Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:21 am BST

PDB ID	:	3NV9
Title	:	Crystal structure of Entamoeba histolytica Malic Enzyme
Authors	:	Dutta, D.; Chakrabarty, A.; Ghosh, S.K.; Das, A.K.
Deposited on	:	2010-07-08
Resolution	:	2.25 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 ⓘ symbol.

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

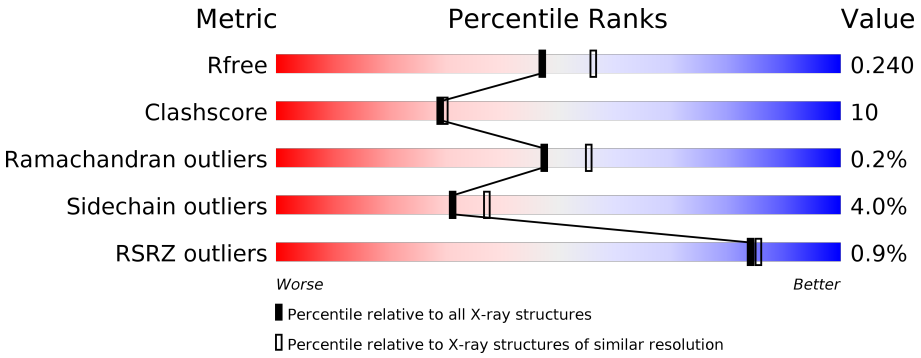
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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	487	% 81% 16% ·
1	B	487	83% 14% ·

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
4	GOL	A	496	-	-	X	-
4	GOL	A	497	-	-	X	-
4	GOL	A	498	-	-	X	-
4	GOL	B	497	-	-	X	-
4	GOL	B	502	-	X	X	-

2 Entry composition

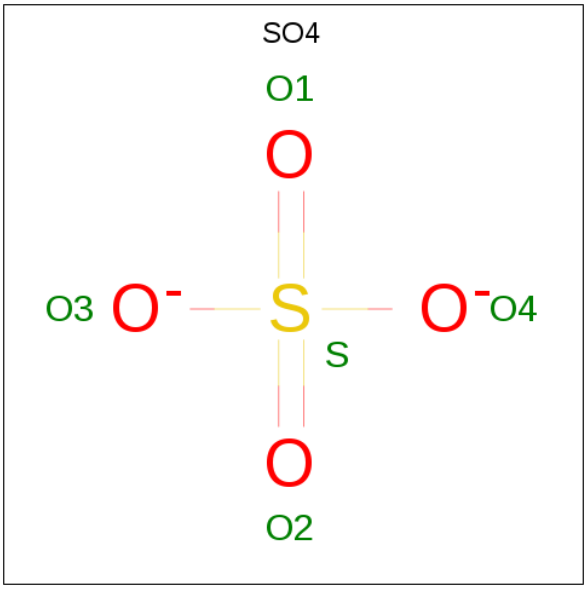
There are 6 unique types of molecules in this entry. The entry contains 8185 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3733	2359	639	713	22			
1	B	486	Total	C	N	O	S	0	0	0
			3733	2359	639	713	22			

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



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

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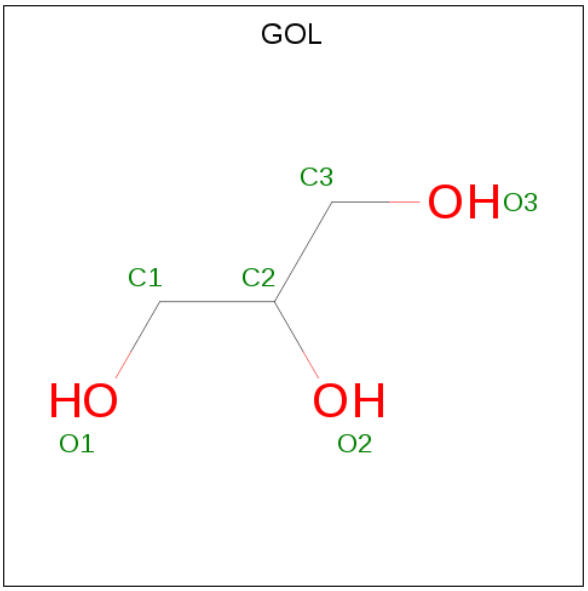
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

