Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 10:52 AM EDT

PDB ID	:	4XZ9
Title	:	Transaldolase variant E60Q/F132Y from T. acidophilum in complex with DHA Schiff base and G3P
Authors	:	Sautner, V.; Tittmann, K.
Deposited on	:	2015-02-04
Resolution	:	1.80 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:

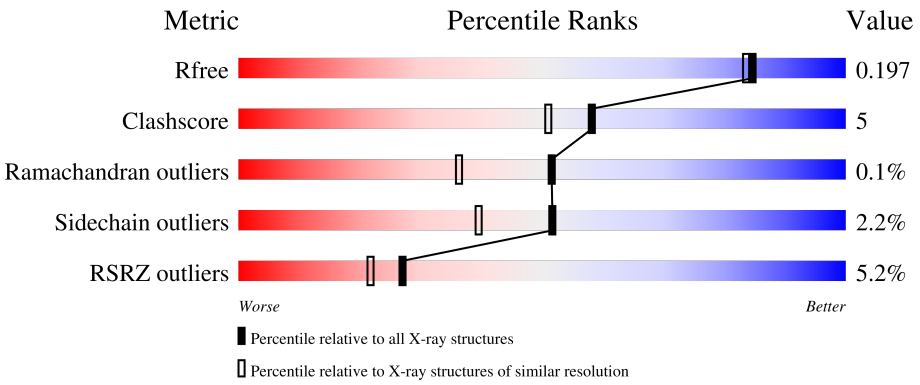
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	223	10% 78% 19% •
1	B	223	92% 5% •
1	C	223	% 93% 7%
1	D	223	6% 84% 14% •
1	E	223	8% 85% 14% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9859 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.

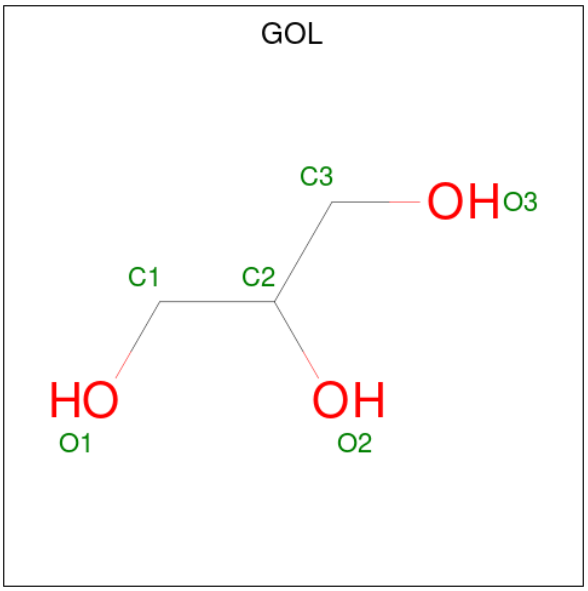
- Molecule 1 is a protein called Probable transaldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1880	1196	316	361	7	0	38	0
1	B	217	1704	1087	289	321	7	0	4	0
1	C	223	1780	1139	300	334	7	0	8	0
1	D	223	1924	1230	323	364	7	0	39	0
1	E	222	1749	1116	295	331	7	0	47	0

There are 15 discrepancies between the modelled and reference sequences:

