



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:54 PM UTC

PDB ID : 8BLU / pdb_00008blu
Title : The PDZ domains of human SDCBP
Authors : Bradshaw, W.J.; Katis, V.L.; Daniel-Mozo, M.; Bountra, C.; von Delft, F.;
Brennan, P.E.
Deposited on : 2022-11-10
Resolution : 1.50 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

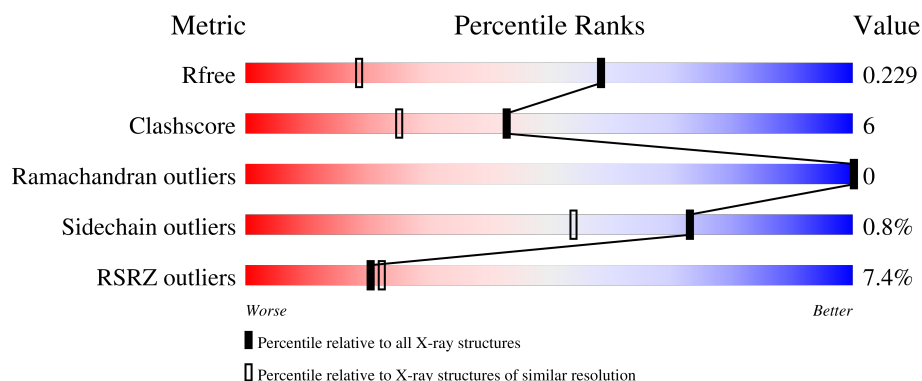
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	195	17% 84% 14% ..
1	B	195	2% 91% 8% .
1	C	195	5% 87% 12% .
1	D	195	5% 89% 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
4	GOL	B	303	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7119 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 Syntenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	4	0
			1508	954	266	279	9			
1	B	195	Total	C	N	O	S	0	13	0
			1578	999	275	293	11			
1	C	193	Total	C	N	O	S	0	11	0
			1537	973	268	286	10			
1	D	193	Total	C	N	O	S	0	18	0
			1597	1014	277	296	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag	UNP O00560
D	105	MET	-	expression tag	UNP O00560

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



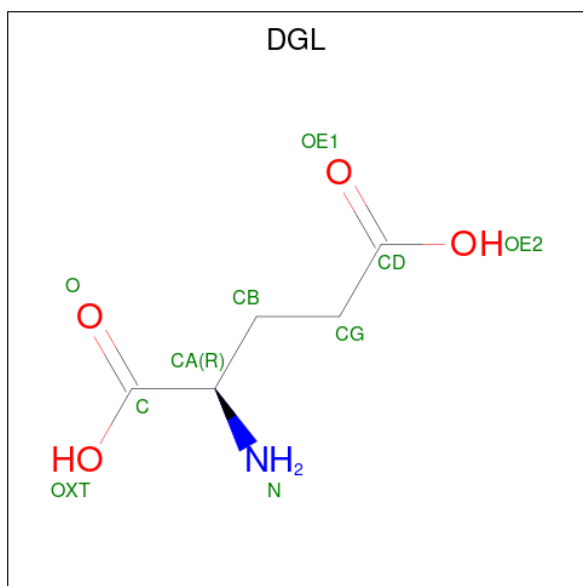
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



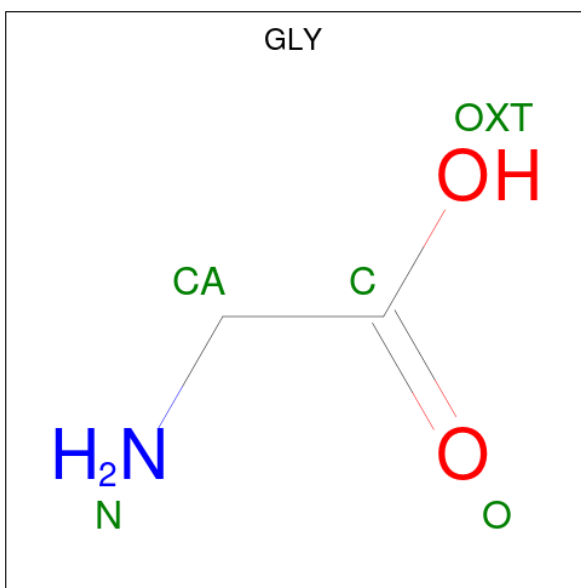
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			10	5	1	4		
5	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	1
			12	6	1	4	1		

