Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 PM GMT

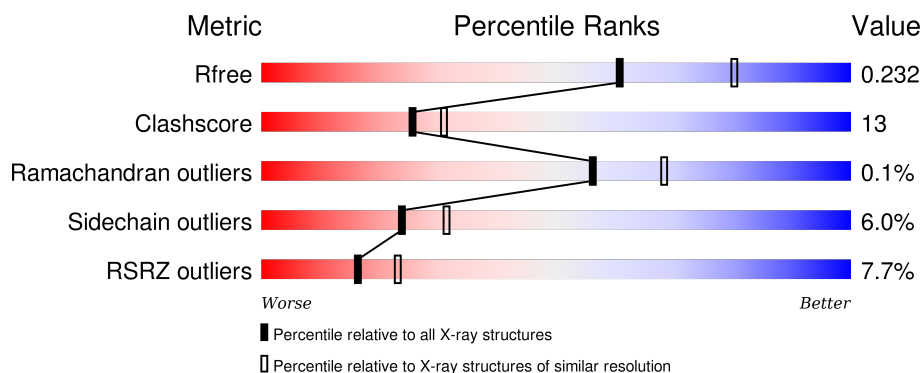|		
PDB ID	:	4R29
Title	:	Crystal structure of bacterial cysteine methyltransferase effector NleE
Authors	:	Yao, Q.; Chen, J.; Hu, L.; Zhang, L.; Shao, F.
Deposited on	:	2014-08-11
Resolution	:	2.31 Å(reported)

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 2.31 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		0.232
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		6.0%
RSRZ outliers		7.7%

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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	224	7% 70% 16% • 11%
1	B	224	6% 70% 18% • 9%
1	C	224	7% 68% 21% • 9%
1	D	224	8% 66% 20% • 11%

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	GOL	C	303	-	-	X	X
4	CIT	B	302	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7034 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1632	1046	267	307	12			
1	B	203	Total	C	N	O	S	0	0	0
			1665	1066	273	314	12			
1	C	203	Total	C	N	O	S	0	0	0
			1657	1060	274	311	12			
1	D	199	Total	C	N	O	S	0	0	0
			1633	1047	269	305	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	GLU	ENGINEERED MUTATION	UNP Q7DBA6
B	181	ALA	GLU	ENGINEERED MUTATION	UNP Q7DBA6
C	181	ALA	GLU	ENGINEERED MUTATION	UNP Q7DBA6
D	181	ALA	GLU	ENGINEERED MUTATION	UNP Q7DBA6

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).
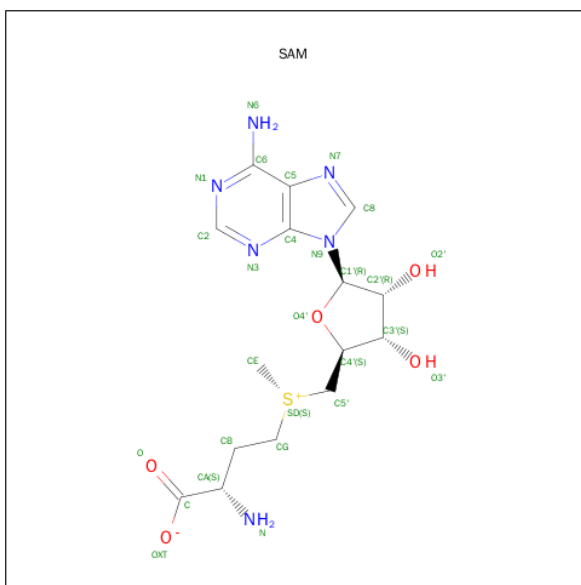
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
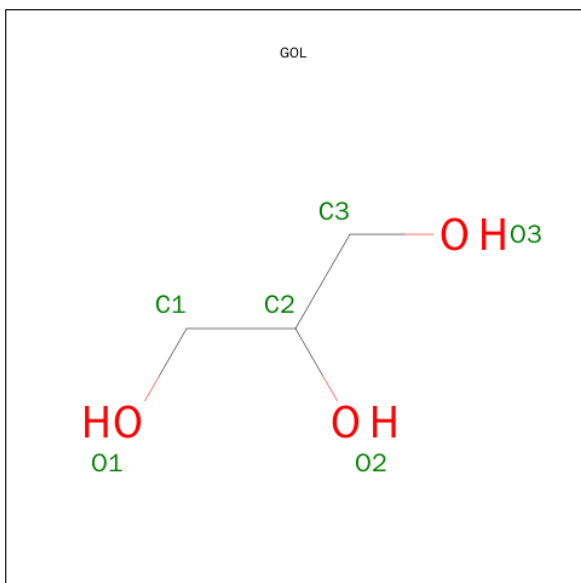
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
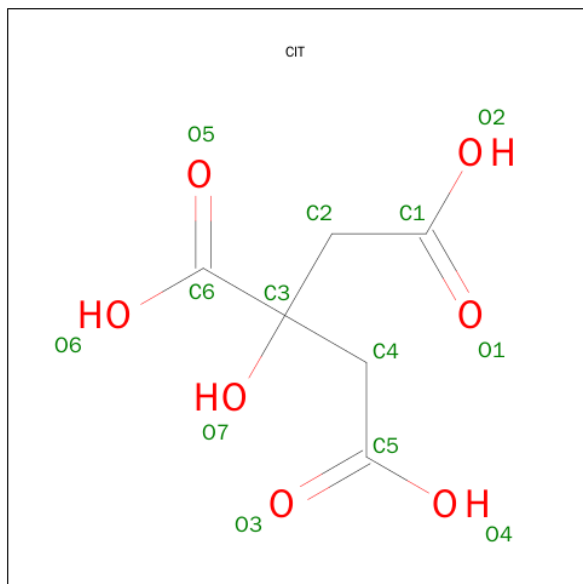
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 13	C 6	O 7	0	0
4	C	1	Total 13	C 6	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total 86	O 86	0	0
5	B	87	Total 87	O 87	0	0
5	C	70	Total 70	O 70	0	0
5	D	52	Total 52	O 52	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: Uncharacterized protein
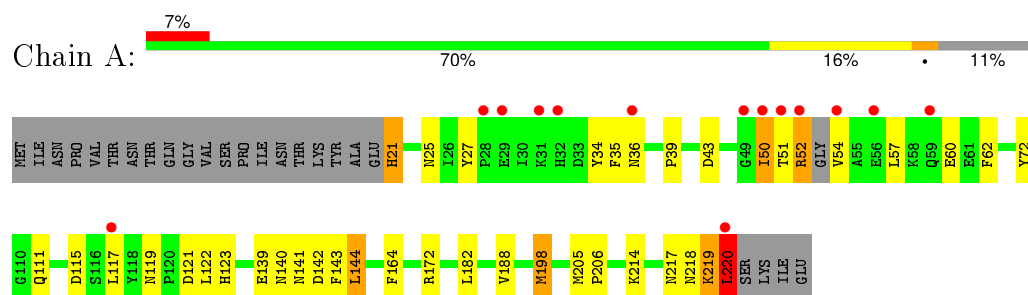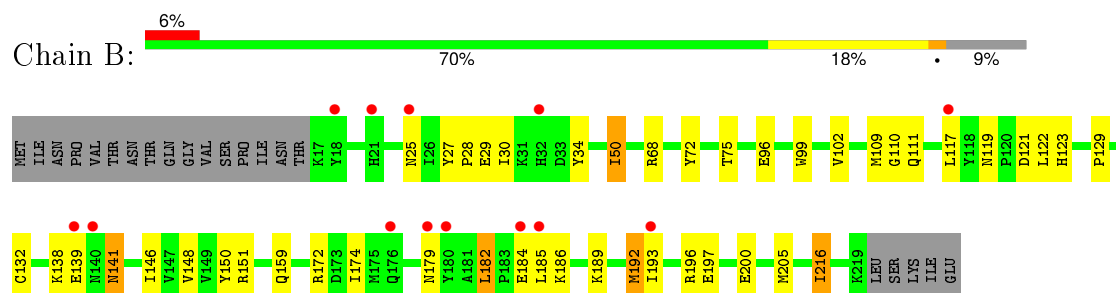