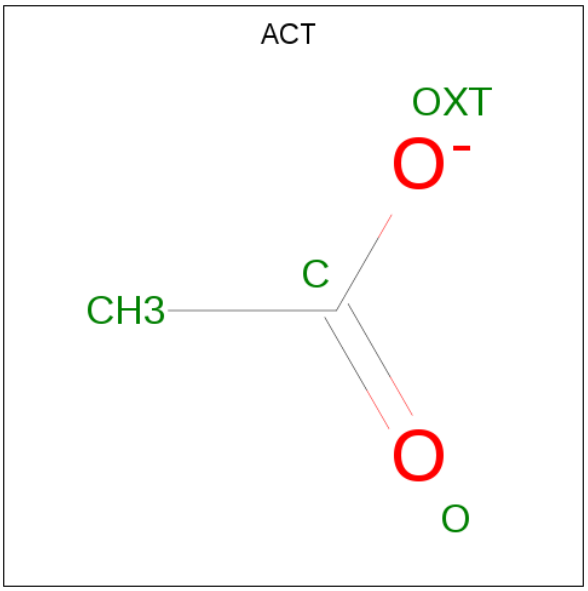
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

- Molecule 6 is water.

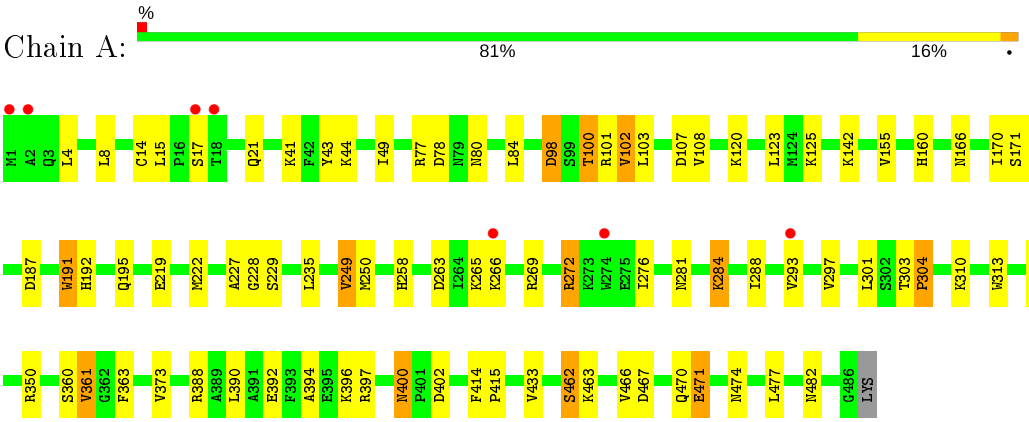
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	268	Total O 268 268	0	0
6	B	314	Total O 314 314	0	0

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 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.