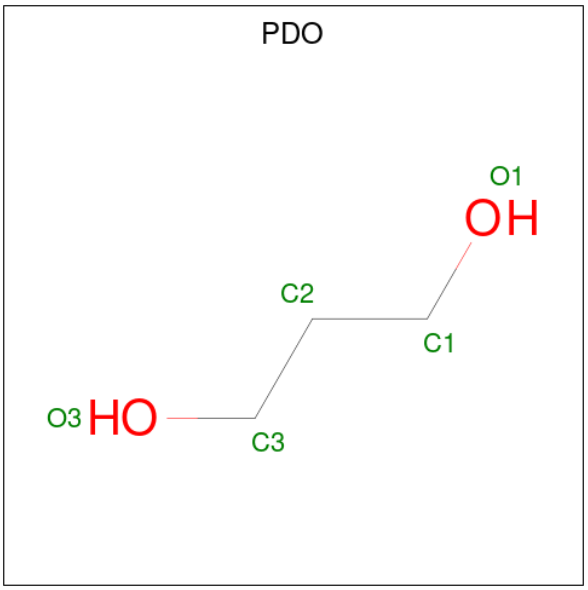
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	engineered mutation	UNP Q9HKI3
A	126	VAL	ALA	conflict	UNP Q9HKI3
A	132	TYR	PHE	engineered mutation	UNP Q9HKI3
B	60	GLN	GLU	engineered mutation	UNP Q9HKI3
B	126	VAL	ALA	conflict	UNP Q9HKI3
B	132	TYR	PHE	engineered mutation	UNP Q9HKI3
C	60	GLN	GLU	engineered mutation	UNP Q9HKI3
C	126	VAL	ALA	conflict	UNP Q9HKI3
C	132	TYR	PHE	engineered mutation	UNP Q9HKI3
D	60	GLN	GLU	engineered mutation	UNP Q9HKI3
D	126	VAL	ALA	conflict	UNP Q9HKI3
D	132	TYR	PHE	engineered mutation	UNP Q9HKI3
E	60	GLN	GLU	engineered mutation	UNP Q9HKI3
E	126	VAL	ALA	conflict	UNP Q9HKI3
E	132	TYR	PHE	engineered mutation	UNP Q9HKI3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



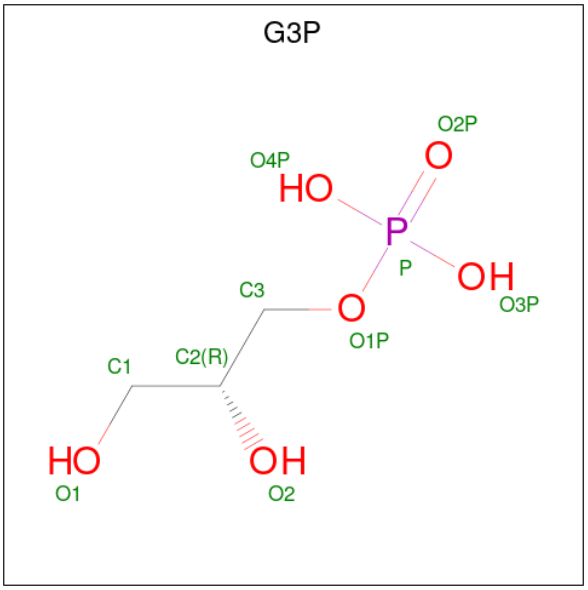
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	1
2	B	1	6	3	3	0	1
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	1
2	E	1	6	3	3	0	1

- Molecule 3 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



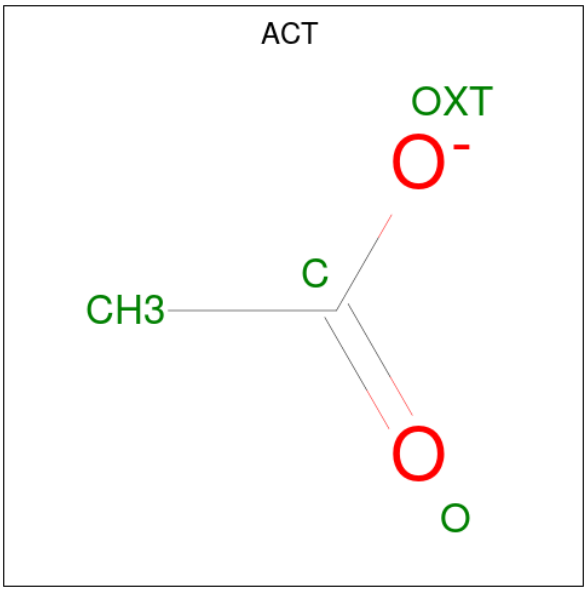
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	B	1	5	3	2		0	0
			Total	C	O			
3	C	1	5	3	2		0	0

