



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:48 PM EDT

PDB ID : 7ACX / pdb_00007acx
Title : H/L (SLPH/SLPL) complex from *C. difficile* (R7404 strain)
Authors : Lanzoni-Mangutchi, P.; Barwinska-Sendra, A.; Basle, A.; El Omari, K.; Wagner, A.; Salgado, P.S.
Deposited on : 2020-09-11
Resolution : 2.65 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

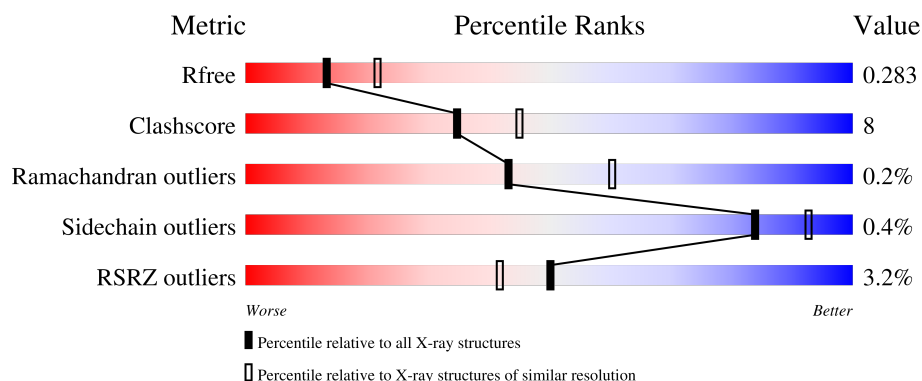
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	317	8% 88% 10% 2%
1	C	317	2% 74% 13% 12%
2	B	373	8% 76% 20%
2	D	373	2% 86% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10096 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.

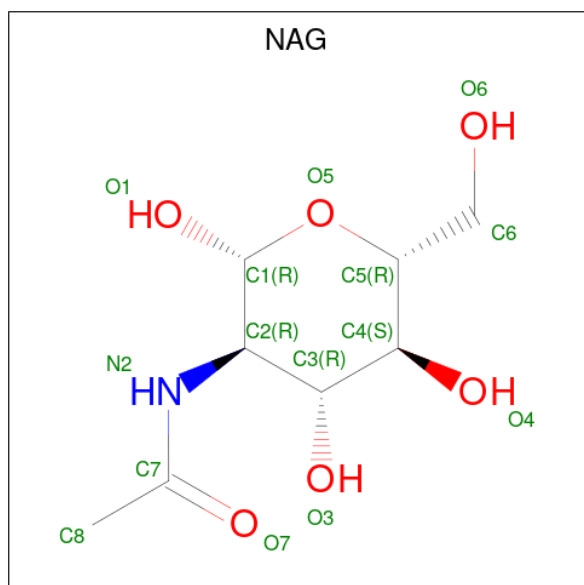
- Molecule 1 is a protein called S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2346	1465	385	493	3			
1	C	278	Total	C	N	O	S	0	0	0
			2103	1315	344	442	2			

- Molecule 2 is a protein called S-layer protein.

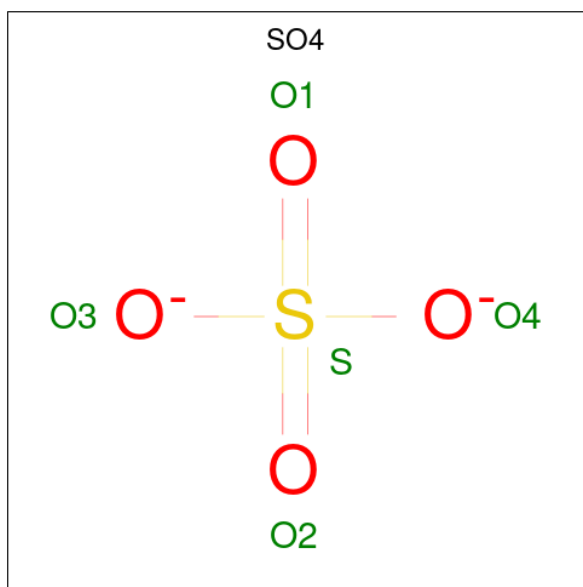
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	369	Total	C	N	O	S	5	0	0
			2732	1690	450	587	5			
2	D	373	Total	C	N	O	S	0	0	0
			2764	1710	456	593	5			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		

