Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 02:29 pm BST

PDB ID	:	4E7C
Title	:	E. cloacae MurA in complex with UTP
Authors	:	Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.
Deposited on	:	2012-03-16
Resolution	:	2.10 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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)	:	2.11

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 2.10 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		0.246
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		0.9%
RSRZ outliers		3.5%

Worse　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
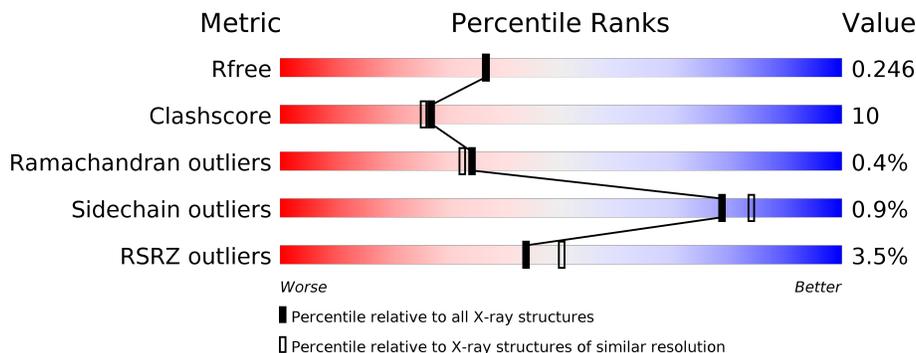
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	419	3%　82%　17%　•
1	B	419	4%　80%　18%　•
1	C	419	4%　85%　15%　•
1	D	419	3%　79%　20%　•

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13738 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	C	N	O	S	0	1	0
			3145	1977	554	600	14			
1	B	419	Total	C	N	O	S	0	0	0
			3143	1976	554	599	14			
1	C	419	Total	C	N	O	S	0	1	0
			3148	1979	554	601	14			
1	D	419	Total	C	N	O	S	0	1	0
			3150	1980	557	599	14			

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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
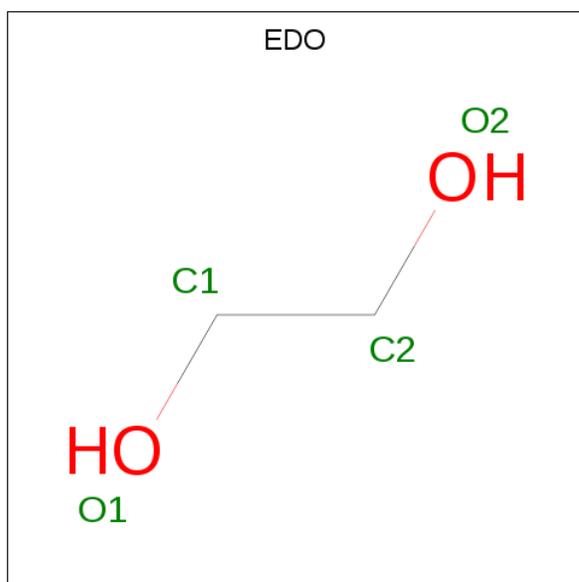
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O^-

C

CH3

O

O
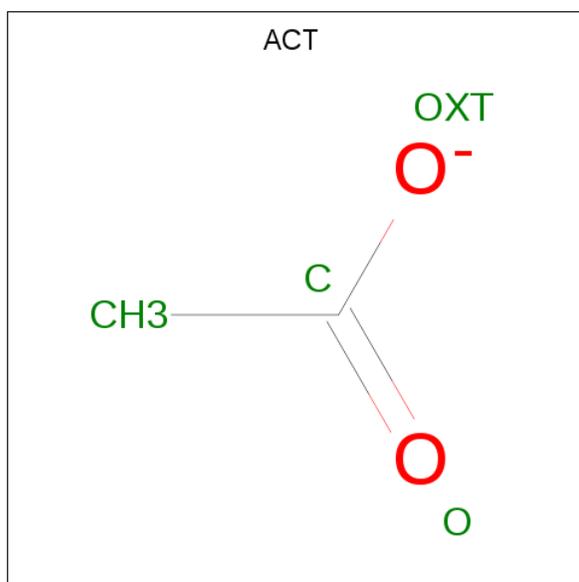
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).

