



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2023 – 06:23 PM EST

PDB ID : 3FMC  
Title : CRYSTAL STRUCTURE OF a putative succinylglutamate desuccinylase / aspartoacylase family protein (SAMA\_0604) FROM SHEWANELLA AMAZONENSIS SB2B AT 1.80 A RESOLUTION  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2008-12-19  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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) : 2.31.2

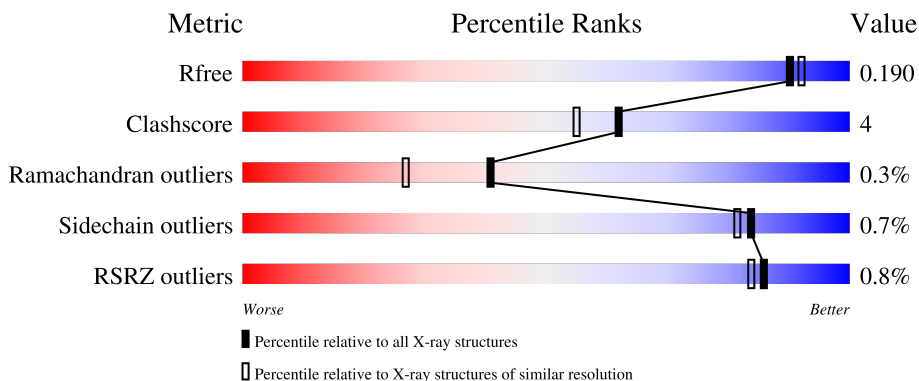
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

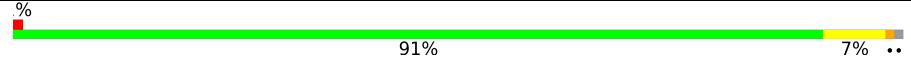
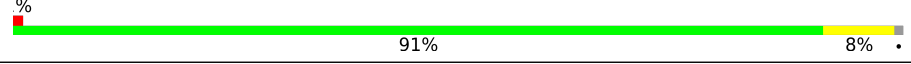
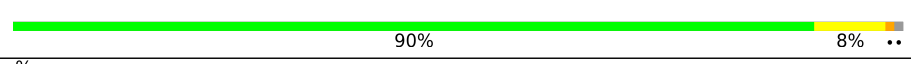

The reported resolution of this entry is 1.80 Å.

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  $\geq 3$ , 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  $\leq 5\%$ . 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	368	
1	B	368	
1	C	368	
1	D	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	370	-	-	X	-
3	GOL	D	370	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13752 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 Putative succinylglutamate desuccinylase / aspartoacylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	365	2949	1885	509	541	5	9	0	10	0
1	B	365	2952	1888	507	544	4	9	0	10	0
1	C	366	2980	1904	515	548	4	9	0	12	0
1	D	365	3002	1917	520	552	4	9	0	16	0

There are 4 discrepancies between the modelled and reference sequences:

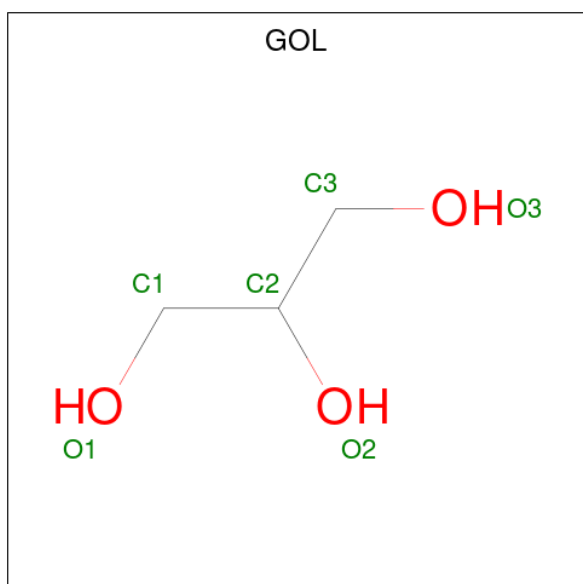
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A1S356
B	0	GLY	-	expression tag	UNP A1S356
C	0	GLY	-	expression tag	UNP A1S356
D	0	GLY	-	expression tag	UNP A1S356