- Molecule 1: Uncharacterized protein

- Molecule 1: Uncharacterized protein
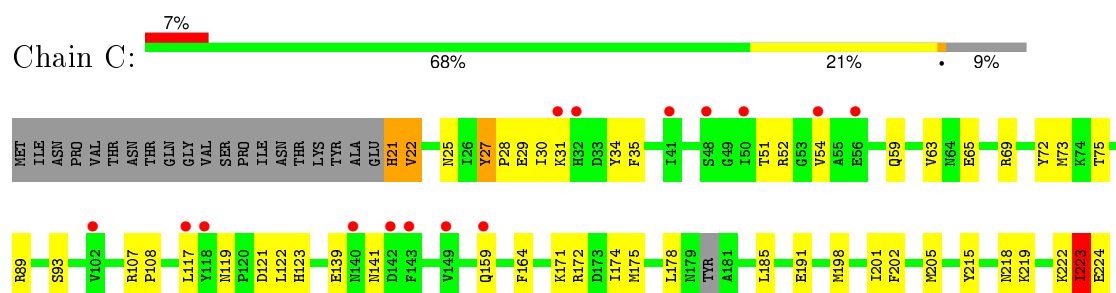
- Molecule 1: Uncharacterized protein
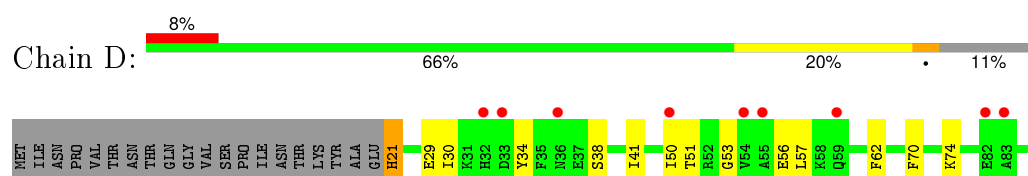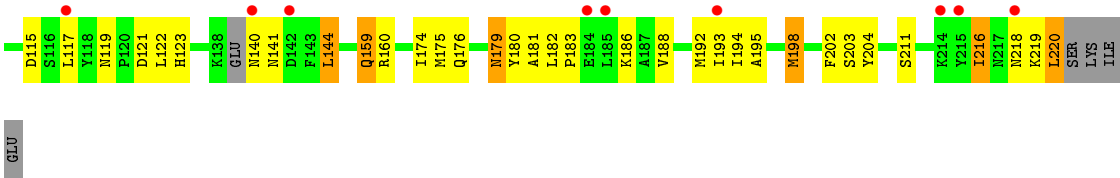
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 53.98Å 134.79Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.02 – 2.31 20.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.02-2.31) 96.3 (20.02-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.197 , 0.234 0.193 , 0.232	Depositor DCC
R_{free} test set	1944 reflections (4.72%)	DCC
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.0	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 41201 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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, 0.375 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: GOL, SAM, CIT

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	0.45	0/1669	0.58	1/2251 (0.0%)
1	B	0.42	0/1705	0.52	0/2302
1	C	0.40	0/1694	0.51	0/2283
1	D	0.39	0/1671	0.53	0/2254
All	All	0.41	0/6739	0.54	1/9090 (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	220	LEU	CA-CB-CG	5.17	127.19	115.30

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	1632	0	1607	45	0
1	B	1665	0	1628	44	0
1	C	1657	0	1637	43	0
1	D	1633	0	1610	42	0
2	A	27	0	22	1	0
2	B	27	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	22	4	0
2	D	27	0	22	2	0
3	A	6	0	8	1	0
3	C	6	0	8	4	0
3	D	6	0	8	0	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
5	A	86	0	0	1	0
5	B	87	0	0	3	0
5	C	70	0	0	3	0
5	D	52	0	0	3	0
All	All	7034	0	6604	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG22	1:A:52:ARG:N	1.54	1.18
1:A:39:PRO:HD3	1:A:51:THR:O	1.45	1.17
1:A:51:THR:CG2	1:A:52:ARG:H	1.62	1.10
1:B:50:ILE:H	1:B:50:ILE:HD12	1.29	0.97
1:D:219:LYS:O	1:D:220:LEU:HB2	1.71	0.91
1:A:51:THR:HG22	1:A:52:ARG:H	0.76	0.89
1:A:220:LEU:HD23	1:A:220:LEU:O	1.75	0.86