UTP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	259	Total	O	0	0
			259	259		
5	C	247	Total	O	0	0
			247	247		
5	D	264	Total	O	0	0
			264	264		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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
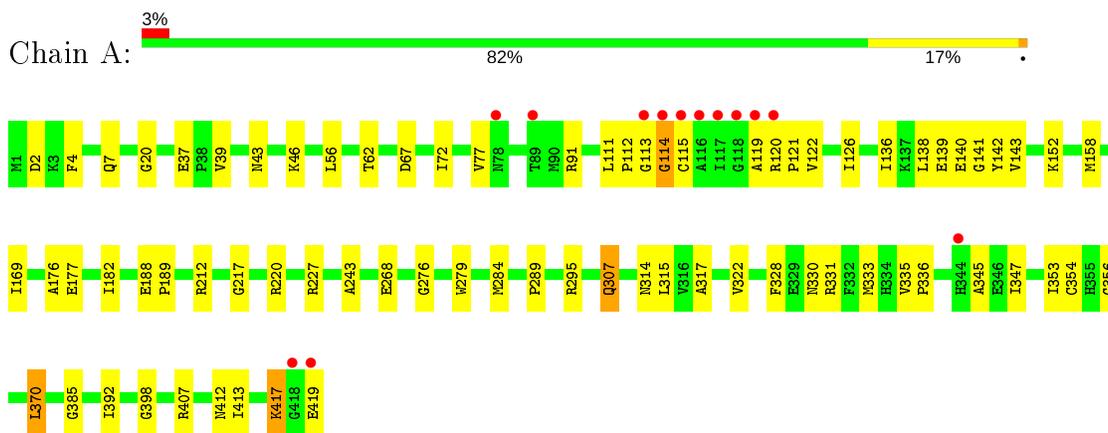
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase
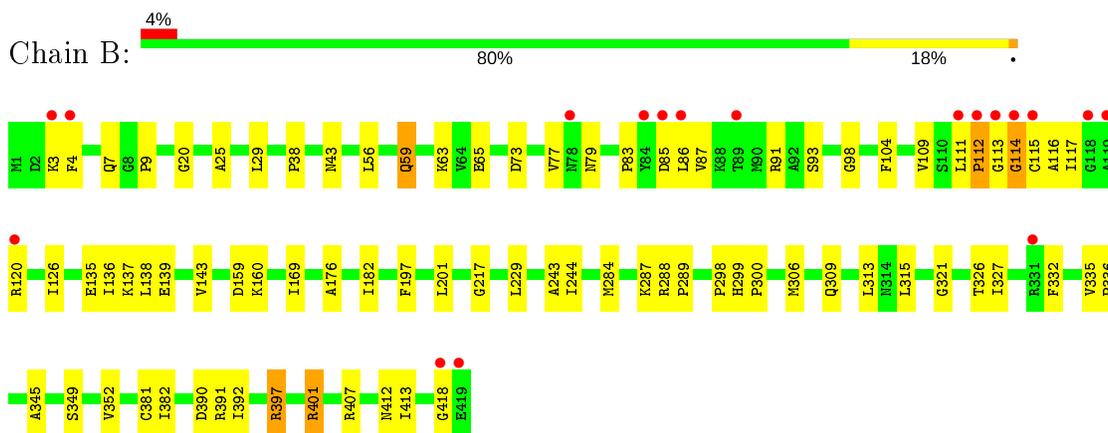
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase
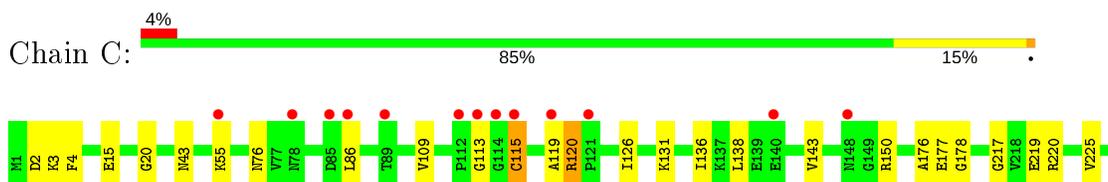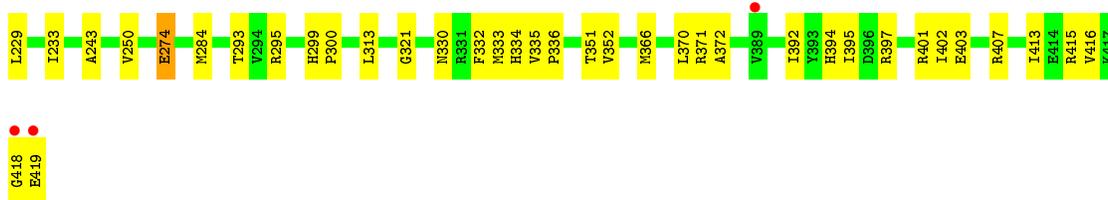
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase
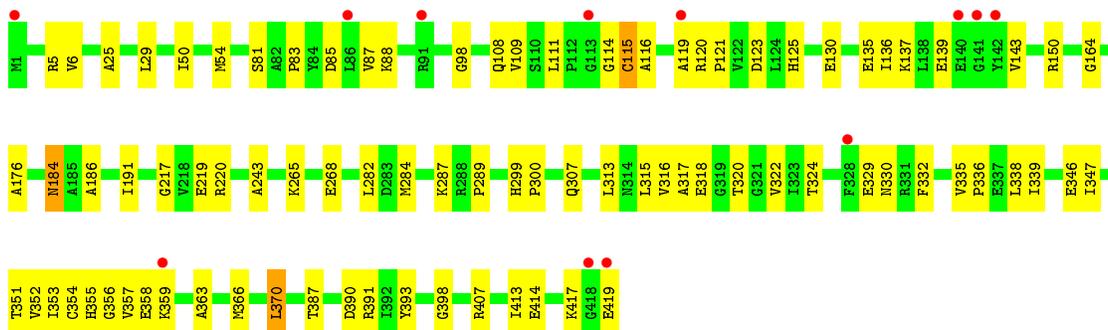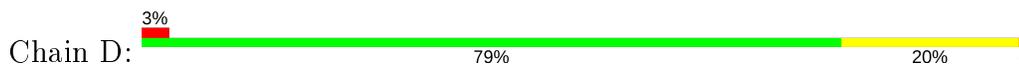
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.94Å 101.27Å 213.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.10 19.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.76-2.10) 97.5 (19.76-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	3.55 (at 2.09Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.199 , 0.250 0.194 , 0.246	Depositor DCC
R_{free} test set	1206 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.8	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13738	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: UTP, EDO, IAS, ACT

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	0.60	1/3185 (0.0%)	0.88	5/4313 (0.1%)
1	B	0.49	0/3179	0.84	0/4305
1	C	0.55	2/3188 (0.1%)	0.84	1/4317 (0.0%)
1	D	0.54	0/3190	0.85	1/4319 (0.0%)
All	All	0.54	3/12742 (0.0%)	0.85	7/17254 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	PRO	N-CD	-14.70	1.27	1.47
1	C	274[A]	GLU	CA-CB	-7.12	1.38	1.53
1	C	274[B]	GLU	CA-CB	-7.12	1.38	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLY	N-CA-C	-8.19	92.62	113.10
1	A	112	PRO	CA-N-CD	7.91	122.77	111.70
1	A	122	VAL	CA-CB-CG1	6.09	120.03	110.90
1	D	115	CYS	N-CA-C	6.06	127.37	111.00
1	A	122	VAL	N-CA-CB	-5.92	98.49	111.50
1	A	122	VAL	CA-CB-CG2	5.67	119.41	110.90
1	C	115	CYS	N-CA-C	5.05	124.65	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	3145	0	3217	66	0
1	B	3143	0	3216	79	0
1	C	3148	0	3218	66	0
1	D	3150	0	3225	69	0
2	A	12	0	18	1	0
2	B	4	0	6	0	0
2	C	20	0	30	9	0
2	D	12	0	18	2	0
3	A	8	0	6	0	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	8	0	6	0	0
4	A	29	0	11	0	0
4	B	29	0	11	0	0
5	A	252	0	0	5	0
5	B	259	0	0	12	0
5	C	247	0	0	8	0
5	D	264	0	0	8	0
All	All	13738	0	12988	262	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 10.

