



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:13 AM UTC

PDB ID : 1N0U / pdb_00001n0u
Title : Crystal structure of yeast elongation factor 2 in complex with sordarin
Authors : Joergensen, R.; Ortiz, P.A.; Carr-Schmid, A.; Nissen, P.; Kinzy, T.G.; Andersen, G.R.
Deposited on : 2002-10-15
Resolution : 2.12 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

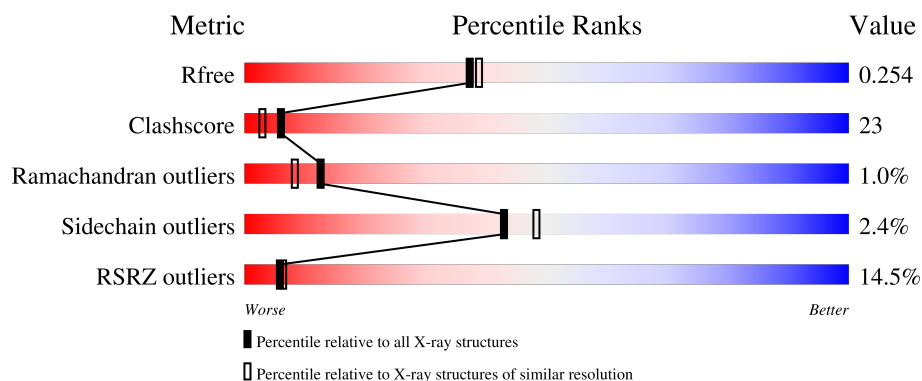
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	842	14% 61% 34% ..

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
2	SO1	A	843	X	-	-	-

2 Entry composition [i](#)

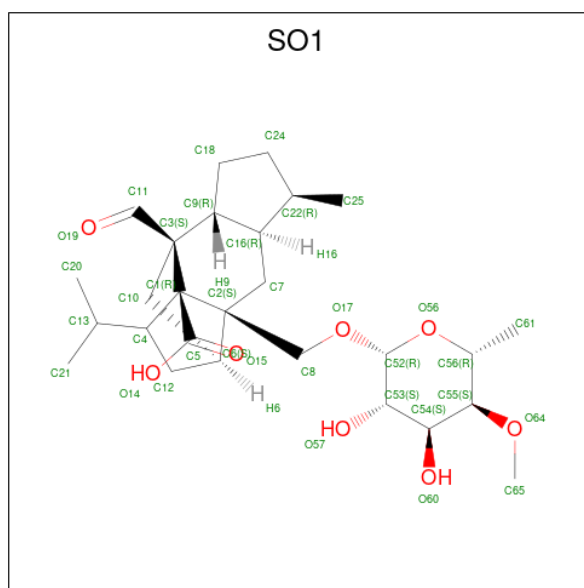
There are 3 unique types of molecules in this entry. The entry contains 6904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	819	6375	4057	1086	1202	30	0	0	0

- Molecule 2 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (CCD ID: SO1) (formula: C₂₇H₄₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	35	27	8	0	0