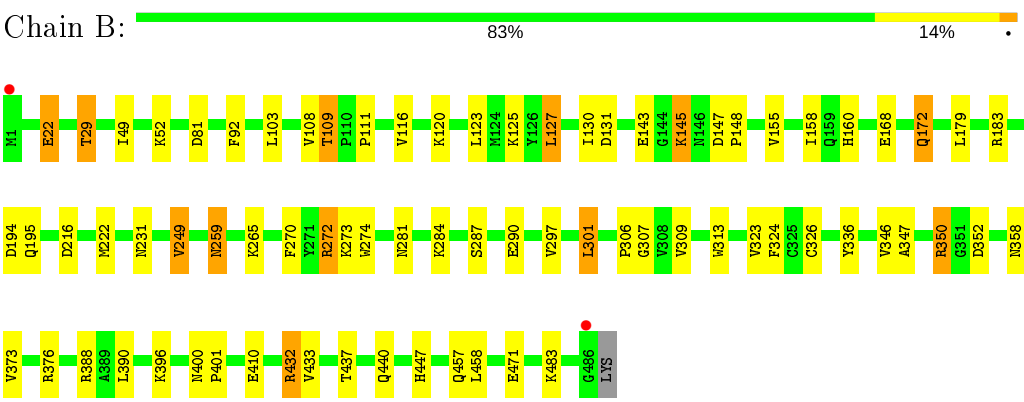
- Molecule 1: Malic enzyme

Chain A:



- Molecule 1: Malic enzyme

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.73Å 117.73Å 157.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.16 – 2.25 47.16 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.16-2.25) 100.0 (47.16-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.24 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0095	Depositor
R, R_{free}	0.179 , 0.245 0.176 , 0.240	Depositor DCC
R_{free} test set	2704 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8185	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

5.1 Standard geometry

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

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	0.95	2/3803 (0.1%)	0.91	5/5148 (0.1%)
1	B	0.95	0/3803	0.90	10/5148 (0.2%)
All	All	0.95	2/7606 (0.0%)	0.91	15/10296 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	CB-CG	5.22	1.62	1.52
1	A	471	GLU	CG-CD	5.17	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	350	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	A	272	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	272	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	B	350	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	216	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	272	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	350	ARG	CA-CB-CG	6.07	126.76	113.40
1	A	107	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	350	ARG	CB-CG-CD	-5.66	96.89	111.60
1	B	390	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	B	259	ASN	CB-CA-C	-5.39	99.62	110.40
1	B	432	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	249	VAL	CB-CA-C	-5.31	101.31	111.40
1	B	272	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	98	ASP	CB-CG-OD2	5.23	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3733	0	3743	74	0
1	B	3733	0	3742	75	0
2	A	35	0	0	1	0
2	B	40	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	32	20	0
4	B	24	0	31	16	0
5	A	4	0	3	0	0
5	B	8	0	6	1	0
6	A	268	0	0	6	0
6	B	314	0	0	13	0
All	All	8185	0	7557	145	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 10.