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

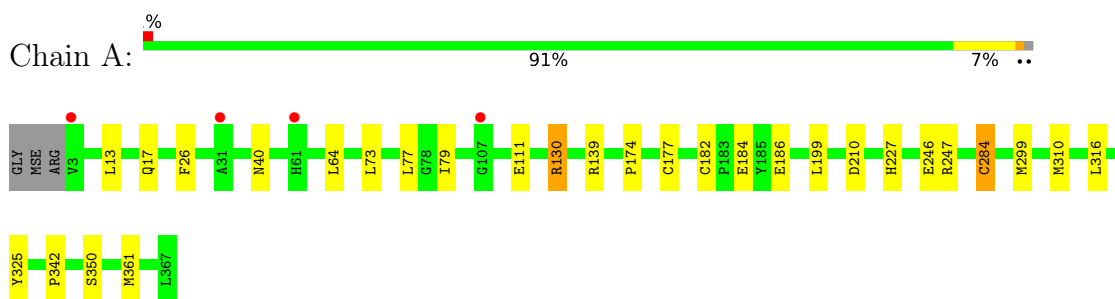
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	459	Total O 469 469	0	10
4	B	425	Total O 433 433	0	8
4	C	436	Total O 446 446	0	10
4	D	439	Total O 448 448	0	9

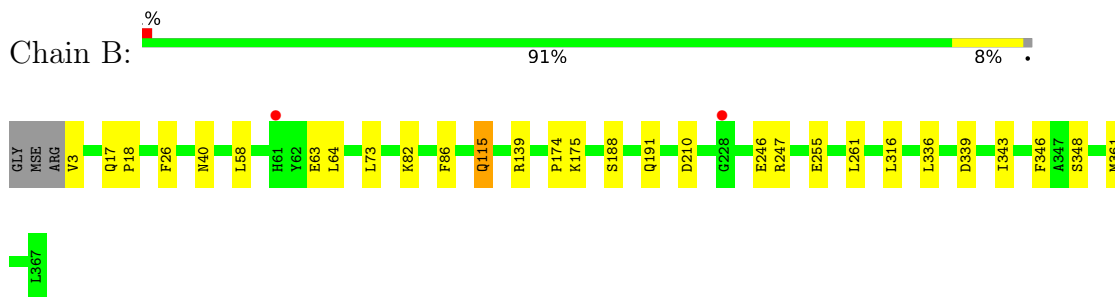
### 3 Residue-property plots [i](#)

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.

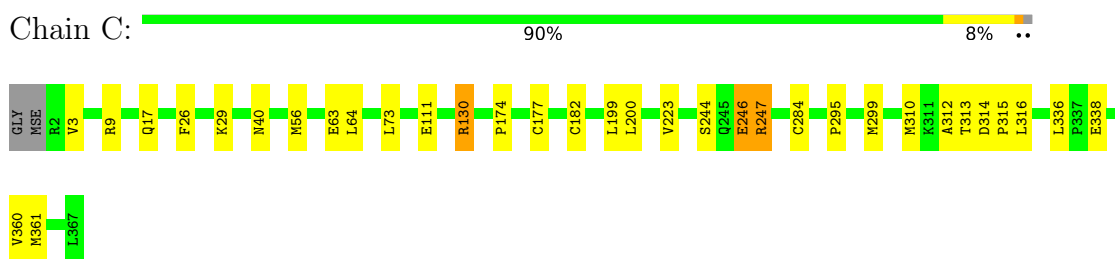
- Molecule 1: Putative succinylglutamate desuccinylase / aspartoacylase



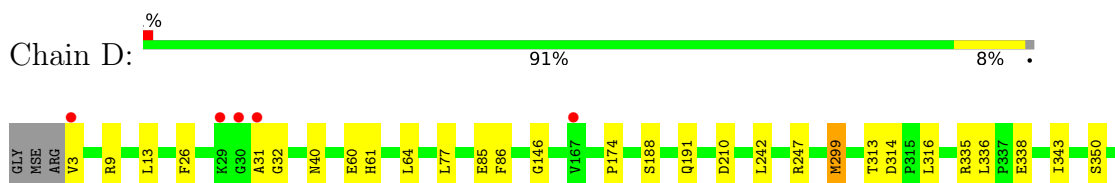
- Molecule 1: Putative succinylglutamate desuccinylase / aspartoacylase



