Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:52 PM JST

PDB ID	:	6J9S
Title	:	Penta mutant of Lactobacillus casei lactate dehydrogenase
Authors	:	Arai, K.; Miyanaga, A.; Uchikoba, H.; Fushinobu, S.; Taguchi, H.
Deposited on	:	2019-01-24
Resolution	:	2.00 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:

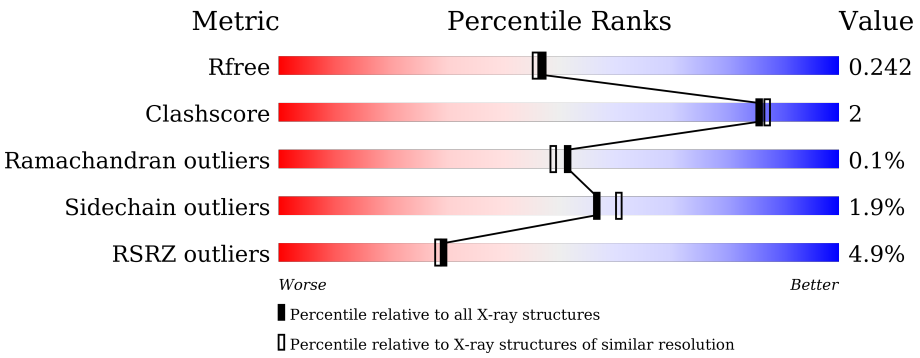
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	326	6% 83% 6% • 10%
1	B	326	4% 89% 8% •
1	C	326	3% 85% 6% • 8%
1	D	326	5% 84% 6% • 9%
1	E	326	5% 90% 5% • •
1	F	326	5% 89% 6% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14730 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2263	1447	375	435	6	0	0	0
1	B	315	2422	1547	403	466	6	0	0	0
1	C	299	2302	1472	382	442	6	0	0	0
1	D	297	2287	1463	379	439	6	0	0	0
1	E	315	2422	1547	403	466	6	0	0	0
1	F	315	2422	1547	403	466	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLU	SER	engineered mutation	UNP S6C1Z0
A	56	ASP	ASN	engineered mutation	UNP S6C1Z0
A	164	LYS	GLU	engineered mutation	UNP S6C1Z0
A	223	ASN	ASP	engineered mutation	UNP S6C1Z0
A	224	LYS	ALA	engineered mutation	UNP S6C1Z0
B	55	GLU	SER	engineered mutation	UNP S6C1Z0
B	56	ASP	ASN	engineered mutation	UNP S6C1Z0
B	164	LYS	GLU	engineered mutation	UNP S6C1Z0
B	223	ASN	ASP	engineered mutation	UNP S6C1Z0
B	224	LYS	ALA	engineered mutation	UNP S6C1Z0
C	55	GLU	SER	engineered mutation	UNP S6C1Z0
C	56	ASP	ASN	engineered mutation	UNP S6C1Z0
C	164	LYS	GLU	engineered mutation	UNP S6C1Z0
C	223	ASN	ASP	engineered mutation	UNP S6C1Z0
C	224	LYS	ALA	engineered mutation	UNP S6C1Z0
D	55	GLU	SER	engineered mutation	UNP S6C1Z0
D	56	ASP	ASN	engineered mutation	UNP S6C1Z0

