Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:34 PM GMT

PDB ID	:	4IQF
Title	:	Crystal Structure of Methyionyl-tRNA Formyltransferase from Bacillus anthracis
Authors	:	Kim, Y.; Makowska-Grzyska, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-01-11
Resolution	:	2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the symbol.

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

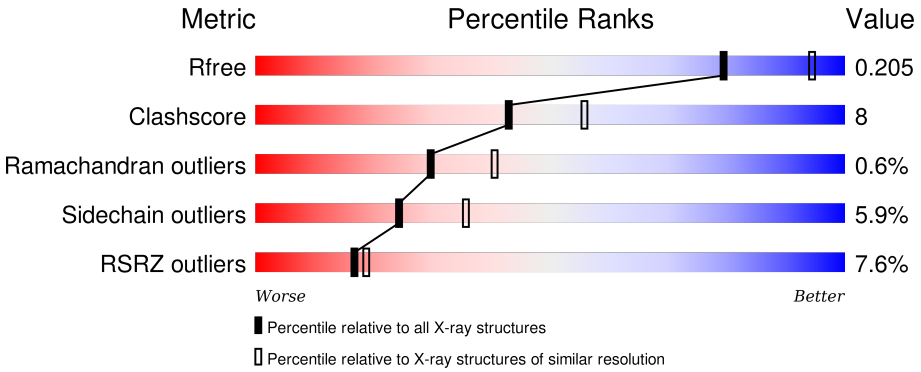
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	317	5% 79% 19%
1	B	317	11% 75% 23%
1	C	317	8% 72% 25%
1	D	317	6% 75% 23%

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	A	402	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10413 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.

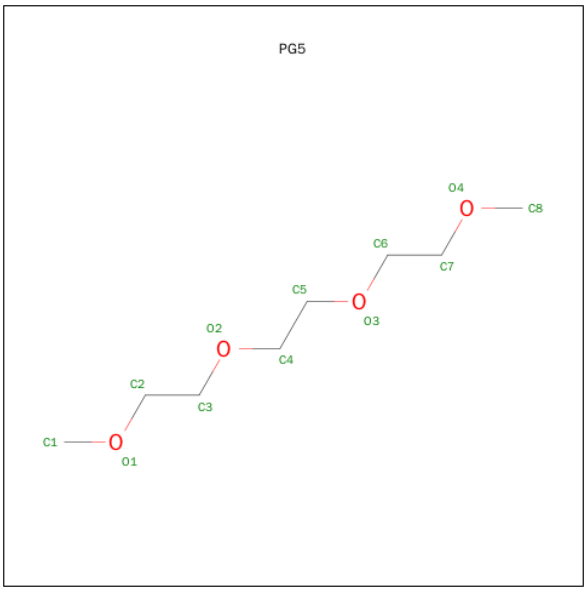
- Molecule 1 is a protein called Methionyl-tRNA formyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	Se	0	1	0
			2450	1567	409	466	2	6			
1	B	314	Total	C	N	O	S	Se	0	1	0
			2458	1575	410	465	2	6			
1	C	315	Total	C	N	O	S	Se	0	1	0
			2464	1578	411	467	2	6			
1	D	315	Total	C	N	O	S	Se	10	3	0
			2483	1589	415	471	2	6			

There are 12 discrepancies between the modelled and reference sequences:

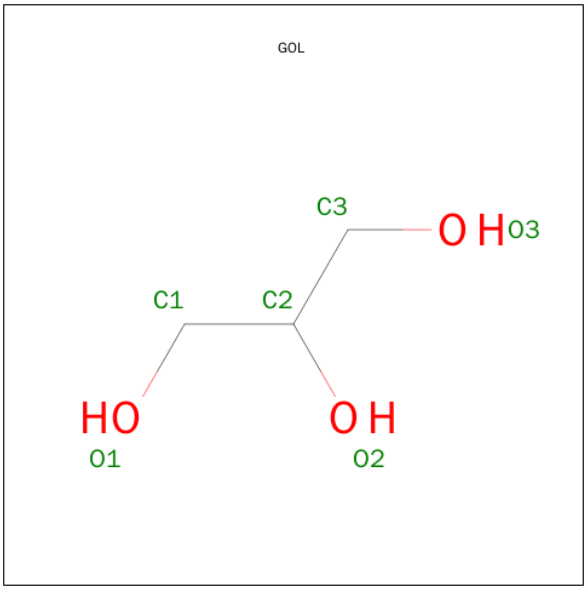
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81WH2
A	-1	ASN	-	EXPRESSION TAG	UNP Q81WH2
A	0	ALA	-	EXPRESSION TAG	UNP Q81WH2
B	-2	SER	-	EXPRESSION TAG	UNP Q81WH2
B	-1	ASN	-	EXPRESSION TAG	UNP Q81WH2
B	0	ALA	-	EXPRESSION TAG	UNP Q81WH2
C	-2	SER	-	EXPRESSION TAG	UNP Q81WH2
C	-1	ASN	-	EXPRESSION TAG	UNP Q81WH2
C	0	ALA	-	EXPRESSION TAG	UNP Q81WH2
D	-2	SER	-	EXPRESSION TAG	UNP Q81WH2
D	-1	ASN	-	EXPRESSION TAG	UNP Q81WH2
D	0	ALA	-	EXPRESSION TAG	UNP Q81WH2