- Molecule 1: Putative succinylglutamate desuccinylase / aspartoacylase



- Molecule 1: Putative succinylglutamate desuccinylase / aspartoacylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.28Å 140.10Å 164.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 1.80 29.73 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.73-1.80) 88.2 (29.73-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, $R_{free}$	0.155 , 0.187 0.160 , 0.190	Depositor DCC
$R_{free}$ test set	9270 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.82	3/3013 (0.1%)	0.87	6/4081 (0.1%)
1	B	0.76	2/3017 (0.1%)	0.84	4/4088 (0.1%)
1	C	0.78	2/3044 (0.1%)	0.84	3/4124 (0.1%)
1	D	0.75	0/3068	0.82	2/4158 (0.0%)
All	All	0.78	7/12142 (0.1%)	0.85	15/16451 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	GLU	CD-OE2	-6.21	1.18	1.25
1	A	284	CYS	CB-SG	-6.14	1.71	1.82
1	A	177	CYS	CB-SG	-6.00	1.72	1.82
1	B	246	GLU	CG-CD	5.72	1.60	1.51
1	C	177	CYS	CB-SG	-5.62	1.72	1.81
1	C	246	GLU	CD-OE2	-5.50	1.19	1.25
1	A	246	GLU	CD-OE2	-5.02	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	D	210	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	130	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	247[A]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	247[B]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	247[A]	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	247[B]	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	316	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	339	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	210	ASP	CB-CG-OD1	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	175[A]	LYS	N-CA-C	-5.12	97.18	111.00
1	B	175[B]	LYS	N-CA-C	-5.12	97.18	111.00
1	A	210	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	130	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2949	0	2917	21	0
1	B	2952	0	2909	27	0
1	C	2980	0	2952	34	0
1	D	3002	0	2950	34	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	6	0	8	1	0
3	B	18	0	24	4	0
3	C	6	0	8	1	0
3	D	18	0	24	7	0
4	A	469	0	0	3	0
4	B	433	0	0	5	0
4	C	446	0	0	3	0
4	D	448	0	0	9	0
All	All	13752	0	11792	104	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 4.