All (145) 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:270:PHE:CA	4:B:497:GOL:H11	1.86	1.06
1:A:103:LEU:CD2	4:A:497:GOL:H11	1.88	1.04
1:B:270:PHE:HA	4:B:497:GOL:C1	1.88	1.01
1:A:192:HIS:CD2	1:A:195:GLN:HE21	1.79	0.98
1:B:270:PHE:HA	4:B:497:GOL:H11	0.96	0.96
1:A:103:LEU:HD23	4:A:497:GOL:H11	1.49	0.95
1:B:29:THR:CG2	1:B:350:ARG:HH22	1.79	0.95
1:A:192:HIS:HD2	1:A:195:GLN:HE21	0.96	0.91
1:A:313:TRP:HE1	4:A:496:GOL:H11	1.37	0.89
1:B:192:HIS:HD2	1:B:195:GLN:HE21	1.22	0.88
1:A:482:ASN:HB2	6:A:586:HOH:O	1.76	0.84
1:A:192:HIS:HD2	1:A:195:GLN:NE2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:HE2	4:B:502:GOL:H12	1.60	0.83
1:B:116:VAL:HG13	4:B:502:GOL:H11	1.59	0.82
1:A:100:THR:CG2	1:A:171:SER:H	1.92	0.81
1:A:103:LEU:HD21	4:A:497:GOL:H11	1.62	0.80
1:A:166:ASN:HD22	1:A:191:TRP:HE1	1.31	0.79
1:B:29:THR:HG21	1:B:350:ARG:HH22	1.48	0.76
1:A:103:LEU:HD21	4:A:497:GOL:C1	2.15	0.76
1:B:109:THR:HG23	1:B:111:PRO:HD2	1.67	0.75
1:A:310:LYS:NZ	4:A:496:GOL:H12	2.01	0.75
1:A:98:ASP:OD2	1:A:100:THR:HB	1.87	0.75
1:A:172:GLN:HG2	4:A:498:GOL:H2	1.71	0.72
1:B:29:THR:HB	1:B:350:ARG:NH2	2.06	0.71
1:B:307:GLY:HA2	6:B:626:HOH:O	1.92	0.70
1:A:471:GLU:HG3	6:A:612:HOH:O	1.92	0.69
1:B:447:HIS:HE1	6:B:779:HOH:O	1.76	0.67
1:B:29:THR:CB	1:B:350:ARG:HH22	2.06	0.67
1:A:250:MET:HE2	1:A:276:ILE:HG21	1.77	0.67
1:B:265:LYS:HE3	1:B:274:TRP:CZ2	2.31	0.66
1:B:287:SER:OG	1:B:290:GLU:HG3	1.96	0.65
1:B:222:MET:HG2	1:B:297:VAL:HB	1.77	0.65
1:A:269:ARG:HD2	4:A:499:GOL:H2	1.79	0.65
1:B:306:PRO:HA	6:B:699:HOH:O	1.95	0.65
1:B:457:GLN:HG3	6:B:811:HOH:O	1.96	0.65
1:A:100:THR:HG23	1:A:171:SER:HB3	1.80	0.64
1:A:462:SER:O	1:A:463:LYS:HB2	1.97	0.64
1:A:313:TRP:NE1	4:A:496:GOL:H11	2.11	0.64
1:A:303:THR:CG2	4:A:498:GOL:H31	2.27	0.63
1:B:116:VAL:CG1	4:B:502:GOL:H11	2.29	0.62
1:A:222:MET:HG2	1:A:297:VAL:HB	1.81	0.61
1:A:192:HIS:CD2	1:A:195:GLN:NE2	2.58	0.60
1:A:310:LYS:HZ2	4:A:496:GOL:H12	1.66	0.60
1:A:361:VAL:HG13	1:A:390:LEU:HD21	1.83	0.60
1:A:103:LEU:CD2	4:A:497:GOL:C1	2.69	0.60
1:A:77:ARG:HD2	1:A:78:ASP:OD1	2.02	0.60
1:A:400:ASN:HD22	1:A:402:ASP:H	1.49	0.58
1:B:81:ASP:OD1	5:B:499:ACT:H3	2.04	0.58
1:A:317:MET:HE1	1:A:321:PRO:HB3	1.85	0.58
1:B:376:ARG:HD2	6:B:515:HOH:O	2.03	0.58
1:A:229:SER:HB3	4:A:498:GOL:H12	1.86	0.58
1:B:179:LEU:HD11	1:B:183:ARG:HD3	1.86	0.56
1:B:192:HIS:CD2	1:B:195:GLN:HE21	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASN:HD21	4:B:502:GOL:H32	1.70	0.56
1:B:259:ASN:HB2	1:B:284:LYS:NZ	2.20	0.55
1:A:462:SER:OG	1:B:458:LEU:HD21	2.05	0.55
1:B:388:ARG:NH2	6:B:769:HOH:O	2.39	0.55
1:A:14:CYS:HB3	1:A:477:LEU:HD21	1.87	0.55
1:B:29:THR:HB	1:B:350:ARG:HH22	1.65	0.55
1:B:123:LEU:O	1:B:127:LEU:HB2	2.06	0.55
1:A:100:THR:HG22	1:A:171:SER:H	1.71	0.54
1:B:103:LEU:HD21	4:B:502:GOL:C2	2.37	0.54
1:B:130:ILE:CD1	1:B:368:LYS:HD3	2.38	0.54
1:B:120:LYS:CE	4:B:502:GOL:H12	2.36	0.53
1:A:43:TYR:O	1:B:52:LYS:HE3	2.07	0.53
1:A:310:LYS:HZ3	4:A:496:GOL:H12	1.69	0.53
1:B:172:GLN:O	1:B:172:GLN:HG3	2.09	0.52
1:B:183:ARG:HD2	6:B:519:HOH:O	2.08	0.52
1:A:360:SER:HA	1:A:363:PHE:CE1	2.44	0.51
1:A:373:VAL:HA	1:A:433:VAL:HB	1.92	0.51
1:B:130:ILE:HD11	1:B:368:LYS:HD3	1.92	0.51
1:B:350:ARG:HD3	1:B:352:ASP:OD1	2.11	0.51
1:B:324:PHE:CD2	1:B:347:ALA:HB3	2.45	0.51
1:B:130:ILE:HD12	1:B:371:LEU:HD12	1.93	0.51