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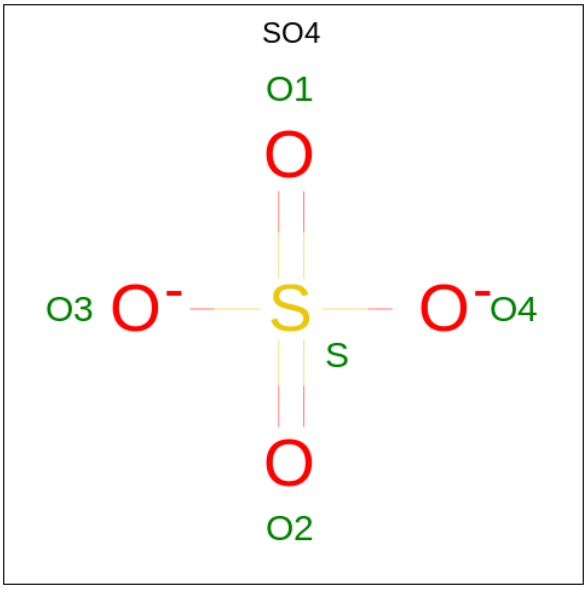
Chain	Residue	Modelled	Actual	Comment	Reference
D	164	LYS	GLU	engineered mutation	UNP S6C1Z0
D	223	ASN	ASP	engineered mutation	UNP S6C1Z0
D	224	LYS	ALA	engineered mutation	UNP S6C1Z0
E	55	GLU	SER	engineered mutation	UNP S6C1Z0
E	56	ASP	ASN	engineered mutation	UNP S6C1Z0
E	164	LYS	GLU	engineered mutation	UNP S6C1Z0
E	223	ASN	ASP	engineered mutation	UNP S6C1Z0
E	224	LYS	ALA	engineered mutation	UNP S6C1Z0
F	55	GLU	SER	engineered mutation	UNP S6C1Z0
F	56	ASP	ASN	engineered mutation	UNP S6C1Z0
F	164	LYS	GLU	engineered mutation	UNP S6C1Z0
F	223	ASN	ASP	engineered mutation	UNP S6C1Z0
F	224	LYS	ALA	engineered mutation	UNP S6C1Z0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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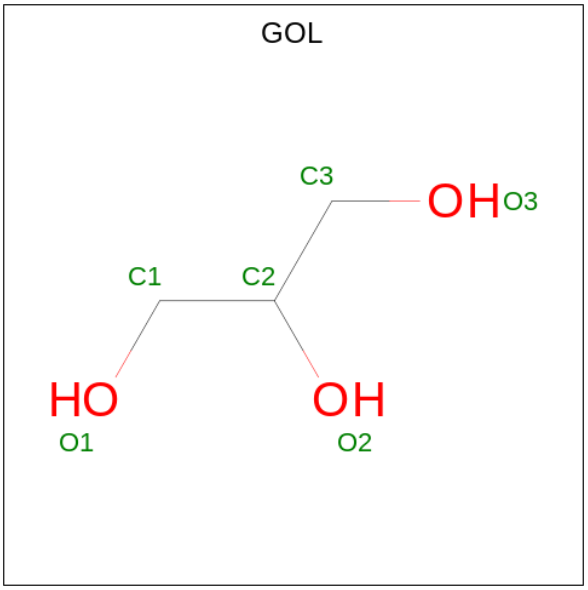
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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



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

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

- Molecule 4 is water.

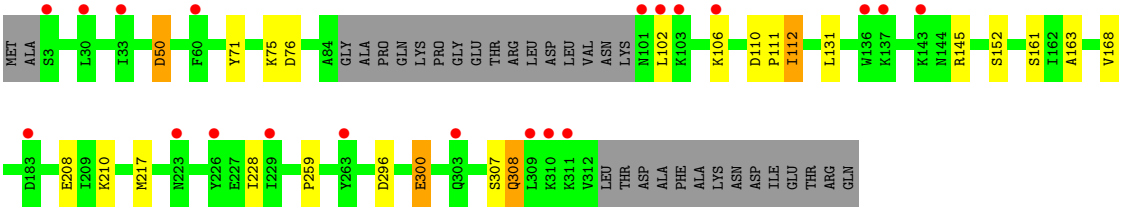
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	52	52	52	0	0
			Total	O		
4	B	111	111	111	0	0
			Total	O		
4	C	69	69	69	0	0
			Total	O		
4	D	82	82	82	0	0
			Total	O		
4	E	117	117	117	0	0
			Total	O		
4	F	79	79	79	0	0

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.