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



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

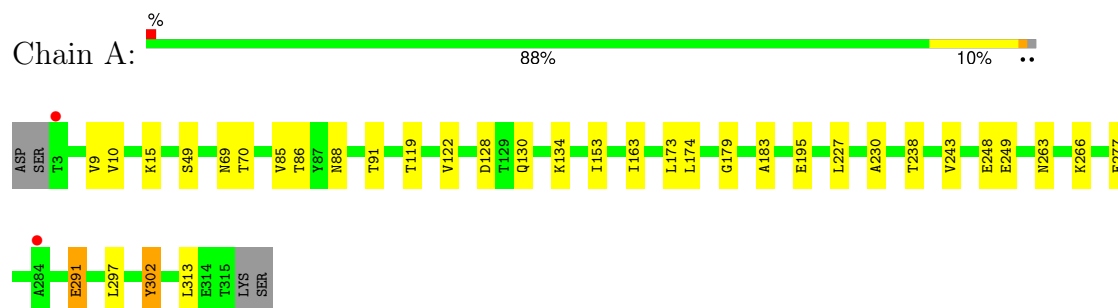
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	21	Total	O	0	0
			21	21		
5	C	31	Total	O	0	0
			31	31		
5	D	21	Total	O	0	0
			21	21		

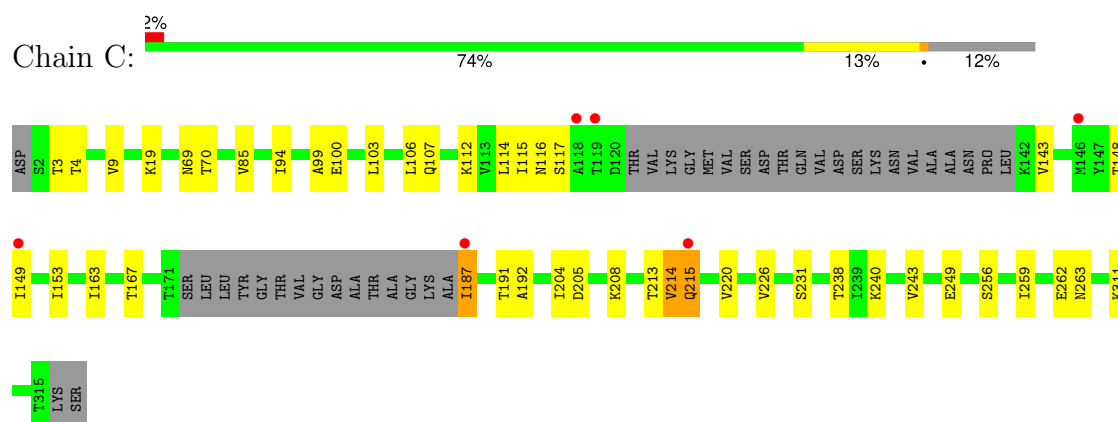
3 Residue-property plots [i](#)

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.