1:A:317:MET:CE	1:A:321:PRO:HB3	2.41	0.50
1:A:303:THR:HG22	4:A:498:GOL:H31	1.91	0.50
1:A:172:GLN:HG2	4:A:498:GOL:C2	2.41	0.50
1:A:388:ARG:O	1:A:392:GLU:HG3	2.11	0.50
1:A:466:VAL:HG12	1:A:467:ASP:O	2.12	0.50
1:B:192:HIS:CE1	1:B:194:ASP:HB2	2.48	0.49
1:A:329:PRO:O	1:A:350:ARG:HD2	2.13	0.49
1:A:361:VAL:HG13	1:A:390:LEU:CD2	2.42	0.49
1:B:22:GLU:HB3	1:B:336:TYR:OH	2.13	0.49
1:A:227:ALA:HB3	2:A:492:SO4:O2	2.13	0.49
1:A:41:LYS:O	1:A:44:LYS:HD3	2.13	0.48
1:B:270:PHE:HD1	4:B:497:GOL:H31	1.78	0.48
1:A:187:ASP:HB2	6:A:614:HOH:O	2.14	0.48
1:B:309:VAL:HA	1:B:313:TRP:CZ3	2.49	0.47
1:A:394:ALA:O	1:A:397:ARG:HD2	2.15	0.47
1:B:249:VAL:HG13	1:B:281:ASN:CG	2.34	0.47
1:B:273:LYS:N	4:B:497:GOL:O2	2.33	0.47
1:A:125:LYS:HE2	1:B:49:ILE:O	2.14	0.47
1:B:160:HIS:HD2	6:B:524:HOH:O	1.97	0.46
1:A:249:VAL:HG13	1:A:281:ASN:CG	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:170:ILE:HA	1.96	0.46
1:A:49:ILE:O	1:B:125:LYS:HE2	2.15	0.46
1:A:228:GLY:HA3	4:A:498:GOL:H32	1.97	0.46
1:B:179:LEU:O	1:B:183:ARG:HB2	2.15	0.46
1:B:187:ASP:HB2	6:B:613:HOH:O	2.15	0.46
1:B:301:LEU:HD22	1:B:326:CYS:HB2	1.98	0.46
1:B:400:ASN:HB2	1:B:401:PRO:CD	2.45	0.46
1:B:270:PHE:HD1	4:B:497:GOL:C3	2.29	0.46
1:A:155:VAL:HG11	1:A:182:LEU:HD13	1.97	0.45
1:B:437:THR:OG1	1:B:440:GLN:HG3	2.16	0.45
1:A:175:CYS:HB2	1:A:192:HIS:CD2	2.50	0.45
1:B:108:VAL:O	1:B:109:THR:HG22	2.16	0.45
1:A:102:VAL:HG13	1:A:108:VAL:HG22	1.99	0.45
1:B:396:LYS:HB2	6:B:760:HOH:O	2.17	0.45
1:B:155:VAL:HA	1:B:158:ILE:HG22	1.99	0.45
4:B:498:GOL:H32	6:B:809:HOH:O	2.18	0.44
1:A:361:VAL:CG1	1:A:390:LEU:HD21	2.48	0.44
1:B:147:ASP:HA	1:B:148:PRO:HD2	1.91	0.44
1:B:183:ARG:HD2	6:B:529:HOH:O	2.17	0.44
1:B:172:GLN:OE1	4:B:498:GOL:H31	2.16	0.44
1:A:414:PHE:N	1:A:415:PRO:HD2	2.33	0.43
1:B:400:ASN:HB2	1:B:401:PRO:HD2	2.01	0.43
1:A:258:HIS:HB2	1:A:284:LYS:HD2	2.01	0.43
1:B:168:GLU:OE1	1:B:193:ASP:OD2	2.36	0.42
1:A:120:LYS:NZ	4:A:497:GOL:H2	2.34	0.42
1:A:266:LYS:HB3	6:A:823:HOH:O	2.19	0.42
1:B:270:PHE:C	4:B:497:GOL:H11	2.38	0.42
1:B:273:LYS:CD	4:B:497:GOL:H31	2.49	0.42
1:B:123:LEU:HD22	1:B:127:LEU:HD22	2.02	0.42
1:A:313:TRP:HE1	4:A:496:GOL:C1	2.21	0.42
1:A:288:ILE:HD13	1:A:313:TRP:CH2	2.55	0.42
6:A:567:HOH:O	1:B:160:HIS:HE1	2.03	0.41
1:B:179:LEU:CD1	1:B:183:ARG:HD3	2.50	0.41
1:B:92:PHE:HA	1:B:131:ASP:O	2.19	0.41
1:A:400:ASN:ND2	1:A:402:ASP:H	2.16	0.41
1:B:410:GLU:HA	2:B:493:SO4:O1	2.19	0.41
1:A:172:GLN:HG3	1:A:172:GLN:O	2.21	0.41
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.85	0.41
1:B:447:HIS:CE1	6:B:779:HOH:O	2.61	0.41
1:A:235:LEU:HD22	1:A:276:ILE:HG12	2.03	0.41
1:A:123:LEU:HD13	1:A:360:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:VAL:HA	1:B:433:VAL:HB	2.01	0.41
1:A:258:HIS:CD2	1:A:284:LYS:HG3	2.55	0.41
1:A:470:GLN:HE21	1:A:474:ASN:HD21	1.69	0.41
1:B:172:GLN:HB2	1:B:172:GLN:HE21	1.71	0.41
1:A:101:ARG:HD2	1:A:304:PRO:HD3	2.03	0.41
1:A:80:ASN:OD1	1:B:109:THR:HG21	2.21	0.40
1:A:160:HIS:HD2	6:A:527:HOH:O	2.03	0.40
1:B:323:VAL:O	1:B:346:VAL:HA	2.21	0.40
1:A:172:GLN:CG	4:A:498:GOL:H2	2.43	0.40
1:B:143:GLU:O	1:B:145:LYS:HE3	2.22	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	484/487 (99%)	463 (96%)	19 (4%)	2 (0%)	34 37
1	B	484/487 (99%)	459 (95%)	25 (5%)	0	100 100
All	All	968/974 (99%)	922 (95%)	44 (4%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	304	PRO