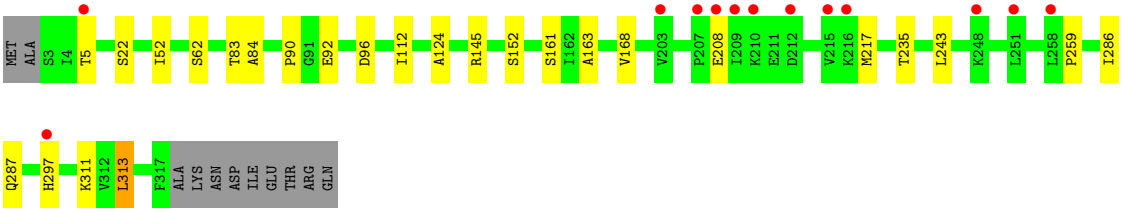
• Molecule 1: L-lactate dehydrogenase

Chain A:



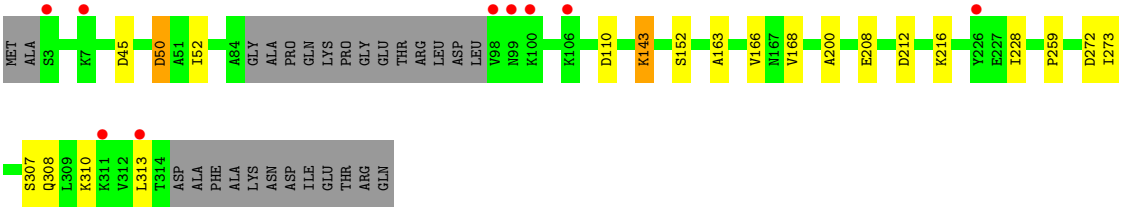
• Molecule 1: L-lactate dehydrogenase

Chain B:



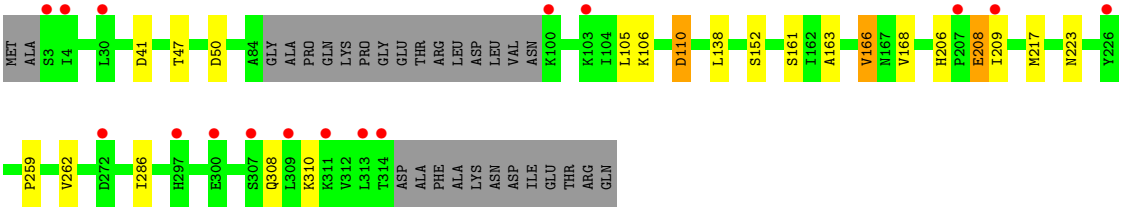
• Molecule 1: L-lactate dehydrogenase

Chain C:



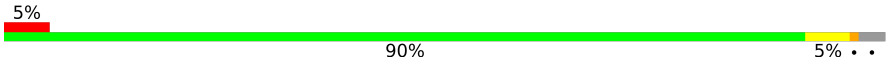
• Molecule 1: L-lactate dehydrogenase

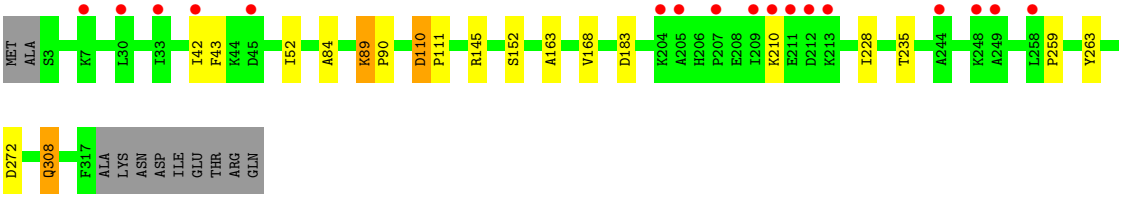
Chain D:



- Molecule 1: L-lactate dehydrogenase

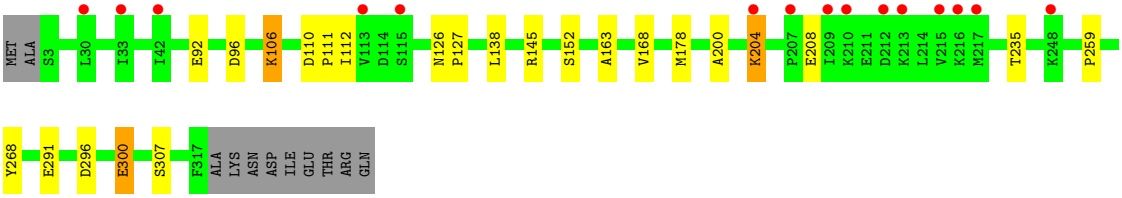
Chain E:





- Molecule 1: L-lactate dehydrogenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.57Å 82.89Å 180.83Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (41.07-2.00) 97.0 (41.03-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.234 0.216 , 0.242	Depositor DCC
R_{free} test set	7948 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14730	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: SO4, GOL

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	0.85	0/2303	0.88	5/3120 (0.2%)
1	B	0.94	3/2466 (0.1%)	0.92	6/3343 (0.2%)
1	C	0.86	0/2342	0.89	7/3173 (0.2%)
1	D	0.96	1/2327 (0.0%)	0.90	4/3152 (0.1%)
1	E	0.95	0/2466	0.92	6/3343 (0.2%)
1	F	0.88	1/2466 (0.0%)	0.82	2/3343 (0.1%)
All	All	0.91	5/14370 (0.0%)	0.89	30/19474 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	ALA	N-CA	10.20	1.66	1.46
1	B	22	SER	CB-OG	-5.88	1.34	1.42
1	D	208	GLU	CB-CG	5.04	1.61	1.52
1	F	291	GLU	CD-OE2	-5.04	1.20	1.25
1	B	62	SER	CB-OG	-5.02	1.35	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	THR	C-N-CA	-12.35	90.82	121.70
1	A	112	ILE	CG1-CB-CG2	-8.45	92.81	111.40
1	B	83	THR	O-C-N	-8.28	109.46	122.70
1	E	145	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	A	145	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	E	183	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	E	145	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	45	ASP	CB-CG-OD1	6.93	124.54	118.30
1	F	145	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	B	145	ARG	NE-CZ-NH1	-6.56	117.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	E	183	ASP	CB-CG-OD2	6.25	123.92	118.30
1	C	272	ASP	CB-CG-OD1	6.16	123.84	118.30
1	E	110	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	272	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	143	LYS	CD-CE-NZ	5.68	124.77	111.70
1	C	313	LEU	CB-CG-CD1	5.61	120.54	111.00
1	B	145	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	B	313	LEU	CA-CB-CG	5.50	127.96	115.30
1	D	110	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	308	GLN	N-CA-CB	-5.34	100.99	110.60
1	D	208	GLU	CB-CA-C	5.33	121.05	110.40
1	E	308	GLN	N-CA-CB	-5.30	101.06	110.60
1	F	112	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	A	50	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	105	LEU	N-CA-C	5.20	125.04	111.00
1	C	110	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	166	VAL	N-CA-CB	-5.11	100.26	111.50
1	C	50	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	112	ILE	CA-CB-CG1	-5.01	101.48	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	2263	0	2288	12	0
1	B	2422	0	2451	11	0
1	C	2302	0	2334	8	0
1	D	2287	0	2319	15	0
1	E	2422	0	2451	9	0
1	F	2422	0	2451	12	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	10	0	0	1	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	12	0	16	0	0
3	F	6	0	8	0	0
4	A	52	0	0	0	0
4	B	111	0	0	0	0
4	C	69	0	0	0	0
4	D	82	0	0	2	0
4	E	117	0	0	0	0
4	F	79	0	0	0	0
All	All	14730	0	14350	63	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 2.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:THR:HG21	2:B:401:SO4:O3	1.71	0.89
