D:340:ARG:NH2	1:D:364:GLN:O	2.47	0.48
1:C:138:LEU:N	1:C:138:LEU:HD22	2.29	0.47
1:A:139:GLU:O	1:A:140:GLU:HG2	2.14	0.47
1:C:21:ALA:HB2	1:C:231:ASP:HA	1.95	0.47
1:D:30:PHE:O	1:D:33:LEU:HB2	2.14	0.47
1:B:150:ARG:HD2	1:B:177:GLU:HG2	1.96	0.47
1:A:150:ARG:HH22	1:A:219:GLU:HA	1.78	0.47
1:B:299:HIS:CG	1:B:300:PRO:HA	2.49	0.47
1:C:120:ARG:NH2	1:D:348:GLU:OE1	2.48	0.47
1:C:91:ARG:HG2	1:C:91:ARG:HH11	1.79	0.46
1:B:348:GLU:O	1:B:349:SER:HB3	2.15	0.46
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.98	0.46
1:A:282:LEU:HD23	1:A:282:LEU:C	2.36	0.46
1:C:348:GLU:O	1:C:349:SER:HB3	2.16	0.46
1:D:11:ARG:HA	1:D:245:SER:HB2	1.98	0.46
1:A:156:ILE:HD13	1:A:169:ILE:HG21	1.98	0.46
1:B:150:ARG:HD3	1:B:175:LEU:O	2.16	0.45
1:B:304:THR:CG2	1:B:325:GLU:OE2	2.64	0.45
1:A:297:ALA:HB3	1:A:301:ALA:CB	2.47	0.45
1:C:124:LEU:CD1	1:C:124:LEU:N	2.79	0.45
1:C:120:ARG:HA	1:C:120:ARG:HD3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CD1	1:B:392:ILE:HG21	2.52	0.45
1:C:2:ASP:OD1	1:C:417:LYS:HD3	2.17	0.45
1:A:160:LYS:NZ	1:A:160:LYS:CB	2.79	0.45
1:D:215:ILE:HD12	1:D:215:ILE:N	2.31	0.45
1:C:294:VAL:HB	1:C:323:ILE:HD13	1.99	0.45
1:C:150:ARG:NH1	1:C:150:ARG:HG2	2.32	0.45
1:C:215:ILE:HD12	1:C:215:ILE:N	2.31	0.45
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.99	0.45
1:D:29:LEU:HD23	1:D:41:ILE:HD12	1.99	0.44
1:A:56:LEU:C	1:A:56:LEU:HD23	2.38	0.44
1:D:126:ILE:HG23	1:D:136:ILE:HG13	2.00	0.44
1:B:370:LEU:HD12	1:B:395:ILE:HA	1.99	0.44
1:A:359:LYS:CE	1:A:384:GLU:HB2	2.47	0.44
1:C:27:PRO:HD3	1:C:95:TRP:CZ3	2.52	0.44
1:C:333:MET:O	1:C:336:PRO:HD2	2.17	0.44
1:D:256:PRO:HG3	1:D:280:ILE:CG1	2.48	0.44
1:A:59:GLN:HG2	1:A:86:LEU:HD12	2.00	0.44
1:C:403:GLU:CB	4:C:446:HOH:O	2.65	0.43
1:C:176:ALA:O	1:C:217:GLY:HA3	2.18	0.43
1:D:56:LEU:O	1:D:56:LEU:HD23	2.19	0.43
1:C:124:LEU:HD12	1:C:124:LEU:N	2.34	0.43
1:C:313:LEU:HD23	1:C:313:LEU:C	2.38	0.43
1:C:160:LYS:HB2	1:C:160:LYS:NZ	2.34	0.43
1:C:64:VAL:HG13	1:C:72:ILE:HD13	2.01	0.43
1:A:161:VAL:CG1	1:A:186:ALA:HA	2.49	0.43
1:B:325:GLU:O	1:B:350:ASN:ND2	2.44	0.43
1:C:299:HIS:CG	1:C:300:PRO:HA	2.54	0.43
1:D:278:ASP:OD2	1:D:278:ASP:N	2.52	0.43
1:C:294:VAL:HB	1:C:323:ILE:CD1	2.49	0.42
1:C:282:LEU:C	1:C:282:LEU:HD23	2.40	0.42
1:C:403:GLU:HB3	4:C:446:HOH:O	2.17	0.42
1:C:370:LEU:HD12	1:C:395:ILE:HA	2.01	0.42
1:C:417:LYS:O	1:C:418:GLY:O	2.36	0.42
1:D:324:THR:HG23	1:D:351:THR:HG22	2.01	0.42
1:B:56:LEU:HD23	1:B:56:LEU:C	2.39	0.42
1:B:3:LYS:HG2	1:B:390:ASP:OD1	2.19	0.42
