



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 PM UTC

PDB ID : 6O63 / pdb_00006o63
Title : Crystal Structure of Arabidopsis thaliana Spermidine Synthase isoform 1 (At-SPDS1)
Authors : Sekula, B.; Dauter, Z.
Deposited on : 2019-03-05
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

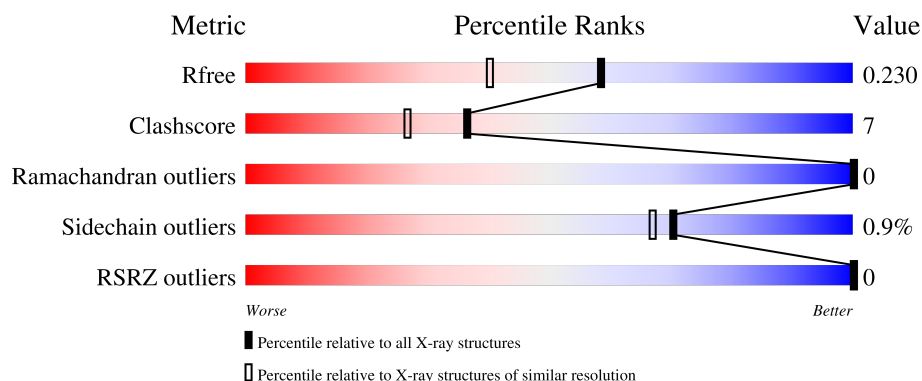
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

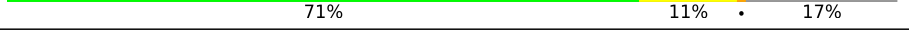
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	337	
1	B	337	
1	C	337	
1	D	337	

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	C	402	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9923 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 Spermidine synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	3	0
			2256	1452	361	427	16			
1	B	286	Total	C	N	O	S	0	4	0
			2228	1434	358	421	15			
1	C	282	Total	C	N	O	S	0	3	0
			2195	1417	352	411	15			
1	D	281	Total	C	N	O	S	0	5	0
			2196	1414	352	415	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9ZUB3
A	-1	ASN	-	expression tag	UNP Q9ZUB3
A	0	ALA	-	expression tag	UNP Q9ZUB3
B	-2	SER	-	expression tag	UNP Q9ZUB3
B	-1	ASN	-	expression tag	UNP Q9ZUB3
B	0	ALA	-	expression tag	UNP Q9ZUB3
C	-2	SER	-	expression tag	UNP Q9ZUB3
C	-1	ASN	-	expression tag	UNP Q9ZUB3
C	0	ALA	-	expression tag	UNP Q9ZUB3
D	-2	SER	-	expression tag	UNP Q9ZUB3
D	-1	ASN	-	expression tag	UNP Q9ZUB3
D	0	ALA	-	expression tag	UNP Q9ZUB3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



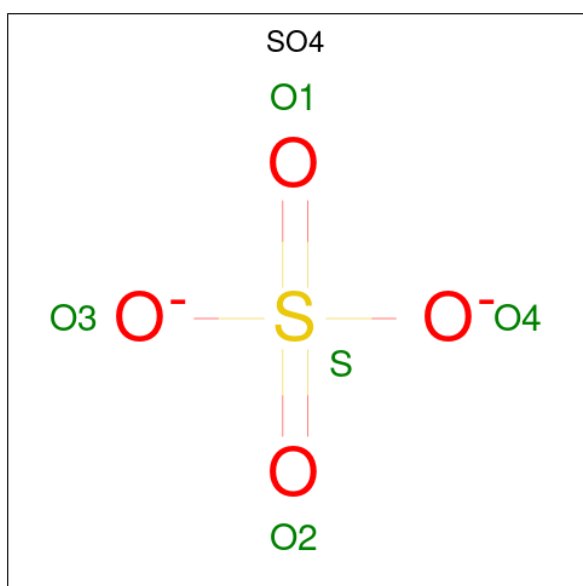
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