- Molecule 2 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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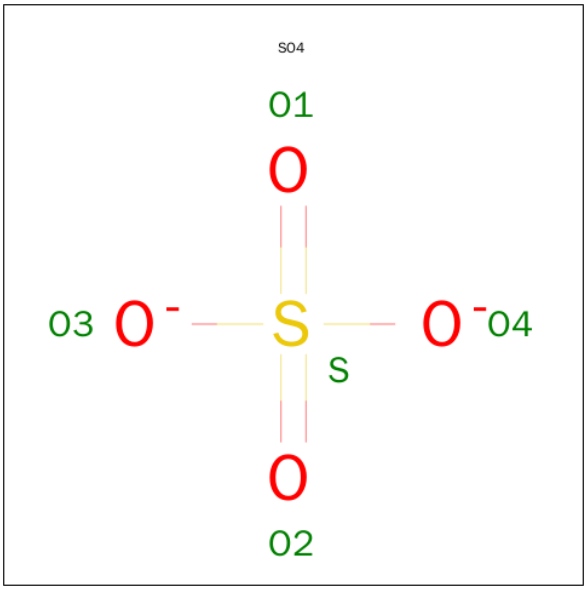
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

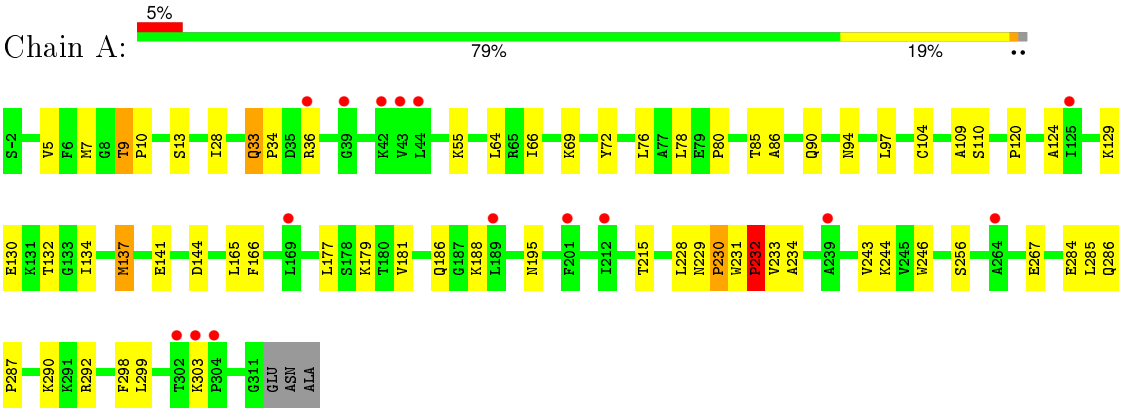
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	122	Total O 122 122	0	0
5	C	97	Total O 97 97	0	0
5	D	135	Total O 135 135	0	0

3 Residue-property plots (i)

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.

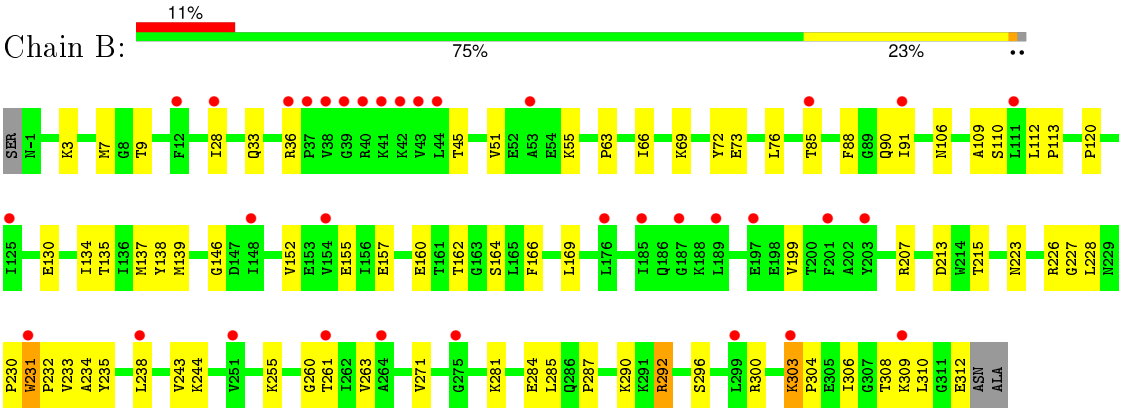
- Molecule 1: Methionyl-tRNA formyltransferase