1:F:235:THR:HG21	2:F:401:SO4:O2	1.77	0.84
1:D:262:VAL:HG12	1:D:286:ILE:CD1	2.10	0.82
1:D:262:VAL:HG12	1:D:286:ILE:HD13	1.71	0.71
1:D:262:VAL:HG12	1:D:286:ILE:HD11	1.77	0.65
1:F:106:LYS:HG2	1:F:138:LEU:HD22	1.79	0.64
1:B:5:THR:O	1:B:5:THR:OG1	2.14	0.63
1:F:106:LYS:HG2	1:F:138:LEU:CD2	2.30	0.61
1:F:296:ASP:O	1:F:300:GLU:HG2	2.02	0.60
1:D:262:VAL:CG1	1:D:286:ILE:HD13	2.33	0.58
1:A:296:ASP:O	1:A:300:GLU:HG2	2.02	0.58
1:D:106:LYS:HD3	1:D:138:LEU:HD22	1.85	0.58
1:C:273:ILE:HG21	1:C:310:LYS:HG2	1.85	0.57
1:F:200:ALA:O	1:F:204:LYS:HD3	2.06	0.56
1:B:90:PRO:HG3	1:C:200:ALA:HB2	1.87	0.55
1:E:235:THR:HG21	2:E:401:SO4:O3	2.07	0.54
1:D:106:LYS:HD2	1:D:110:ASP:OD1	2.11	0.50
1:D:161:SER:OG	1:D:217:MET:HG3	2.13	0.49
1:A:75:LYS:CG	1:A:76:ASP:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:LYS:HE3	1:D:310:LYS:HB2	1.61	0.48
1:A:71:TYR:CD1	1:A:112:ILE:HD12	2.50	0.46
1:E:42:ILE:HD11	1:E:43:PHE:CE1	2.50	0.46
1:A:102:LEU:HD23	1:A:131:LEU:CD2	2.46	0.46
1:F:296:ASP:O	1:F:300:GLU:CG	2.63	0.46
1:A:75:LYS:HG3	1:A:76:ASP:N	2.29	0.46
1:E:163:ALA:HB1	1:E:168:VAL:O	2.15	0.46
1:C:152:SER:HA	1:C:259:PRO:HG2	1.98	0.45
1:F:92:GLU:HG2	1:F:96:ASP:HB3	1.99	0.45
1:D:310:LYS:NZ	4:D:504:HOH:O	2.48	0.45
1:F:110:ASP:HB2	1:F:111:PRO:HD3	1.99	0.44
1:B:161:SER:OG	1:B:217:MET:HG3	2.16	0.44
1:A:296:ASP:O	1:A:300:GLU:CG	2.65	0.44
1:F:126:ASN:ND2	1:F:127:PRO:HA	2.32	0.44
1:A:161:SER:OG	1:A:217:MET:HG3	2.18	0.44
1:B:152:SER:HA	1:B:259:PRO:HG2	2.00	0.44
1:D:106:LYS:HD3	1:D:138:LEU:CD2	2.48	0.44
1:F:163:ALA:HB1	1:F:168:VAL:O	2.18	0.43
1:D:286:ILE:HD12	4:D:564:HOH:O	2.17	0.43
1:A:71:TYR:CD1	1:A:112:ILE:CD1	3.01	0.43
1:A:163:ALA:HB1	1:A:168:VAL:O	2.19	0.43
1:A:228:ILE:HG12	1:B:52:ILE:HG13	1.99	0.43
1:C:163:ALA:HB1	1:C:168:VAL:O	2.18	0.43
1:D:152:SER:HA	1:D:259:PRO:HG2	2.00	0.42
1:B:286:ILE:HG22	1:B:287:GLN:O	2.18	0.42
1:B:163:ALA:HB1	1:B:168:VAL:O	2.19	0.42
1:E:89:LYS:HB2	1:E:90:PRO:HD2	2.00	0.42
1:B:92:GLU:HG2	1:B:96:ASP:HB3	2.02	0.42
1:C:228:ILE:HG12	1:E:52:ILE:HG13	2.02	0.42
1:B:311:LYS:O	1:B:311:LYS:HD2	2.20	0.41
1:C:212:ASP:O	1:C:216:LYS:HG3	2.20	0.41
1:A:152:SER:HA	1:A:259:PRO:HG2	2.02	0.41
1:D:41:ASP:HB3	1:D:47:THR:CG2	2.50	0.41
1:E:263:TYR:CZ	1:E:272:ASP:HA	2.56	0.41
1:D:206:HIS:HB3	1:D:209:ILE:HG12	2.02	0.41
1:C:52:ILE:HG13	1:E:228:ILE:HG12	2.03	0.41
1:F:152:SER:HA	1:F:259:PRO:HG2	2.02	0.41
1:C:273:ILE:CG2	1:C:310:LYS:HG2	2.49	0.40
1:E:152:SER:HA	1:E:259:PRO:HG2	2.02	0.40
1:B:124:ALA:HB2	1:B:243:LEU:HD21	2.04	0.40
1:D:163:ALA:HB1	1:D:168:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:HB2	1:A:111:PRO:HD3	2.04	0.40
1:E:110:ASP:HB2	1:E:111:PRO:HD3	2.03	0.40
1:F:178:MET:HE1	1:F:268:TYR:CZ	2.56	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	290/326 (89%)	282 (97%)	8 (3%)	0	100	100
1	B	313/326 (96%)	303 (97%)	10 (3%)	0	100	100
1	C	295/326 (90%)	288 (98%)	7 (2%)	0	100	100
1	D	293/326 (90%)	285 (97%)	8 (3%)	0	100	100
1	E	313/326 (96%)	305 (97%)	7 (2%)	1 (0%)	41	37
1	F	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
All	All	1817/1956 (93%)	1767 (97%)	49 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	84	ALA