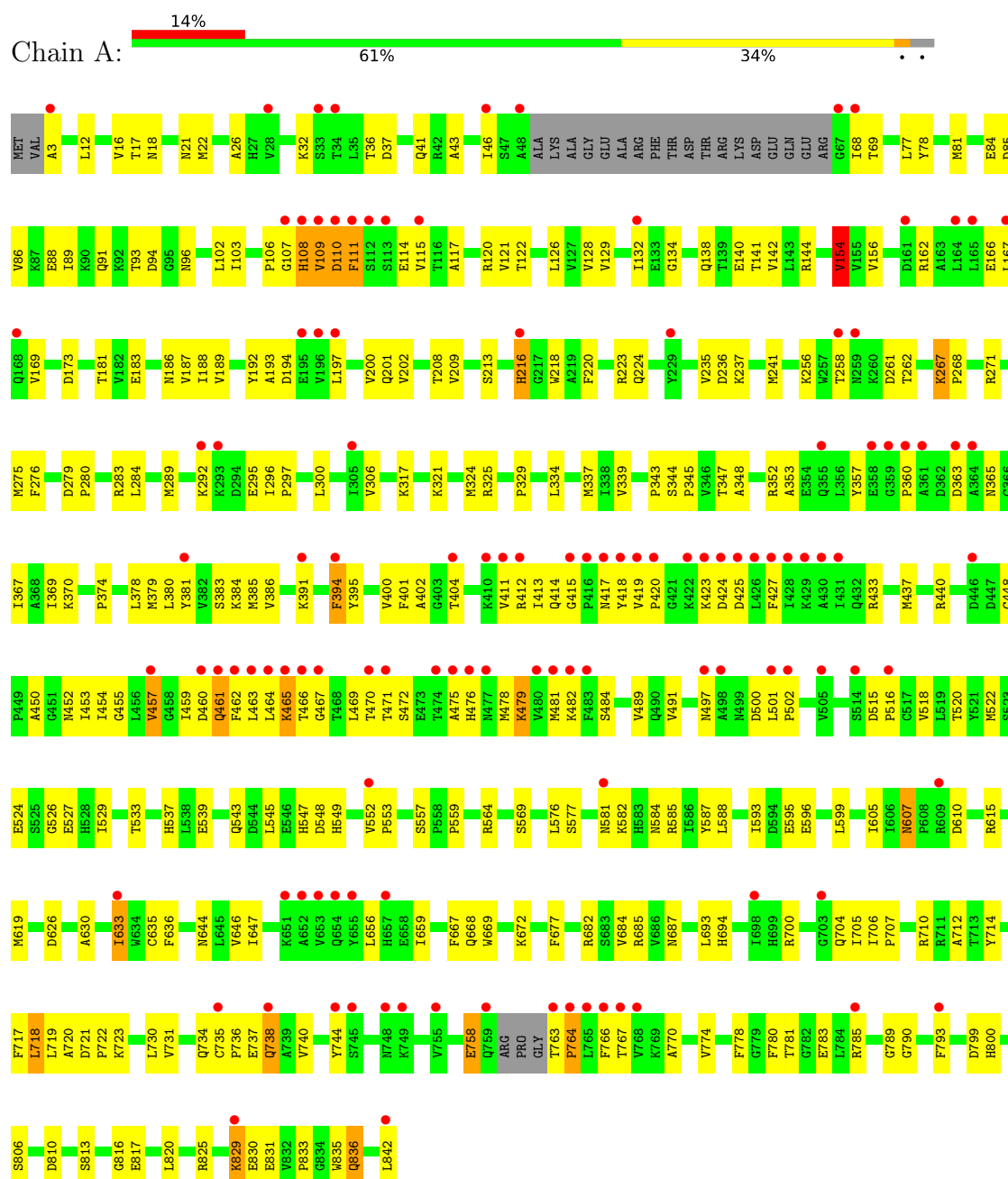
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	494	Total	O	0	0
			494	494		

3 Residue-property plots

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: Elongation factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.96Å 150.83Å 65.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.12 31.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.0 (31.00-2.12) 98.0 (31.00-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.254 0.236 , 0.254	Depositor DCC
R_{free} test set	1962 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: SO1

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	0.45	0/6497	0.93	20/8797 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	N-CA-C	-11.96	96.46	113.21
1	A	109	VAL	N-CA-C	7.43	120.29	108.85
1	A	461	GLN	N-CA-C	6.15	117.98	111.28
1	A	348	ALA	N-CA-C	6.10	118.01	111.36
1	A	557	SER	N-CA-C	5.95	113.58	108.22
1	A	187	VAL	N-CA-C	-5.81	105.06	110.53
1	A	593	ILE	N-CA-C	-5.80	100.07	108.36
1	A	154	VAL	N-CA-C	-5.73	99.97	108.45
1	A	721	ASP	CA-C-N	5.71	125.64	119.76
1	A	721	ASP	C-N-CA	5.71	125.64	119.76
1	A	267	LYS	CA-C-N	5.68	125.96	119.83
1	A	267	LYS	C-N-CA	5.68	125.96	119.83
1	A	636	PHE	N-CA-C	-5.58	101.49	110.14
1	A	626	ASP	N-CA-C	-5.40	101.18	109.76
1	A	192	TYR	N-CA-C	5.34	119.95	113.38
1	A	607	ASN	N-CA-C	5.34	118.20	110.14
1	A	17	THR	N-CA-C	-5.26	105.71	111.82
1	A	730	LEU	N-CA-C	-5.09	99.49	108.20
1	A	607	ASN	CA-C-N	5.06	125.09	119.32
1	A	607	ASN	C-N-CA	5.06	125.09	119.32

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	6375	0	6441	293	0
2	A	35	0	40	2	0
3	A	494	0	0	48	0
All	All	6904	0	6481	293	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 23.