Chain A:



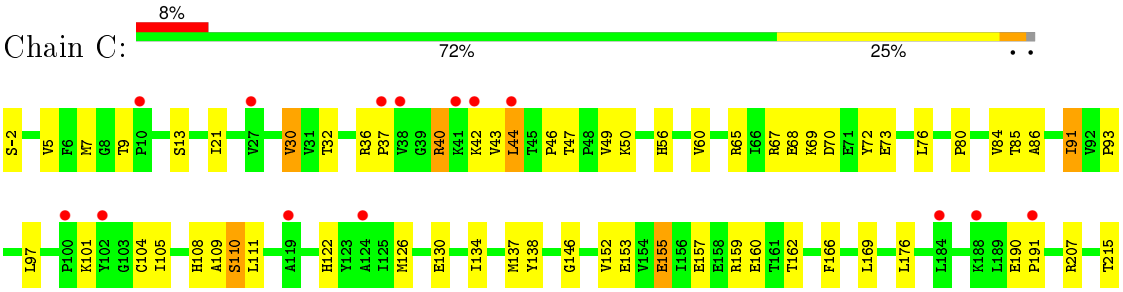
- Molecule 1: Methionyl-tRNA formyltransferase

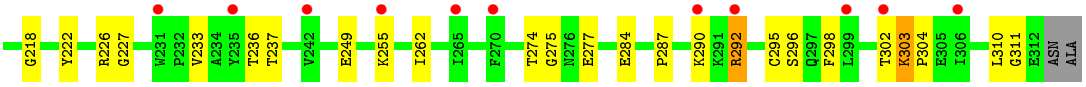
Chain B:



- Molecule 1: Methionyl-tRNA formyltransferase

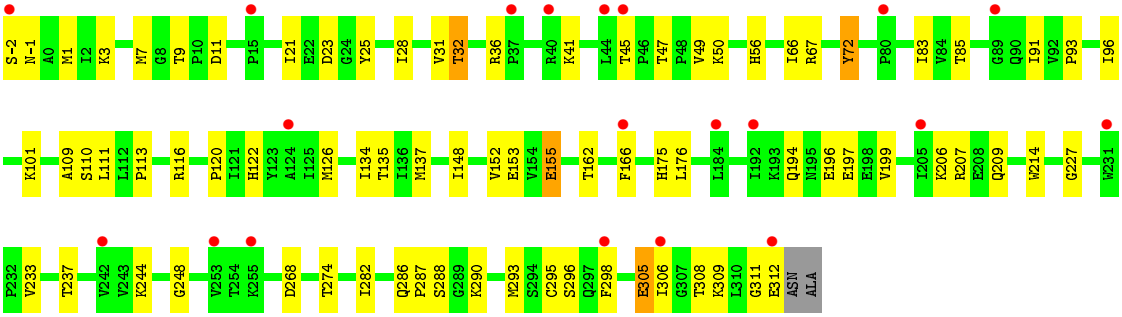
Chain C:





- Molecule 1: Methionyl-tRNA formyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.86Å 191.50Å 89.95Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	36.59 – 2.38 36.59 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.5 (36.59-2.38) 97.5 (36.59-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.181 , 0.210 0.180 , 0.205	Depositor DCC
R_{free} test set	4126 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.0	EDS
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 82905 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10413	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 35.26 % 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 5.9941e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG5, SO4

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	0.30	2/2491 (0.1%)	0.46	0/3369
1	B	0.27	1/2501 (0.0%)	0.45	1/3385 (0.0%)
1	C	0.28	1/2507 (0.0%)	0.45	1/3393 (0.0%)
1	D	0.23	0/2527	0.44	0/3420
All	All	0.27	4/10026 (0.0%)	0.45	2/13567 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	PRO	N-CD	5.41	1.55	1.47
1	C	304	PRO	N-CD	5.20	1.55	1.47
1	B	304	PRO	N-CD	5.13	1.55	1.47
1	A	230	PRO	N-CD	5.02	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	303	LYS	C-N-CD	5.59	140.14	128.40
1	C	303	LYS	C-N-CD	5.55	140.06	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2450	0	2516	36	0
1	B	2458	0	2522	41	0
1	C	2464	0	2527	46	0
1	D	2483	0	2538	43	0
2	A	10	0	12	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	10	0	0	0	0
5	A	150	0	0	2	0
5	B	122	0	0	0	0
5	C	97	0	0	3	0
5	D	135	0	0	2	0
All	All	10413	0	10147	164	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 8.