1:B:119:ASN:HD22	1:B:122:LEU:H	1.23	0.83
1:C:164:PHE:HD1	1:C:198:MET:HE2	1.45	0.81
1:A:35:PHE:O	1:A:51:THR:CG2	2.30	0.80
1:C:119:ASN:HD22	1:C:122:LEU:H	1.27	0.79
1:B:192:MET:HE3	1:B:193:ILE:HD13	1.65	0.77
1:B:109:MET:CE	1:B:148:VAL:HG13	2.14	0.77
1:C:89:ARG:HG3	2:C:301:SAM:N1	2.00	0.76
1:B:192:MET:CE	1:D:192:MET:HE2	2.16	0.76
1:A:218:ASN:HB3	5:A:462:HOH:O	1.84	0.75
1:C:223:ILE:N	1:C:224:GLU:HA	2.04	0.73
1:B:119:ASN:HD21	1:B:121:ASP:HB2	1.53	0.72
1:D:188:VAL:HG21	1:D:219:LYS:HE3	1.71	0.71
1:D:179:ASN:HB2	1:D:186:LYS:HZ2	1.55	0.71
1:A:35:PHE:HA	1:A:52:ARG:HB3	1.71	0.71
1:C:29:GLU:CD	1:C:29:GLU:H	1.94	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:CD	1:A:51:THR:O	2.34	0.70
1:A:188:VAL:HG21	1:A:219:LYS:HG2	1.73	0.70
1:D:119:ASN:HD21	1:D:121:ASP:HB2	1.57	0.70
1:A:51:THR:CG2	1:A:52:ARG:N	2.30	0.70
1:C:21:HIS:HD1	1:C:21:HIS:N	1.90	0.69
1:B:138:LYS:HD2	1:B:146:ILE:HD11	1.75	0.68
1:A:117:LEU:O	1:A:123:HIS:HE1	1.76	0.68
1:B:192:MET:HE1	1:D:192:MET:HE2	1.76	0.68
1:B:109:MET:HE2	1:B:148:VAL:HG13	1.74	0.68
1:C:164:PHE:CD1	1:C:198:MET:HE2	2.28	0.68
1:B:50:ILE:H	1:B:50:ILE:CD1	2.06	0.67
1:D:50:ILE:HG22	1:D:51:THR:HG23	1.76	0.67
1:A:54:VAL:HG23	1:A:54:VAL:O	1.95	0.67
1:A:119:ASN:HD21	1:A:121:ASP:HB2	1.61	0.66
1:B:68:ARG:HD3	5:B:484:HOH:O	1.95	0.66
1:D:174:ILE:HD13	1:D:193:ILE:HG13	1.79	0.65
1:A:143:PHE:CE1	1:A:144:LEU:HD13	2.32	0.65
1:C:164:PHE:HD1	1:C:198:MET:CE	2.10	0.65
1:B:109:MET:HE3	1:B:148:VAL:HG13	1.79	0.65
1:D:188:VAL:HG23	5:D:441:HOH:O	1.96	0.64
1:B:117:LEU:O	1:B:123:HIS:HE1	1.80	0.64
1:C:219:LYS:HE2	5:D:401:HOH:O	1.97	0.64
1:C:119:ASN:ND2	1:C:122:LEU:H	1.95	0.64
1:C:171:LYS:HE2	1:C:191:GLU:OE1	1.98	0.63
1:A:188:VAL:HG11	1:A:219:LYS:HB3	1.79	0.63
1:A:119:ASN:HD22	1:A:122:LEU:H	1.45	0.63
1:B:72:TYR:O	1:B:75:THR:HB	1.98	0.62
1:D:117:LEU:O	1:D:123:HIS:HE1	1.81	0.62
1:A:43:ASP:OD2	1:A:52:ARG:NH2	2.19	0.62
1:C:172:ARG:HD3	5:C:447:HOH:O	1.99	0.62
1:B:192:MET:CE	1:B:193:ILE:HD13	2.30	0.61
2:A:301:SAM:HN2	3:A:302:GOL:H2	1.65	0.61
1:A:35:PHE:O	1:A:51:THR:HG22	2.01	0.61