All (262) 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:55:LYS:CE	1:C:86:LEU:HD21	1.78	1.13
1:C:55:LYS:HE3	1:C:86:LEU:HD21	1.31	1.10
1:C:55:LYS:HD3	1:C:86:LEU:CD2	1.87	1.03
1:C:55:LYS:CD	1:C:86:LEU:HD21	1.94	0.97
1:C:55:LYS:CD	1:C:86:LEU:CD2	2.46	0.94
1:A:158:MET:HE3	5:A:601:HOH:O	1.69	0.92
1:B:137:LYS:HE2	1:D:137:LYS:HD3	1.51	0.91
1:C:15:GLU:HG2	1:C:250:VAL:HB	1.53	0.91
1:C:178:GLY:H	2:C:505:EDO:H11	1.35	0.89

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150[B]:ARG:NH1	1:D:219:GLU:HA	1.92	0.83
1:C:397:ARG:HH21	2:C:501:EDO:H11	1.44	0.82
1:B:85:ASP:HB2	5:B:728:HOH:O	1.80	0.81
1:B:137:LYS:HG2	1:D:137:LYS:HG2	1.63	0.81
1:A:62:THR:HG22	1:A:77:VAL:HG22	1.63	0.80
1:D:121:PRO:HD2	5:D:656:HOH:O	1.81	0.79
1:B:309:GLN:HG2	5:B:812:HOH:O	1.81	0.79
1:B:407:ARG:HD3	5:B:813:HOH:O	1.85	0.76
1:B:135:GLU:HG3	1:D:139:GLU:HB3	1.67	0.76
1:D:88:LYS:HD2	5:D:745:HOH:O	1.84	0.76
1:C:55:LYS:CE	1:C:86:LEU:CD2	2.64	0.75
1:C:55:LYS:HD3	1:C:86:LEU:HD22	1.74	0.70
1:A:120:ARG:HA	1:A:120:ARG:NE	2.05	0.69
1:B:326:THR:OG1	1:B:327:ILE:HD12	1.92	0.69
1:B:298:PRO:HD3	1:B:327:ILE:HD11	1.75	0.69
1:A:417:LYS:CE	1:A:417:LYS:H	2.06	0.68
1:A:115:CYS:HB3	1:C:131:LYS:HD2	1.74	0.68
1:D:150[B]:ARG:HH12	1:D:219:GLU:HA	1.56	0.67
1:D:358:GLU:HG3	1:D:359:LYS:HG3	1.77	0.67
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.78	0.65
1:A:268:GLU:OE2	3:B:502:ACT:H1	1.96	0.65
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.79	0.65
1:D:407:ARG:HD3	5:D:635:HOH:O	1.95	0.65
1:A:295:ARG:NH2	5:A:705:HOH:O	2.30	0.64
1:A:113:GLY:C	1:A:115:CYS:N	2.52	0.63
1:B:83:PRO:HD2	1:B:86:LEU:HD12	1.79	0.63
1:B:79:ASN:ND2	5:B:727:HOH:O	2.17	0.62
1:D:413:ILE:HD12	1:D:414:GLU:H	1.65	0.62
1:C:397:ARG:NH2	2:C:501:EDO:H11	2.14	0.61
1:C:109:VAL:O	1:C:143:VAL:HG12	1.99	0.61
1:A:335:VAL:HB	1:A:347:ILE:HD11	1.83	0.61
1:A:417:LYS:HE3	1:A:417:LYS:H	1.65	0.61
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.82	0.60
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.83	0.60
1:A:115:CYS:HB2	1:A:140:GLU:OE2	2.02	0.60
1:A:115:CYS:HB3	1:C:131:LYS:CD	2.30	0.60
1:B:176:ALA:O	1:B:217:GLY:HA3	2.03	0.59
1:B:336:PRO:HG2	1:C:333:MET:CE	2.32	0.59
1:C:177:GLU:HG3	2:C:505:EDO:O2	2.02	0.59
1:D:370:LEU:CD1	1:D:398:GLY:HA3	2.34	0.58
1:A:417:LYS:N	1:A:417:LYS:CE	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.86	0.58
1:A:2:ASP:HB3	1:A:392:ILE:HD11	1.86	0.58
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.19	0.57
1:B:143:VAL:HG13	1:B:143:VAL:O	2.05	0.57
1:A:227:ARG:HE	2:A:503:EDO:C2	2.17	0.57
1:B:65:GLU:HG2	5:B:851:HOH:O	2.05	0.57
1:A:113:GLY:C	1:A:115:CYS:H	2.06	0.56
1:B:114:GLY:C	1:B:116:ALA:H	2.09	0.56
1:A:114:GLY:O	1:A:119:ALA:HB3	2.05	0.56
1:B:4:PHE:CD2	1:B:392:ILE:HG21	2.40	0.56
1:C:274[B]:GLU:HG3	5:C:762:HOH:O	2.05	0.56
1:B:38:PRO:HG3	1:B:73:ASP:OD2	2.06	0.55
1:A:417:LYS:HE2	1:A:417:LYS:N	2.21	0.55
1:D:135:GLU:OE2	1:D:137:LYS:HE2	2.07	0.55