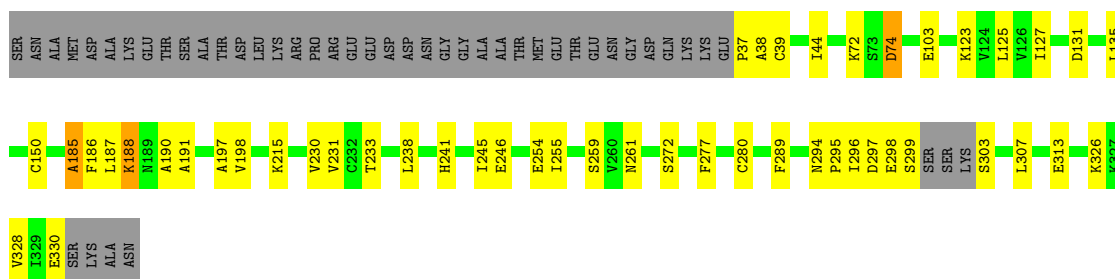
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	287	Total O 287 287	0	0
5	B	230	Total O 230 230	0	0
5	C	237	Total O 237 237	0	0
5	D	232	Total O 232 232	0	0

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.

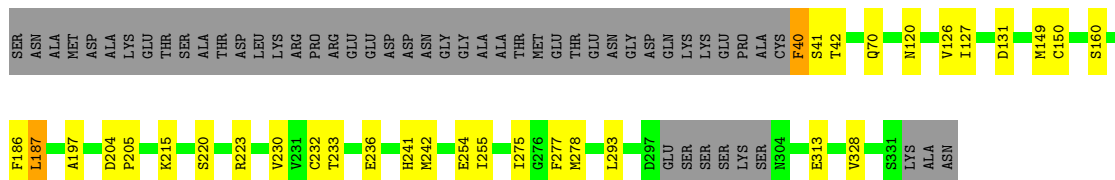
• Molecule 1: Spermidine synthase 1

Chain A: 



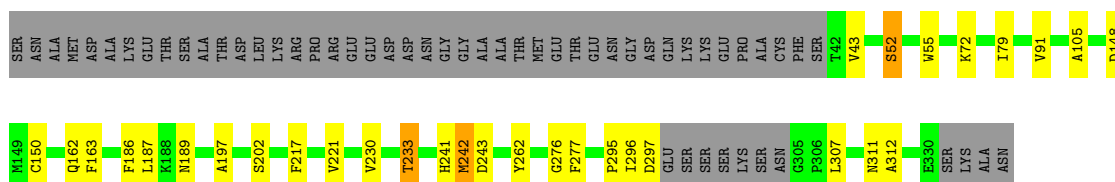
• Molecule 1: Spermidine synthase 1

Chain B: 



• Molecule 1: Spermidine synthase 1

Chain C: 



• Molecule 1: Spermidine synthase 1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.54Å 76.34Å 90.19Å 90.00° 104.68° 90.00°	Depositor
Resolution (Å)	43.46 – 1.80 43.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.9 (43.46-1.80) 88.0 (43.46-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.165 , 0.222 0.174 , 0.230	Depositor DCC
R_{free} test set	1178 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.078 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9923	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.21	5/2321 (0.2%)	1.33	6/3153 (0.2%)
1	B	1.15	1/2292 (0.0%)	1.32	2/3114 (0.1%)
1	C	1.19	5/2259 (0.2%)	1.32	5/3069 (0.2%)
1	D	1.16	3/2261 (0.1%)	1.33	3/3069 (0.1%)
All	All	1.18	14/9133 (0.2%)	1.33	16/12405 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	HIS	CE1-NE2	8.16	1.40	1.32
1	D	279	LEU	C-O	7.00	1.32	1.24
1	A	198	VAL	C-O	6.03	1.30	1.24
1	C	148	ASP	C-O	5.94	1.31	1.23
1	D	311	ASN	C-O	5.94	1.30	1.23
1	C	242	MET	C-O	-5.68	1.17	1.24
1	A	135	LEU	C-O	-5.46	1.17	1.24
1	A	241	HIS	CE1-NE2	5.45	1.38	1.32
1	A	191	ALA	C-O	5.38	1.30	1.23
1	C	105	ALA	C-O	5.23	1.30	1.24
1	D	272	SER	CA-CB	-5.19	1.48	1.54
1	B	293	LEU	C-O	5.12	1.30	1.24
1	C	52	SER	CA-CB	-5.04	1.46	1.53
1	A	231	VAL	C-O	5.01	1.29	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASN	O-C-N	8.20	126.97	121.23
1	D	131	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	74	ASP	CA-CB-CG	7.29	119.89	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ASN	CB-CA-C	6.69	116.82	111.00
1	D	209	ALA	N-CA-C	-5.70	105.59	112.54
1	D	42	THR	CA-CB-OG1	-5.69	101.07	109.60
1	C	243	ASP	CB-CA-C	5.60	120.37	110.85
1	C	72	LYS	CB-CA-C	5.60	118.76	110.14
1	A	72	LYS	CB-CA-C	5.42	118.53	110.62
1	A	272	SER	O-C-N	5.42	127.56	121.87
1	C	233	THR	CA-CB-OG1	-5.41	101.48	109.60
1	C	189	ASN	CB-CA-C	5.32	118.97	110.09
1	A	185	ALA	CA-C-O	-5.32	115.42	121.00
1	A	188	LYS	CB-CA-C	5.29	119.56	110.79
1	C	163	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	42	THR	CA-C-O	-5.08	115.97	121.36