All (104) 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:73:LEU:HD21	1:C:299[C]:MSE:HE3	1.47	0.96
1:C:295:PRO:HB3	3:D:370:GOL:H2	1.55	0.87
1:B:115:GLN:HE21	1:B:115:GLN:HA	1.41	0.86
1:C:316:LEU:HD22	1:C:336[A]:LEU:HD23	1.56	0.85
1:A:73:LEU:CD2	1:C:299[C]:MSE:HE3	2.12	0.79
1:A:299[C]:MSE:HE3	1:C:73:LEU:CD2	2.15	0.76
1:C:29:LYS:O	1:C:29:LYS:HG3	1.85	0.75
1:A:299[C]:MSE:HE3	1:C:73:LEU:HD21	1.70	0.74
1:D:146:GLY:N	3:D:370:GOL:H11	2.03	0.73
1:B:58:LEU:HD13	1:B:261:LEU:HD12	1.70	0.72
1:B:58:LEU:HD13	1:B:261:LEU:CD1	2.21	0.71
1:B:316:LEU:HD13	1:B:336[B]:LEU:HD13	1.72	0.70
1:B:73:LEU:CD2	1:D:299[C]:MSE:HE3	2.22	0.69
1:C:29:LYS:NZ	1:C:63:GLU:OE2	2.26	0.68
1:C:199:LEU:HG	1:C:361:MSE:HE2	1.75	0.66
1:D:3:VAL:HG22	1:D:26:PHE:CE2	2.30	0.66
1:B:316:LEU:HD13	1:B:336[B]:LEU:CD1	2.25	0.66
1:C:246:GLU:OE1	4:C:1023:HOH:O	2.14	0.65
1:B:73:LEU:HD21	1:D:299[C]:MSE:HE3	1.78	0.64
1:D:31:ALA:C	4:D:1048:HOH:O	2.35	0.64
1:C:29:LYS:O	1:C:29:LYS:CG	2.46	0.63
1:B:17[A]:GLN:HE22	1:C:17:GLN:HG2	1.63	0.63
1:C:3:VAL:HG22	1:C:26:PHE:CE2	2.35	0.62
1:C:316:LEU:HD22	1:C:336[A]:LEU:CD2	2.30	0.62
4:C:1205:HOH:O	3:D:370:GOL:H32	2.01	0.60
1:D:60[B]:GLU:HG2	1:D:61[B]:HIS:CE1	2.37	0.60
1:B:73:LEU:CD2	1:D:299[C]:MSE:CE	2.80	0.59
1:A:199:LEU:HG	1:A:361:MSE:HE2	1.85	0.57
1:D:146:GLY:HA3	3:D:370:GOL:H12	1.86	0.57
1:B:188:SER:O	1:B:191[A]:GLN:HG2	2.04	0.57
1:A:182[B]:CYS:SG	1:A:186:GLU:O	2.63	0.56
1:D:146:GLY:CA	3:D:370:GOL:H11	2.36	0.56
1:B:139:ARG:HD3	4:B:963:HOH:O	2.06	0.56
1:B:17[A]:GLN:HE22	1:C:17:GLN:CG	2.17	0.55
1:B:115:GLN:HA	1:B:115:GLN:NE2	2.18	0.55
1:B:3:VAL:HG22	1:B:26:PHE:CE2	2.41	0.55
1:D:314[A]:ASP:O	4:D:1458:HOH:O	2.16	0.53
1:D:85:GLU:O	1:D:86[A]:PHE:CG	2.62	0.53
1:B:247[A]:ARG:CD	3:B:370:GOL:H2	2.40	0.52
1:D:188:SER:O	1:D:191[B]:GLN:HG2	2.08	0.52
1:A:111:GLU:OE2	1:A:227:HIS:CE1	2.62	0.52
1:D:313[B]:THR:O	1:D:335:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:D:299[C]:MSE:CE	2.38	0.52
1:B:86[A]:PHE:HZ	4:D:1189:HOH:O	1.92	0.52
1:D:146:GLY:HA3	3:D:370:GOL:C1	2.41	0.51
1:A:13:LEU:HD21	1:A:77:LEU:HD13	1.93	0.50
1:D:336[A]:LEU:HG	1:D:338:GLU:O	2.11	0.50
1:D:146:GLY:CA	3:D:370:GOL:C1	2.90	0.50
1:A:139[A]:ARG:CZ	1:A:139[A]:ARG:HB2	2.42	0.50
1:A:299[A]:MSE:SE	1:A:350:SER:HB3	2.61	0.50
1:C:316:LEU:CD2	1:C:336[A]:LEU:HD23	2.35	0.49
1:D:3:VAL:HG22	1:D:26:PHE:CZ	2.48	0.49
1:B:247[B]:ARG:HD3	3:B:370:GOL:H2	1.95	0.49
1:D:343:ILE:CD1	1:D:361:MSE:HE3	2.43	0.48
1:C:130:ARG:HE	3:C:369:GOL:H32	1.77	0.48
1:C:17:GLN:NE2	4:C:444:HOH:O	2.45	0.48
1:C:26:PHE:HB3	1:C:64:LEU:HD22	1.94	0.48
1:D:32:GLY:N	4:D:1048:HOH:O	2.47	0.48
1:C:336[A]:LEU:HD11	1:C:360:VAL:HG21	1.95	0.47
1:D:299[B]:MSE:SE	1:D:350:SER:HB3	2.64	0.46
1:D:316:LEU:HD22	1:D:336[B]:LEU:CD2	2.44	0.46
1:B:17[A]:GLN:HG2	1:B:18:PRO:HD2	1.98	0.46
1:B:82:LYS:HD3	1:B:86[A]:PHE:O	2.16	0.46
