



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 10:43 AM EDT

PDB ID : 2QAA  
Title : Crystal structure of the second tetrahedral intermediates of SGPB at pH 7.3  
Authors : Lee, T.W.; James, M.N.G.  
Deposited on : 2007-06-14  
Resolution : 1.23 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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
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

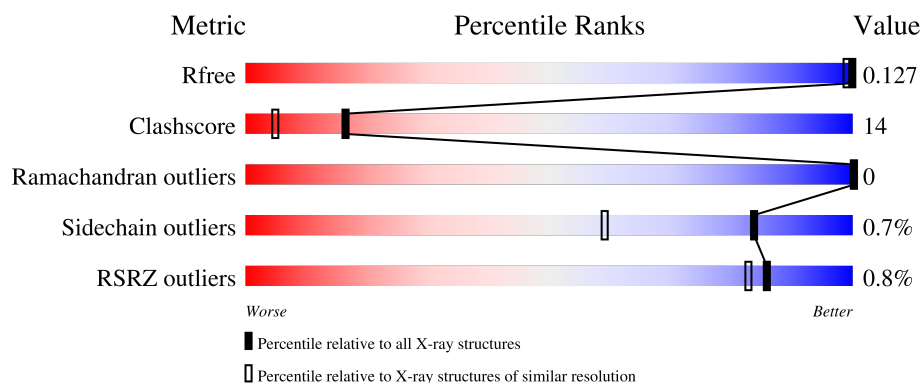
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.23 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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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	185	 90% 10%
1	B	185	 2% 90% 9%

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	CL	A	945[A]	-	-	X	-
3	CL	A	957[A]	-	-	X	-
3	CL	A	957[B]	-	-	X	-
4	TYR	A	1[A]	-	-	X	-
4	TYR	B	1[A]	-	-	X	-
5	LEU	A	2[B]	-	-	X	-
5	LEU	B	2[B]	-	X	X	-
6	EDO	A	921	-	-	X	-
6	EDO	A	923	-	X	X	-
7	EPE	A	961	-	-	X	-
9	ACY	A	931	-	-	X	-
9	ACY	A	933[A]	-	-	X	-
9	ACY	A	933[B]	-	X	X	-
9	ACY	B	932	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3397 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 Streptogrisin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	15	0
			1353	823	229	293	8			
1	B	185	Total	C	N	O	S	0	10	0
			1342	816	231	288	7			

- 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	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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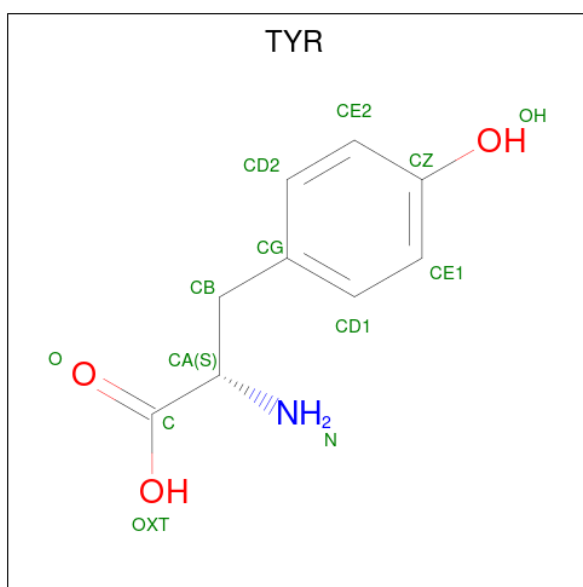
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

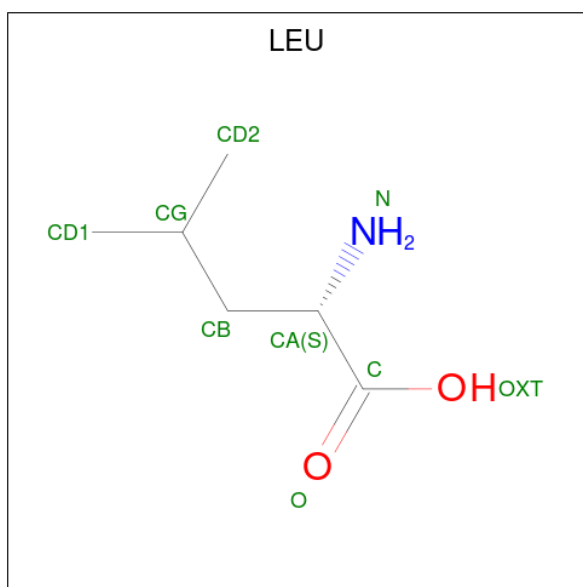
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	3
			7	7		
3	B	6	Total	Cl	0	5
			11	11		