- Molecule 4 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	8	2	5	1	0	0
			Total	C	O	P		
4	C	1	8	2	5	1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

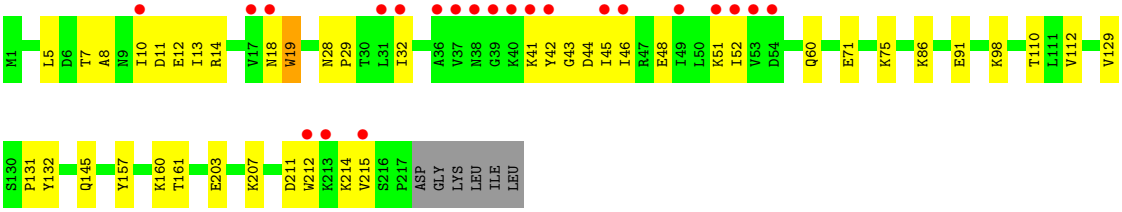
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	133	133	133	0	0
			Total	O		
6	B	162	162	162	0	0
			Total	O		
6	C	178	178	178	0	0
			Total	O		
6	D	148	148	148	0	0
			Total	O		
6	E	129	129	129	0	0

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.

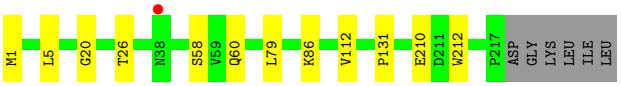
• Molecule 1: Probable transaldolase

Chain A:



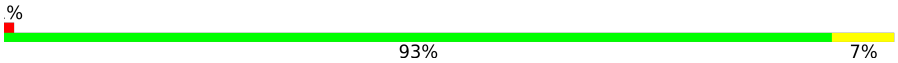
• Molecule 1: Probable transaldolase

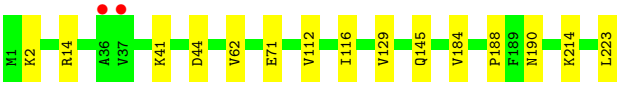
Chain B:



• Molecule 1: Probable transaldolase

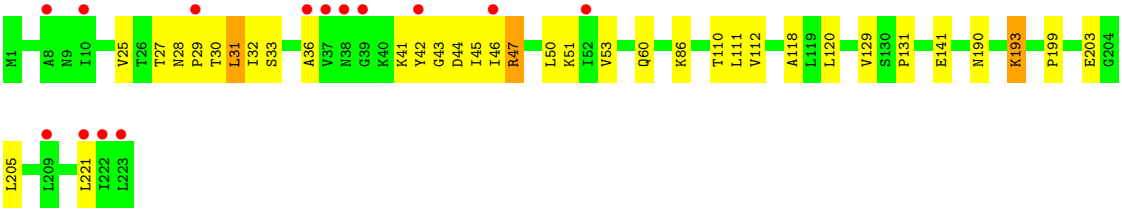
Chain C:





• Molecule 1: Probable transaldolase

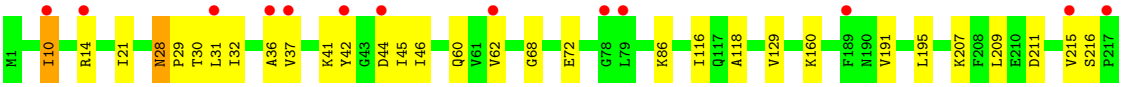
Chain D:

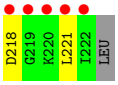


• Molecule 1: Probable transaldolase

Chain E:

8%
85%
14%


M1
I10
R14
I21
N28
P29
T30
L31
I32
A36
V37
K41
Y42
G43
D44
I45
I46
Q60
V61
V62
G68
E72
G78
L79
K86
I116
Q117
A118
V129
K160
F189
N190
V191
L195
K207
F208
L209
E210
D211
V215
S216
P217


D218
G219
K220
L221
I222
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	148.87Å 172.07Å 100.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 1.80 49.08 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.08-1.80) 96.6 (49.08-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.162 , 0.194 0.164 , 0.197	Depositor DCC
R_{free} test set	5904 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9859	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: GOL, G3P, ACT, PDO

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	0.57	0/1908	0.68	0/2594
1	B	0.62	0/1730	0.66	0/2347
1	C	0.62	0/1806	0.67	0/2451
1	D	0.61	1/1952 (0.1%)	0.66	0/2647
1	E	0.57	0/1775	0.68	0/2407
All	All	0.60	1/9171 (0.0%)	0.67	0/12446

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	GLU	CB-CG	-5.27	1.42	1.52

There are no bond angle outliers.

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	1880	0	1930	31	0
1	B	1704	0	1768	8	0
1	C	1780	0	1860	10	0
1	D	1924	0	2008	28	0
1	E	1749	0	1816	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
3	B	5	0	7	1	0
3	C	5	0	6	0	0
4	B	8	0	2	0	0
4	C	8	0	2	0	0
5	B	4	0	3	1	0
5	C	4	0	3	1	0
5	E	8	0	6	0	0
6	A	133	0	0	3	0
6	B	162	0	0	1	0
6	C	178	0	0	4	0
6	D	148	0	0	1	0
6	E	129	0	0	1	0
All	All	9859	0	9451	90	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 5.