1:B:30:ILE:HD11	1:B:34:TYR:CG	2.35	0.61
1:D:119:ASN:HD22	1:D:122:LEU:H	1.49	0.60
1:C:117:LEU:O	1:C:123:HIS:HE1	1.84	0.60
1:C:119:ASN:HD21	1:C:121:ASP:HB2	1.66	0.60
1:B:50:ILE:HD12	1:B:50:ILE:N	2.10	0.60
1:B:174:ILE:HD12	1:B:193:ILE:HG13	1.83	0.60
1:B:119:ASN:ND2	1:B:122:LEU:H	1.99	0.60
1:B:28:PRO:HD2	1:B:29:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ASP:HA	1:D:144:LEU:HD12	1.85	0.59
1:D:21:HIS:HE1	1:D:53:GLY:HA2	1.69	0.58
1:B:197:GLU:HG2	1:D:182:LEU:HD21	1.85	0.58
1:D:30:ILE:HD11	1:D:34:TYR:CD2	2.39	0.57
1:D:179:ASN:HB2	1:D:186:LYS:NZ	2.18	0.57
1:B:109:MET:HE1	1:B:111:GLN:HB2	1.86	0.57
1:C:164:PHE:CD1	1:C:198:MET:CE	2.87	0.56
1:D:194:ILE:HD12	1:D:195:ALA:N	2.21	0.56
1:A:139:GLU:O	1:A:140:ASN:CG	2.44	0.56
1:B:184:GLU:HG2	1:B:185:LEU:HD12	1.87	0.55
1:C:159:GLN:HG3	5:C:448:HOH:O	2.06	0.55
1:C:21:HIS:ND1	1:C:21:HIS:N	2.50	0.54
1:C:30:ILE:HD11	1:C:34:TYR:CG	2.42	0.54
1:B:182:LEU:HD22	5:B:476:HOH:O	2.08	0.54
1:A:111:GLN:HG3	1:A:164:PHE:CZ	2.43	0.54
1:D:159:GLN:HG3	1:D:160:ARG:N	2.23	0.53
1:D:30:ILE:HD11	1:D:34:TYR:CG	2.44	0.53
1:A:220:LEU:C	1:A:220:LEU:HD23	2.30	0.53
1:C:222:LYS:C	1:C:223:ILE:HG13	2.28	0.53
1:B:159:GLN:NE2	1:C:218:ASN:HD22	2.05	0.53
1:A:115:ASP:HA	1:A:144:LEU:HD12	1.91	0.52
1:A:217:ASN:O	1:A:220:LEU:HB3	2.09	0.52
1:D:204:TYR:OH	2:D:301:SAM:HB2	2.10	0.52
1:A:143:PHE:CD1	1:A:144:LEU:HD13	2.45	0.51
1:A:35:PHE:O	1:A:51:THR:HG21	2.10	0.51
1:C:139:GLU:HB3	1:C:172:ARG:NH1	2.25	0.51
1:D:194:ILE:HD12	1:D:194:ILE:C	2.30	0.51
1:A:72:TYR:CD1	1:B:129:PRO:CB	2.94	0.51
1:D:182:LEU:N	1:D:183:PRO:HD3	2.26	0.51
1:A:21:HIS:ND1	1:A:21:HIS:N	2.57	0.51
1:C:198:MET:CE	1:C:201:ILE:HD11	2.41	0.50
1:A:220:LEU:CD2	1:A:220:LEU:O	2.55	0.50
1:C:174:ILE:O	1:C:178:LEU:HG	2.12	0.50
1:D:96:GLU:HB2	5:D:411:HOH:O	2.12	0.49
1:B:123:HIS:HD2	5:B:419:HOH:O	1.95	0.49
1:C:35:PHE:HA	1:C:52:ARG:HB2	1.93	0.49
1:C:198:MET:HG3	1:C:202:PHE:CE2	2.48	0.49
1:D:198:MET:HB3	2:D:301:SAM:H1'	1.94	0.49
1:A:34:TYR:CE2	1:A:52:ARG:HD3	2.48	0.49