1:B:113:GLY:O	1:B:114:GLY:O	2.25	0.55
1:A:4:PHE:CD2	1:A:392:ILE:HG21	2.41	0.55
1:D:324:THR:HG23	1:D:351:THR:HG22	1.89	0.55
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.72	0.55
1:B:391:ARG:HD3	5:B:827:HOH:O	2.05	0.54
1:A:333:MET:O	1:A:336:PRO:HD2	2.06	0.54
1:C:3:LYS:HB2	1:C:416:VAL:CG1	2.38	0.54
1:D:85:ASP:HA	1:D:88:LYS:HE2	1.88	0.54
1:D:322:VAL:HG13	1:D:353:ILE:HD13	1.89	0.54
1:C:299:HIS:CG	1:C:300:PRO:HA	2.42	0.54
1:A:330:ASN:HB2	2:D:502:EDO:O2	2.08	0.54
1:B:56:LEU:C	1:B:56:LEU:HD23	2.29	0.54
1:D:282:LEU:HD23	1:D:282:LEU:C	2.28	0.54
1:C:176:ALA:O	1:C:217:GLY:HA3	2.08	0.54
1:B:332:PHE:CD1	1:B:352:VAL:HG21	2.44	0.53
1:B:109:VAL:O	1:B:143:VAL:HG12	2.07	0.53
1:B:397:ARG:HD3	5:B:695:HOH:O	2.08	0.53
1:B:135:GLU:OE2	1:B:137:LYS:HE3	2.09	0.53
1:C:407:ARG:HD3	5:C:657:HOH:O	2.09	0.53
1:A:417:LYS:HE2	1:A:417:LYS:H	1.73	0.53
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.89	0.53
1:A:317:ALA:O	1:A:356:GLY:HA3	2.09	0.52
1:C:293:THR:OG1	2:C:503:EDO:H11	2.08	0.52
1:D:186:ALA:HB3	1:D:191:ILE:CD1	2.39	0.52
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.75	0.52
1:D:120:ARG:HB2	1:D:123:ASP:OD2	2.09	0.52
1:A:176:ALA:O	1:A:217:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:O	1:A:56:LEU:HD23	2.10	0.51
1:A:370:LEU:CD1	1:A:398:GLY:HA3	2.40	0.51
1:C:3:LYS:HB2	1:C:416:VAL:HG13	1.93	0.51
1:A:314:ASN:HB3	1:A:354:CYS:HB2	1.91	0.51
1:D:289:PRO:HG2	1:D:317:ALA:HA	1.92	0.51
1:C:295:ARG:HE	1:D:184:ASN:HD21	1.56	0.51
1:B:336:PRO:HG2	1:C:333:MET:HE1	1.93	0.51
1:A:111:LEU:O	1:A:141:GLY:HA2	2.11	0.50
1:D:391:ARG:HD2	1:D:393:TYR:HE2	1.75	0.50
1:C:401:ARG:HD2	5:C:845:HOH:O	2.11	0.50
1:C:402:ILE:HG23	1:C:403:GLU:N	2.25	0.50
1:B:313:LEU:HD23	1:B:313:LEU:C	2.31	0.50
1:B:126:ILE:HG23	1:B:136:ILE:HG21	1.93	0.49
1:C:3:LYS:HE2	1:C:419:GLU:HG2	1.93	0.49
1:C:332:PHE:CZ	1:C:352:VAL:HG23	2.48	0.49
1:B:20:GLY:HA3	1:B:43:ASN:O	2.13	0.49
1:D:315:LEU:HD23	1:D:354:CYS:HB3	1.94	0.49
1:C:143:VAL:O	1:C:143:VAL:HG13	2.13	0.49
1:D:318:GLU:HB3	5:D:853:HOH:O	2.12	0.49
1:A:315:LEU:HD23	1:A:354:CYS:HB3	1.95	0.48
1:A:91:ARG:NH2	1:A:121:PRO:O	2.44	0.48
1:A:212:ARG:NH2	1:B:321:GLY:HA2	2.27	0.48
1:B:115:CYS:SG	1:D:130:GLU:HG2	2.53	0.48
1:B:137:LYS:HG2	1:D:137:LYS:CG	2.40	0.48
1:D:114:GLY:O	1:D:116:ALA:N	2.46	0.48
1:C:4:PHE:CD2	1:C:392:ILE:HG21	2.48	0.48
1:B:332:PHE:CD1	1:B:352:VAL:CG2	2.97	0.48
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.48	0.48
1:A:62:THR:CG2	1:A:77:VAL:HG22	2.41	0.48
1:B:298:PRO:HD3	1:B:327:ILE:CD1	2.42	0.48
1:B:87:VAL:CG1	5:B:830:HOH:O	2.62	0.48
1:A:7:GLN:HE22	1:A:385:GLY:HA2	1.78	0.48
1:B:59:GLN:CG	1:B:86:LEU:HD11	2.44	0.48
1:B:3:LYS:HG2	1:B:390:ASP:OD2	2.13	0.47
1:B:56:LEU:O	1:B:56:LEU:HD23	2.14	0.47
1:C:243:ALA:HA	1:C:284:MET:CG	2.45	0.47
1:B:160:LYS:HD3	5:B:762:HOH:O	2.13	0.47
1:D:335:VAL:O	1:D:339:ILE:HG12	2.15	0.47
1:A:331:ARG:HB3	1:A:331:ARG:NH2	2.30	0.47
1:B:349:SER:O	1:C:330:ASN:ND2	2.44	0.47