All (90) 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:29[B]:PRO:HD3	1:D:60:GLN:HG3	1.49	0.93
1:D:43[B]:GLY:O	1:D:47[B]:ARG:HG3	1.84	0.77
1:A:203:GLU:OE1	6:A:401:HOH:O	2.07	0.73
1:A:48:GLU:O	1:A:52:ILE:HG13	1.93	0.69
1:A:41[A]:LYS:NZ	1:A:44[A]:ASP:OD1	2.27	0.66
1:D:28[B]:ASN:O	1:D:32[B]:ILE:HG12	1.95	0.66
1:E:41[A]:LYS:HG2	1:E:42[A]:TYR:N	2.11	0.65
1:A:86:LYS:NZ	6:A:402:HOH:O	2.29	0.65
1:D:60:GLN:HG2	1:D:86:LYS:HD3	1.79	0.64
1:D:41[A]:LYS:HG2	1:D:44[A]:ASP:H	1.63	0.63
1:A:129[B]:VAL:HG23	1:A:161:THR:HG21	1.80	0.63
1:C:190[A]:ASN:ND2	6:C:402:HOH:O	2.31	0.63
1:C:2:LYS:HE3	6:C:416:HOH:O	2.01	0.61
1:A:212:TRP:CD2	1:E:62:VAL:HG11	2.39	0.58
1:D:25:VAL:HG21	1:D:53[B]:VAL:HG21	1.85	0.58
1:D:30[B]:THR:OG1	1:E:211:ASP:OD2	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:O	1:E:21[A]:ILE:HD11	2.03	0.57
1:A:32[A]:ILE:HD13	1:A:46:ILE:HD11	1.86	0.57
1:A:98:LYS:NZ	6:A:403:HOH:O	2.37	0.57
1:E:41[A]:LYS:O	1:E:45[A]:ILE:HD12	2.05	0.56
1:D:60:GLN:HA	1:D:86:LYS:HB2	1.87	0.56
1:A:5:LEU:HB3	1:A:7[A]:THR:HG22	1.87	0.55
1:C:14:ARG:NH1	6:C:401:HOH:O	2.24	0.55
1:E:207:LYS:NZ	6:E:401:HOH:O	2.39	0.54
1:A:60:GLN:HA	1:A:86:LYS:HB2	1.91	0.53
1:C:112:VAL:HG21	1:C:129[B]:VAL:HG13	1.90	0.53
1:A:7[A]:THR:HG1	1:A:8[A]:ALA:N	2.07	0.53
1:D:33[B]:SER:CB	1:E:215:VAL:HG12	2.39	0.53
1:A:41[A]:LYS:HG2	1:A:43[A]:GLY:N	2.23	0.53
1:D:42[B]:TYR:CE1	1:E:221:LEU:HD12	2.45	0.52
1:E:60:GLN:HA	1:E:86:LYS:HB2	1.90	0.52
1:D:32[A]:ILE:HD13	1:D:46[A]:ILE:HD11	1.92	0.52
1:A:41[A]:LYS:HG2	1:A:43[A]:GLY:H	1.75	0.52
1:A:112:VAL:HG21	1:A:129[B]:VAL:HG13	1.93	0.51
5:C:304:ACT:H1	6:C:501:HOH:O	2.10	0.51
1:A:212:TRP:CZ3	1:E:29[A]:PRO:HB3	2.47	0.50
1:E:41[A]:LYS:HG2	1:E:42[A]:TYR:H	1.77	0.50
1:D:118:ALA:HA	1:D:129[A]:VAL:HG21	1.92	0.50
1:D:27[B]:THR:O	1:D:86:LYS:NZ	2.31	0.49
1:A:7[B]:THR:HG21	1:A:12[B]:GLU:OE1	2.13	0.49
1:A:18[B]:ASN:O	1:A:19:TRP:CG	2.66	0.48
1:D:28[B]:ASN:HB2	6:D:437:HOH:O	2.13	0.48
1:D:190:ASN:O	1:D:193:LYS:HG3	2.13	0.48
1:E:41[A]:LYS:HB3	1:E:44[A]:ASP:OD1	2.14	0.47
1:D:190:ASN:HA	1:D:193:LYS:CG	2.44	0.47
1:D:25:VAL:CG2	1:D:53[B]:VAL:HG21	2.45	0.47
1:D:199:PRO:O	1:D:203[A]:GLU:HG3	2.14	0.47
1:E:28[A]:ASN:ND2	1:E:30[A]:THR:H	2.13	0.47
1:B:79:LEU:HD11	1:C:223:LEU:HD13	1.96	0.46