1:A:72:TYR:CD1	1:B:129:PRO:HB2	2.48	0.49
1:A:50:ILE:CG2	1:A:51:THR:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HG3	1:B:139:GLU:N	2.29	0.48
1:D:202:PHE:O	1:D:203:SER:HB2	2.14	0.48
2:C:301:SAM:HN2	3:C:303:GOL:H11	1.79	0.48
1:B:102:VAL:O	1:B:151:ARG:HD3	2.14	0.48
1:A:141:ASN:OD1	1:A:144:LEU:HB2	2.14	0.48
1:A:72:TYR:HD1	1:B:129:PRO:CB	2.27	0.47
1:D:57:LEU:HD13	1:D:62:PHE:CE2	2.49	0.47
1:C:72:TYR:O	1:C:75:THR:HB	2.14	0.47
1:C:93:SER:C	3:C:303:GOL:H12	2.35	0.47
1:D:140:ASN:CG	1:D:141:ASN:H	2.17	0.47
1:D:70:PHE:CD2	1:D:74:LYS:HE2	2.49	0.47
1:B:109:MET:HE1	1:B:110:GLY:C	2.36	0.46
1:C:29:GLU:CD	1:C:29:GLU:N	2.66	0.46
2:C:301:SAM:HN2	3:C:303:GOL:H32	1.81	0.46
1:B:159:GLN:HE22	1:C:215:TYR:HA	1.81	0.46
1:B:179:ASN:OD1	1:B:186:LYS:NZ	2.49	0.46
1:A:21:HIS:HD1	1:A:21:HIS:N	2.14	0.45
1:D:192:MET:CE	1:D:193:ILE:HD13	2.47	0.45
1:C:223:ILE:HA	1:C:224:GLU:HG3	1.98	0.45
1:C:198:MET:HE3	1:C:201:ILE:HD11	1.98	0.45
1:B:216:ILE:HA	1:B:216:ILE:HD12	1.83	0.45
1:D:38:SER:HA	1:D:51:THR:HA	1.98	0.45
1:B:109:MET:HE2	1:B:110:GLY:O	2.16	0.45
1:B:192:MET:SD	1:D:192:MET:HE2	2.56	0.44
1:C:185:LEU:CD2	1:D:183:PRO:HG2	2.47	0.44
1:C:107:ARG:HB2	1:C:108:PRO:HD2	2.00	0.44
1:A:119:ASN:ND2	1:A:121:ASP:HB2	2.30	0.44
1:C:31:LYS:HE2	1:C:31:LYS:HB3	1.77	0.44
1:B:139:GLU:HA	1:B:139:GLU:OE1	2.17	0.44
1:B:139:GLU:OE1	1:B:172:ARG:CZ	2.66	0.43
1:A:144:LEU:HA	1:A:144:LEU:HD12	1.89	0.43
1:C:22:VAL:HG13	1:C:123:HIS:NE2	2.33	0.43
1:C:159:GLN:CG	5:C:448:HOH:O	2.64	0.43
1:C:51:THR:OG1	1:C:54:VAL:HG22	2.19	0.43
1:D:194:ILE:CD1	1:D:194:ILE:C	2.86	0.43
1:A:164:PHE:CD1	1:A:198:MET:HE1	2.53	0.43
1:D:180:TYR:C	1:D:180:TYR:CD1	2.92	0.43
1:D:56:GLU:O	1:D:56:GLU:HG2	2.18	0.43
1:A:54:VAL:CG2	1:A:54:VAL:O	2.66	0.43
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.18	0.43
1:D:216:ILE:O	1:D:219:LYS:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LYS:O	1:D:220:LEU:CB	2.54	0.42
1:A:57:LEU:HD13	1:A:62:PHE:CE2	2.55	0.42
1:C:119:ASN:HD22	1:C:122:LEU:N	2.07	0.42
1:B:96:GLU:HG3	1:B:99:TRP:CZ2	2.55	0.42