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:GLY:N	2:C:505:EDO:H11	2.15	0.47
1:D:176:ALA:O	1:D:217:GLY:HA3	2.15	0.47
1:B:243:ALA:HA	1:B:284:MET:CG	2.44	0.47
1:D:317:ALA:O	1:D:356:GLY:HA3	2.15	0.47
1:C:2:ASP:OD2	1:C:415:ARG:HD3	2.14	0.47
1:D:320:THR:HA	1:D:354:CYS:O	2.15	0.47
1:D:366:MET:HB2	1:D:390:ASP:HB3	1.96	0.47
1:B:59:GLN:CB	1:B:86:LEU:HD11	2.45	0.46
1:D:150[B]:ARG:HH12	1:D:219:GLU:CA	2.26	0.46
1:A:322:VAL:HG13	1:A:353:ILE:HD13	1.97	0.46
1:B:336:PRO:HG2	1:C:333:MET:HE2	1.96	0.46
1:A:139:GLU:HB2	1:A:142:TYR:CE2	2.50	0.46
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.97	0.46
1:D:299:HIS:CG	1:D:300:PRO:HA	2.50	0.46
1:D:332:PHE:CZ	1:D:352:VAL:HG23	2.50	0.46
1:A:333:MET:HE1	1:D:347:ILE:HG21	1.98	0.46
1:D:120:ARG:HD3	5:D:738:HOH:O	2.15	0.46
1:C:330:ASN:HB3	5:C:672:HOH:O	2.15	0.46
1:C:220:ARG:NH1	1:C:220:ARG:HG3	2.31	0.46
1:D:120:ARG:HA	1:D:121:PRO:HD3	1.86	0.46
1:D:125:HIS:CE1	1:D:164:GLY:C	2.89	0.46
1:A:20:GLY:HA3	1:A:43:ASN:O	2.16	0.45
1:D:25:ALA:O	1:D:29:LEU:HG	2.16	0.45
1:C:120:ARG:NH1	5:C:780:HOH:O	2.49	0.45
1:D:265:LYS:HD3	1:D:268:GLU:OE1	2.17	0.45
1:A:62:THR:HG22	1:A:77:VAL:CG2	2.40	0.45
1:B:98:GLY:HA3	5:B:642:HOH:O	2.17	0.45
1:A:126:ILE:HG12	1:A:143:VAL:HG21	1.97	0.45
1:B:288:ARG:HG3	1:B:289:PRO:HD2	1.97	0.45
1:C:418:GLY:HA2	5:C:828:HOH:O	2.16	0.45
1:D:220:ARG:NH1	1:D:220:ARG:HG3	2.31	0.45
1:D:6:VAL:HG22	1:D:413:ILE:HD13	1.97	0.45
1:B:287:LYS:HE2	1:B:287:LYS:HB3	1.77	0.45
1:B:7:GLN:HB3	1:B:412:ASN:ND2	2.32	0.45
1:C:138:LEU:N	1:C:138:LEU:HD22	2.32	0.45
1:C:313:LEU:HD23	1:C:313:LEU:C	2.37	0.45
1:A:407:ARG:NH1	1:A:413:ILE:O	2.50	0.45
1:B:91:ARG:HH11	1:B:91:ARG:HG2	1.81	0.45
1:D:98:GLY:HA3	5:D:780:HOH:O	2.17	0.45
1:A:7:GLN:HB3	1:A:412:ASN:ND2	2.32	0.45
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HG22	1:A:182:ILE:HD11	1.99	0.45
1:A:419:GLU:OE1	1:A:419:GLU:HA	2.17	0.45
1:B:77:VAL:HB	1:B:104:PHE:CZ	2.52	0.45
1:A:243:ALA:HA	1:A:284:MET:CG	2.47	0.44
1:C:402:ILE:CG2	1:C:403:GLU:N	2.80	0.44
1:C:225:VAL:H	2:C:504:EDO:H21	1.82	0.44
1:C:4:PHE:CD1	1:C:413:ILE:HD11	2.52	0.44
1:C:321:GLY:HA2	2:C:503:EDO:H12	2.00	0.44
1:A:353:ILE:HD11	5:A:832:HOH:O	2.17	0.44
1:A:91:ARG:NH1	1:A:91:ARG:HG3	2.33	0.44
1:B:120:ARG:NH2	5:B:714:HOH:O	2.51	0.44
1:D:109:VAL:O	1:D:143:VAL:HG12	2.18	0.44
1:D:137:LYS:HD2	1:D:139:GLU:OE1	2.18	0.44
1:A:56:LEU:C	1:A:56:LEU:HD23	2.38	0.44
1:D:111:LEU:HD12	1:D:111:LEU:O	2.18	0.44
1:D:135:GLU:HB2	5:D:699:HOH:O	2.16	0.44
1:D:85:ASP:HA	1:D:88:LYS:CE	2.48	0.44
1:A:315:LEU:HD21	1:A:345:ALA:HB2	1.99	0.44
1:B:87:VAL:HG12	5:B:830:HOH:O	2.16	0.44
1:D:315:LEU:HD12	1:D:338:LEU:HD13	2.00	0.43
1:D:50:ILE:O	1:D:54:MET:HG3	2.17	0.43
1:B:117:ILE:HD13	2:C:503:EDO:O1	2.18	0.43
1:B:390:ASP:OD2	1:B:391:ARG:N	2.47	0.43
1:A:37:GLU:OE1	1:A:220:ARG:NH2	2.52	0.43
1:D:313:LEU:HD23	1:D:313:LEU:C	2.39	0.43
1:D:83:PRO:O	1:D:87:VAL:HG13	2.18	0.43
1:D:316:VAL:HA	1:D:357:VAL:O	2.19	0.43
1:D:5:ARG:O	1:D:413:ILE:HD12	2.19	0.43