- Molecule 7 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



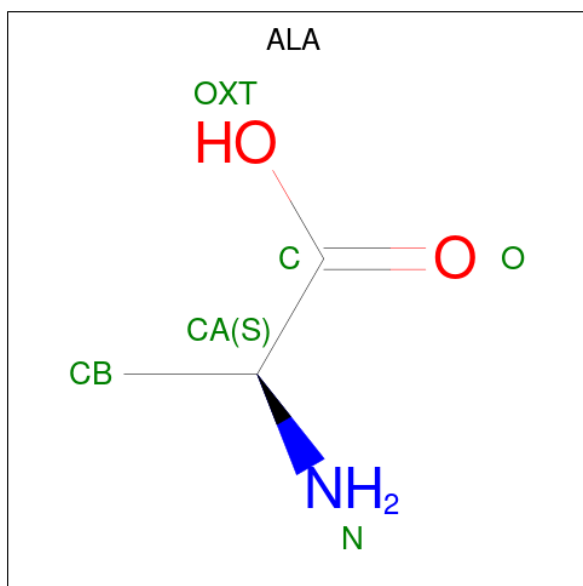
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O		0	0
			5	2	1	2			
7	C	1	Total	C	N	O		0	0
			5	2	1	2			
7	C	1	Total	C	N	O		0	0
			5	2	1	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 8 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			6	3	1	2		

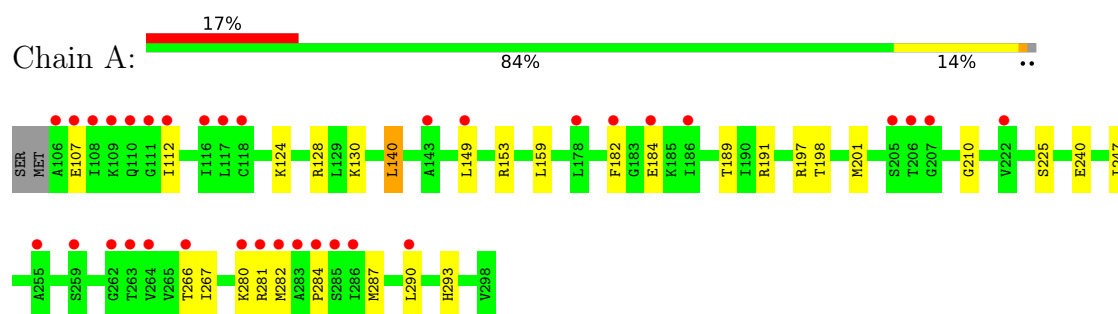
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	127	Total	O	0	0
			127	127		
9	B	234	Total	O	0	5
			236	236		
9	C	193	Total	O	0	4
			195	195		
9	D	220	Total	O	0	2
			220	220		

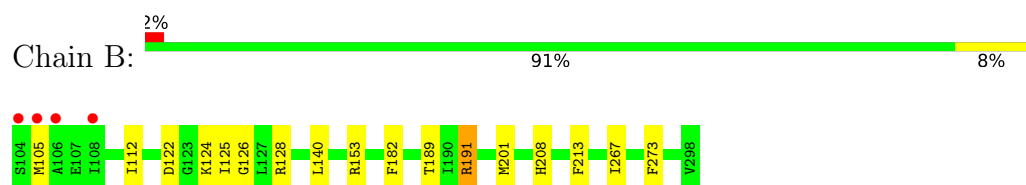
3 Residue-property plots [i](#)

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.