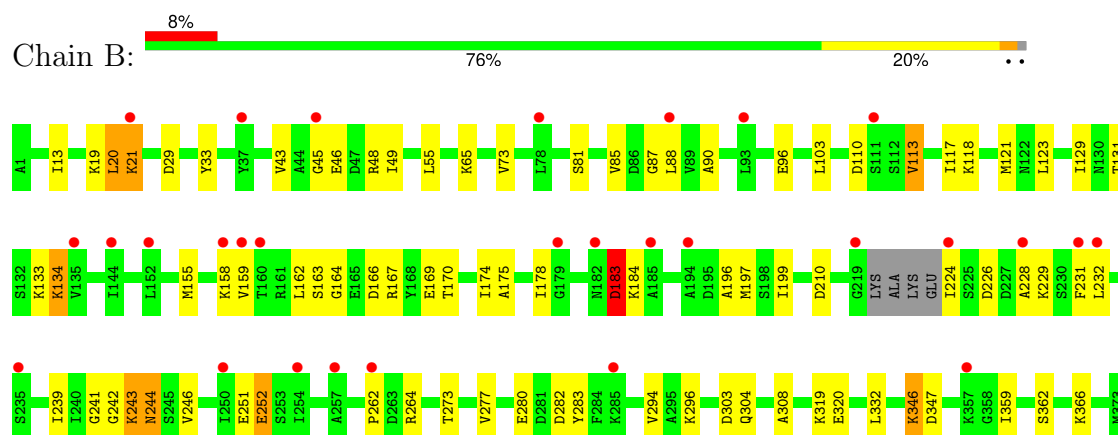
• Molecule 1: S-layer protein



• Molecule 1: S-layer protein

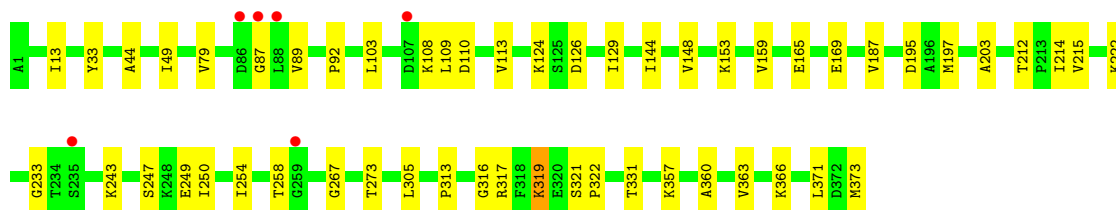


• Molecule 2: S-layer protein



● Molecule 2: S-layer protein

Chain D:  2% 86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.05Å 137.94Å 84.73Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	83.26 – 2.65 83.26 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (83.26-2.65) 99.9 (83.26-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.225 , 0.278 0.231 , 0.283	Depositor DCC
R_{free} test set	2592 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 31.93 % 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 1.0205e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.30	1/2374 (0.0%)	0.57	2/3219 (0.1%)
1	C	0.30	0/2127	0.69	7/2879 (0.2%)
2	B	0.36	0/2754	0.80	17/3725 (0.5%)
2	D	0.35	0/2787	0.62	2/3769 (0.1%)
All	All	0.33	1/10042 (0.0%)	0.68	28/13592 (0.2%)

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	C	0	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLU	CB-CG	5.61	1.69	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLU	CA-CB-CG	10.51	135.12	114.10
1	C	112	LYS	CB-CG-CD	8.32	130.44	111.30
1	C	19	LYS	CB-CA-C	-8.30	96.57	110.68
1	C	215	GLN	CA-CB-CG	-7.74	98.63	114.10
2	B	244	ASN	CA-C-N	7.46	137.54	121.64
2	B	244	ASN	C-N-CA	7.46	137.54	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLU	CB-CA-C	-7.37	96.43	109.62
2	B	183	ASP	CA-C-N	-7.08	111.70	122.81
2	B	183	ASP	C-N-CA	-7.08	111.70	122.81
2	B	332	LEU	CB-CG-CD2	-6.92	89.94	110.70
2	B	134	LYS	CB-CG-CD	-6.71	95.88	111.30
2	B	45	GLY	CA-C-N	-6.52	112.79	122.83
2	B	45	GLY	C-N-CA	-6.52	112.79	122.83
2	B	46	GLU	CA-CB-CG	-6.28	101.55	114.10
1	C	214	VAL	CA-C-N	-6.09	111.86	123.32
1	C	214	VAL	C-N-CA	-6.09	111.86	123.32
2	D	222	LYS	CA-C-N	6.05	132.22	121.75
2	D	222	LYS	C-N-CA	6.05	132.22	121.75
2	B	244	ASN	N-CA-C	-5.93	105.13	112.90
2	B	183	ASP	N-CA-C	5.93	123.42	110.80
2	B	243	LYS	CA-CB-CG	-5.89	102.32	114.10
2	B	282	ASP	CA-C-N	5.78	134.28	121.80
2	B	282	ASP	C-N-CA	5.78	134.28	121.80
1	C	19	LYS	N-CA-CB	5.67	118.57	110.06
1	C	19	LYS	CA-CB-CG	5.66	125.42	114.10
2	B	183	ASP	CB-CA-C	-5.32	99.84	110.42
2	B	346	LYS	CG-CD-CE	5.03	122.87	111.30
2	B	252	GLU	CA-CB-CG	-5.00	104.10	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	LEU	Peptide
1	C	117	SER	Peptide

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	2346	0	2351	27	1
1	C	2103	0	2100	31	0
2	B	2732	0	2753	64	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2764	0	2791	35	0
3	A	15	0	15	1	0
3	C	15	0	15	1	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	38	0	0	6	0
5	B	21	0	0	1	0
5	C	31	0	0	4	0
5	D	21	0	0	4	0
All	All	10096	0	10025	150	1

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 8.