- Molecule 4 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



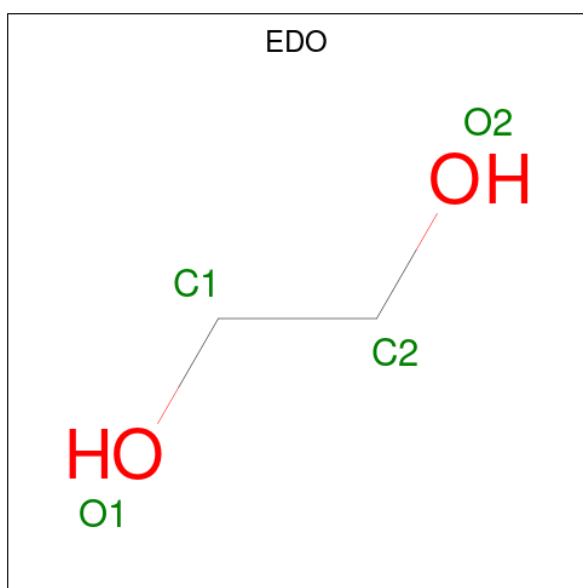
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			13	9	1	3		
4	B	1	Total	C	N	O	0	1
			13	9	1	3		

- Molecule 5 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			9	6	1	2		
5	B	1	Total	C	N	O	0	1
			9	6	1	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



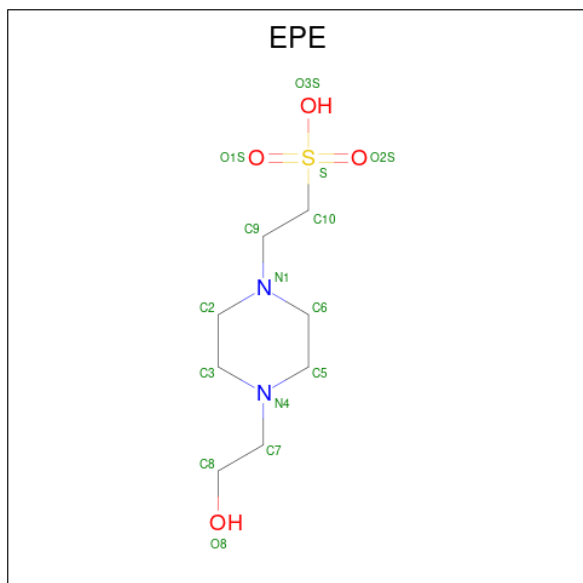
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



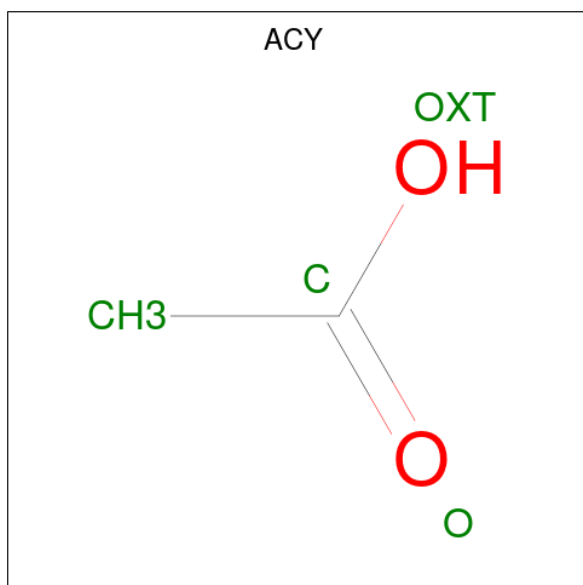
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	1
			8	4	4		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 8 4 4	0	1
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	278	Total O 290 290	0	12
10	B	243	Total O 252 252	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: Streptogrisin-B