1:B:138:LEU:HD23	1:D:136:ILE:HB	2.00	0.43
1:B:111:LEU:HA	1:B:112:PRO:HD2	1.82	0.42
1:B:114:GLY:O	1:B:116:ALA:N	2.45	0.42
1:D:320:THR:HG23	1:D:354:CYS:O	2.20	0.42
1:D:417:LYS:C	1:D:419:GLU:N	2.73	0.42
1:A:46:LYS:HZ1	1:A:67:IAS:C	2.31	0.42
1:C:150:ARG:NH2	1:C:219:GLU:O	2.44	0.42
1:B:243:ALA:HA	1:B:284:MET:HG3	2.01	0.42
1:D:83:PRO:HB2	1:D:85:ASP:OD1	2.20	0.42
5:A:717:HOH:O	1:C:119:ALA:HB3	2.19	0.42
1:D:81:SER:HB2	1:D:108:GLN:CG	2.50	0.42
1:D:329:GLU:HA	2:D:502:EDO:H21	2.02	0.42
1:B:299:HIS:CG	1:B:300:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLN:HB3	1:B:412:ASN:CG	2.40	0.42
1:C:15:GLU:CG	1:C:250:VAL:HB	2.39	0.42
1:C:351:THR:HG22	1:C:352:VAL:N	2.35	0.42
1:C:370:LEU:CD1	1:C:395:ILE:HA	2.50	0.42
1:D:363:ALA:O	1:D:387:THR:HG23	2.19	0.42
1:B:169:ILE:HG22	1:B:182:ILE:HD11	2.02	0.42
1:B:288:ARG:CG	1:B:289:PRO:HD2	2.50	0.41
1:A:152:LYS:HE3	1:A:177:GLU:OE1	2.19	0.41
1:D:287:LYS:HE3	5:D:835:HOH:O	2.20	0.41
1:C:274[A]:GLU:HG2	5:C:689:HOH:O	2.20	0.41
1:B:306:MET:HE3	1:B:309:GLN:HB2	2.02	0.41
1:B:9:PRO:HA	1:B:381:CYS:O	2.20	0.41
1:D:346:GLU:OE2	1:D:355:HIS:NE2	2.51	0.41
1:A:39:VAL:CG2	1:A:72:ILE:HB	2.50	0.41
1:B:25:ALA:O	1:B:29:LEU:HG	2.20	0.41
1:C:20:GLY:HA3	1:C:43:ASN:O	2.20	0.41
1:C:76:ASN:HA	5:C:728:HOH:O	2.19	0.41
1:A:188:GLU:HA	1:A:189:PRO:HD3	1.96	0.41
1:B:114:GLY:C	1:B:116:ALA:N	2.74	0.41
1:B:401:ARG:HG3	1:B:401:ARG:HH11	1.84	0.41
1:C:366:MET:SD	1:C:366:MET:C	2.99	0.41
1:D:243:ALA:HA	1:D:284:MET:CG	2.50	0.41
1:A:136:ILE:HB	1:C:138:LEU:HD23	2.03	0.41
1:A:289:PRO:HG2	1:A:317:ALA:HA	2.01	0.41
1:B:327:ILE:N	1:B:327:ILE:HD12	2.36	0.41
1:A:335:VAL:HB	1:A:336:PRO:HD3	2.03	0.41
1:B:159:ASP:OD2	1:D:119:ALA:HB3	2.20	0.41
1:B:59:GLN:HB3	1:B:86:LEU:HD11	2.03	0.41
1:A:126:ILE:HD13	1:A:138:LEU:HD21	2.02	0.41
1:A:331:ARG:HB3	1:A:331:ARG:CZ	2.51	0.40
1:B:197:PHE:CZ	1:B:201:LEU:HD11	2.56	0.40
1:B:332:PHE:CG	1:B:352:VAL:CG2	3.04	0.40
1:C:233:ILE:HG21	1:C:371:ARG:CZ	2.51	0.40
1:C:4:PHE:CZ	1:C:403:GLU:HB3	2.55	0.40
1:C:407:ARG:NH1	1:C:413:ILE:O	2.53	0.40
1:B:139:GLU:HB3	1:D:135:GLU:HG3	2.03	0.40
1:A:289:PRO:HD3	5:A:632:HOH:O	2.20	0.40
1:A:307:GLN:HE21	1:A:331:ARG:NH2	2.19	0.40
1:B:7:GLN:O	1:B:412:ASN:HB3	2.22	0.40
1:B:87:VAL:HG22	1:B:93:SER:HB3	2.02	0.40
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ARG:NH1	1:B:413:ILE:O	2.55	0.40
1:A:139:GLU:HB2	1:A:142:TYR:CZ	2.57	0.40
1:A:328:PHE:HB2	1:A:331:ARG:HD2	2.04	0.40
1:C:370:LEU:HD13	1:C:394:HIS:O	2.22	0.40
1:D:413:ILE:HD12	1:D:414:GLU:N	2.34	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	416/419 (99%)	404 (97%)	12 (3%)	0	100	100
1	B	415/419 (99%)	395 (95%)	17 (4%)	3 (1%)	22	18
1	C	416/419 (99%)	403 (97%)	10 (2%)	3 (1%)	22	18
1	D	416/419 (99%)	398 (96%)	17 (4%)	1 (0%)	47	49
All	All	1663/1676 (99%)	1600 (96%)	56 (3%)	7 (0%)	34	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	115	CYS
1	B	114	GLY
1	C	113	GLY
1	C	120	ARG
1	C	115	CYS
1	B	112	PRO
1	B	418	GLY