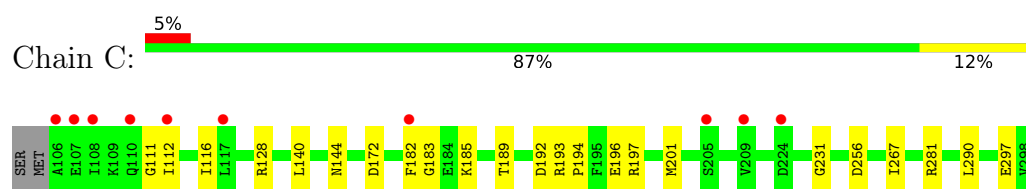
• Molecule 1: Syntenin-1



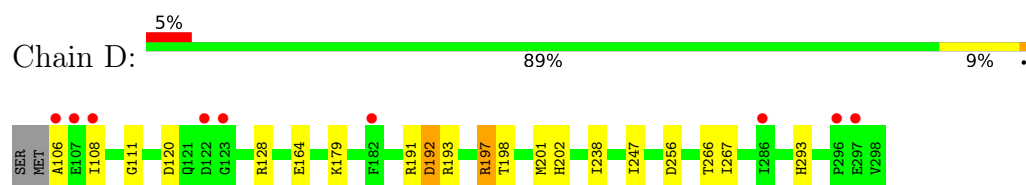
• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.60Å 49.59Å 118.19Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	63.95 – 1.50 63.95 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.95-1.50) 100.0 (63.95-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.183 , 0.223 0.191 , 0.229	Depositor DCC
R_{free} test set	2055 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7119	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4404e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, SO4, MES, DGL, 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	0.71	0/1541	1.04	1/2071 (0.0%)
1	B	0.82	0/1641	1.06	4/2202 (0.2%)
1	C	0.77	0/1591	1.00	0/2138
1	D	0.81	0/1660	1.04	1/2229 (0.0%)
All	All	0.78	0/6433	1.03	6/8640 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	6
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	CG-CD-NE	6.62	126.56	112.00
1	B	208	HIS	CA-CB-CG	-6.37	107.43	113.80
1	D	120	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	105	MET	CA-C-N	5.47	132.25	121.58
1	B	105	MET	C-N-CA	5.47	132.25	121.58
1	A	107	GLU	CB-CA-C	5.15	118.46	109.65

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191[A]	ARG	Sidechain
1	A	191[B]	ARG	Sidechain
1	D	128	ARG	Sidechain
1	D	191[A]	ARG	Sidechain
1	D	191[B]	ARG	Sidechain
1	D	192	ASP	Sidechain
1	D	197[A]	ARG	Sidechain
1	D	197[B]	ARG	Sidechain

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	1508	0	1571	24	0
1	B	1578	0	1661	29	0
1	C	1537	0	1614	18	0
1	D	1597	0	1690	16	0
2	A	8	0	12	1	0
2	B	8	0	12	0	0
2	C	12	0	18	3	0
2	D	8	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	B	6	0	8	14	0
4	D	6	0	8	1	0
5	B	10	0	7	0	0
5	D	10	0	7	0	0
6	B	12	0	13	1	0
7	C	15	0	6	0	0
7	D	5	0	2	1	0
8	D	6	0	4	0	0
9	A	127	0	0	1	0
9	B	236	0	0	6	0
9	C	195	0	0	8	0
9	D	220	0	0	6	0
All	All	7119	0	6645	81	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 6.