All (164) 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:D:237:THR:OG1	1:D:311:GLY:HA2	1.85	0.76
1:D:268:ASP:HA	1:D:296:SER:HB3	1.72	0.70
1:C:152:VAL:HG12	1:C:176:LEU:HD22	1.79	0.64
1:C:295:CYS:HA	1:C:298:PHE:HB3	1.80	0.63
1:B:7:MSE:HB2	1:B:85:THR:HG22	1.79	0.63
1:B:243:VAL:HG11	1:B:285:LEU:HD12	1.82	0.62
1:B:63:PRO:HG3	1:B:66:ILE:HD13	1.82	0.61
1:C:237:THR:OG1	1:C:311:GLY:HA2	2.01	0.60
1:B:157:GLU:HB2	1:B:160:GLU:HG2	1.84	0.59
1:A:7:MSE:HB2	1:A:85:THR:HG22	1.85	0.58
1:D:111:LEU:HD11	1:D:153:GLU:HG2	1.85	0.58
1:A:66:ILE:H	1:A:90:GLN:NE2	2.01	0.57
1:C:47:THR:HG22	1:C:49:VAL:H	1.69	0.57
1:C:237:THR:O	1:C:311:GLY:N	2.26	0.56
1:C:32:THR:OG1	1:C:47:THR:HG21	2.05	0.56
1:B:287:PRO:HG2	1:B:290:LYS:HB2	1.87	0.56
1:A:195:ASN:HA	1:D:41:LYS:HE3	1.87	0.55
1:A:287:PRO:HG2	1:A:290:LYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PHE:CE2	1:B:90:GLN:HB2	2.42	0.55
1:A:228:LEU:HD22	1:A:232:PRO:HD2	1.88	0.54
1:B:213:ASP:OD1	1:B:215:THR:OG1	2.25	0.54
1:A:109:ALA:HA	1:A:134:ILE:HD13	1.89	0.54
1:A:69:LYS:NZ	1:A:72:TYR:OH	2.30	0.54
1:B:228:LEU:HD12	1:B:234:ALA:HB2	1.90	0.53
1:D:287:PRO:HG2	1:D:290:LYS:HB2	1.90	0.53
1:C:284:GLU:OE2	1:C:292:ARG:NH2	2.40	0.53
1:D:32:THR:OG1	1:D:47:THR:HG21	2.09	0.52
1:A:299:LEU:O	1:A:303:LYS:HG3	2.09	0.52
1:B:263:VAL:O	1:B:306:ILE:HD12	2.09	0.52
1:D:3:LYS:HB3	1:D:28:ILE:HD13	1.92	0.52
1:B:284:GLU:OE2	1:B:292:ARG:NH2	2.44	0.51
1:D:109:ALA:HA	1:D:134:ILE:HD13	1.93	0.51
1:D:7:MSE:HB2	1:D:85:THR:HG22	1.93	0.51
1:B:51:VAL:O	1:B:55:LYS:HG3	2.11	0.51
1:A:179:LYS:NZ	5:A:574:HOH:O	2.43	0.51
1:B:271:VAL:HG22	1:B:281:LYS:HB2	1.93	0.51
1:B:261:THR:OG1	1:B:309:LYS:HG3	2.10	0.50
1:B:260:GLY:O	1:B:310:LEU:N	2.42	0.50
1:D:21:ILE:HG21	1:D:56:HIS:CD2	2.46	0.50
1:D:135:THR:HG23	1:D:148:ILE:HG23	1.92	0.50
1:A:94:ASN:HD21	1:A:141:GLU:HG3	1.77	0.49
1:C:109:ALA:HA	1:C:134:ILE:HD13	1.93	0.49
1:A:243:VAL:HG11	1:A:285:LEU:HD12	1.93	0.49
1:C:134:ILE:HD11	1:C:169:LEU:HB3	1.94	0.49
1:D:122:HIS:HB3	1:D:126:MSE:HE3	1.94	0.49
1:C:162:THR:OG1	1:C:227:GLY:O	2.27	0.49
1:C:97:LEU:HA	1:C:104:CYS:SG	2.53	0.48
1:D:237:THR:OG1	1:D:311:GLY:CA	2.59	0.48
1:C:159:ARG:NH1	1:C:249:GLU:OE2	2.38	0.48
1:C:5:VAL:HG23	1:C:80:PRO:HB3	1.94	0.48
1:A:228:LEU:HD12	1:A:234:ALA:HB2	1.95	0.48
1:C:218:GLY:HA2	1:C:274:THR:HG21	1.95	0.48
1:B:261:THR:HA	1:B:309:LYS:HA	1.95	0.48
1:D:155:GLU:CD	1:D:155:GLU:H	2.16	0.48
1:A:132:THR:HG21	1:A:165:LEU:HD21	1.95	0.47
1:B:110:SER:HB3	1:B:120:PRO:HB2	1.95	0.47
1:B:109:ALA:HA	1:B:134:ILE:HD13	1.96	0.47