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	2256	0	2224	37	0
1	B	2228	0	2197	22	0
1	C	2195	0	2170	29	0
1	D	2196	0	2171	39	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
2	C	7	0	10	1	0
2	D	7	0	10	0	0
3	A	6	0	8	3	0
3	B	6	0	8	0	0
3	C	6	0	8	13	0
3	D	6	0	8	2	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	287	0	0	10	0
5	B	230	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	237	0	0	4	0
5	D	232	0	0	8	0
All	All	9923	0	8834	128	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 7.

All (128) 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:C:297:ASP:HA	3:C:402:GOL:C1	1.80	1.12
1:C:297:ASP:HA	3:C:402:GOL:H12	1.29	1.11
1:C:296:ILE:CG2	1:C:307:LEU:HD11	1.83	1.07
1:A:295:PRO:HG2	1:A:298:GLU:HG3	1.30	1.07
1:D:161:LYS:HA	1:D:167:VAL:HG21	1.14	1.07
1:A:296:ILE:HG23	1:A:307[A]:LEU:HD11	1.32	1.06
1:C:312:ALA:H	3:C:402:GOL:H32	1.22	1.03
1:C:296:ILE:HG23	1:C:307:LEU:HD11	1.03	1.03
1:C:296:ILE:HG23	1:C:307:LEU:CD1	1.88	1.01
1:B:127:ILE:HD11	1:B:187:LEU:HD21	1.52	0.91
1:C:311:ASN:HA	3:C:402:GOL:H11	1.54	0.90
1:A:44:ILE:HD11	1:B:41:SER:HB3	1.53	0.90
1:C:312:ALA:N	3:C:402:GOL:H32	1.86	0.89
1:A:295:PRO:HG2	1:A:298:GLU:CG	2.03	0.88
1:C:297:ASP:HA	3:C:402:GOL:C2	2.06	0.85
1:C:297:ASP:CA	3:C:402:GOL:H12	2.08	0.83
1:C:187:LEU:HD21	1:C:221:VAL:HG22	1.59	0.83
1:D:135:LEU:HG	1:D:149:MET:CE	2.10	0.81
1:D:286:ASP:HB3	5:D:699:HOH:O	1.83	0.79
1:D:131:ASP:HA	1:D:160:SER:HB3	1.67	0.77
1:A:299:SER:HB3	5:A:713:HOH:O	1.86	0.75
1:A:297:ASP:HB3	1:A:307[A]:LEU:HD12	1.70	0.74
1:D:207:GLY:O	1:D:210:LYS:HB2	1.88	0.74
1:C:312:ALA:H	3:C:402:GOL:C3	2.00	0.73
1:A:38:ALA:HA	1:B:70:GLN:HE22	1.55	0.72
1:B:223:ARG:NH1	5:B:501:HOH:O	2.25	0.70
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.21	0.70
1:A:295:PRO:CG	1:A:298:GLU:HG3	2.16	0.68
1:C:297:ASP:HA	3:C:402:GOL:H2	1.74	0.68
3:A:402:GOL:H32	5:A:571:HOH:O	1.95	0.67
1:A:297:ASP:HB3	1:A:307[A]:LEU:CD1	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:N	5:A:504:HOH:O	2.29	0.65
1:C:162:GLN:NE2	5:C:502:HOH:O	2.30	0.64
1:D:162:GLN:NE2	5:D:506:HOH:O	2.31	0.64
1:A:297:ASP:CB	1:A:307[A]:LEU:HD12	2.28	0.63
1:A:150[B]:CYS:SG	1:A:186:PHE:CG	2.92	0.63
1:A:297:ASP:CA	1:A:307[A]:LEU:HD12	2.30	0.62
1:D:161:LYS:HA	1:D:167:VAL:CG2	2.08	0.62