1:B:346:PHE:CE2	1:B:348:SER:HB3	2.50	0.46
1:C:29:LYS:CE	1:C:63:GLU:OE2	2.63	0.46
1:C:316:LEU:HD13	1:C:336[A]:LEU:HG	1.97	0.46
1:D:316:LEU:HD13	1:D:336[B]:LEU:HG	1.97	0.46
1:B:73:LEU:HD23	1:D:299[C]:MSE:HE3	1.98	0.46
1:D:13:LEU:HD21	1:D:77:LEU:HD13	1.97	0.46
1:C:336[A]:LEU:CD1	1:C:360:VAL:HG11	2.46	0.46
1:A:17:GLN:HG2	4:A:845:HOH:O	2.16	0.45
1:C:312[B]:ALA:C	1:C:313[B]:THR:HG23	2.37	0.45
1:A:79:ILE:CG2	1:C:299[B]:MSE:HE1	2.47	0.45
1:C:310:MSE:HE3	1:C:314[A]:ASP:HB2	1.99	0.45
1:B:343:ILE:HG13	1:B:361:MSE:HE3	1.98	0.45
1:A:17:GLN:NE2	4:A:942:HOH:O	2.49	0.45
1:D:9[B]:ARG:NH1	4:D:1329:HOH:O	2.50	0.45
3:B:370:GOL:H12	4:B:1104:HOH:O	2.17	0.44
1:A:310:MSE:SE	1:A:342:PRO:HG3	2.67	0.44
1:C:244:SER:O	1:C:247[A]:ARG:HD3	2.17	0.44
1:C:314[A]:ASP:HA	1:C:315:PRO:HD3	1.87	0.44
1:D:316:LEU:HD22	1:D:336[B]:LEU:HD23	1.99	0.44
1:B:63:GLU:OE1	4:B:1401:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17[A]:GLN:HE22	1:C:17:GLN:HB3	1.83	0.43
1:A:139[A]:ARG:HB2	1:A:139[A]:ARG:NH1	2.33	0.43
1:D:191[A]:GLN:HG2	4:D:806:HOH:O	2.17	0.43
1:A:299[B]:MSE:SE	1:A:299[B]:MSE:N	3.02	0.42
1:C:182:CYS:O	1:C:200:LEU:HA	2.19	0.42
1:B:255[B]:GLU:HG3	4:B:426:HOH:O	2.19	0.42
1:A:184:GLU:OE2	4:A:705:HOH:O	2.22	0.42
1:D:242:LEU:O	1:D:247[A]:ARG:NH2	2.53	0.42
1:D:336[A]:LEU:CB	4:D:1458:HOH:O	2.67	0.42
1:A:73:LEU:CD2	1:C:299[C]:MSE:CE	2.93	0.41
1:A:130:ARG:HH11	3:A:369:GOL:C1	2.33	0.41
1:C:336[B]:LEU:HG	1:C:338[B]:GLU:O	2.20	0.41
1:B:26:PHE:HB3	1:B:64:LEU:HD22	2.02	0.41
3:B:370:GOL:C1	4:B:1104:HOH:O	2.67	0.41
1:A:26:PHE:HB3	1:A:64:LEU:CD2	2.49	0.41
1:D:343:ILE:HG13	1:D:361:MSE:HE3	2.02	0.41
1:D:31:ALA:CA	4:D:1048:HOH:O	2.69	0.40
1:C:111:GLU:OE1	1:C:223:VAL:HG13	2.22	0.40
1:D:31:ALA:HB1	4:D:1048:HOH:O	2.21	0.40
1:A:325:TYR:CD1	1:C:56:MSE:HE3	2.56	0.40
1:D:26:PHE:HB3	1:D:64:LEU:HD22	2.03	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	374/368 (102%)	367 (98%)	6 (2%)	1 (0%)	41	27
1	B	374/368 (102%)	368 (98%)	5 (1%)	1 (0%)	41	27
1	C	377/368 (102%)	370 (98%)	6 (2%)	1 (0%)	41	27
1	D	380/368 (103%)	374 (98%)	5 (1%)	1 (0%)	41	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1505/1472 (102%)	1479 (98%)	22 (2%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	PRO
1	C	174	PRO
1	D	174	PRO
1	A	174	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	313/298 (105%)	311 (99%)	2 (1%)	86	84
1	B	313/298 (105%)	311 (99%)	2 (1%)	86	84
1	C	316/298 (106%)	313 (99%)	3 (1%)	78	75
1	D	317/298 (106%)	313 (99%)	4 (1%)	69	62
All	All	1259/1192 (106%)	1248 (99%)	11 (1%)	84	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	284	CYS
1	B	40	ASN
1	B	115	GLN
1	C	9	ARG
1	C	40	ASN
1	C	284	CYS
1	D	40	ASN
1	D	299[A]	MSE
1	D	299[B]	MSE
1	D	299[C]	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	B	115	GLN
1	C	115	GLN
1	C	227	HIS
1	D	6	HIS
1	D	227	HIS