1:C:27:TYR:N	1:C:28:PRO:HD3	2.35	0.42
1:D:180:TYR:HD1	1:D:181:ALA:HB2	1.84	0.42
1:C:69:ARG:O	1:C:73:MET:HG3	2.19	0.41
1:A:205:MET:HA	1:A:206:PRO:HD3	1.92	0.41
1:A:36:ASN:O	1:A:51:THR:HG23	2.20	0.41
1:A:21:HIS:HE1	1:A:35:PHE:CE1	2.38	0.41
1:B:196:ARG:O	1:B:200:GLU:HG3	2.20	0.41
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.20	0.41
1:D:29:GLU:OE1	1:D:29:GLU:N	2.52	0.41
1:B:138:LYS:HG2	1:B:141:ASN:HB2	2.02	0.41
1:D:140:ASN:CG	1:D:141:ASN:N	2.74	0.41
1:A:217:ASN:O	1:A:220:LEU:HD13	2.20	0.40
1:C:59:GLN:O	1:C:63:VAL:HB	2.21	0.40
1:C:185:LEU:HD23	1:D:183:PRO:HG2	2.03	0.40
1:B:132:CYS:HB2	1:B:150:TYR:CZ	2.56	0.40
1:B:189:LYS:O	1:B:192:MET:HG3	2.21	0.40
2:C:301:SAM:N	3:C:303:GOL:H11	2.36	0.40
1:D:192:MET:HE1	1:D:193:ILE:HD13	2.03	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	195/224 (87%)	186 (95%)	9 (5%)	0	100	100
1	B	201/224 (90%)	195 (97%)	6 (3%)	0	100	100
1	C	199/224 (89%)	190 (96%)	8 (4%)	1 (0%)	34	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	195/224 (87%)	186 (95%)	9 (5%)	0	100	100
All	All	790/896 (88%)	757 (96%)	32 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	ILE

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	182/205 (89%)	168 (92%)	14 (8%)	16	19
1	B	184/205 (90%)	176 (96%)	8 (4%)	35	48
1	C	185/205 (90%)	177 (96%)	8 (4%)	35	48
1	D	182/205 (89%)	168 (92%)	14 (8%)	16	19
All	All	733/820 (89%)	689 (94%)	44 (6%)	24	31

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	25	ASN
1	A	27	TYR
1	A	50	ILE
1	A	52	ARG
1	A	109	MET
1	A	142	ASP
1	A	144	LEU
1	A	172	ARG
1	A	182	LEU
1	A	198	MET
1	A	214	LYS
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	220	LEU
1	B	25	ASN
1	B	27	TYR
1	B	50	ILE
1	B	141	ASN
1	B	182	LEU
1	B	192	MET
1	B	205	MET
1	B	216	ILE
1	C	21	HIS
1	C	22	VAL
1	C	25	ASN
1	C	27	TYR
1	C	141	ASN
1	C	175	MET
1	C	205	MET
1	C	223	ILE
1	D	21	HIS
1	D	41	ILE
1	D	89	ARG
1	D	109	MET
1	D	144	LEU
1	D	159	GLN
1	D	175	MET
1	D	176	GLN
1	D	179	ASN
1	D	198	MET
1	D	211	SER
1	D	216	ILE