All (150) 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:187:ILE:HG23	1:C:220:VAL:HB	1.39	1.03
2:B:226:ASP:HA	2:B:229:LYS:HD2	1.58	0.86
2:D:313:PRO:O	5:D:401:HOH:O	1.92	0.86
1:C:231:SER:O	5:C:501:HOH:O	1.99	0.80
1:C:100:GLU:OE2	5:C:502:HOH:O	2.00	0.79
2:B:231:PHE:HD2	2:B:232:LEU:HD12	1.49	0.78
1:C:214:VAL:C	1:C:215:GLN:HG2	2.09	0.78
1:A:277:GLU:OE1	5:A:601:HOH:O	2.02	0.76
2:B:251:GLU:OE2	5:B:401:HOH:O	2.04	0.75
2:B:296:LYS:HE2	2:B:304:GLN:HB3	1.68	0.74
2:B:85:VAL:HG11	2:B:167:ARG:HD2	1.69	0.73
1:A:313:LEU:HB3	2:D:129:ILE:HD11	1.71	0.71
1:A:302:TYR:CE2	2:B:20:LEU:HD23	2.26	0.70
2:B:252:GLU:HG3	2:B:252:GLU:O	1.90	0.70
2:D:195:ASP:OD2	5:D:403:HOH:O	2.11	0.68
2:B:131:THR:HA	2:B:158:LYS:HE2	1.74	0.67
2:B:183:ASP:O	2:B:184:LYS:HD2	1.95	0.67
1:A:173:LEU:O	5:A:602:HOH:O	2.14	0.66
1:A:49:SER:N	5:A:607:HOH:O	2.29	0.65
2:B:239:ILE:HD11	2:B:262:PRO:HB2	1.78	0.65
2:D:317:ARG:N	5:D:401:HOH:O	2.06	0.65
2:B:48:ARG:HH22	2:B:303:ASP:HB3	1.62	0.64
2:B:49:ILE:HD13	2:B:110:ASP:OD2	1.97	0.64
3:C:401:NAG:O6	5:C:504:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:VAL:HG13	2:D:214:ILE:HB	1.80	0.62
2:B:88:LEU:HD21	2:B:196:ALA:CB	2.30	0.62
1:C:3:THR:HG22	1:C:4:THR:H	1.65	0.62
1:A:134:LYS:NZ	1:A:179:GLY:O	2.27	0.61
1:C:114:LEU:HD11	1:C:143:VAL:HG12	1.81	0.61
1:C:69:ASN:OD1	1:C:70:THR:N	2.33	0.61
1:A:69:ASN:OD1	1:A:70:THR:N	2.35	0.59
2:D:79:VAL:HG13	2:D:103:LEU:HD23	1.84	0.59
2:D:110:ASP:HB2	2:D:113:VAL:HG12	1.84	0.59
1:C:256:SER:N	5:C:508:HOH:O	2.35	0.58
2:B:243:LYS:HA	2:B:246:VAL:O	2.02	0.58
2:B:65:LYS:HE3	2:D:126:ASP:OD2	2.03	0.58
1:C:106:LEU:HD11	1:C:204:ILE:HD13	1.86	0.57
2:D:316:GLY:HA2	2:D:322:PRO:HB3	1.86	0.57
2:D:363:VAL:HA	2:D:366:LYS:HE3	1.85	0.57
2:B:164:GLY:H	2:B:170:THR:HG22	1.70	0.56
1:A:230:ALA:O	5:A:603:HOH:O	2.17	0.56
2:B:117:ILE:HG23	2:B:121:MET:HE2	1.87	0.56
1:A:297:LEU:HD13	1:A:302:TYR:CD1	2.40	0.56
2:D:79:VAL:HG21	2:D:87:GLY:HA3	1.86	0.56
2:B:273:THR:O	2:B:277:VAL:HG23	2.06	0.55
2:B:87:GLY:HA2	2:B:90:ALA:HB3	1.87	0.55
2:B:48:ARG:NH2	2:B:303:ASP:HB3	2.22	0.55
2:B:129:ILE:HG12	1:C:311:LYS:O	2.07	0.54
1:C:107:GLN:HG2	1:C:149:ILE:HD12	1.89	0.54
1:A:15:LYS:NZ	5:A:612:HOH:O	2.40	0.54
1:A:302:TYR:HD1	1:A:302:TYR:N	2.05	0.54
1:C:103:LEU:O	1:C:107:GLN:HG3	2.08	0.54
2:D:89:VAL:O	2:D:92:PRO:HD2	2.08	0.54
2:B:81:SER:HA	2:B:103:LEU:HD13	1.89	0.54
2:B:199:ILE:HD11	2:B:283:TYR:CE1	2.43	0.53
2:B:242:GLY:C	2:B:264:ARG:HH12	2.17	0.53
2:B:280:GLU:HG2	2:B:283:TYR:CD2	2.44	0.52
1:C:94:ILE:HD12	1:C:99:ALA:HB2	1.91	0.52
1:C:213:THR:HG22	1:C:215:GLN:HE21	1.73	0.52
1:A:302:TYR:CD1	1:A:302:TYR:N	2.78	0.52
1:A:302:TYR:CD2	2:B:20:LEU:HD23	2.45	0.51
2:D:108:LYS:HD3	2:D:109:LEU:O	2.10	0.51
1:C:208:LYS:HB3	1:C:226:VAL:HG21	1.92	0.51
2:B:118:LYS:HE2	2:B:155:MET:HE3	1.93	0.50
2:B:346:LYS:HG3	2:B:347:ASP:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLU:OE1	2:B:210:ASP:HA	2.11	0.50
2:D:153:LYS:HD3	2:D:159:VAL:HB	1.92	0.50
2:B:88:LEU:HD21	2:B:196:ALA:HB3	1.91	0.50
2:D:243:LYS:N	2:D:243:LYS:HD2	2.26	0.50
2:D:371:LEU:HB2	2:D:373:MET:HE2	1.93	0.50
2:D:124:LYS:HB3	2:D:126:ASP:OD1	2.11	0.50
1:A:195:GLU:OE2	1:A:227:LEU:HD12	2.12	0.50
2:B:73:VAL:O	2:B:121:MET:HG2	2.12	0.50
2:B:163:SER:OG	2:B:164:GLY:N	2.44	0.49
2:D:267:GLY:N	2:D:273:THR:HG22	2.27	0.49
2:B:110:ASP:HB2	2:B:113:VAL:HG12	1.94	0.49