All (293) 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:615:ARG:HG2	1:A:619:MET:HE2	1.45	0.99
1:A:463:LEU:HD21	1:A:467:GLY:HA3	1.46	0.97
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.50	0.93
1:A:284:LEU:HD13	1:A:324:MET:HE1	1.51	0.93
1:A:667:PHE:HB3	3:A:1142:HOH:O	1.69	0.91
1:A:109:VAL:HG11	1:A:142:VAL:HG22	1.52	0.88
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.55	0.87
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.40	0.86
1:A:685:ARG:HE	1:A:687:ASN:HD21	1.20	0.85
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.59	0.85
1:A:533:THR:H	1:A:537:HIS:HD2	1.26	0.84
1:A:109:VAL:HG22	1:A:138:GLN:HG3	1.60	0.82
1:A:216:HIS:HA	3:A:1026:HOH:O	1.80	0.81
1:A:694:HIS:O	1:A:700:ARG:HD3	1.81	0.80
1:A:18:ASN:HD21	1:A:94:ASP:H	1.27	0.79
1:A:829:LYS:HE2	3:A:905:HOH:O	1.83	0.78
1:A:91:GLN:NE2	1:A:344:SER:H	1.81	0.78
1:A:91:GLN:HE22	1:A:344:SER:H	1.32	0.78
1:A:109:VAL:HG21	1:A:142:VAL:HG23	1.65	0.77
1:A:734:GLN:HE21	1:A:767:THR:HG22	1.50	0.77
1:A:433:ARG:HB3	1:A:457:VAL:CG1	2.17	0.75
1:A:378:LEU:H	1:A:471:THR:HG22	1.52	0.74
1:A:780:PHE:HA	3:A:1144:HOH:O	1.88	0.74
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.18	0.73
1:A:718:LEU:HB3	1:A:835:TRP:HB3	1.70	0.73
1:A:829:LYS:HE3	1:A:830:GLU:H	1.50	0.73
1:A:799:ASP:OD1	1:A:800:HIS:HD2	1.72	0.72
1:A:522:MET:HE2	1:A:526:GLY:C	2.15	0.72
1:A:763:THR:N	1:A:764:PRO:HD3	2.04	0.72
1:A:466:THR:HB	3:A:943:HOH:O	1.89	0.71
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.20	0.71
1:A:533:THR:H	1:A:537:HIS:CD2	2.09	0.70
1:A:630:ALA:O	1:A:633:ILE:HG23	1.91	0.70
1:A:194:ASP:HB2	1:A:197:LEU:HD13	1.73	0.70
1:A:386:VAL:HG11	1:A:437:MET:HE1	1.75	0.69
1:A:189:VAL:CG1	1:A:200:VAL:HG13	2.24	0.68
1:A:202:VAL:HG12	1:A:209:VAL:CG2	2.23	0.68
1:A:103:ILE:HD11	1:A:453:ILE:HD11	1.76	0.68
1:A:482:LYS:HB2	1:A:793:PHE:CZ	2.29	0.67
1:A:836:GLN:H	1:A:836:GLN:NE2	1.90	0.67
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.59	0.67
1:A:386:VAL:HG12	1:A:395:TYR:O	1.94	0.67
1:A:424:ASP:O	1:A:425:ASP:HB2	1.92	0.67
1:A:417:ASN:HB2	1:A:425:ASP:OD2	1.94	0.67
1:A:284:LEU:CD1	1:A:324:MET:HE1	2.23	0.66
1:A:324:MET:HE2	1:A:324:MET:HA	1.77	0.66
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.78	0.66
1:A:734:GLN:HE21	1:A:767:THR:CG2	2.09	0.66
1:A:785:ARG:HG3	1:A:785:ARG:HH11	1.61	0.66
1:A:91:GLN:HE21	1:A:347:THR:CB	2.09	0.65
1:A:813:SER:O	1:A:817:GLU:HG3	1.97	0.65
1:A:374:PRO:O	1:A:404:THR:HG23	1.97	0.65
1:A:522:MET:HE3	1:A:527:GLU:C	2.22	0.65
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.26	0.65
1:A:378:LEU:N	1:A:471:THR:HG22	2.12	0.65
1:A:385:MET:HG2	3:A:1102:HOH:O	1.97	0.64
1:A:497:ASN:HB3	1:A:500:ASP:OD2	1.97	0.64
1:A:369:ILE:HD13	1:A:402:ALA:HB2	1.79	0.64
1:A:202:VAL:HG12	1:A:209:VAL:HG23	1.78	0.64
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.80	0.64