1:B:131:ASP:HA	1:B:160:SER:HB3	1.84	0.60
1:D:131:ASP:HA	1:D:160:SER:CB	2.33	0.58
1:A:39:CYS:H	1:B:40:PHE:HB3	1.70	0.57
1:D:135:LEU:CG	1:D:149:MET:CE	2.82	0.57
1:D:135:LEU:CG	1:D:149:MET:HE3	2.34	0.57
5:C:652:HOH:O	3:D:402:GOL:H12	2.04	0.57
1:D:135:LEU:HG	1:D:149:MET:HE3	1.87	0.56
1:D:161:LYS:CA	1:D:167:VAL:HG21	2.10	0.54
1:A:215:LYS:NZ	1:A:254:GLU:OE1	2.40	0.54
1:D:215:LYS:HG3	1:D:255:ILE:HD11	1.90	0.54
1:B:150[A]:CYS:SG	1:B:186:PHE:CD2	3.00	0.54
1:D:254:GLU:O	1:D:257:LYS:NZ	2.42	0.52
1:A:313:GLU:HG3	5:A:720:HOH:O	2.09	0.52
1:C:297:ASP:CA	3:C:402:GOL:C1	2.69	0.52
1:C:295:PRO:HB2	3:C:402:GOL:O1	2.09	0.52
5:C:652:HOH:O	3:D:402:GOL:C1	2.58	0.52
1:C:187:LEU:HD23	1:C:217:PHE:CE1	2.45	0.51
1:D:111[A]:THR:CG2	1:D:134:VAL:HG13	2.40	0.51
1:A:187:LEU:O	1:A:190:ALA:HB3	2.09	0.51
1:B:242:MET:HE2	1:B:328:VAL:HG11	1.93	0.51
1:D:243:ASP:HB2	5:D:645:HOH:O	2.11	0.51
1:C:296:ILE:CG2	1:C:307:LEU:CD1	2.67	0.51
1:B:197:ALA:HA	1:B:230:VAL:O	2.11	0.51
1:D:129:GLY:N	1:D:151:GLU:OE1	2.43	0.51
1:D:160:SER:O	1:D:167:VAL:HG11	2.11	0.50
1:B:150[A]:CYS:SG	1:B:186:PHE:CG	3.03	0.50
1:D:203:SER:HB2	5:D:638:HOH:O	2.12	0.50
1:D:54:MET:HE1	1:D:204:ASP:HB3	1.92	0.50
1:D:166:ASP:O	1:D:167:VAL:C	2.54	0.50
1:A:297:ASP:HA	1:A:307[A]:LEU:HD12	1.95	0.49
1:C:150[A]:CYS:SG	1:C:186:PHE:CG	3.04	0.49
1:C:242:MET:HG3	5:C:732:HOH:O	2.13	0.49
1:D:135:LEU:HD11	1:D:149:MET:HE3	1.94	0.49
1:A:246:GLU:HG3	1:A:328:VAL:CG1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:GOL:C3	5:A:571:HOH:O	2.58	0.48
1:A:37:PRO:C	5:A:504:HOH:O	2.56	0.48
1:D:111[A]:THR:HG22	1:D:134:VAL:HG13	1.95	0.47
1:A:261:ASN:HD22	1:A:289:PHE:HD2	1.62	0.47
1:A:326:LYS:O	1:A:330:GLU:HG2	2.14	0.47
1:A:215:LYS:HG2	1:A:255:ILE:HD11	1.96	0.47
1:D:131:ASP:O	1:D:167:VAL:HG12	2.15	0.46
1:A:38:ALA:HB3	1:B:40:PHE:HD2	1.80	0.46
1:A:150[B]:CYS:SG	1:A:186:PHE:CD2	3.09	0.46
1:B:204:ASP:HB3	1:B:205:PRO:HD2	1.97	0.46
1:C:52:SER:HB3	1:C:55:TRP:CE2	2.51	0.46
1:C:262:TYR:OH	1:C:276:GLY:HA3	2.16	0.46
1:D:207:GLY:O	1:D:210:LYS:CB	2.61	0.46
1:D:215:LYS:NZ	1:D:254:GLU:OE1	2.50	0.45
1:D:288:ASP:OD1	5:D:501:HOH:O	2.20	0.45
1:C:297:ASP:CA	3:C:402:GOL:H2	2.43	0.45
1:C:197:ALA:HA	1:C:230:VAL:O	2.17	0.44
1:D:251:ASN:OD1	5:D:503:HOH:O	2.21	0.44
1:B:126:VAL:O	1:B:149:MET:HA	2.17	0.44