1:C:153:ILE:HG22	1:C:163:ILE:HD13	1.93	0.49
2:B:164:GLY:HA3	2:B:169:GLU:HG3	1.94	0.49
3:A:501:NAG:O7	3:A:501:NAG:O3	2.29	0.48
1:C:9:VAL:HB	1:C:243:VAL:HG22	1.94	0.48
2:B:29:ASP:O	2:B:33:TYR:HD1	1.96	0.48
2:B:197:MET:HE2	2:B:308:ALA:HB3	1.95	0.48
2:B:164:GLY:N	2:B:170:THR:HG22	2.28	0.48
1:C:249:GLU:HB2	2:D:13:ILE:HG12	1.96	0.48
2:B:19:LYS:HB3	2:B:21:LYS:HB3	1.96	0.47
1:A:10:VAL:HG11	1:A:248:GLU:HB2	1.96	0.47
2:B:88:LEU:HD21	2:B:196:ALA:HB1	1.96	0.47
1:A:153:ILE:HG22	1:A:163:ILE:HD13	1.97	0.47
2:D:233:GLY:O	2:D:258:THR:HG22	2.14	0.47
2:B:159:VAL:HG23	2:B:159:VAL:O	2.14	0.47
1:A:9:VAL:HB	1:A:243:VAL:HG22	1.97	0.47
1:A:86:THR:OG1	1:A:238:THR:HG22	2.15	0.46
1:A:119:THR:OG1	1:A:122:VAL:HG22	2.15	0.46
1:A:88:ASN:ND2	1:A:91:THR:HG23	2.31	0.46
2:D:360:ALA:O	2:D:363:VAL:HG12	2.16	0.46
1:A:183:ALA:O	5:A:604:HOH:O	2.21	0.46
2:B:239:ILE:HG21	2:B:246:VAL:HG11	1.97	0.46
1:C:214:VAL:O	1:C:215:GLN:HG2	2.15	0.46
2:B:199:ILE:HD11	2:B:283:TYR:HE1	1.81	0.46
2:B:224:ILE:O	2:B:229:LYS:HE3	2.16	0.46
1:C:115:ILE:HG22	1:C:116:ASN:O	2.16	0.46
2:D:165:GLU:CD	2:D:169:GLU:OE2	2.59	0.46
1:A:128:ASP:HA	1:A:174:LEU:HD12	1.98	0.45
2:B:162:LEU:HD22	2:B:174:ILE:HA	1.98	0.45
1:C:262:GLU:HG3	2:D:33:TYR:CD1	2.51	0.45
2:B:362:SER:O	2:B:366:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:GLU:CG	2:B:283:TYR:CD2	2.99	0.45
1:C:114:LEU:HD12	1:C:114:LEU:N	2.32	0.45
1:C:213:THR:HG22	1:C:215:GLN:NE2	2.32	0.45
2:D:250:ILE:O	2:D:254:ILE:HG13	2.17	0.45
2:B:224:ILE:HG22	2:B:228:ALA:HB3	1.99	0.45
2:B:239:ILE:CD1	2:B:262:PRO:HB2	2.45	0.44
2:D:49:ILE:HD13	2:D:110:ASP:OD2	2.17	0.44
1:C:240:LYS:HB3	1:C:240:LYS:HE2	1.81	0.44
2:D:321:SER:OG	5:D:402:HOH:O	1.98	0.44
2:D:331:THR:OG1	2:D:366:LYS:NZ	2.51	0.44
2:B:199:ILE:HD12	2:B:199:ILE:HA	1.69	0.44
2:B:19:LYS:CB	2:B:21:LYS:HB3	2.48	0.44
2:B:43:VAL:HG11	2:B:55:LEU:HD23	1.99	0.44
1:C:85:VAL:O	1:C:238:THR:HA	2.18	0.44
2:D:247:SER:OG	2:D:249:GLU:HG3	2.18	0.44
2:D:203:ALA:HB1	2:D:212:THR:O	2.19	0.43
1:A:85:VAL:O	1:A:238:THR:HA	2.18	0.43
2:B:175:ALA:HA	2:B:178:ILE:HD12	1.99	0.43
2:D:197:MET:HG3	2:D:305:LEU:HD22	2.00	0.43
1:C:3:THR:HG22	1:C:4:THR:N	2.31	0.43
1:C:262:GLU:HG3	2:D:33:TYR:CE1	2.53	0.43
2:D:144:ILE:HG22	2:D:148:VAL:HG21	2.00	0.42
2:D:187:VAL:HG22	2:D:215:VAL:CG2	2.49	0.42
2:B:319:LYS:HB3	2:B:320:GLU:H	1.63	0.42
2:B:199:ILE:CD1	2:B:283:TYR:HE1	2.32	0.42
2:B:241:GLY:O	2:B:264:ARG:NH1	2.52	0.42
1:A:266:LYS:HB3	1:A:266:LYS:HE3	1.85	0.42
2:D:319:LYS:HD2	2:D:319:LYS:HA	1.73	0.42
2:B:134:LYS:HB3	2:B:134:LYS:HE2	1.32	0.42
1:C:148:THR:HB	1:C:167:THR:OG1	2.20	0.42
2:B:174:ILE:HG22	2:B:178:ILE:HD11	2.00	0.41
1:C:205:ASP:HB3	1:C:226:VAL:HG23	2.01	0.41
2:B:121:MET:HE3	2:B:123:LEU:HD11	2.02	0.41
1:A:249:GLU:HB2	2:B:13:ILE:HD13	2.02	0.41
1:A:134:LYS:HG2	1:A:179:GLY:HA2	2.03	0.41
2:D:44:ALA:HB1	2:D:357:LYS:HG3	2.03	0.41
2:B:231:PHE:CD2	2:B:232:LEU:HD12	2.41	0.41
1:A:263:ASN:HA	1:A:266:LYS:HE3	2.03	0.41
2:B:133:LYS:O	2:B:158:LYS:HG2	2.21	0.41
1:C:191:THR:O	1:C:192:ALA:HB3	2.21	0.41
2:B:85:VAL:HG11	2:B:167:ARG:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:VAL:HG12	2:B:359:ILE:HD13	2.04	0.40
1:C:259:ILE:HD11	1:C:263:ASN:HB3	2.02	0.40
2:B:166:ASP:O	2:B:170:THR:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLN:O	2:B:244:ASN:ND2[2_543]	1.95	0.25

