Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:12 AM JST

PDB ID	:	6IQV
Title	:	Crystal Structure of Cell Surface Glyceraldehyde-3-Phosphate Dehydrogenase Complexed with Hg2+ from Lactobacillus plantarum
Authors	:	Yoneda, K.; Kinoshita, H.
Deposited on	:	2018-11-09
Resolution	:	2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

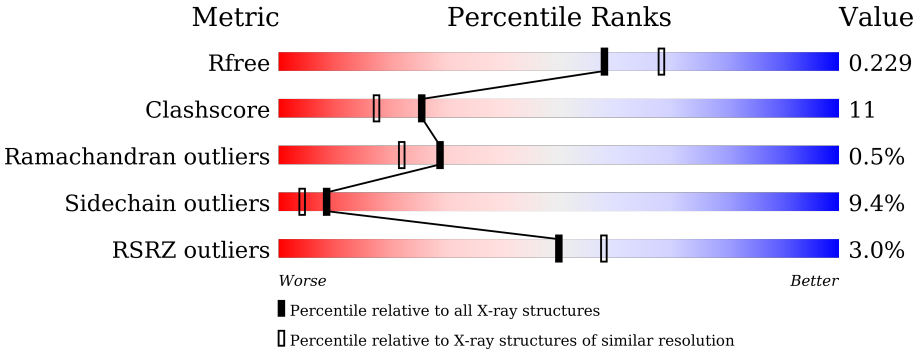
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.13 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	.% 84% 14% •
1	B	340	.% 81% 14% • •
1	C	340	7% 70% 22% • •
1	D	340	2% 75% 19% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	405	-	-	X	X
3	HG	A	404	-	-	X	-
4	TRS	B	401	-	X	X	-

2 Entry composition (i)

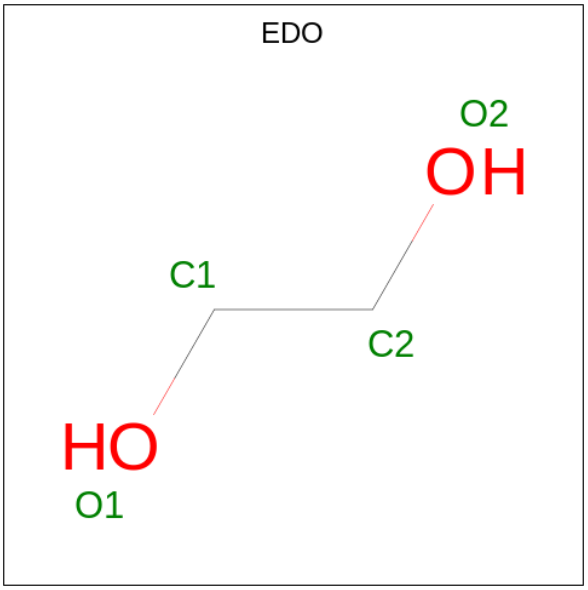
There are 5 unique types of molecules in this entry. The entry contains 10725 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase, type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2564	1609	439	508	8	0	0	0
1	B	336	2536	1594	435	500	7	0	0	0
1	C	326	2463	1550	422	483	8	0	0	0
1	D	333	2515	1579	431	497	8	0	0	0

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



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

Continued on next page...

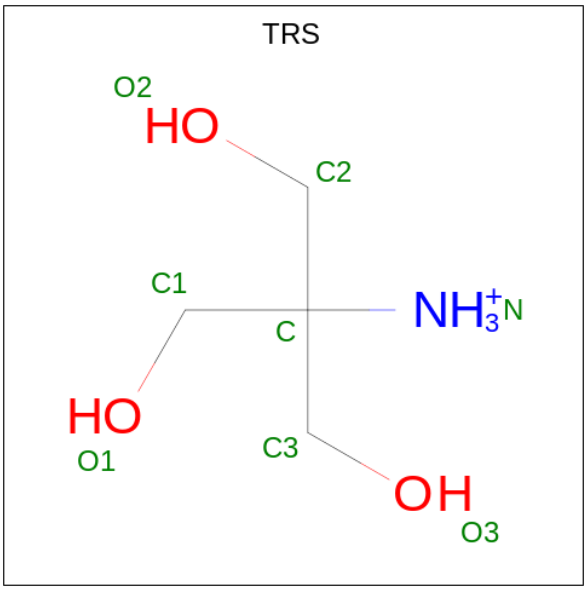
Continued from previous page...

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	8	4	1	3	0	0

- Molecule 5 is water.