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	244/270 (90%)	237 (97%)	7 (3%)	42	43
1	B	261/270 (97%)	258 (99%)	3 (1%)	73	78
1	C	249/270 (92%)	243 (98%)	6 (2%)	49	51
1	D	247/270 (92%)	242 (98%)	5 (2%)	55	58
1	E	261/270 (97%)	258 (99%)	3 (1%)	73	78
1	F	261/270 (97%)	256 (98%)	5 (2%)	57	61
All	All	1523/1620 (94%)	1494 (98%)	29 (2%)	57	61

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	106	LYS
1	A	208	GLU
1	A	210	LYS
1	A	300	GLU
1	A	307	SER
1	A	308	GLN
1	B	208	GLU
1	B	297	HIS
1	B	313	LEU
1	C	50	ASP
1	C	143	LYS
1	C	166	VAL
1	C	208	GLU
1	C	307	SER
1	C	308	GLN
1	D	50	ASP
1	D	166	VAL
1	D	208	GLU
1	D	223	ASN
1	D	308	GLN
1	E	89	LYS
1	E	210	LYS
1	E	308	GLN
1	F	106	LYS
1	F	204	LYS
1	F	208	GLU
1	F	300	GLU
1	F	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	ASN
1	D	118	ASN
1	F	126	ASN
1	F	223	ASN

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)