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	311/317 (98%)	306 (98%)	5 (2%)	0	100	100
1	C	272/317 (86%)	263 (97%)	9 (3%)	0	100	100
2	B	365/373 (98%)	351 (96%)	12 (3%)	2 (0%)	24	39
2	D	371/373 (100%)	362 (98%)	8 (2%)	1 (0%)	36	52
All	All	1319/1380 (96%)	1282 (97%)	34 (3%)	3 (0%)	43	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	LYS
2	B	183	ASP
2	D	319	LYS

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	259/263 (98%)	257 (99%)	2 (1%)	73	85
1	C	233/263 (89%)	232 (100%)	1 (0%)	84	93
2	B	307/310 (99%)	306 (100%)	1 (0%)	86	94
2	D	310/310 (100%)	310 (100%)	0	100	100
All	All	1109/1146 (97%)	1105 (100%)	4 (0%)	84	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	A	302	TYR
2	B	113	VAL
1	C	187	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	287	ASN
1	A	299	ASN
2	B	39	ASN
2	B	291	ASN
2	B	337	ASN
2	B	351	ASN
1	C	107	GLN
1	C	215	GLN
2	D	39	ASN
2	D	354	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NAG	C	401	-	15,15,15	0.29	0	21,21,21	0.44	0
3	NAG	A	501	-	15,15,15	0.27	0	21,21,21	0.67	0
4	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.15	0
4	SO4	C	402	-	4,4,4	0.21	0	6,6,6	0.26	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	NAG	C	401	-	-	2/6/26/26	0/1/1/1
3	NAG	A	501	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C1-C2-N2-C7
3	A	501	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	A	501	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	NAG	1	0
3	A	501	NAG	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 ⓘ