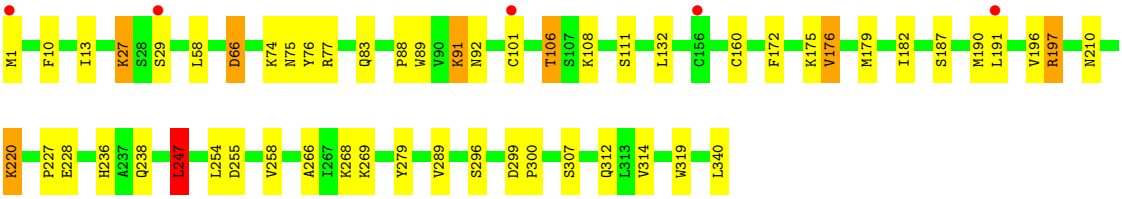
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	169	169	169	0	0
			Total	O		
5	B	163	163	163	0	0
			Total	O		
5	C	122	122	122	0	0
			Total	O		
5	D	150	150	150	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

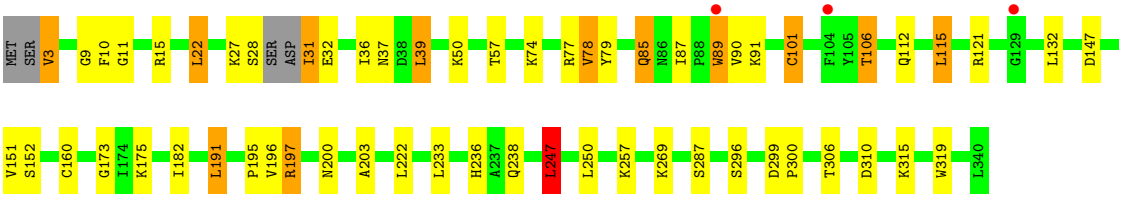
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain A:



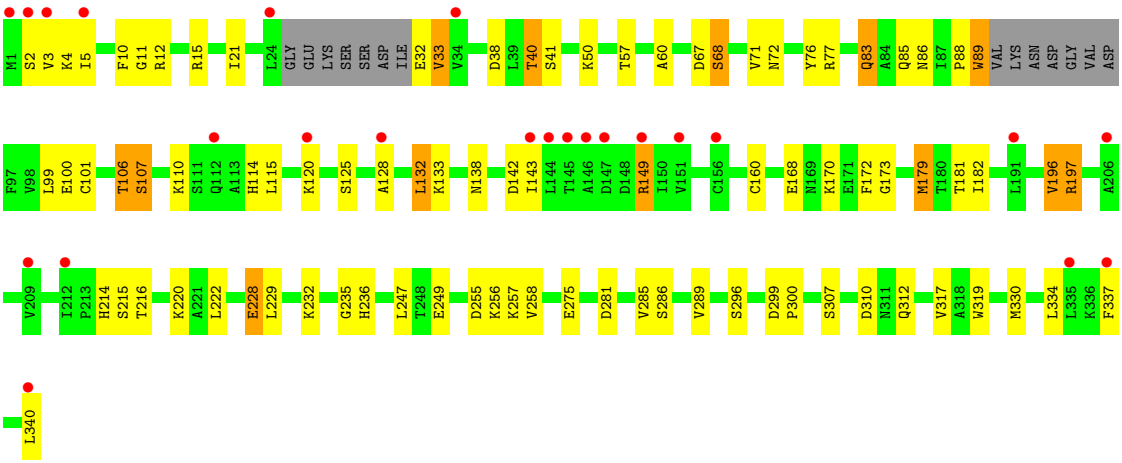
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain B:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain C:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain D: 2% 75% 19%

M1 S2 V3 K4 F10 R15 E23 L24 G25 E26 LYS SER SER ASP ILE E32 V33 V34 L39 K50 I69 N86 I87 P88 W89 V90 K91 G94 V95 D96 F97 C101 F104 Y105 T106 S107 K108 A109 K110 A117 K120 R121 I124 S125 A126 PRO ALA

G129 S130 D131 L132 N138 D141 R149 C160 L161 A162 P163 E168 M169 K170 G173 V176 M179 T180 T181 Q189 M190 G194 R197 A207 I212 E228 K232 G235 H236 A237 Q238 V243 L247 L254 V258 K269 E275

Y279 S286 V289 S296 D299 P300 Q312 L313 V314 L334 L335 K336 F337 A338 T339 L340

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.04Å 172.95Å 149.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.86 – 2.13 49.46 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (101.86-2.13) 99.3 (49.46-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.229 0.214 , 0.229	Depositor DCC
R_{free} test set	4550 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10725	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HG, EDO, TRS