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	330/329 (100%)	327 (99%)	3 (1%)	78	84
1	B	329/329 (100%)	325 (99%)	4 (1%)	71	77
1	C	330/329 (100%)	329 (100%)	1 (0%)	92	95
1	D	330/329 (100%)	326 (99%)	4 (1%)	71	77
All	All	1319/1316 (100%)	1307 (99%)	12 (1%)	78	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	A	370	LEU
1	A	417	LYS
1	B	59	GLN
1	B	229	LEU
1	B	397	ARG
1	B	401	ARG
1	C	229	LEU
1	D	184	ASN
1	D	307	GLN
1	D	330	ASN
1	D	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN

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	C	67	1	4,7,8	0.76	0	2,8,10	1.18	0
1	IAS	D	67	1	4,7,8	0.82	0	2,8,10	1.08	0
1	IAS	A	67	1	4,7,8	0.72	0	2,8,10	1.17	0
1	IAS	B	67	1	4,7,8	0.75	0	2,8,10	1.18	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	C	67	1	-	0/3/7/8	-
1	IAS	D	67	1	-	0/3/7/8	-
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	67	IAS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

20 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	#$|Z| > 2$
3	ACT	A	504	-	1,3,3	1.81	0	0,3,3	0.00	-
3	ACT	C	506	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
3	ACT	B	502	-	1,3,3	1.88	0	0,3,3	0.00	-
2	EDO	B	501	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	C	503	-	3,3,3	0.41	0	2,2,2	0.39	0
3	ACT	A	505	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
2	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	C	505	-	3,3,3	0.47	0	2,2,2	0.32	0
3	ACT	D	505	-	1,3,3	1.49	0	0,3,3	0.00	-
2	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	D	503	-	3,3,3	0.55	0	2,2,2	0.28	0
4	UTP	B	503	-	26,30,30	1.93	3 (11%)	34,47,47	1.05	1 (2%)
2	EDO	D	502	-	3,3,3	0.41	0	2,2,2	0.27	0
2	EDO	A	501	-	3,3,3	0.50	0	2,2,2	0.31	0
3	ACT	D	504	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
2	EDO	C	502	-	3,3,3	0.47	0	2,2,2	0.32	0
4	UTP	A	506	-	26,30,30	1.93	5 (19%)	34,47,47	1.10	3 (8%)
2	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	D	501	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.35	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
4	UTP	B	503	-	-	4/22/38/38	0/2/2/2
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	C	503	-	-	1/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	C	505	-	-	1/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	D	503	-	-	1/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	C	502	-	-	1/1/1/1	-
4	UTP	A	506	-	-	9/22/38/38	0/2/2/2
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	UTP	C6-C5	-6.40	1.35	1.52
4	A	506	UTP	C6-C5	-6.24	1.35	1.52
4	A	506	UTP	C2-N1	5.07	1.42	1.35
4	B	503	UTP	C2-N1	4.69	1.42	1.35
4	B	503	UTP	C6-N1	-3.45	1.40	1.47
4	A	506	UTP	C6-N1	-3.00	1.41	1.47
3	C	506	ACT	CH3-C	2.61	1.52	1.48
3	A	505	ACT	CH3-C	2.06	1.51	1.48
4	A	506	UTP	PB-O1B	-2.05	1.45	1.55
4	A	506	UTP	C4-N3	2.04	1.41	1.37
3	D	504	ACT	CH3-C	2.03	1.51	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	UTP	C5-C6-N1	3.49	123.13	111.61
4	B	503	UTP	C5-C6-N1	3.47	123.04	111.61
4	A	506	UTP	N3-C2-N1	-2.10	114.44	116.65
4	A	506	UTP	C3'-C2'-C1'	2.04	105.31	101.43

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	UTP	O4'-C4'-C5'-O5'
4	B	503	UTP	C3'-C4'-C5'-O5'
2	C	504	EDO	O1-C1-C2-O2
2	C	505	EDO	O1-C1-C2-O2
2	D	503	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
2	A	502	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2
4	A	506	UTP	PB-O3B-PG-O2G
4	A	506	UTP	PB-O3A-PA-O1A
2	C	503	EDO	O1-C1-C2-O2
4	A	506	UTP	O4'-C4'-C5'-O5'
4	B	503	UTP	PB-O3A-PA-O1A
4	A	506	UTP	PB-O3B-PG-O1G
4	A	506	UTP	PB-O3B-PG-O3G
4	B	503	UTP	PB-O3A-PA-O2A
4	A	506	UTP	PB-O3A-PA-O2A
4	A	506	UTP	PA-O3A-PB-O1B
4	A	506	UTP	PA-O3A-PB-O2B
4	A	506	UTP	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ACT	1	0
2	C	503	EDO	3	0
2	C	504	EDO	1	0
2	C	505	EDO	3	0
2	C	501	EDO	2	0
2	D	502	EDO	2	0
2	A	503	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UTP B 503

Bond lengths   Bond angles

Torsions   Rings

Ligand UTP A 506

Bond lengths   Bond angles

Torsions   Rings
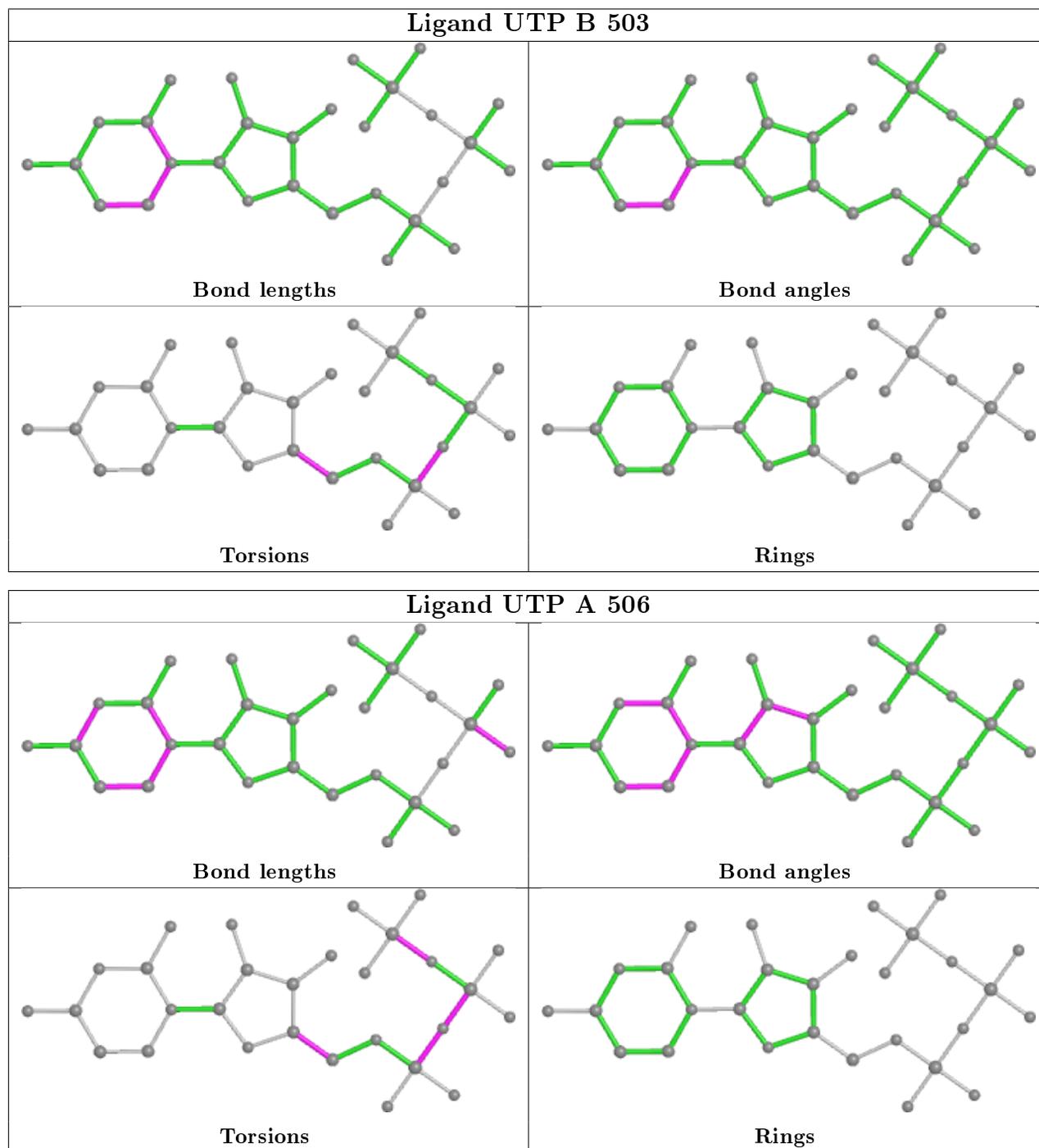
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	67:IAS	C	68:GLY	N	4.43
1	D	67:IAS	C	68:GLY	N	4.39
1	A	67:IAS	C	68:GLY	N	4.37
1	B	67:IAS	C	68:GLY	N	4.37