1:B:58:SER:HB3	1:B:86:LYS:HG3	1.97	0.46
1:A:157:TYR:CZ	1:B:1:MET:HB2	2.50	0.46
1:D:28[B]:ASN:HB3	1:D:31[B]:LEU:HD12	1.98	0.45
1:B:26:THR:HB	3:B:301:PDO:H22	1.98	0.45
1:D:46[A]:ILE:O	1:D:50[A]:LEU:HD23	2.16	0.45
1:A:98:LYS:NZ	1:B:20:GLY:O	2.50	0.45
1:A:211[A]:ASP:O	1:A:214:LYS:HB2	2.17	0.45
1:A:41[A]:LYS:HZ3	1:A:41[A]:LYS:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110[A]:THR:HG1	1:A:132:TYR:HE2	1.65	0.44
1:D:112:VAL:O	1:D:131:PRO:HA	2.17	0.44
1:D:25:VAL:HG21	1:D:53[B]:VAL:CG2	2.47	0.44
1:E:191:VAL:O	1:E:195:LEU:HG	2.17	0.44
1:B:60:GLN:HA	1:B:86:LYS:HB2	1.99	0.44
1:C:2:LYS:HE2	1:C:184:VAL:HG22	1.99	0.44
1:E:160:LYS:HA	1:E:160:LYS:HD3	1.84	0.44
1:E:68:GLY:O	1:E:72:GLU:HG3	2.18	0.43
1:E:10[A]:ILE:HD13	1:E:10[A]:ILE:N	2.34	0.43
1:E:10[A]:ILE:O	1:E:14[A]:ARG:HG3	2.19	0.43
1:A:10[A]:ILE:HA	1:A:13[A]:ILE:HD12	2.00	0.43
1:A:11[B]:ASP:HA	1:A:14[B]:ARG:HG2	2.00	0.43
1:D:36:ALA:HB2	1:D:45[B]:ILE:HG13	2.00	0.43
1:E:32[A]:ILE:HD13	1:E:46[A]:ILE:HD11	1.99	0.43
1:A:41[A]:LYS:HE2	1:A:43[A]:GLY:HA3	2.00	0.42
1:A:71:GLU:O	1:A:75:LYS:HG2	2.19	0.42
1:C:188:PRO:HB2	1:C:190[A]:ASN:OD1	2.20	0.42
1:D:51[B]:LYS:HE3	1:D:51[B]:LYS:HB3	1.86	0.42
1:D:110[A]:THR:HG23	1:D:111:LEU:HG	2.00	0.42
1:A:29[A]:PRO:HB3	1:B:212:TRP:HZ3	1.84	0.42
1:D:112:VAL:HG21	1:D:129[B]:VAL:HG13	2.00	0.42
1:E:36[A]:ALA:HA	1:E:45[A]:ILE:HD11	2.00	0.42
1:A:42[A]:TYR:O	1:A:45[A]:ILE:HB	2.20	0.41
1:A:51:LYS:HE2	1:A:51:LYS:HB3	1.83	0.41
1:B:112:VAL:O	1:B:131:PRO:HA	2.20	0.41
1:C:62:VAL:HG22	1:D:221:LEU:HB2	2.02	0.41
1:E:118:ALA:HA	1:E:129[A]:VAL:HG21	2.02	0.41
1:A:112:VAL:O	1:A:131:PRO:HA	2.21	0.41
1:E:116:ILE:HD13	1:E:116:ILE:HA	1.91	0.41
1:C:41:LYS:HE3	1:C:44:ASP:OD1	2.20	0.41
5:B:304:ACT:H1	6:B:509:HOH:O	2.20	0.40
1:C:116:ILE:HD13	1:C:116:ILE:HA	1.95	0.40
1:A:160:LYS:HA	1:A:160:LYS:HD3	1.79	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	242/223 (108%)	227 (94%)	14 (6%)	1 (0%)	34	21
1	B	219/223 (98%)	215 (98%)	4 (2%)	0	100	100
1	C	229/223 (103%)	227 (99%)	2 (1%)	0	100	100
1	D	247/223 (111%)	239 (97%)	8 (3%)	0	100	100
1	E	225/223 (101%)	222 (99%)	3 (1%)	0	100	100
All	All	1162/1115 (104%)	1130 (97%)	31 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	TRP