Chain A:  90% 10%



- Molecule 1: Streptogrisin-B

Chain B:  2% 90% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.29Å 142.29Å 142.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.23 38.03 – 1.23	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-1.23) 99.0 (38.03-1.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.23Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.113 , 0.127 0.113 , 0.127	Depositor DCC
$R_{free}$ test set	6843 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: CL, EDO, ACY, SO4, GOL, EPE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.08	6/1448 (0.4%)	1.03	3/1972 (0.2%)
1	B	1.16	7/1413 (0.5%)	1.12	9/1924 (0.5%)
All	All	1.12	13/2861 (0.5%)	1.08	12/3896 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	-7.39	1.36	1.77
1	B	126	SER	CA-CB	6.63	1.62	1.52
1	A	161[A]	SER	CB-OG	-6.16	1.34	1.42
1	A	161[B]	SER	CB-OG	-6.16	1.34	1.42
1	B	103	TYR	CE1-CZ	-6.02	1.30	1.38
1	A	200	TYR	CD1-CE1	5.97	1.48	1.39
1	B	222	SER	CA-CB	-5.78	1.44	1.52
1	B	222	SER	CB-OG	-5.38	1.35	1.42
1	B	42[A]	CYS	CB-SG	5.36	1.91	1.82
1	B	42[B]	CYS	CB-SG	5.36	1.91	1.82
1	A	201	SER	CB-OG	-5.36	1.35	1.42
1	B	221	SER	CB-OG	-5.29	1.35	1.42
1	A	129	ASN	CG-OD1	-5.26	1.12	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	208	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	208	ARG	CA-CB-CG	7.55	130.02	113.40
1	B	208[A]	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	B	208[B]	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	B	81	ARG	NE-CZ-NH2	-6.71	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	182	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	81	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	60[A]	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	60[B]	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	81	ARG	CB-CA-C	5.04	120.47	110.40

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	1353	0	1249	20	0
1	B	1342	0	1251	17	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	A	7	0	0	12	0
3	B	11	0	0	3	0
4	A	13	0	11	7	0
4	B	13	0	11	8	0
5	A	9	0	10	6	0
5	B	9	0	10	12	0
6	A	12	0	18	12	0
6	B	4	0	6	0	0
7	A	15	0	17	7	0
8	A	6	0	7	2	0
8	B	20	0	23	2	0
9	A	12	0	10	8	0
9	B	4	0	3	6	0
10	A	290	0	0	18	0
10	B	252	0	0	9	0
All	All	3397	0	2626	78	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 14.