### 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	$\# Z  > 2$
3	GOL	D	371	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	D	372	-	5,5,5	0.37	0	5,5,5	0.44	0
2	SO4	A	368	-	4,4,4	0.38	0	6,6,6	0.62	0
3	GOL	B	371	-	5,5,5	0.54	0	5,5,5	0.84	0
3	GOL	D	370	-	5,5,5	0.59	0	5,5,5	1.00	1 (20%)
2	SO4	C	368	-	4,4,4	0.26	0	6,6,6	0.59	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	370	-	5,5,5	0.70	0	5,5,5	0.79	0
3	GOL	C	369	-	5,5,5	0.42	0	5,5,5	0.59	0
2	SO4	D	369	-	4,4,4	0.23	0	6,6,6	0.20	0
3	GOL	A	369	-	5,5,5	0.56	0	5,5,5	1.05	0
2	SO4	B	368	-	4,4,4	0.26	0	6,6,6	0.86	0
2	SO4	D	368	-	4,4,4	0.28	0	6,6,6	0.80	0
3	GOL	B	369	-	5,5,5	0.50	0	5,5,5	0.35	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
3	GOL	D	371	-	-	0/4/4/4	-
3	GOL	D	372	-	-	0/4/4/4	-
3	GOL	B	371	-	-	1/4/4/4	-
3	GOL	D	370	-	-	2/4/4/4	-
3	GOL	B	370	-	-	4/4/4/4	-
3	GOL	C	369	-	-	3/4/4/4	-
3	GOL	A	369	-	-	4/4/4/4	-
3	GOL	B	369	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	370	GOL	O1-C1-C2	2.04	119.99	110.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	369	GOL	O1-C1-C2-C3
3	A	369	GOL	C1-C2-C3-O3
3	B	370	GOL	O1-C1-C2-O2
3	B	370	GOL	O1-C1-C2-C3
3	B	370	GOL	C1-C2-C3-O3
3	C	369	GOL	C1-C2-C3-O3
3	C	369	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	370	GOL	C1-C2-C3-O3
3	A	369	GOL	O2-C2-C3-O3
3	A	369	GOL	O1-C1-C2-O2
3	B	370	GOL	O2-C2-C3-O3
3	D	370	GOL	O2-C2-C3-O3
3	B	371	GOL	O1-C1-C2-O2
3	C	369	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	370	GOL	7	0
3	B	370	GOL	4	0
3	C	369	GOL	1	0
3	A	369	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/368 (97%)	-0.56	4 (1%) 80 78	12, 17, 32, 46	0
1	B	358/368 (97%)	-0.50	2 (0%) 89 87	11, 19, 38, 58	0
1	C	359/368 (97%)	-0.57	0 100 100	11, 18, 35, 54	0
1	D	358/368 (97%)	-0.46	5 (1%) 75 72	11, 19, 39, 49	0
All	All	1433/1472 (97%)	-0.52	11 (0%) 86 84	11, 18, 36, 58	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	4.4
1	D	3	VAL	4.3
1	A	61	HIS	2.7
1	B	61	HIS	2.6
1	A	3	VAL	2.4
1	A	31	ALA	2.3
1	B	228	GLY	2.3
1	D	29	LYS	2.2
1	A	107	GLY	2.2
1	D	167	VAL	2.2
1	D	30	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	B	369	6/6	0.68	0.16	56,60,63,65	0
2	SO4	D	369	5/5	0.74	0.21	88,91,93,94	0
3	GOL	D	372	6/6	0.85	0.18	32,46,56,57	0
3	GOL	A	369	6/6	0.86	0.16	29,45,47,53	0
3	GOL	C	369	6/6	0.87	0.20	26,41,44,48	0
3	GOL	B	370	6/6	0.89	0.16	16,38,48,48	0
3	GOL	D	371	6/6	0.90	0.12	27,37,43,47	0
3	GOL	D	370	6/6	0.91	0.22	25,45,50,55	0
3	GOL	B	371	6/6	0.93	0.23	15,36,45,50	0
2	SO4	D	368	5/5	0.98	0.06	24,36,37,43	0
2	SO4	B	368	5/5	0.99	0.06	17,25,30,38	0
2	SO4	C	368	5/5	0.99	0.10	19,29,39,43	0
2	SO4	A	368	5/5	0.99	0.06	20,29,34,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.