1:D:36:GLU:HG3	1:D:221:LEU:O	2.20	0.42
1:B:159:ASP:OD1	1:B:160:LYS:N	2.52	0.42
1:A:111:LEU:CD2	1:A:112:PRO:O	2.68	0.42
1:C:312:LEU:O	1:C:316:VAL:HG22	2.20	0.42
1:D:127:PHE:O	1:D:130:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD11	1:A:399:TYR:CD1	2.55	0.42
1:A:160:LYS:HZ1	1:A:160:LYS:HB2	1.85	0.42
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.85	0.42
1:A:320:THR:HA	1:A:354:CYS:O	2.19	0.42
1:C:322:VAL:HG22	1:C:353:ILE:CD1	2.49	0.42
1:B:143:VAL:O	1:B:143:VAL:HG13	2.19	0.41
1:D:208:GLN:HG2	1:D:208:GLN:O	2.20	0.41
1:C:298:PRO:O	1:C:301:ALA:HB3	2.20	0.41
1:D:314:ASN:ND2	1:D:323:ILE:HD11	2.35	0.41
1:A:359:LYS:HE3	1:A:384:GLU:HB2	2.02	0.41
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.78	0.41
1:C:362:GLY:HA2	1:C:387:THR:OG1	2.21	0.41
1:C:9:PRO:HB3	1:C:382:ILE:O	2.19	0.41
1:A:138:LEU:HD22	2:A:500:TR9:C2	2.45	0.41
1:C:91:ARG:HG2	1:C:91:ARG:NH1	2.35	0.41
1:D:56:LEU:C	1:D:56:LEU:HD23	2.40	0.41
1:D:307:GLN:HG3	1:D:325:GLU:HG2	2.02	0.41
1:A:111:LEU:HD11	1:A:122:VAL:HG11	2.01	0.41
1:C:41:ILE:HG22	1:C:44:VAL:CG2	2.50	0.41
1:A:370:LEU:HD11	1:A:399:TYR:HD1	1.85	0.41
1:A:320:THR:HG23	1:A:354:CYS:O	2.21	0.41
1:A:329:GLU:HB3	1:A:350:ASN:CB	2.50	0.41
1:A:329:GLU:HB3	1:A:350:ASN:HB3	2.02	0.41
1:B:119:ALA:C	1:B:120:ARG:HG3	2.41	0.41
1:A:111:LEU:HD22	1:A:112:PRO:O	2.21	0.41
1:D:170:MET:O	1:D:174:THR:HG23	2.21	0.41
1:D:63:LYS:HB2	1:D:73:ASP:HB3	2.02	0.40
1:C:4:PHE:CD1	1:C:392:ILE:HG21	2.55	0.40
1:D:25:ALA:O	1:D:29:LEU:HG	2.21	0.40
1:A:297:ALA:HB3	1:A:301:ALA:HB3	2.03	0.40
1:D:108:GLN:CG	1:D:144:LYS:HG2	2.52	0.40
1:A:138:LEU:CD2	2:A:500:TR9:H2	2.45	0.40
1:A:150:ARG:HD3	1:A:177:GLU:N	2.37	0.40
1:D:297:ALA:HB1	1:D:298:PRO:CD	2.52	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	415/419 (99%)	408 (98%)	7 (2%)	0	100	100
1	B	415/419 (99%)	409 (99%)	5 (1%)	1 (0%)	52	61
1	C	415/419 (99%)	407 (98%)	6 (1%)	2 (0%)	34	34
1	D	415/419 (99%)	404 (97%)	8 (2%)	3 (1%)	26	26
All	All	1660/1676 (99%)	1628 (98%)	26 (2%)	6 (0%)	39	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	330	ASN
1	B	418	GLY
1	C	418	GLY
1	D	114	GLY
1	D	417	LYS
1	D	111	LEU

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	329/329 (100%)	322 (98%)	7 (2%)	61	71
1	B	329/329 (100%)	318 (97%)	11 (3%)	45	56
1	C	329/329 (100%)	321 (98%)	8 (2%)	57	67
1	D	329/329 (100%)	321 (98%)	8 (2%)	57	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1316/1316 (100%)	1282 (97%)	34 (3%)	54 65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	85	ASP