All (78) 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)
6:A:923:EDO:C2	6:A:923:EDO:O2	1.67	1.42
6:A:921:EDO:O2	6:A:921:EDO:C2	1.66	1.40
1:B:195:SER:OG	5:B:2[B]:LEU:C	1.69	1.30
1:B:195:SER:OG	4:B:1[A]:TYR:C	1.69	1.30
3:A:957[A]:CL:CL	9:A:933[A]:ACY:CH3	2.21	1.25
3:A:957[A]:CL:CL	9:A:933[A]:ACY:H3	1.76	1.23
1:A:60[B]:ASP:OD1	10:A:1220:HOH:O	1.58	1.15
4:A:1[A]:TYR:CE1	10:A:1146:HOH:O	2.00	1.14
1:A:60[C]:ASP:OD2	10:A:1050:HOH:O	1.68	1.10
3:A:957[B]:CL:CL	10:A:1238:HOH:O	2.05	1.09
4:A:1[A]:TYR:O	10:A:1235:HOH:O	1.81	0.98
5:A:2[B]:LEU:O	10:A:1235:HOH:O	1.81	0.98
1:B:126:SER:OG	1:B:208[A]:ARG:NE	2.00	0.93
4:A:1[A]:TYR:OXT	10:A:1235:HOH:O	1.88	0.91
5:A:2[B]:LEU:OXT	10:A:1235:HOH:O	1.88	0.91
1:B:195:SER:HG	5:B:2[B]:LEU:C	1.70	0.89
1:B:195:SER:HG	4:B:1[A]:TYR:C	1.70	0.89
3:A:957[A]:CL:CL	9:A:933[A]:ACY:H2	2.09	0.87
1:B:208[A]:ARG:NH2	10:B:1184:HOH:O	1.86	0.87
3:A:957[A]:CL:CL	10:A:1239:HOH:O	2.30	0.85
3:A:945[A]:CL:CL	9:A:931:ACY:H2	2.19	0.80
4:A:1[A]:TYR:CD1	10:A:1146:HOH:O	2.30	0.80
3:B:944:CL:CL	10:B:1006:HOH:O	2.37	0.78
3:A:945[A]:CL:CL	10:A:1203:HOH:O	2.42	0.73
4:A:1[A]:TYR:HE2	10:A:1046:HOH:O	1.70	0.73
3:A:957[B]:CL:CL	10:A:1239:HOH:O	2.43	0.73
3:A:957[B]:CL:CL	9:A:933[B]:ACY:H3	2.27	0.72
4:A:1[A]:TYR:CE2	10:A:1046:HOH:O	2.45	0.69
7:A:961:EPE:N4	9:B:932:ACY:H1	2.08	0.68
1:A:48(A):ARG:HE	6:A:923:EDO:C2	2.07	0.67
3:A:950[B]:CL:CL	10:A:1213:HOH:O	2.51	0.65
3:A:945[A]:CL:CL	9:A:931:ACY:CH3	2.84	0.63
1:A:166[A]:ASN:HD22	1:A:179:GLY:HA2	1.63	0.62
1:A:48(A):ARG:HE	6:A:923:EDO:H21	1.63	0.62
4:B:1[A]:TYR:HE1	10:B:1013:HOH:O	1.84	0.61
1:A:19:GLY:O	6:A:921:EDO:H22	2.00	0.60
5:B:2[B]:LEU:N	10:B:1178:HOH:O	2.35	0.60
1:B:195:SER:OG	4:B:1[A]:TYR:CA	2.50	0.60
1:A:240[A]:SER:OG	6:A:923:EDO:H22	2.03	0.58
6:A:921:EDO:C2	6:A:921:EDO:HO2	2.10	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1[A]:TYR:N	8:B:902:GOL:O1	2.37	0.57
5:B:2[B]:LEU:N	8:B:902:GOL:O1	2.37	0.57
1:A:87[A]:THR:HG21	7:A:961:EPE:H92	1.86	0.56
5:A:2[B]:LEU:N	8:A:901:GOL:O1	2.38	0.55
4:B:1[A]:TYR:CE1	10:B:1013:HOH:O	2.53	0.55
1:A:87[A]:THR:HG21	7:A:961:EPE:H62	1.88	0.55
4:A:1[A]:TYR:N	8:A:901:GOL:O1	2.38	0.54
1:B:195:SER:OG	5:B:2[B]:LEU:HD23	2.08	0.54
7:A:961:EPE:H22	9:B:932:ACY:H1	1.89	0.53
7:A:961:EPE:N4	9:B:932:ACY:CH3	2.72	0.53
1:A:233[B]:GLU:HG3	10:A:1123:HOH:O	2.08	0.53
1:B:213:THR:HG22	5:B:2[B]:LEU:HD21	1.90	0.52
1:A:48(A):ARG:NE	6:A:923:EDO:H21	2.25	0.51
1:B:64[A]:THR:OG1	3:B:946[A]:CL:CL	2.66	0.50
5:B:2[B]:LEU:HA	10:B:1178:HOH:O	2.12	0.50
6:A:923:EDO:C2	6:A:923:EDO:HO2	2.11	0.49
1:B:195:SER:CB	4:B:1[A]:TYR:C	2.76	0.48
1:B:195:SER:CB	5:B:2[B]:LEU:C	2.76	0.48
5:B:2[B]:LEU:CA	10:B:1178:HOH:O	2.62	0.47
1:A:215:GLY:HA2	5:A:2[B]:LEU:HD22	1.96	0.47
1:B:215:GLY:HA2	5:B:2[B]:LEU:HD22	1.97	0.47
1:B:240:SER:OG	9:B:932:ACY:H3	2.15	0.46
5:B:2[B]:LEU:N	5:B:2[B]:LEU:HD22	2.29	0.46
1:A:233[B]:GLU:CG	10:A:1123:HOH:O	2.63	0.46
1:A:202:GLY:HA3	9:A:933[B]:ACY:H1	1.97	0.45
1:A:60[C]:ASP:CG	10:A:1050:HOH:O	2.36	0.45
1:B:107:ARG:HD2	10:B:1187[A]:HOH:O	2.16	0.45
1:B:158:HIS:HE1	3:B:952[A]:CL:CL	2.37	0.44
7:A:961:EPE:C2	9:B:932:ACY:H1	2.49	0.43
1:A:240[B]:SER:HB2	6:A:923:EDO:H22	2.00	0.43
1:A:48(A):ARG:HH21	6:A:923:EDO:C1	2.30	0.43
1:B:192(B):PRO:HA	5:B:2[B]:LEU:HB2	2.01	0.43
4:B:1[A]:TYR:N	10:B:1178:HOH:O	2.35	0.42
1:A:213:THR:HG22	5:A:2[B]:LEU:HD21	2.01	0.41
3:A:957[B]:CL:CL	9:A:933[B]:ACY:CH3	3.04	0.41
1:A:140:GLY:O	6:A:921:EDO:H11	2.20	0.41
7:A:961:EPE:C3	9:B:932:ACY:H1	2.52	0.40
1:A:215:GLY:HA2	5:A:2[B]:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	200/185 (108%)	192 (96%)	8 (4%)	0	100	100
1	B	194/185 (105%)	185 (95%)	9 (5%)	0	100	100
All	All	394/370 (106%)	377 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	155/138 (112%)	155 (100%)	0	100	100
1	B	149/138 (108%)	149 (100%)	0	100	100
All	All	304/276 (110%)	304 (100%)	0	84	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	129	ASN
1	B	100	ASN
1	B	101	ASN