All (81) 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:140:LEU:HD22	1:B:182:PHE:CE1	1.91	1.04
1:A:140:LEU:HD22	1:B:182:PHE:HE1	1.23	1.00
1:B:125:ILE:H	4:B:303:GOL:H11	1.23	0.98
1:B:125:ILE:N	4:B:303:GOL:H11	1.94	0.82
1:B:126:GLY:H	4:B:303:GOL:H32	1.51	0.74
1:C:201:MET:HE1	1:C:267:ILE:HD12	1.73	0.70
1:A:198:THR:CG2	1:A:266:THR:CG2	2.70	0.69
1:C:172:ASP:HB3	2:C:303:EDO:H21	1.74	0.68
1:D:198[A]:THR:CG2	1:D:266[A]:THR:CG2	2.70	0.68
4:B:303:GOL:O1	9:B:601:HOH:O	2.13	0.66
1:A:281:ARG:O	2:A:302:EDO:H22	1.96	0.65
1:D:256[B]:ASP:OD1	9:D:401:HOH:O	2.14	0.65
1:A:140:LEU:CD2	1:B:182:PHE:CE1	2.77	0.65
1:C:111:GLY:O	9:C:401:HOH:O	2.14	0.64
1:C:172:ASP:O	2:C:303:EDO:O2	2.14	0.64
1:C:256[A]:ASP:OD1	9:C:402:HOH:O	2.15	0.63
1:D:201:MET:HE1	1:D:267[A]:ILE:HD12	1.80	0.63
1:B:125:ILE:H	4:B:303:GOL:C1	2.05	0.62
1:B:153[B]:ARG:NH1	9:B:603:HOH:O	2.27	0.61
1:A:201:MET:HE1	1:A:267[B]:ILE:HD12	1.84	0.59
1:C:290:LEU:O	9:C:403:HOH:O	2.17	0.58
1:B:153[A]:ARG:NH1	9:B:605:HOH:O	2.36	0.58
1:A:182:PHE:CE1	1:A:184:GLU:HB3	2.39	0.57
1:A:198:THR:HG23	1:A:266:THR:CG2	2.34	0.57
1:D:111:GLY:O	9:D:402:HOH:O	2.17	0.56
1:C:172:ASP:CG	2:C:303:EDO:H11	2.31	0.56
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.87	0.55
1:A:124:LYS:HD3	9:B:617:HOH:O	2.07	0.55
1:A:198:THR:CG2	1:A:266:THR:HG23	2.38	0.54
1:D:108:ILE:HG21	9:D:507:HOH:O	2.08	0.54
1:A:140:LEU:CD2	1:B:182:PHE:HE1	2.10	0.53
1:B:122:ASP:HB2	1:B:124[B]:LYS:HD3	1.92	0.52
1:D:198[A]:THR:HG23	1:D:266[A]:THR:CG2	2.40	0.52
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.10	0.52
1:D:238:ILE:HG12	1:D:267[B]:ILE:HD11	1.92	0.52
1:D:164[A]:GLU:OE2	9:D:403:HOH:O	2.18	0.52
1:A:159:LEU:HD22	1:C:231:GLY:HA3	1.92	0.51
1:C:116:ILE:HG21	1:C:185:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PHE:HA	9:C:404:HOH:O	2.11	0.51
1:C:183:GLY:O	9:C:404:HOH:O	2.20	0.50
1:B:126:GLY:N	4:B:303:GOL:H32	2.24	0.50
1:A:140:LEU:HB2	1:A:282:MET:HE1	1.92	0.50
1:B:191:ARG:HG3	9:B:710:HOH:O	2.11	0.50
1:A:198:THR:HG23	1:A:266:THR:HG22	1.94	0.50
1:A:197:ARG:HD3	1:C:194:PRO:O	2.12	0.49
1:B:112:ILE:CG2	1:B:189[A]:THR:CG2	2.90	0.48