1:B:187:LEU:HB3	1:B:220[A]:SER:OG	2.17	0.44
5:A:781:HOH:O	1:B:313:GLU:HG2	2.17	0.44
1:A:197:ALA:HA	1:A:230:VAL:O	2.17	0.44
1:A:326:LYS:HE2	5:A:719:HOH:O	2.16	0.44
1:D:135:LEU:CD1	1:D:149:MET:HE3	2.47	0.44
1:A:185:ALA:O	1:A:188:LYS:N	2.46	0.43
1:D:135:LEU:CD1	1:D:149:MET:CE	2.96	0.43
1:D:233:THR:O	1:D:277:PHE:HA	2.18	0.43
1:C:187:LEU:HD21	1:C:221:VAL:CG2	2.40	0.43
1:A:125:LEU:HD21	1:A:127:ILE:HD11	2.01	0.43
1:A:299:SER:C	5:A:713:HOH:O	2.61	0.43
1:A:74:ASP:CG	5:A:506:HOH:O	2.61	0.42
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.54	0.42
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.34	0.42
1:C:233:THR:O	1:C:277:PHE:HA	2.19	0.42
1:A:238:LEU:HD23	1:A:245:ILE:HD13	2.02	0.42
1:A:295:PRO:HG2	1:A:298:GLU:CD	2.44	0.42
1:B:233:THR:O	1:B:277:PHE:HA	2.18	0.42
1:C:79:ILE:HB	1:C:91:VAL:HB	2.02	0.42
1:B:215:LYS:HG3	1:B:255:ILE:HD11	2.01	0.42
1:A:233:THR:O	1:A:277:PHE:HA	2.19	0.42
1:D:54:MET:HE2	1:D:206:ILE:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:MET:HE3	1:B:242:MET:HA	2.02	0.42
1:D:48:PHE:O	1:D:61:SER:HA	2.19	0.41
1:D:203:SER:CB	5:D:638:HOH:O	2.68	0.41
1:A:103:GLU:OE1	1:A:131:ASP:OD2	2.38	0.41
1:C:311:ASN:HA	3:C:402:GOL:C1	2.38	0.41
1:D:293:LEU:C	1:D:293:LEU:HD12	2.45	0.41
1:D:198:VAL:O	1:D:231:VAL:HA	2.20	0.41
1:D:166:ASP:OD1	1:D:167:VAL:N	2.54	0.41
1:B:232:CYS:HA	1:B:278:MET:O	2.20	0.41
1:C:202:SER:O	2:C:401:PEG:H12	2.22	0.40
1:D:210:LYS:CD	5:D:660:HOH:O	2.68	0.40
1:A:259:SER:O	1:A:280:CYS:HA	2.21	0.40
3:A:402:GOL:H12	5:B:573:HOH:O	2.21	0.40
1:B:215:LYS:NZ	1:B:254:GLU:OE1	2.52	0.40
1:A:296:ILE:HD12	1:A:296:ILE:HA	1.95	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	290/337 (86%)	282 (97%)	8 (3%)	0	100	100
1	B	286/337 (85%)	279 (98%)	7 (2%)	0	100	100
1	C	281/337 (83%)	271 (96%)	10 (4%)	0	100	100
1	D	280/337 (83%)	270 (96%)	10 (4%)	0	100	100
All	All	1137/1348 (84%)	1102 (97%)	35 (3%)	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	252/286 (88%)	250 (99%)	2 (1%)	73	70
1	B	249/286 (87%)	246 (99%)	3 (1%)	63	57
1	C	244/286 (85%)	243 (100%)	1 (0%)	84	83
1	D	246/286 (86%)	243 (99%)	3 (1%)	63	57
All	All	991/1144 (87%)	982 (99%)	9 (1%)	70	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	303	SER
1	B	40	PHE
1	B	187	LEU