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	404/405 (100%)	386 (96%)	18 (4%)	27	31
1	B	404/405 (100%)	390 (96%)	14 (4%)	36	43
All	All	808/810 (100%)	776 (96%)	32 (4%)	31	37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	15	LEU
1	A	17	SER
1	A	21	GLN
1	A	84	LEU
1	A	100	THR
1	A	102	VAL
1	A	142	LYS
1	A	191	TRP
1	A	265	LYS
1	A	272	ARG
1	A	284	LYS
1	A	293	VAL
1	A	301	LEU
1	A	361	VAL
1	A	396	LYS
1	A	400	ASN
1	A	462	SER
1	B	22	GLU
1	B	29	THR
1	B	109	THR
1	B	127	LEU
1	B	145	LYS
1	B	172	GLN
1	B	191	TRP
1	B	231	ASN
1	B	249	VAL
1	B	272	ARG
1	B	301	LEU
1	B	432	ARG
1	B	471	GLU
1	B	483	LYS

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

Mol	Chain	Res	Type
1	A	91	ASN
1	A	146	ASN
1	A	160	HIS
1	A	166	ASN
1	A	192	HIS
1	A	195	GLN
1	A	328	ASN
1	A	356	GLN
1	A	400	ASN
1	A	474	ASN
1	B	59	ASN
1	B	75	ASN
1	B	91	ASN
1	B	160	HIS
1	B	192	HIS
1	B	457	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