1:B:126:GLY:H	4:B:303:GOL:C3	2.22	0.48
1:D:198[A]:THR:CG2	1:D:266[A]:THR:HG23	2.43	0.48
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.95	0.48
1:D:198[A]:THR:HG23	1:D:266[A]:THR:HG22	1.95	0.47
1:B:124[A]:LYS:HD2	4:B:303:GOL:H12	1.97	0.47
1:C:281:ARG:NH1	9:C:405:HOH:O	2.27	0.46
1:A:112:ILE:CG2	1:A:189:THR:CG2	2.94	0.46
1:D:197[A]:ARG:HD2	4:D:303[A]:GOL:O1	2.15	0.46
1:A:153:ARG:NH2	1:A:240:GLU:OE1	2.49	0.46
1:A:130:LYS:NZ	9:A:405:HOH:O	2.49	0.45
1:D:179[B]:LYS:HD2	1:D:179[B]:LYS:HA	1.83	0.44
1:A:284:PRO:HA	1:A:287:MET:HE3	1.98	0.44
1:A:210:GLY:HA3	1:A:225:SER:HB2	2.00	0.44
1:A:182:PHE:CZ	1:A:184:GLU:HB3	2.53	0.44
1:D:202:HIS:CD2	9:D:447:HOH:O	2.71	0.44
1:B:124[B]:LYS:HA	4:B:303:GOL:C1	2.49	0.43
1:C:128:ARG:HD3	9:C:421:HOH:O	2.19	0.43
1:D:247:ILE:O	1:D:293:HIS:HE1	2.02	0.42
1:B:112:ILE:CG2	1:B:189[A]:THR:HG22	2.49	0.42
1:B:124[A]:LYS:CA	4:B:303:GOL:H11	2.49	0.42
1:B:124[B]:LYS:HA	4:B:303:GOL:H11	2.01	0.42
1:A:247:ILE:O	1:A:293:HIS:HE1	2.03	0.42
1:B:124[B]:LYS:CA	4:B:303:GOL:H11	2.49	0.42
1:D:192:ASP:O	1:D:193:ARG:C	2.63	0.42
1:C:144:ASN:HB3	9:C:553:HOH:O	2.19	0.41
1:A:128:ARG:HG2	1:B:182:PHE:CZ	2.55	0.41
1:B:213:PHE:O	6:B:306[A]:MES:H61	2.20	0.41
1:B:124[A]:LYS:HA	4:B:303:GOL:C1	2.50	0.41
1:D:106:ALA:O	1:D:198[B]:THR:HG21	2.21	0.41
1:B:128:ARG:HD3	1:B:140:LEU:HD22	2.03	0.41
1:B:124[A]:LYS:HA	4:B:303:GOL:H11	2.03	0.40
1:B:273[A]:PHE:HD1	9:B:715:HOH:O	2.03	0.40
7:D:305:GLY:HA2	9:D:462:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:CG2	1:C:189:THR:CG2	2.99	0.40
1:C:192:ASP:O	1:C:193:ARG:C	2.64	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	195/195 (100%)	192 (98%)	3 (2%)	0	100	100
1	B	207/195 (106%)	204 (99%)	3 (1%)	0	100	100
1	C	202/195 (104%)	199 (98%)	3 (2%)	0	100	100
1	D	209/195 (107%)	206 (99%)	3 (1%)	0	100	100
All	All	813/780 (104%)	801 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	170/168 (101%)	167 (98%)	3 (2%)	51	24
1	B	182/168 (108%)	182 (100%)	0	100	100
1	C	177/168 (105%)	175 (99%)	2 (1%)	65	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	185/168 (110%)	185 (100%)	0	100	100
All	All	714/672 (106%)	709 (99%)	5 (1%)	73	57