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	418/419 (99%)	0.04	13 (3%)	49	55	16, 28, 43, 69	0
1	B	418/419 (99%)	0.15	18 (4%)	35	41	17, 28, 46, 79	0
1	C	418/419 (99%)	0.07	16 (3%)	40	46	16, 27, 46, 73	0
1	D	418/419 (99%)	0.06	12 (2%)	51	57	15, 26, 45, 78	0
All	All	1672/1676 (99%)	0.08	59 (3%)	44	50	15, 27, 45, 79	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	419	GLU	7.0
1	B	115	CYS	6.4
1	B	419	GLU	6.1
1	B	112	PRO	6.1
1	B	418	GLY	5.7
1	A	116	ALA	5.1
1	A	419	GLU	5.1
1	B	113	GLY	4.9
1	D	119	ALA	4.3
1	C	419	GLU	4.3
1	D	86	LEU	4.2
1	A	114	GLY	4.2
1	A	120	ARG	4.1
1	C	119	ALA	3.9
1	C	113	GLY	3.8
1	D	418	GLY	3.7
1	A	418	GLY	3.7
1	B	120	ARG	3.6
1	C	112	PRO	3.5
1	A	118	GLY	3.4
1	A	113	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	418	GLY	3.3
1	C	115	CYS	3.3
1	A	115	CYS	3.2
1	A	119	ALA	3.1
1	D	141	GLY	3.1
1	D	140	GLU	3.1
1	C	85	ASP	2.9
1	B	86	LEU	2.9
1	B	89	THR	2.8
1	C	121	PRO	2.8
1	B	78	ASN	2.8
1	D	113	GLY	2.8
1	C	86	LEU	2.8
1	B	85	ASP	2.7
1	C	140	GLU	2.5
1	A	117	ILE	2.5
1	D	142	TYR	2.4
1	D	1	MET	2.4
1	C	114	GLY	2.4
1	C	78	ASN	2.4
1	B	119	ALA	2.3
1	B	114	GLY	2.3
1	B	118	GLY	2.3
1	A	78	ASN	2.3
1	D	359	LYS	2.3
1	A	89	THR	2.3
1	C	89	THR	2.3
1	D	91	ARG	2.3
1	D	328	PHE	2.2
1	A	344	HIS	2.2
1	B	111	LEU	2.1
1	B	331	ARG	2.1
1	C	55	LYS	2.1
1	C	148	ASN	2.1
1	B	84	TYR	2.1
1	B	4	PHE	2.1
1	B	3	LYS	2.0
1	C	389	VAL	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. 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
1	IAS	B	67	8/9	0.89	0.15	36,37,39,40	0
1	IAS	C	67	8/9	0.93	0.23	35,36,37,39	0
1	IAS	A	67	8/9	0.94	0.18	35,37,39,39	0
1	IAS	D	67	8/9	0.95	0.11	20,22,24,24	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. 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
3	ACT	D	504	4/4	0.58	0.39	75,75,75,75	0
2	EDO	B	501	4/4	0.65	0.33	55,57,57,58	0
4	UTP	B	503	29/29	0.73	0.24	60,68,92,92	0
2	EDO	C	501	4/4	0.75	0.29	60,60,60,60	0
2	EDO	D	501	4/4	0.78	0.28	52,53,54,54	0
4	UTP	A	506	29/29	0.79	0.21	40,52,77,78	0
2	EDO	A	501	4/4	0.80	0.19	44,46,46,48	0
2	EDO	D	503	4/4	0.80	0.18	41,44,44,44	0
2	EDO	C	502	4/4	0.86	0.22	63,63,63,63	0
3	ACT	A	504	4/4	0.87	0.23	60,61,61,62	0
2	EDO	C	504	4/4	0.88	0.52	65,66,66,66	0
2	EDO	C	505	4/4	0.89	0.25	48,49,50,50	0
2	EDO	C	503	4/4	0.90	0.20	39,41,43,45	0
3	ACT	B	502	4/4	0.91	0.20	47,47,48,49	0
2	EDO	A	502	4/4	0.91	0.25	42,43,44,44	0
3	ACT	D	505	4/4	0.91	0.17	51,51,51,52	0
3	ACT	A	505	4/4	0.92	0.31	76,76,76,76	0
2	EDO	A	503	4/4	0.92	0.26	35,36,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	D	502	4/4	0.93	0.16	36,37,37,38	0
3	ACT	C	506	4/4	0.95	0.14	49,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UTP B 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around UTP A 506:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.