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 18 are monoatomic - leaving 23 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	913	-	4,4,4	1.03	0	6,6,6	1.49	1 (16%)
4	TYR	A	1[A]	-	12,13,13	3.61	6 (50%)	13,17,17	3.38	6 (46%)
4	TYR	B	1[A]	-	12,13,13	2.57	4 (33%)	13,17,17	3.02	6 (46%)
5	LEU	B	2[B]	-	6,8,8	2.87	2 (33%)	5,10,10	4.02	2 (40%)
8	GOL	B	904	-	5,5,5	1.42	1 (20%)	5,5,5	2.01	2 (40%)
6	EDO	A	921	-	3,3,3	3.18	2 (66%)	2,2,2	0.14	0
2	SO4	B	911	-	4,4,4	0.76	0	6,6,6	1.09	0
2	SO4	B	915	-	4,4,4	1.21	1 (25%)	6,6,6	1.21	0
9	ACY	A	931	-	3,3,3	3.24	2 (66%)	3,3,3	1.34	0
5	LEU	A	2[B]	-	6,8,8	3.44	2 (33%)	5,10,10	5.06	2 (40%)
8	GOL	B	903[B]	-	5,5,5	2.05	2 (40%)	5,5,5	1.09	1 (20%)
9	ACY	A	933[A]	-	3,3,3	3.04	2 (66%)	3,3,3	1.20	0
2	SO4	B	914	-	4,4,4	0.39	0	6,6,6	1.88	2 (33%)
7	EPE	A	961	-	15,15,15	1.66	2 (13%)	19,20,20	1.87	3 (15%)
2	SO4	A	912	-	4,4,4	0.90	0	6,6,6	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ACY	B	932	-	3,3,3	1.24	0	3,3,3	2.75	1 (33%)
6	EDO	A	922	-	3,3,3	0.95	0	2,2,2	0.85	0
6	EDO	B	924	-	3,3,3	0.87	0	2,2,2	0.75	0
8	GOL	A	901	-	5,5,5	2.07	1 (20%)	5,5,5	1.46	1 (20%)
8	GOL	B	902	-	5,5,5	1.24	0	5,5,5	2.37	2 (40%)
6	EDO	A	923	-	3,3,3	3.89	3 (100%)	2,2,2	0.66	0
9	ACY	A	933[B]	-	3,3,3	3.28	2 (66%)	3,3,3	1.88	2 (66%)
8	GOL	B	903[A]	-	5,5,5	1.46	1 (20%)	5,5,5	1.57	2 (40%)