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	149	LEU
1	A	280	LYS
1	C	140	LEU
1	C	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	HIS
1	D	157	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 ⓘ

22 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	$\# Z > 2$
5	DGL	B	305	-	8,9,9	0.80	0	8,11,11	1.11	1 (12%)
4	GOL	D	303[A]	-	5,5,5	0.47	0	5,5,5	0.95	0
3	SO4	A	303	-	4,4,4	0.43	0	6,6,6	0.15	0
2	EDO	C	301	-	3,3,3	0.57	0	2,2,2	0.27	0
2	EDO	A	301	-	3,3,3	0.14	0	2,2,2	0.25	0
2	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.76	0
7	GLY	C	305	-	4,4,4	0.93	0	3,4,4	1.07	0
7	GLY	C	306	-	4,4,4	0.81	0	3,4,4	1.08	0
2	EDO	A	302	-	3,3,3	0.54	0	2,2,2	0.31	0
7	GLY	C	304	-	4,4,4	1.16	1 (25%)	3,4,4	1.09	0
2	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.47	0
6	MES	B	306[A]	-	12,12,12	0.99	0	15,16,16	1.14	1 (6%)
2	EDO	D	302	-	3,3,3	0.75	0	2,2,2	0.26	0
8	ALA	D	307	-	5,5,5	1.79	1 (20%)	6,6,6	1.49	2 (33%)
7	GLY	D	305	-	4,4,4	1.36	0	3,4,4	0.77	0
3	SO4	B	304	-	4,4,4	0.86	0	6,6,6	0.32	0
2	EDO	B	301	-	3,3,3	0.67	0	2,2,2	0.25	0
5	DGL	D	306	-	8,9,9	1.23	1 (12%)	8,11,11	0.98	0
3	SO4	D	304	-	4,4,4	0.25	0	6,6,6	0.19	0
2	EDO	D	301	-	3,3,3	0.21	0	2,2,2	0.27	0
4	GOL	B	303	-	5,5,5	0.45	0	5,5,5	0.70	0
2	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DGL	B	305	-	-	0/9/9/9	-
4	GOL	D	303[A]	-	-	4/4/4/4	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
7	GLY	C	305	-	-	2/2/2/2	-
7	GLY	C	306	-	-	2/2/2/2	-
2	EDO	A	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLY	C	304	-	-	2/2/2/2	-
2	EDO	B	302	-	-	0/1/1/1	-
6	MES	B	306[A]	-	-	0/6/14/14	0/1/1/1
2	EDO	D	302	-	-	1/1/1/1	-
8	ALA	D	307	-	-	0/4/4/4	-
7	GLY	D	305	-	-	0/2/2/2	-
2	EDO	B	301	-	-	0/1/1/1	-
5	DGL	D	306	-	-	4/9/9/9	-
2	EDO	D	301	-	-	0/1/1/1	-
4	GOL	B	303	-	-	1/4/4/4	-
2	EDO	C	302	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	307	ALA	O-C	3.59	1.32	1.22
5	D	306	DGL	O-C	2.69	1.30	1.22
7	C	304	GLY	OXT-C	-2.02	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	306[A]	MES	O1S-S-C8	-2.98	102.22	106.73
8	D	307	ALA	OXT-C-O	2.65	130.10	124.08
8	D	307	ALA	O-C-CA	-2.37	114.79	122.07
5	B	305	DGL	CB-CA-C	2.12	116.05	110.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303[A]	GOL	C1-C2-C3-O3
7	C	306	GLY	OXT-C-CA-N
7	C	304	GLY	O-C-CA-N
7	C	306	GLY	O-C-CA-N
7	C	304	GLY	OXT-C-CA-N
4	D	303[A]	GOL	O1-C1-C2-C3
4	D	303[A]	GOL	O2-C2-C3-O3
2	C	303	EDO	O1-C1-C2-O2
7	C	305	GLY	O-C-CA-N
5	D	306	DGL	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	B	303	GOL	C1-C2-C3-O3
5	D	306	DGL	O-C-CA-CB
4	D	303[A]	GOL	O1-C1-C2-O2
5	D	306	DGL	OE2-CD-CG-CB
7	C	305	GLY	OXT-C-CA-N
2	A	302	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
5	D	306	DGL	OE1-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303[A]	GOL	1	0
2	C	303	EDO	3	0
2	A	302	EDO	1	0
6	B	306[A]	MES	1	0
7	D	305	GLY	1	0
4	B	303	GOL	14	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 ⓘ