1	A	159	ASP
1	A	160	LYS
1	A	307	GLN
1	A	359	LYS
1	A	414	GLU
1	B	7	GLN
1	B	59	GLN
1	B	78	ASN
1	B	85	ASP
1	B	106	GLN
1	B	111	LEU
1	B	158	MET
1	B	229	LEU
1	B	304	THR
1	B	307	GLN
1	B	330	ASN
1	C	1	MET
1	C	3	LYS
1	C	59	GLN
1	C	111	LEU
1	C	159	ASP
1	C	229	LEU
1	C	307	GLN
1	C	361	SER
1	D	85	ASP
1	D	110	SER
1	D	148	ASN
1	D	184	ASN
1	D	229	LEU
1	D	307	GLN
1	D	325	GLU
1	D	419	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	76	ASN
1	A	148	ASN
1	A	184	ASN
1	B	7	GLN
1	B	43	ASN
1	B	59	GLN
1	B	78	ASN
1	B	106	GLN
1	B	148	ASN
1	B	184	ASN
1	B	330	ASN
1	C	59	GLN
1	C	76	ASN
1	C	148	ASN
1	C	155	HIS
1	C	184	ASN
1	D	59	GLN
1	D	76	ASN
1	D	184	ASN
1	D	344	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)

4 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	IAS	A	67	1	4,7,8	0.64	0	1,8,10	1.14	0
1	IAS	B	67	1	4,7,8	0.64	0	1,8,10	1.76	0
1	IAS	C	67	1	4,7,8	0.61	0	1,8,10	1.36	0
1	IAS	D	67	1	4,7,8	0.59	0	1,8,10	1.46	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
1	IAS	A	67	1	-	0/3/7/8	0/0/0/0
1	IAS	B	67	1	-	0/3/7/8	0/0/0/0
1	IAS	C	67	1	-	0/3/7/8	0/0/0/0
1	IAS	D	67	1	-	0/3/7/8	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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	#$|Z| > 2$
2	TR9	A	500	1,3	9,11,11	6.23	6 (66%)	9,16,16	1.55	2 (22%)
2	TR9	B	500	1,3	9,11,11	6.40	6 (66%)	9,16,16	1.30	1 (11%)
2	TR9	C	500	1,3	9,11,11	5.98	6 (66%)	9,16,16	1.82	2 (22%)
2	TR9	D	500	1,3	9,11,11	6.30	6 (66%)	9,16,16	1.58	2 (22%)

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	TR9	A	500	1,3	-	0/0/20/20	0/1/1/1
2	TR9	B	500	1,3	-	0/0/20/20	0/1/1/1
2	TR9	C	500	1,3	-	0/0/20/20	0/1/1/1
2	TR9	D	500	1,3	-	0/0/20/20	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	TR9	C7-C4	-6.17	1.38	1.50
2	D	500	TR9	C7-C4	-5.95	1.38	1.50
2	A	500	TR9	C7-C4	-5.73	1.38	1.50
2	B	500	TR9	C7-C4	-5.53	1.39	1.50
2	A	500	TR9	C5-C6	-4.78	1.38	1.46
2	B	500	TR9	C5-C6	-4.19	1.39	1.46
2	D	500	TR9	C5-C6	-3.71	1.40	1.46
2	C	500	TR9	C5-C6	-3.13	1.41	1.46
2	D	500	TR9	C1-C6	2.68	1.55	1.50
2	B	500	TR9	C1-C6	3.52	1.56	1.50
2	C	500	TR9	C1-C6	3.71	1.56	1.50
2	A	500	TR9	C1-C6	4.21	1.57	1.50
2	D	500	TR9	O4-C6	5.50	1.35	1.23
2	B	500	TR9	O4-C6	6.25	1.36	1.23
2	C	500	TR9	O4-C6	6.37	1.37	1.23
2	A	500	TR9	O4-C6	6.64	1.37	1.23
2	C	500	TR9	O3-C3	7.75	1.36	1.22
2	B	500	TR9	O3-C3	7.79	1.36	1.22
2	A	500	TR9	O3-C3	7.83	1.36	1.22
2	D	500	TR9	O3-C3	8.49	1.37	1.22
2	C	500	TR9	C5-C4	12.36	1.52	1.35
2	A	500	TR9	C5-C4	12.86	1.52	1.35