1	B	275	ILE
1	C	43	VAL
1	D	159	VAL
1	D	203	SER
1	D	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	97	GLN
1	A	261	ASN
1	B	70	GLN
1	B	76	GLN
1	B	162	GLN
1	B	294	ASN
1	C	162	GLN
1	C	189	ASN
1	C	261	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	76	GLN
1	D	162	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	PEG	A	401	-	6,6,6	0.78	0	5,5,5	0.33	0
2	PEG	B	401	-	6,6,6	0.82	0	5,5,5	0.52	0
2	PEG	C	401	-	6,6,6	0.79	0	5,5,5	0.37	0
3	GOL	D	402	-	5,5,5	0.12	0	5,5,5	0.36	0
2	PEG	D	401	-	6,6,6	0.57	0	5,5,5	0.29	0
4	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.14	0
4	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.14	0
3	GOL	B	402	-	5,5,5	0.08	0	5,5,5	0.34	0
3	GOL	A	402	-	5,5,5	0.25	0	5,5,5	0.40	0
3	GOL	C	402	-	5,5,5	0.17	0	5,5,5	0.58	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	PEG	A	401	-	-	0/4/4/4	-
2	PEG	B	401	-	-	0/4/4/4	-
2	PEG	C	401	-	-	0/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
2	PEG	D	401	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	402	-	-	3/4/4/4	-
3	GOL	C	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	C1-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	D	402	GOL	O2-C2-C3-O3
3	C	402	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PEG	1	0
3	D	402	GOL	2	0
3	A	402	GOL	3	0
3	C	402	GOL	13	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 [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	291/337 (86%)	-1.50	0 100 100	11, 21, 41, 74	3 (1%)
1	B	286/337 (84%)	-1.50	0 100 100	11, 24, 41, 61	4 (1%)
1	C	282/337 (83%)	-1.46	0 100 100	10, 25, 42, 60	3 (1%)
1	D	281/337 (83%)	-1.45	0 100 100	11, 26, 44, 60	5 (1%)
All	All	1140/1348 (84%)	-1.48	0 100 100	10, 24, 43, 74	15 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	402	6/6	0.98	0.04	28,29,31,33	0
4	SO4	D	403	5/5	0.98	0.04	39,50,54,55	5
2	PEG	A	401	7/7	0.99	0.02	16,18,22,22	0
3	GOL	B	402	6/6	0.99	0.03	33,36,37,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	402	6/6	0.99	0.04	36,37,40,43	0
3	GOL	D	402	6/6	0.99	0.04	48,50,51,55	0
4	SO4	B	403	5/5	0.99	0.03	33,34,42,46	5
2	PEG	C	401	7/7	0.99	0.03	16,18,21,22	0
2	PEG	B	401	7/7	1.00	0.02	18,20,24,25	0
2	PEG	D	401	7/7	1.00	0.02	24,24,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.