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	1.32	1/2605 (0.0%)	0.82	2/3536 (0.1%)
1	B	1.31	0/2576	0.84	3/3496 (0.1%)
1	C	1.28	2/2502 (0.1%)	0.82	0/3395
1	D	1.31	1/2553 (0.0%)	0.82	2/3462 (0.1%)
All	All	1.30	4/10236 (0.0%)	0.82	7/13889 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	LEU	C-OXT	-7.73	1.08	1.23
1	C	168	GLU	CD-OE2	-5.99	1.19	1.25
1	C	168	GLU	CD-OE1	-5.82	1.19	1.25
1	D	168	GLU	CD-OE1	-5.06	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	31	ILE	N-CA-C	-14.84	70.93	111.00
1	D	105	TYR	N-CA-C	-6.20	94.26	111.00
1	D	25	GLY	N-CA-C	-5.76	98.69	113.10
1	A	247	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	247	LEU	CA-CB-CG	5.12	127.09	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	22	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	191	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LYS	Peptide

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	2564	0	2549	42	0
1	B	2536	0	2521	40	0
1	C	2463	0	2452	60	0
1	D	2515	0	2497	72	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	8	0	12	9	0
3	A	3	0	0	2	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	B	8	0	12	6	0
5	A	169	0	0	10	0
5	B	163	0	0	6	0
5	C	122	0	0	11	0
5	D	150	0	0	8	0
All	All	10725	0	10067	214	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 11.