2	D	500	TR9	C5-C4	13.85	1.54	1.35
2	B	500	TR9	C5-C4	14.26	1.54	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	TR9	C7-C4-C3	2.20	119.62	115.69
2	C	500	TR9	C7-C4-C3	2.49	120.13	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	TR9	C7-C4-C3	2.69	120.50	115.69
2	B	500	TR9	O1-C5-C6	2.83	121.38	115.79
2	A	500	TR9	O1-C5-C6	2.96	121.64	115.79
2	D	500	TR9	O1-C5-C6	3.24	122.20	115.79
2	C	500	TR9	O1-C5-C6	3.76	123.23	115.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	TR9	3	0
2	B	500	TR9	1	0
2	D	500	TR9	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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(Å²)	Q<0.9
1	A	418/419 (99%)	-0.42	5 (1%)	81	83	14, 26, 44, 79	0
1	B	418/419 (99%)	-0.46	4 (0%)	84	85	12, 23, 41, 83	0
1	C	418/419 (99%)	-0.27	7 (1%)	73	77	14, 28, 48, 84	0
1	D	418/419 (99%)	-0.07	11 (2%)	59	63	19, 37, 56, 85	0
All	All	1672/1676 (99%)	-0.30	27 (1%)	74	77	12, 28, 50, 85	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	6.0
1	B	419	GLU	5.4
1	A	419	GLU	5.2
1	B	418	GLY	5.0
1	C	418	GLY	4.4
1	D	418	GLY	4.2
1	D	419	GLU	4.1
1	A	418	GLY	3.9
1	C	329	GLU	3.7
1	D	330	ASN	3.5
1	B	329	GLU	3.4
1	D	329	GLU	3.1
1	D	219	GLU	3.0
1	D	328	PHE	2.7
1	D	216	GLU	2.7
1	D	140	GLU	2.7
1	A	330	ASN	2.5
1	B	330	ASN	2.5
1	D	277	GLU	2.5
1	C	348	GLU	2.4
1	D	119	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	148	ASN	2.2
1	C	358	GLU	2.2
1	C	349	SER	2.1
1	D	112	PRO	2.1
1	A	344	HIS	2.1
1	C	216	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	IAS	D	67	8/9	0.91	0.16	-	34,36,42,48	0
1	IAS	C	67	8/9	0.93	0.18	-	32,39,41,44	0
1	IAS	B	67	8/9	0.92	0.19	-	22,28,38,38	0
1	IAS	A	67	8/9	0.94	0.17	-	21,31,43,47	0

6.3 Carbohydrates (i)

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	TR9	A	500	11/11	0.90	0.14	1.88	24,26,29,30	0
2	TR9	B	500	11/11	0.94	0.13	1.16	19,24,28,28	0
2	TR9	D	500	11/11	0.96	0.12	0.11	34,38,40,41	0
2	TR9	C	500	11/11	0.85	0.14	-0.61	44,50,52,52	0
3	CA	B	420	1/1	0.98	0.08	-1.92	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	D	421	1/1	0.96	0.05	-2.17	34,34,34,34	0
3	CA	B	423	1/1	0.95	0.05	-2.27	36,36,36,36	0
3	CA	C	420	1/1	0.97	0.04	-2.46	45,45,45,45	0
3	CA	B	422	1/1	0.99	0.04	-3.03	31,31,31,31	0
3	CA	A	421	1/1	0.99	0.03	-3.65	27,27,27,27	0
3	CA	B	421	1/1	0.96	0.05	-	29,29,29,29	0
3	CA	A	420	1/1	0.96	0.04	-	28,28,28,28	0
3	CA	C	421	1/1	0.90	0.07	-	50,50,50,50	0
3	CA	D	420	1/1	0.97	0.05	-	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.