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
6	EDO	A	923	-	-	1/1/1/1	-
7	EPE	A	961	-	-	1/9/19/19	0/1/1/1
4	TYR	B	1[A]	-	-	5/8/8/8	0/1/1/1
5	LEU	B	2[B]	-	-	7/8/8/8	-
4	TYR	A	1[A]	-	-	3/8/8/8	0/1/1/1
8	GOL	A	901	-	-	1/4/4/4	-
8	GOL	B	904	-	-	0/4/4/4	-
5	LEU	A	2[B]	-	-	5/8/8/8	-
8	GOL	B	903[B]	-	-	1/4/4/4	-
8	GOL	B	903[A]	-	-	0/4/4/4	-
6	EDO	A	922	-	-	0/1/1/1	-
6	EDO	A	921	-	-	0/1/1/1	-
6	EDO	B	924	-	-	1/1/1/1	-
8	GOL	B	902	-	-	0/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1[A]	TYR	O-C	6.42	1.41	1.22
5	A	2[B]	LEU	O-C	6.42	1.41	1.22
4	A	1[A]	TYR	OXT-C	5.19	1.47	1.30
5	A	2[B]	LEU	OXT-C	5.19	1.47	1.30
9	A	933[B]	ACY	OXT-C	-5.18	1.06	1.30
6	A	923	EDO	O2-C2	5.04	1.67	1.42
4	B	1[A]	TYR	O-C	5.03	1.37	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2[B]	LEU	O-C	5.03	1.37	1.22
9	A	931	ACY	O-C	4.95	1.43	1.22
4	A	1[A]	TYR	CE2-CZ	-4.91	1.29	1.39
7	A	961	EPE	C10-S	-4.89	1.70	1.77
4	B	1[A]	TYR	OXT-C	4.82	1.46	1.30
5	B	2[B]	LEU	OXT-C	4.82	1.46	1.30
6	A	921	EDO	O2-C2	4.79	1.66	1.42
4	A	1[A]	TYR	CE1-CZ	4.67	1.47	1.39
9	A	933[A]	ACY	O-C	4.66	1.42	1.22
4	A	1[A]	TYR	CD1-CG	-4.27	1.30	1.38
4	B	1[A]	TYR	OH-CZ	4.18	1.46	1.37
8	A	901	GOL	O2-C2	-4.06	1.31	1.43
4	A	1[A]	TYR	OH-CZ	3.98	1.45	1.37
6	A	923	EDO	O1-C1	3.61	1.60	1.42
8	B	903[B]	GOL	O3-C3	3.11	1.55	1.42
7	A	961	EPE	C9-N1	2.98	1.54	1.47
4	B	1[A]	TYR	CE2-CZ	2.80	1.44	1.39
6	A	923	EDO	C2-C1	2.64	1.69	1.48
8	B	903[A]	GOL	C1-C2	2.44	1.61	1.51
8	B	903[B]	GOL	C1-C2	2.44	1.61	1.51
9	A	933[A]	ACY	CH3-C	2.36	1.58	1.49
6	A	921	EDO	O1-C1	2.35	1.54	1.42
9	A	931	ACY	OXT-C	2.34	1.41	1.30
2	B	915	SO4	O1-S	2.31	1.58	1.44
9	A	933[B]	ACY	O-C	2.31	1.32	1.22
8	B	904	GOL	O1-C1	-2.30	1.32	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1[A]	TYR	OXT-C-O	-9.70	102.08	124.08
5	A	2[B]	LEU	OXT-C-O	-9.70	102.08	124.08
4	B	1[A]	TYR	OXT-C-O	-8.58	104.62	124.08
5	B	2[B]	LEU	OXT-C-O	-8.58	104.62	124.08
5	A	2[B]	LEU	CB-CA-C	5.46	126.96	110.34
7	A	961	EPE	O1S-S-C10	5.10	114.44	106.73
4	B	1[A]	TYR	OH-CZ-CE1	4.12	131.48	120.00
7	A	961	EPE	O2S-S-C10	-4.03	100.63	106.73
9	B	932	ACY	OXT-C-O	-4.00	107.19	122.03
4	A	1[A]	TYR	OH-CZ-CE2	3.60	130.02	120.00
8	B	902	GOL	O2-C2-C1	3.59	124.03	109.18
4	A	1[A]	TYR	CD1-CE1-CZ	3.49	123.57	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1[A]	TYR	CE2-CZ-CE1	-3.48	114.23	119.77
8	B	904	GOL	O1-C1-C2	-3.45	94.82	110.38
8	B	902	GOL	C3-C2-C1	-3.19	100.11	111.80
8	A	901	GOL	O2-C2-C3	-3.10	96.36	109.18
2	B	914	SO4	O3-S-O1	3.01	125.28	109.56
2	B	914	SO4	O4-S-O2	-3.00	93.88	109.56
2	A	913	SO4	O3-S-O2	-2.91	94.35	109.56
7	A	961	EPE	C3-C2-N1	-2.79	105.02	110.65
4	B	1[A]	TYR	CD1-CE1-CZ	2.68	122.71	119.88
4	B	1[A]	TYR	CE2-CZ-CE1	-2.62	115.59	119.77
4	B	1[A]	TYR	OH-CZ-CE2	-2.54	112.92	120.00
9	A	933[B]	ACY	O-C-CH3	-2.42	112.59	122.53
4	A	1[A]	TYR	CE2-CD2-CG	2.39	124.14	121.00
8	B	904	GOL	C3-C2-C1	-2.21	103.69	111.80
9	A	933[B]	ACY	OXT-C-CH3	2.15	124.09	115.05
8	B	903[A]	GOL	O3-C3-C2	-2.14	100.74	110.38
5	B	2[B]	LEU	CB-CA-C	2.12	116.80	110.34
4	A	1[A]	TYR	CE1-CD1-CG	-2.09	118.25	121.00
4	B	1[A]	TYR	CD2-CE2-CZ	2.07	122.07	119.88
8	B	903[A]	GOL	O2-C2-C1	-2.03	100.77	109.18
8	B	903[B]	GOL	O2-C2-C1	-2.03	100.77	109.18