All (214) 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:196:VAL:HB	5:A:657:HOH:O	1.44	1.18
1:C:125:SER:HB3	5:C:562:HOH:O	1.40	1.16
1:D:15:ARG:HE	2:D:405:EDO:H11	1.07	1.13
5:A:556:HOH:O	4:B:401:TRS:H12	1.47	1.12
1:D:39:LEU:HD23	1:D:39:LEU:H	1.15	1.12
1:A:101:CYS:SG	3:A:404:HG:HG	1.70	1.10
1:D:121:ARG:HD3	1:D:337:PHE:CE1	1.85	1.10
1:C:216:THR:HG23	5:C:566:HOH:O	1.51	1.09
1:B:197:ARG:O	1:B:197:ARG:HD3	1.53	1.05
1:D:39:LEU:HB3	5:D:642:HOH:O	1.55	1.04
4:B:401:TRS:H11	5:B:587:HOH:O	1.60	1.01
1:D:108:LYS:HD3	1:D:131:ASP:OD2	1.59	1.00
1:D:97:PHE:CE1	1:D:121:ARG:HB2	1.98	0.99
1:C:142:ASP:HB2	5:C:618:HOH:O	1.62	0.98
1:B:39:LEU:H	1:B:39:LEU:HD23	1.29	0.95
1:C:88:PRO:O	1:C:89:TRP:HB3	1.65	0.95
1:D:15:ARG:NE	2:D:405:EDO:H11	1.83	0.94
1:C:38:ASP:OD2	1:C:40:THR:HG23	1.71	0.91
1:C:83:GLN:NE2	1:C:86:ASN:HD22	1.70	0.89
1:D:124:ILE:HG22	1:D:125:SER:H	1.39	0.88
1:D:97:PHE:HZ	1:D:337:PHE:CD2	1.92	0.87
1:D:96:ASP:OD2	1:D:120:LYS:HE2	1.78	0.82
1:A:101:CYS:HG	3:A:404:HG:HG	1.21	0.82
1:D:39:LEU:HD23	1:D:39:LEU:N	1.93	0.81
1:D:15:ARG:HH21	2:D:405:EDO:C1	1.93	0.80
1:C:88:PRO:O	1:C:89:TRP:CB	2.30	0.79
1:C:106:THR:O	1:C:106:THR:CG2	2.30	0.79
1:A:190:MET:CG	5:A:657:HOH:O	2.31	0.79
4:B:401:TRS:C2	5:D:526:HOH:O	2.31	0.78
1:B:77:ARG:HD2	5:B:518:HOH:O	1.81	0.78
1:D:121:ARG:CD	1:D:337:PHE:CE1	2.66	0.78
1:D:86:ASN:O	1:D:88:PRO:HD3	1.83	0.77
4:B:401:TRS:H22	5:D:526:HOH:O	1.84	0.77
1:A:190:MET:SD	5:A:657:HOH:O	2.42	0.77
1:D:108:LYS:CD	1:D:131:ASP:OD2	2.32	0.76
1:D:39:LEU:H	1:D:39:LEU:CD2	1.87	0.74
1:B:9:GLY:O	1:B:101:CYS:SG	2.46	0.73
1:A:106:THR:HG22	5:A:640:HOH:O	1.89	0.72
1:A:228:GLU:H	1:A:228:GLU:CD	1.90	0.72
1:D:15:ARG:HH21	2:D:405:EDO:H12	1.55	0.72
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.06	0.71
1:B:197:ARG:O	1:B:197:ARG:CD	2.35	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ILE:HG22	1:D:125:SER:N	2.07	0.69
1:D:275:GLU:HG2	5:D:551:HOH:O	1.92	0.69
1:D:121:ARG:HD3	1:D:337:PHE:HE1	1.55	0.68
1:D:258:VAL:H	1:D:312:GLN:HE22	1.39	0.68
1:C:83:GLN:HE21	1:C:86:ASN:HD22	1.39	0.68
1:B:106:THR:HG23	1:B:106:THR:O	1.94	0.67
1:A:266:ALA:HA	1:A:269:LYS:HE2	1.77	0.67
1:C:258:VAL:H	1:C:312:GLN:HE22	1.43	0.67
1:B:195:PRO:HD2	5:B:535:HOH:O	1.94	0.66
1:C:160:CYS:HA	1:C:296:SER:HB2	1.77	0.66
1:B:39:LEU:H	1:B:39:LEU:CD2	2.01	0.66
1:A:182:ILE:HD12	1:A:247:LEU:HD11	1.77	0.65
1:D:24:LEU:O	1:D:25:GLY:C	2.35	0.65
1:A:197:ARG:HG2	1:A:197:ARG:HH11	1.60	0.65
1:D:105:TYR:O	1:D:106:THR:HG23	1.97	0.65
1:C:106:THR:O	1:C:106:THR:HG22	1.96	0.64
1:C:100:GLU:OE1	1:C:114:HIS:HE1	1.80	0.64
1:A:160:CYS:HA	1:A:296:SER:HB2	1.80	0.63
1:B:121:ARG:NH1	5:B:504:HOH:O	2.32	0.63
1:D:228:GLU:O	1:D:232:LYS:HE2	2.00	0.62
1:C:128:ALA:O	1:C:132:LEU:HD11	2.00	0.61
1:C:275:GLU:HG2	5:C:540:HOH:O	2.00	0.61
1:D:3:VAL:HG13	1:D:96:ASP:CB	2.29	0.61
1:A:106:THR:CG2	1:A:106:THR:O	2.48	0.61
1:A:106:THR:O	1:A:106:THR:HG23	2.00	0.61
1:D:125:SER:O	1:D:126:ALA:HB3	2.00	0.61
1:A:91:LYS:HG2	1:A:92:ASN:H	1.66	0.61
1:D:125:SER:O	1:D:126:ALA:CB	2.47	0.61
4:B:401:TRS:H21	5:D:526:HOH:O	1.98	0.60
1:D:90:VAL:HG21	1:D:117:ALA:O	2.01	0.60
1:D:97:PHE:CE1	1:D:121:ARG:CB	2.79	0.59
5:A:556:HOH:O	4:B:401:TRS:H31	2.03	0.59
1:D:97:PHE:CD1	1:D:121:ARG:HB2	2.38	0.59
1:A:66:ASP:OD2	1:A:66:ASP:N	2.36	0.59
1:C:5:ILE:HG12	1:C:334:LEU:HD13	1.84	0.58