1:C:69:LYS:HA	1:C:72:TYR:CE2	2.49	0.47
1:D:66:ILE:O	1:D:72:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-2:SER:HB3	1:D:25:TYR:CE2	2.49	0.47
1:C:65:ARG:NH2	1:C:68:GLU:OE2	2.46	0.47
1:D:309:LYS:O	5:D:535:HOH:O	2.21	0.47
1:C:69:LYS:O	1:C:73:GLU:HG3	2.15	0.47
1:C:237:THR:OG1	1:C:311:GLY:CA	2.61	0.46
1:A:130[B]:GLU:CD	1:A:130[B]:GLU:H	2.17	0.46
1:A:5:VAL:HG23	1:A:80:PRO:HB3	1.98	0.46
1:B:134:ILE:HB	1:B:152:VAL:HG12	1.97	0.46
1:C:7:MSE:HB2	1:C:85:THR:HG22	1.97	0.46
1:A:244:LYS:HB2	1:A:286:GLN:HB3	1.97	0.46
1:C:122:HIS:HB3	1:C:126:MSE:HE3	1.97	0.46
1:C:46:PRO:HB3	1:C:50:LYS:HD3	1.97	0.46
1:D:290:LYS:NZ	5:D:630:HOH:O	2.48	0.46
1:D:7:MSE:HG2	1:D:31:VAL:HB	1.96	0.46
1:D:72:TYR:HB2	1:D:96:ILE:HD11	1.99	0.45
1:A:246:TRP:CD2	1:A:292:ARG:HD3	2.51	0.45
1:D:162:THR:OG1	1:D:227:GLY:O	2.33	0.45
1:B:3:LYS:HB3	1:B:28:ILE:HD13	1.98	0.45
1:D:306:ILE:H	1:D:306:ILE:HD12	1.81	0.45
1:D:47:THR:HG22	1:D:50:LYS:H	1.82	0.45
1:A:231:TRP:HA	1:A:232:PRO:HA	1.71	0.45
1:A:69:LYS:HA	1:A:72:TYR:CE2	2.52	0.45
1:D:93:PRO:HG2	1:D:96:ILE:HG13	1.97	0.45
1:A:55:LYS:HD3	1:C:91:ILE:HD12	1.99	0.45
1:A:28:ILE:HD12	1:A:78:LEU:HB3	1.97	0.45
1:C:222:TYR:O	1:C:226:ARG:HG2	2.17	0.45
1:A:231:TRP:CD1	1:A:231:TRP:O	2.70	0.44
1:D:214:TRP:HE3	1:D:274:THR:HG22	1.82	0.44
1:C:40:ARG:NE	5:C:570:HOH:O	2.43	0.44
1:C:65:ARG:HG2	1:C:67:ARG:HG2	1.99	0.44
1:B:160:GLU:OE1	1:B:164:SER:OG	2.30	0.44
1:C:47:THR:HG22	1:C:49:VAL:N	2.31	0.44
1:C:72:TYR:O	1:C:76:LEU:HG	2.18	0.44
1:B:235:TYR:HB3	1:B:244:LYS:HG2	1.98	0.44
1:A:72:TYR:O	1:A:76:LEU:HG	2.18	0.44
1:C:138:TYR:O	1:C:146:GLY:HA3	2.18	0.44
1:A:284:GLU:OE2	1:A:292:ARG:HD2	2.18	0.44
1:C:122:HIS:CE1	1:C:162:THR:HG21	2.53	0.44
1:B:109:ALA:HB1	1:B:169:LEU:HD13	1.99	0.44
1:B:66:ILE:O	1:B:72:TYR:HB3	2.17	0.44
1:B:223:ASN:HA	1:B:226:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:HG3	1:B:72:TYR:CZ	2.53	0.43
1:B:231[B]:TRP:CG	1:B:232:PRO:HA	2.53	0.43
1:C:255:LYS:HE2	1:C:255:LYS:HB3	1.70	0.43
1:A:137:MSE:HE3	1:A:144:ASP:HA	2.00	0.43
1:A:285:LEU:HD21	1:A:298:PHE:HB2	2.00	0.43
1:C:67:ARG:HA	1:C:93:PRO:HG3	2.00	0.43
1:B:162:THR:OG1	1:B:227:GLY:O	2.27	0.43
1:C:111:LEU:HD11	1:C:153:GLU:HG2	2.00	0.43
1:D:152:VAL:HG12	1:D:176:LEU:HD22	2.01	0.43
1:B:261:THR:HG23	1:B:308:THR:O	2.19	0.43
1:A:13:SER:OG	1:A:86:ALA:O	2.24	0.43
1:A:186:GLN:HB3	1:A:188:LYS:HZ2	1.84	0.43
1:C:157:GLU:N	1:C:160:GLU:HG3	2.33	0.43
1:C:37:PRO:HA	1:C:44:LEU:HA	2.00	0.43
1:B:55:LYS:HB3	1:D:91:ILE:HD13	2.01	0.43
1:C:215:THR:O	1:C:275:GLY:HA3	2.18	0.43