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	313/317 (98%)	-0.18	2 (0%) 85 83	38, 63, 87, 111	0
1	C	278/317 (87%)	0.03	6 (2%) 62 56	40, 68, 108, 126	4 (1%)
2	B	369/373 (98%)	0.55	29 (7%) 18 14	48, 76, 117, 134	8 (2%)
2	D	373/373 (100%)	0.06	6 (1%) 70 66	43, 66, 93, 108	3 (0%)
All	All	1333/1380 (96%)	0.13	43 (3%) 50 42	38, 69, 106, 134	15 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	135	VAL	5.9
2	B	235	SER	4.8
2	B	232	LEU	3.7
2	B	257	ALA	3.1
2	B	262	PRO	3.1
2	B	219	GLY	3.0
2	D	235	SER	3.0
2	B	152	LEU	2.9
2	B	111	SER	2.8
2	D	87	GLY	2.8
2	D	86	ASP	2.8
2	B	88	LEU	2.8
1	C	119	THR	2.8
2	B	159	VAL	2.8
2	B	357	LYS	2.7
2	B	182	ASN	2.7
1	C	215	GLN	2.6
2	B	37	TYR	2.6
1	A	284	ALA	2.6
1	C	187	ILE	2.5
2	B	224	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	185	ALA	2.4
2	B	160	THR	2.4
2	B	158	LYS	2.3
2	B	144	ILE	2.3
2	B	194	ALA	2.3
2	B	78	LEU	2.2
2	B	45	GLY	2.2
2	B	231	PHE	2.2
1	A	3	THR	2.2
2	D	88	LEU	2.1
2	B	285	LYS	2.1
1	C	146	MET	2.1
2	B	93	LEU	2.1
2	D	107	ASP	2.1
2	B	228	ALA	2.1
1	C	118	ALA	2.1
2	D	259	GLY	2.1
2	B	250	ILE	2.1
2	B	254	ILE	2.1
2	B	179	GLY	2.0
2	B	21	LYS	2.0
1	C	149	ILE	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 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	NAG	A	501	15/15	0.78	0.18	53,64,72,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	402	5/5	0.81	0.17	67,72,105,113	0
3	NAG	C	401	15/15	0.83	0.13	47,61,71,75	0
4	SO4	A	502	5/5	0.89	0.08	67,86,112,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.