1:D:121:ARG:HD3	1:D:337:PHE:CD1	2.35	0.58
1:B:191:LEU:HD21	1:D:207:ALA:HB3	1.86	0.58
1:C:99:LEU:HD11	5:C:562:HOH:O	2.03	0.58
1:C:214:HIS:CD2	1:C:215:SER:O	2.58	0.57
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.18	0.57
1:B:257:LYS:NZ	1:B:310:ASP:HB3	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:C	1:D:25:GLY:O	2.39	0.57
1:C:179:MET:HG3	1:C:235:GLY:HA3	1.87	0.56
1:A:91:LYS:HG2	1:A:92:ASN:N	2.20	0.56
1:A:77:ARG:HH11	1:A:77:ARG:HG3	1.70	0.56
5:A:620:HOH:O	2:D:401:EDO:H12	2.05	0.56
1:A:74:LYS:HG2	1:A:76:TYR:CZ	2.40	0.56
1:C:196:VAL:CG2	1:C:197:ARG:N	2.69	0.55
1:D:15:ARG:CZ	2:D:405:EDO:H11	2.36	0.55
1:C:106:THR:O	1:C:106:THR:HG23	2.05	0.55
1:C:99:LEU:CD1	5:C:562:HOH:O	2.55	0.55
1:D:121:ARG:CD	1:D:337:PHE:CD1	2.90	0.55
1:A:196:VAL:CG2	5:A:657:HOH:O	2.53	0.55
1:C:83:GLN:NE2	1:C:86:ASN:ND2	2.48	0.54
1:D:96:ASP:CG	1:D:120:LYS:HE2	2.27	0.54
1:A:106:THR:HB	5:A:630:HOH:O	2.07	0.53
1:A:254:LEU:HD12	1:A:314:VAL:HG21	1.90	0.53
1:A:258:VAL:H	1:A:312:GLN:HE22	1.57	0.53
1:D:90:VAL:O	1:D:94:GLY:HA2	2.09	0.52
1:D:279:TYR:CE1	1:D:300:PRO:HG3	2.44	0.52
1:B:3:VAL:N	5:B:508:HOH:O	2.42	0.52
1:D:97:PHE:CZ	1:D:337:PHE:CD2	2.84	0.52
1:C:256:LYS:CE	5:C:602:HOH:O	2.56	0.52
1:C:286:SER:O	1:C:289:VAL:HG22	2.10	0.52
1:B:247:LEU:HD12	1:B:247:LEU:O	2.10	0.52
1:C:100:GLU:OE1	1:C:114:HIS:CE1	2.62	0.52
1:D:3:VAL:HG13	1:D:96:ASP:HB3	1.92	0.51
1:B:151:VAL:HG12	1:B:152:SER:N	2.25	0.51
1:B:106:THR:O	1:B:106:THR:CG2	2.56	0.51
1:C:11:GLY:O	1:C:15:ARG:HG3	2.09	0.51
1:D:254:LEU:HD12	1:D:314:VAL:HG21	1.93	0.51
1:C:229:LEU:HA	1:C:232:LYS:HD2	1.92	0.51
1:C:249:GLU:HG2	1:C:317:VAL:HG22	1.92	0.51
1:C:334:LEU:O	1:C:337:PHE:HB2	2.11	0.51
1:D:15:ARG:HH21	2:D:405:EDO:H11	1.73	0.51
1:B:197:ARG:HD3	1:B:197:ARG:N	2.24	0.51
1:D:141:ASP:O	1:D:336:LYS:NZ	2.41	0.51
1:B:250:LEU:O	1:B:315:LYS:HA	2.11	0.50
1:C:125:SER:HB2	1:C:330:MET:SD	2.51	0.50
1:D:15:ARG:NH2	2:D:405:EDO:H11	2.27	0.50
1:D:24:LEU:O	1:D:25:GLY:O	2.30	0.50
1:A:227:PRO:HD2	1:A:228:GLU:OE1	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:SER:CB	1:C:330:MET:SD	2.99	0.50
1:A:190:MET:HG3	5:A:657:HOH:O	2.05	0.50
1:B:36:ILE:HG22	1:B:37:ASN:N	2.27	0.50
1:D:15:ARG:NH2	2:D:405:EDO:C1	2.70	0.49
1:B:112:GLN:O	1:B:115:LEU:N	2.43	0.49
1:A:13:ILE:HB	1:A:101:CYS:SG	2.52	0.49
1:B:247:LEU:HD12	1:B:247:LEU:C	2.32	0.49
1:D:189:GLN:HG2	5:D:573:HOH:O	2.12	0.49
1:D:179:MET:HG3	1:D:235:GLY:HA3	1.95	0.49
1:B:247:LEU:HD23	1:B:319:TRP:CH2	2.48	0.49
1:C:99:LEU:HG	1:C:101:CYS:SG	2.53	0.48
1:B:200:ASN:HB3	1:B:203:ALA:HB3	1.95	0.48
1:C:67:ASP:OD1	1:C:68:SER:HB3	2.14	0.48
1:A:238:GLN:HG3	1:B:182:ILE:CD1	2.43	0.48
1:C:67:ASP:OD1	1:C:67:ASP:C	2.49	0.48
1:D:97:PHE:CD2	1:D:334:LEU:HD21	2.48	0.48
1:C:256:LYS:HE2	5:C:602:HOH:O	2.13	0.47
1:C:285:VAL:HG11	1:D:212:ILE:HG12	1.96	0.47
1:D:3:VAL:HG13	1:D:96:ASP:HB2	1.96	0.47
1:C:216:THR:CG2	5:C:566:HOH:O	2.28	0.47
1:C:21:ILE:HG21	1:C:33:VAL:HG12	1.98	0.46
1:C:50:LYS:HE3	1:C:57:THR:CG2	2.44	0.46
1:B:257:LYS:HZ1	1:B:310:ASP:HB3	1.80	0.46
1:B:160:CYS:HA	1:B:296:SER:HB2	1.97	0.46
1:A:182:ILE:HD13	1:B:238:GLN:HG3	1.96	0.46
1:C:247:LEU:HD23	1:C:319:TRP:CZ3	2.51	0.46
1:B:11:GLY:O	1:B:15:ARG:HG3	2.16	0.46
1:B:85:GLN:H	1:B:85:GLN:HG3	1.32	0.46
1:C:12:ARG:HH11	1:C:12:ARG:HG2	1.80	0.46