1:A:33:GLN:HE21	1:A:34:PRO:HD2	1.83	0.43
1:B:113:PRO:HB2	1:B:199:VAL:HA	2.01	0.43
1:A:97:LEU:HA	1:A:104:CYS:SG	2.58	0.42
1:D:244:LYS:N	1:D:286:GLN:O	2.51	0.42
1:B:106:ASN:HB2	1:B:139:MSE:HG2	2.02	0.42
1:C:262:ILE:HD11	1:C:310:LEU:HD11	2.01	0.42
1:C:30:VAL:HG12	1:C:60:VAL:HG13	2.01	0.42
1:C:84:VAL:HG22	1:C:105:ILE:HD11	2.01	0.42
1:C:13:SER:OG	1:C:86:ALA:O	2.23	0.42
1:D:110:SER:HB3	1:D:120:PRO:HB3	2.01	0.42
1:D:286:GLN:HA	1:D:287:PRO:HD2	1.94	0.42
1:B:271:VAL:HA	1:B:281:LYS:HA	2.01	0.42
1:D:305:GLU:O	1:D:308:THR:OG1	2.28	0.42
1:B:69:LYS:NZ	1:B:73:GLU:OE1	2.53	0.42
1:A:110:SER:HB3	1:A:120:PRO:HB2	2.02	0.42
1:A:229:ASN:HA	1:A:230:PRO:HA	1.62	0.42
1:C:190:GLU:HA	1:C:191:PRO:HD3	1.87	0.42
1:B:230:PRO:HG2	1:B:231[A]:TRP:CE2	2.55	0.42
1:B:109:ALA:HB3	3:B:401:GOL:H11	2.00	0.42
1:B:138:TYR:O	1:B:146:GLY:HA3	2.20	0.42
1:D:116:ARG:HE	1:D:194:GLN:HE22	1.68	0.42
1:D:47:THR:HG22	1:D:49:VAL:N	2.35	0.41
1:C:21:ILE:O	5:C:509:HOH:O	2.21	0.41
1:B:243:VAL:HG22	1:B:287:PRO:HA	2.02	0.41
1:A:9:THR:HB	1:A:10:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MSE:HE2	1:D:83:ILE:HG21	2.01	0.41
1:D:122:HIS:CE1	1:D:162:THR:HG21	2.55	0.41
1:D:248:GLY:HA2	1:D:282:ILE:HA	2.03	0.41
1:B:296:SER:O	1:B:300:ARG:HG3	2.21	0.41
1:C:108:HIS:CE1	1:C:110:SER:HB3	2.55	0.41
1:D:206:LYS:HG3	1:D:209:GLN:HE22	1.85	0.41
1:A:124:ALA:O	1:A:129:LYS:HB2	2.21	0.41
1:D:295:CYS:HA	1:D:298:PHE:HB3	2.03	0.41
1:B:72:TYR:O	1:B:76:LEU:HG	2.21	0.41
1:D:47:THR:HG22	1:D:49:VAL:H	1.86	0.41
1:C:287:PRO:HG2	1:C:290:LYS:HE3	2.03	0.41
1:D:113:PRO:HB3	1:D:199:VAL:HG22	2.03	0.41
1:C:-2:SER:N	5:C:553:HOH:O	2.48	0.41
3:A:402:GOL:H31	5:A:624:HOH:O	2.21	0.40
1:B:228:LEU:HD22	1:B:232:PRO:HD2	2.02	0.40
1:D:196:GLU:HA	1:D:199:VAL:HG23	2.03	0.40
1:C:155:GLU:CD	1:C:155:GLU:H	2.23	0.40
1:B:112:LEU:HB2	1:B:135:THR:HG21	2.04	0.40
1:A:66:ILE:H	1:A:90:GLN:HE22	1.69	0.40
1:D:67:ARG:HA	1:D:93:PRO:HG3	2.04	0.40
1:C:21:ILE:HG21	1:C:56:HIS:ND1	2.36	0.40
1:D:1:MSE:HE2	1:D:1:MSE:HA	2.03	0.40
1:A:177:LEU:O	1:A:181:VAL:HG23	2.21	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	313/317 (99%)	302 (96%)	9 (3%)	2 (1%)	30	40
1	B	313/317 (99%)	300 (96%)	11 (4%)	2 (1%)	30	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	314/317 (99%)	299 (95%)	13 (4%)	2 (1%)	30 40
1	D	316/317 (100%)	300 (95%)	14 (4%)	2 (1%)	30 40
All	All	1256/1268 (99%)	1201 (96%)	47 (4%)	8 (1%)	30 40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	233	VAL
1	A	233	VAL
1	D	9	THR
1	D	233	VAL
1	A	9	THR
1	B	9	THR
1	B	233	VAL
1	C	9	THR