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	SO4	A	491	-	4,4,4	0.14	0	6,6,6	0.57	0
5	ACT	B	501	-	1,3,3	1.25	0	0,3,3	0.00	-
4	GOL	A	497	-	5,5,5	0.50	0	5,5,5	0.58	0
5	ACT	B	499	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
2	SO4	B	488	-	4,4,4	0.43	0	6,6,6	0.81	0
4	GOL	A	499	-	5,5,5	0.46	0	5,5,5	0.69	0
2	SO4	A	488	-	4,4,4	0.26	0	6,6,6	0.60	0
4	GOL	B	497	-	5,5,5	0.98	0	5,5,5	1.49	1 (20%)
2	SO4	A	490	-	4,4,4	0.12	0	6,6,6	0.45	0
4	GOL	A	496	-	5,5,5	0.63	0	5,5,5	0.88	0
2	SO4	B	494	-	4,4,4	0.13	0	6,6,6	0.09	0
4	GOL	B	500	-	5,5,5	0.42	0	5,5,5	0.42	0
2	SO4	A	492	-	4,4,4	0.26	0	6,6,6	0.80	0
5	ACT	A	502	-	1,3,3	1.45	0	0,3,3	0.00	-
2	SO4	B	491	-	4,4,4	0.28	0	6,6,6	0.34	0
4	GOL	B	498	-	5,5,5	0.30	0	5,5,5	1.10	0
4	GOL	A	498	-	5,5,5	0.78	0	5,5,5	1.75	1 (20%)
2	SO4	B	489	-	4,4,4	0.25	0	6,6,6	0.70	0
4	GOL	B	502	-	5,5,5	0.64	0	5,5,5	1.92	3 (60%)
2	SO4	A	494	-	4,4,4	0.16	0	6,6,6	0.29	0
2	SO4	B	492	-	4,4,4	0.24	0	6,6,6	0.38	0
2	SO4	B	495	-	4,4,4	0.14	0	6,6,6	0.26	0
2	SO4	A	493	-	4,4,4	0.11	0	6,6,6	0.46	0
2	SO4	B	493	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	B	490	-	4,4,4	0.15	0	6,6,6	0.46	0
2	SO4	A	489	-	4,4,4	0.29	0	6,6,6	0.45	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
4	GOL	B	498	-	-	3/4/4/4	-
4	GOL	A	498	-	-	2/4/4/4	-
4	GOL	A	497	-	-	2/4/4/4	-
4	GOL	B	497	-	-	4/4/4/4	-
4	GOL	B	502	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	496	-	-	4/4/4/4	-
4	GOL	B	500	-	-	2/4/4/4	-
4	GOL	A	499	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	499	ACT	CH3-C	2.68	1.52	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	498	GOL	O3-C3-C2	-2.71	97.21	110.20
4	B	502	GOL	O2-C2-C1	2.48	120.03	109.12
4	B	502	GOL	O2-C2-C3	2.35	119.46	109.12
4	B	502	GOL	C3-C2-C1	2.26	120.50	111.70
4	B	497	GOL	O3-C3-C2	2.24	120.96	110.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	499	GOL	O1-C1-C2-C3
4	B	497	GOL	O1-C1-C2-C3
4	B	497	GOL	C1-C2-C3-O3
4	B	497	GOL	O2-C2-C3-O3
4	A	496	GOL	C1-C2-C3-O3
4	A	498	GOL	O1-C1-C2-C3
4	B	502	GOL	C1-C2-C3-O3
4	B	502	GOL	O1-C1-C2-O2
4	A	499	GOL	C1-C2-C3-O3
4	A	496	GOL	O1-C1-C2-C3
4	B	500	GOL	O1-C1-C2-C3
4	B	498	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-C3
4	A	499	GOL	O1-C1-C2-O2
4	B	497	GOL	O1-C1-C2-O2
4	B	500	GOL	O1-C1-C2-O2
4	B	498	GOL	O1-C1-C2-O2
4	A	498	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	496	GOL	O2-C2-C3-O3
4	A	496	GOL	O1-C1-C2-O2
4	B	498	GOL	C1-C2-C3-O3
4	A	497	GOL	O1-C1-C2-O2
4	A	499	GOL	O2-C2-C3-O3
4	A	497	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	497	GOL	6	0
5	B	499	ACT	1	0
4	A	499	GOL	1	0
4	B	497	GOL	8	0
4	A	496	GOL	6	0
2	A	492	SO4	1	0
4	B	498	GOL	2	0
4	A	498	GOL	7	0
4	B	502	GOL	6	0
2	B	493	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	486/487 (99%)	-0.04	7 (1%)	75	77	16, 27, 46, 63	0
1	B	486/487 (99%)	-0.16	2 (0%)	92	93	16, 26, 40, 52	0
All	All	972/974 (99%)	-0.10	9 (0%)	84	85	16, 27, 44, 63	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.0
1	B	1	MET	3.1
1	A	2	ALA	3.0
1	B	486	GLY	3.0
1	A	266	LYS	2.8
1	A	18	THR	2.7
1	A	17	SER	2.4
1	A	274	TRP	2.3
1	A	293	VAL	2.1