1	D	218	ASN
1	D	220	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	119	ASN
1	A	123	HIS
1	B	64	ASN
1	B	119	ASN
1	B	123	HIS
1	B	159	GLN

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Mol	Chain	Res	Type
1	C	32	HIS
1	C	64	ASN
1	C	119	ASN
1	C	123	HIS
1	D	21	HIS
1	D	64	ASN
1	D	119	ASN
1	D	123	HIS
1	D	176	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	SAM	A	301	-	21,29,29	1.13	2 (9%)	17,42,42	2.79	1 (5%)
3	GOL	A	302	-	5,5,5	0.31	0	5,5,5	0.48	0
2	SAM	B	301	-	21,29,29	1.13	2 (9%)	17,42,42	2.82	2 (11%)
4	CIT	B	302	-	3,12,12	1.04	0	3,17,17	2.80	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SAM	C	301	-	21,29,29	1.26	2 (9%)	17,42,42	2.73	1 (5%)
4	CIT	C	302	-	3,12,12	1.24	0	3,17,17	1.05	0
3	GOL	C	303	-	5,5,5	0.34	0	5,5,5	0.68	0
2	SAM	D	301	-	21,29,29	1.25	2 (9%)	17,42,42	3.09	2 (11%)
3	GOL	D	302	-	5,5,5	0.28	0	5,5,5	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAM	A	301	-	-	0/8/33/33	0/3/3/3
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0
2	SAM	B	301	-	-	0/8/33/33	0/3/3/3
4	CIT	B	302	-	-	0/6/16/16	0/0/0/0
2	SAM	C	301	-	-	0/8/33/33	0/3/3/3
4	CIT	C	302	-	-	0/6/16/16	0/0/0/0
3	GOL	C	303	-	-	0/4/4/4	0/0/0/0
2	SAM	D	301	-	-	0/8/33/33	0/3/3/3
3	GOL	D	302	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SAM	C2-N1	2.43	1.38	1.33
2	B	301	SAM	C2-N1	2.45	1.38	1.33
2	A	301	SAM	C2-N1	2.61	1.38	1.33
2	D	301	SAM	C2-N1	2.77	1.39	1.33
2	B	301	SAM	C2-N3	3.49	1.38	1.32
2	A	301	SAM	C2-N3	3.57	1.38	1.32
2	D	301	SAM	C2-N3	3.78	1.38	1.32
2	C	301	SAM	C2-N3	4.07	1.39	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	SAM	N3-C2-N1	-12.03	119.68	128.89
2	A	301	SAM	N3-C2-N1	-11.04	120.44	128.89
2	B	301	SAM	N3-C2-N1	-10.78	120.64	128.89
2	C	301	SAM	N3-C2-N1	-10.78	120.64	128.89
4	B	302	CIT	C3-C2-C1	-3.43	109.48	114.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	302	CIT	C3-C4-C5	-3.41	109.51	114.96
2	D	301	SAM	C4'-O4'-C1'	2.02	111.94	109.72
2	B	301	SAM	C4'-O4'-C1'	2.91	112.92	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SAM	1	0