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	269/264 (102%)	260 (97%)	9 (3%)	45 64
1	B	269/264 (102%)	253 (94%)	16 (6%)	24 36
1	C	270/264 (102%)	249 (92%)	21 (8%)	16 22
1	D	272/264 (103%)	254 (93%)	18 (7%)	21 30
All	All	1080/1056 (102%)	1016 (94%)	64 (6%)	24 36

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	36	ARG
1	A	64	LEU
1	A	137	MSE

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Mol	Chain	Res	Type
1	A	166	PHE
1	A	215	THR
1	A	232	PRO
1	A	256	SER
1	A	267	GLU
1	B	33	GLN
1	B	36	ARG
1	B	45	THR
1	B	91	ILE
1	B	130	GLU
1	B	137	MSE
1	B	155	GLU
1	B	166	PHE
1	B	207	ARG
1	B	231[A]	TRP
1	B	231[B]	TRP
1	B	238	LEU
1	B	255	LYS
1	B	292	ARG
1	B	303	LYS
1	B	312	GLU
1	C	30	VAL
1	C	36	ARG
1	C	40	ARG
1	C	42	LYS
1	C	43	VAL
1	C	44	LEU
1	C	70	ASP
1	C	91	ILE
1	C	101	LYS
1	C	110	SER
1	C	130	GLU
1	C	137	MSE
1	C	155	GLU
1	C	166	PHE
1	C	207	ARG
1	C	236	THR
1	C	277	GLU
1	C	292	ARG
1	C	296	SER
1	C	302	THR
1	C	303	LYS