1:C:67:ASP:HB2	1:C:77:ARG:NH1	2.30	0.46
1:A:268:LYS:HE3	1:A:279:TYR:CZ	2.50	0.46
1:B:90:VAL:HB	5:B:536:HOH:O	2.15	0.46
1:A:74:LYS:HG3	1:A:75:ASN:N	2.31	0.45
1:C:182:ILE:CD1	1:D:238:GLN:HG3	2.46	0.45
1:A:175:LYS:HE3	1:A:255:ASP:HA	1.97	0.45
1:B:222:LEU:HD23	1:B:233:LEU:HD11	1.97	0.45
1:B:299:ASP:HA	1:B:300:PRO:HD2	1.85	0.45
1:D:337:PHE:O	1:D:338:ALA:C	2.55	0.45
1:A:289:VAL:HG11	1:A:319:TRP:HB3	1.99	0.45
1:D:190:MET:HB2	1:D:190:MET:HE2	1.41	0.45
1:D:254:LEU:CD1	1:D:314:VAL:HG21	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:O	1:C:149:ARG:HD2	2.17	0.44
1:A:172:PHE:O	1:A:255:ASP:HB2	2.17	0.44
1:D:258:VAL:H	1:D:312:GLN:NE2	2.12	0.44
1:D:90:VAL:O	1:D:94:GLY:CA	2.65	0.44
1:D:160:CYS:HA	1:D:296:SER:HB2	1.99	0.44
1:D:39:LEU:N	1:D:39:LEU:CD2	2.62	0.44
1:B:196:VAL:HG22	1:B:197:ARG:N	2.32	0.44
1:C:179:MET:HE3	5:C:566:HOH:O	2.17	0.44
1:D:247:LEU:HD12	1:D:247:LEU:C	2.38	0.44
1:C:196:VAL:HG23	1:C:197:ARG:H	1.82	0.43
1:B:77:ARG:HG2	1:B:79:TYR:CZ	2.54	0.43
1:D:50:LYS:HE2	5:D:627:HOH:O	2.17	0.43
1:A:220:LYS:HE2	1:A:220:LYS:HB3	1.52	0.43
1:B:151:VAL:CG1	1:B:152:SER:N	2.81	0.43
1:C:115:LEU:HD22	1:C:149:ARG:NH1	2.33	0.43
1:A:210:ASN:OD1	1:B:287:SER:HB2	2.18	0.43
1:C:71:VAL:O	1:C:72:ASN:C	2.54	0.43
1:C:107:SER:HB2	1:C:110:LYS:HB2	2.00	0.43
1:A:182:ILE:HD12	1:A:247:LEU:CD1	2.45	0.43
1:B:87:ILE:HG21	1:B:89:TRP:CD2	2.53	0.43
1:B:77:ARG:HG3	1:B:78:VAL:N	2.32	0.43
1:C:50:LYS:NZ	1:C:60:ALA:O	2.51	0.43
1:B:197:ARG:HD3	1:B:197:ARG:C	2.03	0.43
1:C:172:PHE:O	1:C:255:ASP:HB2	2.19	0.42
1:D:286:SER:O	1:D:289:VAL:HG22	2.18	0.42
1:C:222:LEU:HA	1:C:222:LEU:HD12	1.83	0.42
1:D:162:ALA:HB3	1:D:163:PRO:HD3	2.01	0.42
1:A:247:LEU:HD23	1:A:319:TRP:CZ3	2.55	0.42
1:D:190:MET:HE1	1:D:194:GLY:O	2.20	0.42
1:A:74:LYS:HG2	1:A:76:TYR:CE1	2.55	0.42
1:C:133:LYS:HD3	1:C:143:ILE:HG13	2.01	0.42
1:A:176:VAL:HG22	1:B:306:THR:HG22	2.02	0.42
1:C:76:TYR:CD1	1:C:76:TYR:N	2.87	0.41
1:D:97:PHE:HE1	1:D:121:ARG:HD2	1.85	0.41
1:D:120:LYS:HZ3	1:D:120:LYS:HG3	1.55	0.41
1:D:299:ASP:HA	1:D:300:PRO:HD2	1.82	0.41
1:C:228:GLU:CD	1:C:228:GLU:H	2.23	0.41
1:B:50:LYS:HE3	1:B:57:THR:CG2	2.51	0.41
1:D:232:LYS:NZ	5:D:511:HOH:O	2.52	0.41
1:D:69:ILE:HD12	1:D:69:ILE:HG21	1.59	0.41
1:D:69:ILE:HG23	1:D:69:ILE:HD13	1.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:HG2	1:C:12:ARG:NH1	2.36	0.40
1:C:299:ASP:HA	1:C:300:PRO:HD2	1.89	0.40
1:D:4:LYS:HD3	1:D:34:VAL:HG11	2.03	0.40
1:D:121:ARG:HD2	1:D:337:PHE:CD1	2.56	0.40
1:C:133:LYS:NZ	1:C:143:ILE:O	2.45	0.40
1:A:88:PRO:O	1:A:91:LYS:HG2	2.22	0.40
1:C:101:CYS:HB3	5:C:591:HOH:O	2.22	0.40
1:A:299:ASP:HA	1:A:300:PRO:HD2	1.93	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	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	B	332/340 (98%)	311 (94%)	20 (6%)	1 (0%)	41	36
1	C	320/340 (94%)	305 (95%)	14 (4%)	1 (0%)	41	36
1	D	327/340 (96%)	309 (94%)	14 (4%)	4 (1%)	13	6
All	All	1317/1360 (97%)	1246 (95%)	65 (5%)	6 (0%)	29	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	THR
1	D	91	LYS
1	D	173	GLY
1	C	173	GLY
1	D	88	PRO
1	B	173	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	277/277 (100%)	256 (92%)	21 (8%)	13 7
1	B	273/277 (99%)	249 (91%)	24 (9%)	10 5
1	C	265/277 (96%)	235 (89%)	30 (11%)	6 2
1	D	271/277 (98%)	244 (90%)	27 (10%)	7 3
All	All	1086/1108 (98%)	984 (91%)	102 (9%)	8 4