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2[B]	LEU	CA-CB-CG-CD2
5	B	2[B]	LEU	CA-CB-CG-CD1
5	A	2[B]	LEU	CA-CB-CG-CD1
5	A	2[B]	LEU	CA-CB-CG-CD2
7	A	961	EPE	N4-C7-C8-O8
8	B	903[B]	GOL	C1-C2-C3-O3
6	B	924	EDO	O1-C1-C2-O2
4	A	1[A]	TYR	CA-CB-CG-CD2
6	A	923	EDO	O1-C1-C2-O2
4	A	1[A]	TYR	CA-CB-CG-CD1
5	B	2[B]	LEU	OXT-C-CA-N
8	A	901	GOL	O2-C2-C3-O3
5	B	2[B]	LEU	N-CA-CB-CG
5	A	2[B]	LEU	C-CA-CB-CG
4	B	1[A]	TYR	OXT-C-CA-CB
4	A	1[A]	TYR	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	B	1[A]	TYR	CA-CB-CG-CD1
5	B	2[B]	LEU	C-CA-CB-CG
4	B	1[A]	TYR	O-C-CA-N
4	B	1[A]	TYR	CA-CB-CG-CD2
5	B	2[B]	LEU	OXT-C-CA-CB
5	A	2[B]	LEU	OXT-C-CA-CB
4	B	1[A]	TYR	OXT-C-CA-N
5	B	2[B]	LEU	O-C-CA-CB
5	A	2[B]	LEU	OXT-C-CA-N

There are no ring outliers.