3	A	302	GOL	1	0
2	C	301	SAM	4	0
3	C	303	GOL	4	0
2	D	301	SAM	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	199/224 (88%)	0.21	16 (8%)	15	21	16, 27, 60, 65	0
1	B	203/224 (90%)	0.08	13 (6%)	23	31	16, 28, 55, 77	0
1	C	203/224 (90%)	0.27	15 (7%)	17	25	18, 30, 58, 72	0
1	D	199/224 (88%)	0.33	18 (9%)	12	17	19, 36, 60, 73	0
All	All	804/896 (89%)	0.22	62 (7%)	16	23	16, 30, 59, 77	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	6.8
1	B	140	ASN	6.6
1	A	54	VAL	5.0
1	A	50	ILE	4.8
1	C	41	ILE	4.7
1	B	18	TYR	4.6
1	C	50	ILE	4.4
1	C	143	PHE	4.4
1	D	82	GLU	4.3
1	A	83	ALA	4.3
1	B	32	HIS	3.7
1	A	59	GLN	3.5
1	D	184	GLU	3.4
1	C	117	LEU	3.3
1	D	140	ASN	3.2
1	C	140	ASN	3.2
1	A	220	LEU	3.1
1	B	176	GLN	3.1
1	D	32	HIS	3.0
1	D	218	ASN	3.0
1	A	51	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	117	LEU	3.0
1	A	49	GLY	2.9
1	B	179	ASN	2.8
1	A	36	ASN	2.8
1	D	59	GLN	2.7
1	D	54	VAL	2.7
1	D	214	LYS	2.7
1	C	54	VAL	2.7
1	D	55	ALA	2.6
1	A	31	LYS	2.5
1	B	139	GLU	2.5
1	B	185	LEU	2.5
1	C	48	SER	2.5
1	B	25	ASN	2.5
1	D	50	ILE	2.5
1	D	83	ALA	2.5
1	A	28	PRO	2.5
1	C	149	VAL	2.5
1	C	159	GLN	2.4
1	D	185	LEU	2.4
1	A	82	GLU	2.4
1	D	193	ILE	2.4
1	A	117	LEU	2.3
1	C	56	GLU	2.3
1	D	142	ASP	2.3
1	D	36	ASN	2.3
1	A	32	HIS	2.3
1	C	102	VAL	2.2
1	D	117	LEU	2.2
1	C	118	TYR	2.2
1	A	29	GLU	2.2
1	B	193	ILE	2.2
1	C	31	LYS	2.2
1	A	56	GLU	2.2
1	D	33	ASP	2.1
1	C	142	ASP	2.1
1	B	184	GLU	2.1
1	D	215	TYR	2.0
1	B	21	HIS	2.0
1	C	32	HIS	2.0
1	A	52	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	GOL	C	303	6/6	0.79	0.24	4.32	34,37,41,42	0
4	CIT	B	302	13/13	0.86	0.24	4.20	20,20,20,20	0
2	SAM	B	301	27/27	0.97	0.15	0.56	19,24,29,32	0
4	CIT	C	302	13/13	0.88	0.17	0.46	41,45,50,50	0
2	SAM	D	301	27/27	0.92	0.16	0.04	25,37,40,49	0
2	SAM	A	301	27/27	0.96	0.13	-0.39	19,24,30,36	0
2	SAM	C	301	27/27	0.96	0.12	-0.40	22,25,32,34	0
3	GOL	A	302	6/6	0.91	0.11	-0.47	31,35,36,37	0
3	GOL	D	302	6/6	0.93	0.13	-0.57	43,48,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.