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

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

6.3 Carbohydrates

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. 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	B-factors(Å^2)	Q<0.9
4	GOL	A	499	6/6	0.67	0.25	63,65,65,65	0
4	GOL	B	500	6/6	0.68	0.20	60,61,64,65	0
5	ACT	A	502	4/4	0.72	0.26	54,55,55,55	0
5	ACT	B	499	4/4	0.75	0.20	41,42,42,43	0
2	SO4	B	491	5/5	0.82	0.26	74,76,77,77	0
4	GOL	B	497	6/6	0.84	0.38	37,42,46,46	0
2	SO4	A	494	5/5	0.84	0.21	104,105,105,105	0
4	GOL	A	496	6/6	0.85	0.20	48,50,50,51	0
4	GOL	B	502	6/6	0.86	0.35	31,32,33,38	2
4	GOL	A	497	6/6	0.87	0.30	41,43,43,44	1
2	SO4	A	493	5/5	0.88	0.29	87,87,87,88	0
2	SO4	B	493	5/5	0.89	0.32	104,104,105,106	0
4	GOL	B	498	6/6	0.91	0.15	41,45,48,53	0
2	SO4	B	489	5/5	0.91	0.27	66,67,68,69	0
2	SO4	A	492	5/5	0.91	0.18	68,69,71,71	0
5	ACT	B	501	4/4	0.92	0.15	37,38,38,39	0
2	SO4	B	495	5/5	0.93	0.31	81,82,82,83	0
2	SO4	B	490	5/5	0.93	0.32	66,66,68,68	0
4	GOL	A	498	6/6	0.94	0.18	36,39,40,42	0
2	SO4	A	491	5/5	0.94	0.30	62,62,63,65	0
2	SO4	B	494	5/5	0.95	0.42	87,88,89,89	0
2	SO4	A	488	5/5	0.96	0.13	46,46,49,52	0
3	NA	A	495	1/1	0.97	0.16	28,28,28,28	0
2	SO4	B	492	5/5	0.97	0.12	54,56,58,58	0
2	SO4	A	490	5/5	0.98	0.12	44,46,47,47	0
2	SO4	A	489	5/5	0.98	0.10	44,44,46,47	0
2	SO4	B	488	5/5	0.99	0.12	35,36,39,40	0
3	NA	B	496	1/1	0.99	0.17	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.