19 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	SO4	F	401	-	4,4,4	0.63	0	6,6,6	0.70	0
2	SO4	F	402	-	4,4,4	0.38	0	6,6,6	0.52	0
2	SO4	A	402	-	4,4,4	0.46	0	6,6,6	0.61	0
2	SO4	D	402	-	4,4,4	1.33	1 (25%)	6,6,6	1.11	1 (16%)
3	GOL	C	403	-	5,5,5	0.97	0	5,5,5	0.54	0
2	SO4	B	401	-	4,4,4	0.27	0	6,6,6	0.74	0
2	SO4	D	401	-	4,4,4	0.44	0	6,6,6	1.14	0
2	SO4	C	402	-	4,4,4	0.43	0	6,6,6	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	E	403	-	5,5,5	1.54	1 (20%)	5,5,5	1.41	1 (20%)
2	SO4	E	401	-	4,4,4	0.59	0	6,6,6	0.99	0
3	GOL	D	403	-	5,5,5	1.58	0	5,5,5	2.22	2 (40%)
3	GOL	F	403	-	5,5,5	0.61	0	5,5,5	0.61	0
2	SO4	B	402	-	4,4,4	0.77	0	6,6,6	0.68	0
3	GOL	B	404	-	5,5,5	0.72	0	5,5,5	1.37	1 (20%)
2	SO4	C	401	-	4,4,4	0.40	0	6,6,6	1.17	0
2	SO4	A	401	-	4,4,4	0.71	0	6,6,6	0.57	0
2	SO4	E	402	-	4,4,4	0.88	0	6,6,6	1.05	0
3	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.64	0
3	GOL	E	404	-	5,5,5	0.77	0	5,5,5	1.47	1 (20%)

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
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	D	403	-	-	3/4/4/4	-
3	GOL	F	403	-	-	2/4/4/4	-
3	GOL	E	403	-	-	2/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	E	404	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	GOL	O3-C3	2.20	1.51	1.42
2	D	402	SO4	O2-S	2.02	1.56	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	403	GOL	O1-C1-C2	3.37	126.35	110.20
3	D	403	GOL	O3-C3-C2	2.96	124.37	110.20
3	B	404	GOL	O2-C2-C1	2.63	120.72	109.12
3	E	403	GOL	O1-C1-C2	2.58	122.57	110.20
3	E	404	GOL	O1-C1-C2	-2.22	99.53	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	402	SO4	O3-S-O1	-2.01	98.82	109.31