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Mol	Chain	Res	Type
1	D	-1	ASN
1	D	11	ASP
1	D	23	ASP
1	D	32	THR
1	D	36	ARG
1	D	45	THR
1	D	72	TYR
1	D	101	LYS
1	D	137	MSE
1	D	155	GLU
1	D	166	PHE
1	D	175	HIS
1	D	197	GLU
1	D	207	ARG
1	D	288	SER
1	D	293	MSE
1	D	305	GLU
1	D	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	56	HIS
1	A	90	GLN
1	A	94	ASN
1	A	186	GLN
1	A	204	ASN
1	B	33	GLN
1	B	62	GLN
1	B	90	GLN
1	B	186	GLN
1	B	204	ASN
1	B	241	GLN
1	C	108	HIS
1	C	209	GLN
1	C	224	HIS
1	C	241	GLN
1	C	297	GLN
1	D	194	GLN
1	D	241	GLN
1	D	297	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	PG5	A	401	-	9,9,11	0.66	0	8,8,10	1.48	0
3	GOL	A	402	-	5,5,5	0.35	0	5,5,5	0.37	0
4	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.22	0
4	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	C	401	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	D	401	-	5,5,5	0.39	0	5,5,5	0.21	0
4	SO4	D	402	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.08	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	PG5	A	401	-	-	0/7/7/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	GOL	B	401	-	-	0/4/4/4	0/0/0/0
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	GOL	C	401	-	-	0/4/4/4	0/0/0/0
3	GOL	D	401	-	-	0/4/4/4	0/0/0/0
4	SO4	D	402	-	-	0/0/0/0	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
3	B	401	GOL	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	308/317 (97%)	0.68	15 (4%)	33	38	29, 48, 84, 118	0
1	B	308/317 (97%)	0.92	34 (11%)	7	9	36, 59, 106, 145	0
1	C	309/317 (97%)	0.75	25 (8%)	15	17	35, 56, 97, 125	1 (0%)
1	D	309/317 (97%)	0.79	20 (6%)	22	26	39, 54, 78, 103	1 (0%)
All	All	1234/1268 (97%)	0.78	94 (7%)	17	19	29, 55, 92, 145	2 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	LYS	7.3
1	B	40	ARG	6.8
1	B	36	ARG	6.5
1	A	36	ARG	6.4
1	C	37	PRO	5.6
1	A	43	VAL	5.3
1	B	39	GLY	5.0
1	B	42	LYS	4.6
1	B	43	VAL	4.5
1	B	38	VAL	4.2
1	B	275	GLY	3.9
1	C	255	LYS	3.9
1	C	41	LYS	3.9
1	B	238	LEU	3.8
1	C	242	VAL	3.7
1	D	231[A]	TRP	3.6
1	B	148	ILE	3.6
1	D	-2	SER	3.5
1	D	255	LYS	3.5
1	C	102	TYR	3.4
1	B	189	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	292	ARG	3.4
1	C	302	THR	3.3
1	B	251	VAL	3.3
1	C	184	LEU	3.3
1	A	189	LEU	3.3
1	A	302	THR	3.2
1	B	264	ALA	3.1
1	C	188	LYS	3.1
1	A	239	ALA	3.1
1	B	53	ALA	3.1
1	C	119	ALA	3.1
1	D	45	THR	3.0
1	D	37	PRO	3.0
1	B	44	LEU	2.9
1	D	312	GLU	2.9
1	B	41	LYS	2.9
1	D	40	ARG	2.9
1	D	80	PRO	2.8
1	A	304	PRO	2.8
1	D	44	LEU	2.8
1	B	231[A]	TRP	2.8
1	C	231[A]	TRP	2.8
1	D	89	GLY	2.8
1	B	37	PRO	2.8
1	C	38	VAL	2.8
1	B	187	GLY	2.7
1	B	203	TYR	2.7
1	A	39	GLY	2.7
1	C	191	PRO	2.7
1	D	184	LEU	2.6
1	B	12	PHE	2.6
1	D	242	VAL	2.5
1	D	166	PHE	2.5
1	D	15	PRO	2.5
1	B	261	THR	2.5
1	B	185	ILE	2.5
1	A	201	PHE	2.5
1	C	290	LYS	2.5
1	B	299	LEU	2.5
1	D	192	ILE	2.4
1	A	44	LEU	2.4
1	C	299	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	91	ILE	2.4
1	C	235	TYR	2.3
1	A	125	ILE	2.3
1	C	27	VAL	2.3
1	C	265	ILE	2.3
1	B	197	GLU	2.3
1	C	124	ALA	2.3
1	D	124	ALA	2.3
1	D	253	VAL	2.3
1	A	169	LEU	2.3
1	A	212	ILE	2.2
1	C	44	LEU	2.2
1	A	264	ALA	2.2
1	C	270	PHE	2.2
1	B	85	THR	2.2
1	B	28	ILE	2.1
1	C	306	ILE	2.1
1	C	100	PRO	2.1
1	B	176	LEU	2.1
1	D	306	ILE	2.1
1	C	42	LYS	2.1
1	A	303	LYS	2.1
1	B	201	PHE	2.1
1	D	298	PHE	2.1
1	B	309	LYS	2.1
1	D	205	ILE	2.1
1	B	111	LEU	2.1
1	B	125	ILE	2.0
1	A	42	LYS	2.0
1	C	10	PRO	2.0
1	B	154	VAL	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

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, 95^{th} 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	A	402	6/6	0.93	0.21	2.63	36,46,52,58	0
3	GOL	D	401	6/6	0.94	0.19	0.34	35,37,49,58	0
3	GOL	C	401	6/6	0.96	0.19	0.24	39,45,47,49	0
3	GOL	B	401	6/6	0.94	0.13	-1.39	39,44,44,47	0
4	SO4	D	403	5/5	0.92	0.13	-	85,89,92,96	0
2	PG5	A	401	10/12	0.85	0.11	-	46,50,55,57	0
4	SO4	A	403	5/5	0.87	0.12	-	81,81,92,96	0
4	SO4	D	402	5/5	0.82	0.15	-	94,100,102,103	0
4	SO4	B	402	5/5	0.88	0.20	-	70,72,77,84	0

6.5 Other polymers

There are no such residues in this entry.