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	PHE
1	A	27	LYS
1	A	29	SER
1	A	58	LEU
1	A	66	ASP
1	A	83	GLN
1	A	89	TRP
1	A	91	LYS
1	A	106	THR
1	A	108	LYS
1	A	111	SER
1	A	132	LEU
1	A	176	VAL
1	A	179	MET
1	A	187	SER
1	A	197	ARG
1	A	220	LYS
1	A	236	HIS
1	A	247	LEU
1	A	307	SER
1	B	3	VAL
1	B	10	PHE
1	B	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	27	LYS
1	B	28	SER
1	B	31	ILE
1	B	32	GLU
1	B	39	LEU
1	B	74	LYS
1	B	78	VAL
1	B	85	GLN
1	B	89	TRP
1	B	91	LYS
1	B	101	CYS
1	B	106	THR
1	B	115	LEU
1	B	132	LEU
1	B	147	ASP
1	B	175	LYS
1	B	191	LEU
1	B	197	ARG
1	B	236	HIS
1	B	247	LEU
1	B	269	LYS
1	C	2	SER
1	C	3	VAL
1	C	4	LYS
1	C	10	PHE
1	C	32	GLU
1	C	33	VAL
1	C	40	THR
1	C	41	SER
1	C	68	SER
1	C	83	GLN
1	C	85	GLN
1	C	89	TRP
1	C	106	THR
1	C	107	SER
1	C	132	LEU
1	C	138	ASN
1	C	149	ARG
1	C	170	LYS
1	C	179	MET
1	C	181	THR
1	C	196	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	197	ARG
1	C	220	LYS
1	C	228	GLU
1	C	236	HIS
1	C	257	LYS
1	C	281	ASP
1	C	307	SER
1	C	310	ASP
1	C	340	LEU
1	D	1	MET
1	D	10	PHE
1	D	23	GLU
1	D	26	GLU
1	D	39	LEU
1	D	69	ILE
1	D	89	TRP
1	D	101	CYS
1	D	110	LYS
1	D	120	LYS
1	D	125	SER
1	D	130	SER
1	D	132	LEU
1	D	138	ASN
1	D	149	ARG
1	D	170	LYS
1	D	176	VAL
1	D	179	MET
1	D	181	THR
1	D	190	MET
1	D	197	ARG
1	D	236	HIS
1	D	243	VAL
1	D	269	LYS
1	D	334	LEU
1	D	337	PHE
1	D	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	312	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	85	GLN
1	B	86	ASN
1	B	112	GLN
1	C	83	GLN
1	C	114	HIS
1	C	214	HIS
1	C	312	GLN
1	D	312	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	D	401	-	3,3,3	0.65	0	2,2,2	0.07	0
2	EDO	A	401	-	3,3,3	0.82	0	2,2,2	0.56	0
2	EDO	A	405	-	3,3,3	0.36	0	2,2,2	0.58	0
4	TRS	B	401	-	7,7,7	1.10	1 (14%)	9,9,9	1.46	1 (11%)
2	EDO	B	402	-	3,3,3	0.56	0	2,2,2	0.38	0
2	EDO	C	401	-	3,3,3	0.66	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	D	405	-	3,3,3	1.13	0	2,2,2	1.39	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	EDO	D	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
4	TRS	B	401	-	-	9/9/9/9	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	D	405	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	TRS	C1-C	-2.00	1.47	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	TRS	C2-C-C1	-2.10	104.31	110.81