13 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1[A]	TYR	7	0
4	B	1[A]	TYR	8	0
5	B	2[B]	LEU	12	0
6	A	921	EDO	4	0
9	A	931	ACY	2	0
5	A	2[B]	LEU	6	0
9	A	933[A]	ACY	3	0
7	A	961	EPE	7	0
9	B	932	ACY	6	0
8	A	901	GOL	2	0
8	B	902	GOL	2	0
6	A	923	EDO	8	0
9	A	933[B]	ACY	3	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	185/185 (100%)	-0.35	0 100 100	7, 10, 15, 20	0
1	B	185/185 (100%)	-0.30	3 (1%) 72 67	7, 11, 20, 27	1 (0%)
All	All	370/370 (100%)	-0.32	3 (0%) 86 83	7, 10, 18, 27	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	THR	3.9
1	B	112	THR	2.4
1	B	39	THR	2.1

### 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	CL	B	952[A]	1/1	0.45	0.18	38,38,38,38	1
3	CL	B	952[B]	1/1	0.45	0.18	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	950[A]	1/1	0.80	0.09	52,52,52,52	1
3	CL	A	950[B]	1/1	0.80	0.09	28,28,28,28	1
2	SO4	B	915	5/5	0.81	0.17	9,11,16,18	5
9	ACY	A	933[A]	4/4	0.82	0.16	9,11,14,18	4
9	ACY	A	933[B]	4/4	0.82	0.16	6,11,16,17	4
3	CL	A	945[B]	1/1	0.83	0.08	44,44,44,44	1
3	CL	B	954[A]	1/1	0.83	0.07	38,38,38,38	1
3	CL	B	954[B]	1/1	0.83	0.07	41,41,41,41	1
3	CL	B	944	1/1	0.83	0.09	44,44,44,44	1
3	CL	A	945[A]	1/1	0.83	0.08	27,27,27,27	1
5	LEU	A	2[B]	9/9	0.84	0.14	10,16,25,35	9
3	CL	B	946[B]	1/1	0.85	0.15	19,19,19,19	1
3	CL	B	946[A]	1/1	0.85	0.15	31,31,31,31	1
9	ACY	B	932	4/4	0.86	0.16	9,17,23,29	4
5	LEU	B	2[B]	9/9	0.87	0.12	10,17,23,25	9
3	CL	A	957[A]	1/1	0.88	0.10	23,23,23,23	1
3	CL	A	957[B]	1/1	0.88	0.10	37,37,37,37	1
8	GOL	B	902	6/6	0.89	0.14	20,23,31,36	0
3	CL	A	941	1/1	0.89	0.11	45,45,45,45	0
3	CL	B	943[A]	1/1	0.89	0.10	31,31,31,31	1
3	CL	B	943[B]	1/1	0.89	0.10	42,42,42,42	1
9	ACY	A	931	4/4	0.90	0.13	25,26,30,33	0
6	EDO	A	921	4/4	0.90	0.10	15,18,20,33	4
4	TYR	A	1[A]	13/13	0.91	0.16	15,22,27,35	13
6	EDO	A	923	4/4	0.91	0.20	8,13,16,16	4
8	GOL	A	901	6/6	0.91	0.12	22,23,29,30	0
4	TYR	B	1[A]	13/13	0.91	0.12	15,17,21,25	13
3	CL	B	942[B]	1/1	0.92	0.06	40,40,40,40	1
3	CL	B	942[A]	1/1	0.92	0.06	41,41,41,41	1
6	EDO	B	924	4/4	0.94	0.27	24,31,33,35	0
8	GOL	B	903[A]	6/6	0.95	0.10	3,9,11,12	6
8	GOL	B	903[B]	6/6	0.95	0.10	7,11,12,16	6
2	SO4	B	914	5/5	0.95	0.10	15,18,22,26	5
2	SO4	B	911	5/5	0.96	0.10	15,16,23,26	5
2	SO4	A	912	5/5	0.96	0.08	11,11,18,18	5
2	SO4	A	913	5/5	0.97	0.08	14,19,22,28	5
6	EDO	A	922	4/4	0.97	0.09	13,22,25,25	0
7	EPE	A	961	15/15	0.98	0.13	5,15,29,33	15
8	GOL	B	904	6/6	0.98	0.05	9,13,16,16	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.