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, 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	193/195 (98%)	1.05	34 (17%) 4 3	17, 40, 69, 121	4 (2%)
1	B	195/195 (100%)	0.18	4 (2%) 63 67	14, 28, 44, 62	13 (6%)
1	C	193/195 (98%)	0.44	10 (5%) 33 35	16, 31, 54, 97	11 (5%)
1	D	193/195 (98%)	0.25	9 (4%) 36 40	13, 27, 55, 84	18 (9%)
All	All	774/780 (99%)	0.48	57 (7%) 20 22	13, 31, 58, 121	46 (5%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	PHE	5.9
1	A	106	ALA	5.8
1	C	106	ALA	5.6
1	D	182	PHE	5.3
1	A	286	ILE	4.4
1	D	106	ALA	4.4
1	C	182	PHE	3.8
1	B	106	ALA	3.8
1	C	108	ILE	3.7
1	A	108	ILE	3.6
1	D	108	ILE	3.5
1	A	283	ALA	3.5
1	A	116	ILE	3.4
1	A	149	LEU	3.4
1	A	290	LEU	3.4
1	A	284	PRO	3.3
1	A	107	GLU	3.3
1	B	104	SER	3.3
1	A	118	CYS	3.2
1	A	110	GLN	3.1
1	C	110	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	105	MET	3.1
1	C	117	LEU	3.1
1	D	123	GLY	3.0
1	D	286	ILE	2.9
1	C	209	VAL	2.9
1	C	112	ILE	2.8
1	A	111	GLY	2.7
1	A	262	GLY	2.7
1	A	109	LYS	2.6
1	A	206	THR	2.5
1	A	186	ILE	2.5
1	A	259	SER	2.5
1	A	281	ARG	2.5
1	A	263	THR	2.4
1	A	143	ALA	2.3
1	C	224	ASP	2.3
1	A	280	LYS	2.3
1	D	297[A]	GLU	2.3
1	A	205	SER	2.3
1	A	222	VAL	2.3
1	A	255	ALA	2.3
1	A	282	MET	2.3
1	A	112	ILE	2.3
1	A	117	LEU	2.3
1	A	266	THR	2.2
1	A	207	GLY	2.2
1	C	205	SER	2.2
1	A	184	GLU	2.2
1	B	108	ILE	2.1
1	D	107	GLU	2.1
1	C	107	GLU	2.1
1	D	122	ASP	2.1
1	D	296[A]	PRO	2.1
1	A	285	SER	2.0
1	A	264	VAL	2.0
1	A	178	LEU	2.0

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 [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($\text{\AA}^2$)	Q<0.9
2	EDO	A	302	4/4	0.73	0.21	42,43,44,45	4
7	GLY	C	306	5/5	0.76	0.19	44,59,63,69	0
2	EDO	C	303	4/4	0.83	0.15	43,56,60,60	0
7	GLY	D	305	5/5	0.85	0.13	47,51,59,63	0
7	GLY	C	304	5/5	0.86	0.14	50,66,80,87	0
6	MES	B	306[A]	12/12	0.87	0.14	29,35,47,48	12
3	SO4	A	303	5/5	0.87	0.12	42,52,80,80	0
7	GLY	C	305	5/5	0.88	0.13	35,39,51,62	0
4	GOL	B	303	6/6	0.88	0.12	37,42,59,61	0
4	GOL	D	303[A]	6/6	0.88	0.14	27,31,37,40	6
5	DGL	B	305	10/10	0.90	0.11	31,46,56,72	0
3	SO4	D	304	5/5	0.91	0.11	50,65,71,79	0
5	DGL	D	306	10/10	0.92	0.10	28,39,44,65	0
3	SO4	B	304	5/5	0.93	0.10	36,43,63,70	5
8	ALA	D	307	6/6	0.94	0.09	30,34,48,52	0
2	EDO	D	301	4/4	0.97	0.06	27,27,30,32	0
2	EDO	D	302	4/4	0.97	0.07	26,26,27,28	0
2	EDO	B	301	4/4	0.97	0.06	26,26,28,29	0
2	EDO	C	301	4/4	0.97	0.06	27,27,31,31	0
2	EDO	A	301	4/4	0.97	0.06	32,33,34,37	0
2	EDO	B	302	4/4	0.98	0.05	24,24,30,30	0
2	EDO	C	302	4/4	0.98	0.06	29,33,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.