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	213/193 (110%)	207 (97%)	6 (3%)	43	30
1	B	192/193 (100%)	190 (99%)	2 (1%)	76	71
1	C	201/193 (104%)	198 (98%)	3 (2%)	65	56
1	D	217/193 (112%)	211 (97%)	6 (3%)	43	30
1	E	197/193 (102%)	190 (96%)	7 (4%)	35	20
All	All	1020/965 (106%)	996 (98%)	24 (2%)	52	36

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28[A]	ASN
1	A	28[B]	ASN
1	A	91	GLU
1	A	145	GLN
1	A	207	LYS
1	A	215	VAL
1	B	5	LEU
1	B	210	GLU
1	C	71	GLU
1	C	145	GLN
1	C	214	LYS
1	D	31[A]	LEU
1	D	31[B]	LEU
1	D	47[A]	ARG
1	D	47[B]	ARG
1	D	193	LYS
1	D	205	LEU
1	E	10[A]	ILE
1	E	28[A]	ASN
1	E	31[A]	LEU
1	E	37[A]	VAL
1	E	209	LEU
1	E	216	SER
1	E	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

13 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	GOL	E	301[B]	-	5,5,5	0.28	0	5,5,5	0.63	0
3	PDO	B	301	1	4,4,4	0.68	0	3,3,3	0.36	0
5	ACT	C	304	-	3,3,3	1.11	0	3,3,3	1.91	2 (66%)
2	GOL	A	301[A]	-	5,5,5	0.32	0	5,5,5	0.35	0
4	G3P	B	302	-	7,7,9	1.00	1 (14%)	9,9,12	1.25	0
5	ACT	B	304	-	3,3,3	0.97	0	3,3,3	1.77	1 (33%)
5	ACT	E	302	-	3,3,3	1.13	0	3,3,3	1.89	2 (66%)
2	GOL	B	303[B]	-	5,5,5	0.29	0	5,5,5	0.33	0
2	GOL	D	301[A]	-	5,5,5	0.27	0	5,5,5	0.48	0
4	G3P	C	302	-	7,7,9	0.76	0	9,9,12	1.20	1 (11%)
5	ACT	E	303	-	3,3,3	0.66	0	3,3,3	1.34	0
3	PDO	C	301	1	4,4,4	0.67	0	3,3,3	0.40	0
2	GOL	C	303	-	5,5,5	0.28	0	5,5,5	0.48	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	GOL	E	301[B]	-	-	3/4/4/4	-
3	PDO	B	301	1	-	1/2/2/2	-
2	GOL	A	301[A]	-	-	2/4/4/4	-
4	G3P	B	302	-	-	1/5/5/8	-
2	GOL	B	303[B]	-	-	4/4/4/4	-
2	GOL	D	301[A]	-	-	2/4/4/4	-
4	G3P	C	302	-	-	3/5/5/8	-
3	PDO	C	301	1	-	2/2/2/2	-
2	GOL	C	303	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	G3P	P-O3P	-2.06	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	304	ACT	OXT-C-O	-2.57	112.57	122.05
5	E	302	ACT	OXT-C-O	-2.56	112.61	122.05
4	C	302	G3P	P-O1P-C3	2.41	124.92	118.30
5	B	304	ACT	OXT-C-O	-2.35	113.39	122.05
5	C	304	ACT	OXT-C-CH3	2.04	123.62	115.18
5	E	302	ACT	OXT-C-CH3	2.01	123.48	115.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	303[B]	GOL	O1-C1-C2-C3
2	B	303[B]	GOL	C1-C2-C3-O3
2	D	301[A]	GOL	O1-C1-C2-C3
3	B	301	PDO	O1-C1-C2-C3
3	C	301	PDO	O1-C1-C2-C3
4	B	302	G3P	C3-O1P-P-O4P
4	C	302	G3P	C3-O1P-P-O4P
4	C	302	G3P	C3-O1P-P-O3P
2	A	301[A]	GOL	C1-C2-C3-O3
2	C	303	GOL	O1-C1-C2-C3
2	E	301[B]	GOL	O1-C1-C2-C3
2	E	301[B]	GOL	C1-C2-C3-O3
2	A	301[A]	GOL	O2-C2-C3-O3
2	B	303[B]	GOL	O1-C1-C2-O2
2	D	301[A]	GOL	O1-C1-C2-O2
2	E	301[B]	GOL	O1-C1-C2-O2
4	C	302	G3P	C3-O1P-P-O2P
2	B	303[B]	GOL	O2-C2-C3-O3
2	C	303	GOL	O1-C1-C2-O2
3	C	301	PDO	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	PDO	1	0
5	C	304	ACT	1	0
5	B	304	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	35[B]:GLU	C	36:ALA	N	4.09