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	TRS	C1-C-C2-O2
4	B	401	TRS	C1-C-C3-O3
4	B	401	TRS	C2-C-C3-O3
4	B	401	TRS	N-C-C3-O3
2	C	401	EDO	O1-C1-C2-O2
4	B	401	TRS	C2-C-C1-O1
4	B	401	TRS	N-C-C1-O1
4	B	401	TRS	C3-C-C2-O2
2	B	402	EDO	O1-C1-C2-O2
4	B	401	TRS	C3-C-C1-O1
4	B	401	TRS	N-C-C2-O2

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	EDO	1	0
4	B	401	TRS	6	0
2	D	405	EDO	8	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	340/340 (100%)	-0.18	5 (1%)	73	78	24, 35, 57, 112	0
1	B	336/340 (98%)	-0.18	3 (0%)	84	87	25, 38, 60, 101	0
1	C	326/340 (95%)	0.31	24 (7%)	14	18	25, 42, 71, 105	0
1	D	333/340 (97%)	-0.06	8 (2%)	59	65	25, 36, 72, 115	0
All	All	1335/1360 (98%)	-0.03	40 (2%)	50	58	24, 37, 68, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.7
1	C	3	VAL	5.5
1	C	143	ILE	4.8
1	C	145	THR	4.1
1	D	337	PHE	4.0
1	D	338	ALA	3.8
1	D	104	PHE	3.8
1	C	340	LEU	3.8
1	C	147	ASP	3.6
1	D	3	VAL	3.5
1	D	97	PHE	3.2
1	C	5	ILE	3.2
1	C	337	PHE	3.1
1	C	144	LEU	3.0
1	A	191	LEU	2.9
1	D	340	LEU	2.8
1	C	34	VAL	2.8
1	C	151	VAL	2.7
1	C	156	CYS	2.7
1	C	1	MET	2.6
1	C	335	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	149	ARG	2.5
1	A	29	SER	2.5
1	C	212	ILE	2.4
1	C	128	ALA	2.4
1	D	126	ALA	2.4
1	B	89	TRP	2.4
1	D	39	LEU	2.3
1	B	129	GLY	2.3
1	C	2	SER	2.3
1	B	104	PHE	2.3
1	C	146	ALA	2.2
1	C	24	LEU	2.1
1	A	156	CYS	2.1
1	C	112	GLN	2.1
1	C	120	LYS	2.1
1	A	101	CYS	2.1
1	C	191	LEU	2.0
1	C	206	ALA	2.0
1	C	209	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	D	405	4/4	0.34	0.43	20,20,20,20	0
4	TRS	B	401	8/8	0.79	0.24	24,31,34,39	0
3	HG	A	404	1/1	0.86	0.09	165,165,165,165	0
3	HG	B	405	1/1	0.88	0.16	174,174,174,174	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HG	B	403	1/1	0.90	0.15	181,181,181,181	0
2	EDO	C	401	4/4	0.92	0.14	47,51,53,53	0
2	EDO	A	401	4/4	0.93	0.10	42,43,47,48	0
3	HG	D	402	1/1	0.93	0.07	116,116,116,116	0
2	EDO	B	402	4/4	0.93	0.15	47,50,51,54	0
3	HG	D	403	1/1	0.94	0.07	127,127,127,127	0
2	EDO	A	405	4/4	0.94	0.17	20,20,20,20	0
2	EDO	D	401	4/4	0.95	0.12	38,38,45,47	0
3	HG	A	403	1/1	0.96	0.07	66,66,66,66	0
3	HG	B	404	1/1	0.96	0.07	74,74,74,74	0
3	HG	C	402	1/1	0.97	0.05	74,74,74,74	0
3	HG	C	403	1/1	0.98	0.14	119,119,119,119	0
3	HG	D	404	1/1	0.98	0.07	70,70,70,70	0
3	HG	A	402	1/1	0.98	0.13	117,117,117,117	0

6.5 Other polymers (i)

There are no such residues in this entry.