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	GOL	C1-C2-C3-O3
3	D	403	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-C3
3	E	403	GOL	C1-C2-C3-O3
3	F	403	GOL	C1-C2-C3-O3
3	E	403	GOL	O2-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	F	403	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	SO4	1	0
2	B	401	SO4	1	0
2	E	401	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	294/326 (90%)	0.30	20 (6%)	17	16	34, 52, 78, 124	0
1	B	315/326 (96%)	0.16	13 (4%)	37	36	31, 46, 67, 87	0
1	C	299/326 (91%)	0.10	9 (3%)	50	49	33, 50, 74, 94	0
1	D	297/326 (91%)	0.20	16 (5%)	25	24	31, 44, 75, 95	0
1	E	315/326 (96%)	0.09	17 (5%)	25	24	32, 42, 63, 88	0
1	F	315/326 (96%)	0.20	15 (4%)	30	29	33, 51, 70, 86	0
All	All	1835/1956 (93%)	0.17	90 (4%)	29	28	31, 47, 72, 124	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	LYS	7.5
1	B	212	ASP	4.9
1	A	311	LYS	4.8
1	E	210	LYS	4.6
1	D	313	LEU	4.5
1	F	212	ASP	4.5
1	D	314	THR	4.1
1	D	311	LYS	4.0
1	F	210	LYS	4.0
1	B	203	VAL	3.9
1	D	226	TYR	3.7
1	B	207	PRO	3.6
1	A	3	SER	3.6
1	A	226	TYR	3.5
1	B	215	VAL	3.5
1	A	102	LEU	3.3
1	E	204	LYS	3.2
1	D	100	LYS	3.2
1	E	209	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	209	ILE	3.1
1	F	30	LEU	3.1
1	A	303	GLN	3.0
1	A	106	LYS	3.0
1	B	210	LYS	2.9
1	A	136	TRP	2.9
1	E	212	ASP	2.9
1	D	207	PRO	2.9
1	C	3	SER	2.8
1	F	216	LYS	2.8
1	A	263	TYR	2.8
1	E	45	ASP	2.8
1	D	297	HIS	2.7
1	E	258	LEU	2.7
1	E	207	PRO	2.7
1	A	33	ILE	2.7
1	B	216	LYS	2.6
1	C	311	LYS	2.6
1	E	7	LYS	2.6
1	B	5	THR	2.6
1	C	226	TYR	2.6
1	A	309	LEU	2.6
1	D	30	LEU	2.6
1	D	309	LEU	2.6
1	C	100	LYS	2.5
1	E	213	LYS	2.5
1	E	42	ILE	2.5
1	E	211	GLU	2.5
1	B	258	LEU	2.5
1	F	115	SER	2.5
1	B	208	GLU	2.5
1	A	137	LYS	2.5
1	B	248	LYS	2.4
1	F	204	LYS	2.4
1	D	209	ILE	2.4
1	E	205	ALA	2.4
1	E	30	LEU	2.4
1	E	244	ALA	2.4
1	F	213	LYS	2.4
1	F	248	LYS	2.4
1	D	4	ILE	2.4
1	B	297	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	103	LYS	2.3
1	C	99	ASN	2.3
1	A	60	PHE	2.3
1	C	313	LEU	2.3
1	C	106	LYS	2.3
1	E	248	LYS	2.3
1	B	251	LEU	2.2
1	F	215	VAL	2.2
1	A	310	LYS	2.2
1	F	33	ILE	2.2
1	A	30	LEU	2.2
1	D	307	SER	2.2
1	A	143	LYS	2.2
1	D	3	SER	2.2
1	F	209	ILE	2.1
1	C	7	LYS	2.1
1	C	98	VAL	2.1
1	F	42	ILE	2.1
1	F	113	VAL	2.1
1	E	249	ALA	2.1
1	A	183	ASP	2.1
1	D	300	GLU	2.0
1	A	223	ASN	2.0
1	E	33	ILE	2.0
1	A	101	ASN	2.0
1	D	272	ASP	2.0
1	A	229	ILE	2.0
1	F	217	MET	2.0
1	F	207	PRO	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
3	GOL	E	403	6/6	0.77	0.26	52,55,57,61	0
3	GOL	D	403	6/6	0.84	0.16	44,59,62,63	0
3	GOL	B	403	6/6	0.85	0.18	47,51,53,59	0
3	GOL	B	404	6/6	0.86	0.18	44,50,55,55	0
3	GOL	C	403	6/6	0.86	0.20	49,60,62,62	0
3	GOL	F	403	6/6	0.89	0.27	47,62,64,66	0
3	GOL	E	404	6/6	0.92	0.18	44,45,47,49	0
2	SO4	E	401	5/5	0.96	0.09	51,55,68,81	0
2	SO4	F	401	5/5	0.97	0.09	54,54,63,67	0
2	SO4	C	401	5/5	0.97	0.09	55,57,69,81	0
2	SO4	D	401	5/5	0.97	0.07	49,51,66,70	0
2	SO4	A	401	5/5	0.97	0.07	58,59,72,75	0
2	SO4	D	402	5/5	0.98	0.09	41,42,49,49	0
2	SO4	A	402	5/5	0.98	0.07	47,48,50,51	0
2	SO4	E	402	5/5	0.99	0.07	44,45,48,49	0
2	SO4	B	402	5/5	0.99	0.10	44,45,52,53	0
2	SO4	F	402	5/5	0.99	0.13	52,52,56,62	0
2	SO4	B	401	5/5	0.99	0.06	48,48,64,70	0
2	SO4	C	402	5/5	0.99	0.09	50,51,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.