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	217/223 (97%)	0.20	22 (10%)	7	5	18, 35, 77, 99	10 (4%)
1	B	217/223 (97%)	-0.20	1 (0%)	91	89	17, 34, 61, 83	0
1	C	223/223 (100%)	-0.13	2 (0%)	84	82	18, 30, 59, 79	0
1	D	223/223 (100%)	0.19	14 (6%)	20	15	17, 32, 56, 75	13 (5%)
1	E	222/223 (99%)	0.38	18 (8%)	12	9	18, 38, 61, 106	42 (18%)
All	All	1102/1115 (98%)	0.09	57 (5%)	27	22	17, 33, 64, 106	65 (5%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10[A]	ILE	7.0
1	E	219	GLY	6.9
1	D	37	VAL	5.6
1	E	220	LYS	4.7
1	A	37[A]	VAL	4.7
1	A	39[A]	GLY	4.5
1	D	39[A]	GLY	4.1
1	A	52	ILE	4.0
1	E	78	GLY	4.0
1	E	217	PRO	3.9
1	E	37[A]	VAL	3.9
1	E	221	LEU	3.8
1	D	38[A]	ASN	3.7
1	D	52[A]	ILE	3.7
1	A	51	LYS	3.6
1	D	29[A]	PRO	3.5
1	C	36	ALA	3.5
1	A	41[A]	LYS	3.4
1	D	8[A]	ALA	3.3
1	E	42[A]	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	54	ASP	3.2
1	E	62	VAL	3.1
1	C	37	VAL	3.1
1	A	36[A]	ALA	3.1
1	E	14[A]	ARG	3.1
1	A	42[A]	TYR	3.0
1	E	36[A]	ALA	2.9
1	E	218	ASP	2.9
1	D	223	LEU	2.9
1	E	189	PHE	2.9
1	E	10[A]	ILE	2.8
1	A	31[A]	LEU	2.8
1	D	46[A]	ILE	2.7
1	A	212	TRP	2.7
1	A	53	VAL	2.7
1	A	17[A]	VAL	2.7
1	B	38	ASN	2.6
1	A	32[A]	ILE	2.6
1	D	42[A]	TYR	2.6
1	D	36	ALA	2.5
1	A	45[A]	ILE	2.5
1	A	38[A]	ASN	2.5
1	A	40[A]	LYS	2.5
1	E	222	ILE	2.4
1	E	215	VAL	2.4
1	D	222	ILE	2.3
1	D	221	LEU	2.3
1	A	215	VAL	2.3
1	D	209	LEU	2.3
1	A	18[A]	ASN	2.2
1	A	46	ILE	2.2
1	E	44[A]	ASP	2.2
1	A	10[A]	ILE	2.2
1	A	213	LYS	2.2
1	E	79	LEU	2.2
1	E	31[A]	LEU	2.1
1	A	49	ILE	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
5	ACT	E	303	4/4	0.76	0.22	50,51,53,54	0
3	PDO	C	301	5/5	0.84	0.11	30,34,41,41	0
4	G3P	B	302	8/10	0.85	0.20	31,46,48,54	8
4	G3P	C	302	8/10	0.88	0.18	23,42,45,46	8
2	GOL	B	303[B]	6/6	0.88	0.13	34,37,39,39	6
2	GOL	A	301[A]	6/6	0.89	0.16	40,42,43,43	6
2	GOL	E	301[B]	6/6	0.91	0.13	39,41,43,44	6
3	PDO	B	301	5/5	0.91	0.09	30,36,41,43	0
2	GOL	D	301[A]	6/6	0.91	0.10	33,38,40,40	6
5	ACT	E	302	4/4	0.92	0.17	34,37,38,38	0
5	ACT	C	304	4/4	0.93	0.16	27,29,32,33	4
5	ACT	B	304	4/4	0.94	0.20	38,38,42,45	0
2	GOL	C	303	6/6	0.94	0.13	31,32,35,35	6

6.5 Other polymers (i)

There are no such residues in this entry.