1:A:213:SER:OG	1:A:216:HIS:HB2	1.97	0.63
1:A:619:MET:HE3	1:A:630:ALA:HB1	1.80	0.63
1:A:464:LEU:O	1:A:465:LYS:HB2	1.99	0.63
1:A:783:GLU:HB2	3:A:1144:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD11	1:A:453:ILE:CD1	2.29	0.63
1:A:186:ASN:HB3	1:A:201:GLN:NE2	2.14	0.63
1:A:668:GLN:NE2	3:A:1142:HOH:O	2.32	0.62
1:A:384:LYS:HD2	3:A:1082:HOH:O	1.99	0.62
1:A:685:ARG:NE	1:A:687:ASN:HD21	1.95	0.62
1:A:81:MET:HG3	1:A:339:VAL:HG11	1.81	0.62
1:A:353:ALA:CB	1:A:370:LYS:HG2	2.29	0.62
1:A:644:ASN:HD22	1:A:684:VAL:H	1.45	0.62
1:A:365:ASN:O	1:A:369:ILE:HG12	1.99	0.62
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.28	0.61
1:A:685:ARG:HE	1:A:687:ASN:ND2	1.97	0.61
1:A:378:LEU:H	1:A:471:THR:CG2	2.12	0.60
1:A:284:LEU:HD13	1:A:324:MET:CE	2.27	0.60
1:A:731:VAL:HG12	1:A:770:ALA:O	2.02	0.60
1:A:223:ARG:HD2	3:A:1304:HOH:O	2.02	0.59
1:A:418:TYR:HA	1:A:424:ASP:O	2.02	0.59
1:A:831:GLU:HG3	3:A:905:HOH:O	2.01	0.59
1:A:545:LEU:HA	1:A:549:HIS:HB2	1.85	0.59
1:A:710:ARG:NH1	1:A:714:TYR:OH	2.36	0.59
1:A:321:LYS:HG2	3:A:1026:HOH:O	2.02	0.59
1:A:88:GLU:CD	1:A:223:ARG:HH21	2.12	0.58
1:A:103:ILE:HD12	1:A:122:THR:CG2	2.31	0.58
1:A:829:LYS:HE3	1:A:830:GLU:N	2.18	0.58
1:A:292:LYS:HD3	1:A:295:GLU:OE2	2.03	0.58
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.85	0.58
1:A:413:ILE:HB	1:A:427:PHE:HB2	1.83	0.58
1:A:836:GLN:H	1:A:836:GLN:HE21	1.50	0.58
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.86	0.57
1:A:296:ILE:O	1:A:300:LEU:HD13	2.04	0.57
1:A:585:ARG:NH1	1:A:842:LEU:HD23	2.19	0.57
1:A:646:VAL:C	1:A:647:ILE:HD12	2.29	0.57
1:A:415:GLY:H	1:A:425:ASP:HB3	1.70	0.57
1:A:705:ILE:HD12	3:A:977:HOH:O	2.05	0.56
1:A:810:ASP:O	1:A:816:GLY:HA3	2.05	0.56
1:A:369:ILE:HD12	1:A:401:PHE:HB3	1.87	0.56
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.86	0.56
1:A:581:ASN:O	1:A:582:LYS:HB2	2.06	0.56
1:A:117:ALA:HB1	3:A:968:HOH:O	2.05	0.55
1:A:237:LYS:O	1:A:241:MET:HG2	2.06	0.55
1:A:482:LYS:HB2	1:A:793:PHE:HZ	1.70	0.55
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.88	0.54
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.89	0.54
1:A:412:ARG:HD2	3:A:1010:HOH:O	2.07	0.54
1:A:734:GLN:HG3	1:A:767:THR:HG22	1.89	0.54
1:A:423:LYS:HG2	1:A:423:LYS:O	2.08	0.54
1:A:501:LEU:HB2	1:A:502:PRO:HD3	1.90	0.54
1:A:275:MET:HE2	1:A:276:PHE:CZ	2.43	0.54
1:A:552:VAL:HG13	1:A:553:PRO:HD2	1.89	0.54
1:A:114:GLU:HB2	3:A:1037:HOH:O	2.07	0.54
1:A:200:VAL:HG12	3:A:1237:HOH:O	2.06	0.54
1:A:588:LEU:HD12	1:A:588:LEU:C	2.33	0.53
1:A:88:GLU:OE2	1:A:223:ARG:NH2	2.42	0.53
1:A:829:LYS:HE3	1:A:829:LYS:HA	1.90	0.53
1:A:109:VAL:HG12	1:A:115:VAL:HG21	1.89	0.53
1:A:154:VAL:HG11	1:A:337:MET:HB3	1.91	0.53
1:A:3:ALA:HA	1:A:46:ILE:O	2.09	0.53
1:A:461:GLN:HG2	3:A:904:HOH:O	2.09	0.53
1:A:103:ILE:HD13	1:A:121:VAL:HG23	1.91	0.52
1:A:169:VAL:CG1	1:A:173:ASP:HB2	2.39	0.52
1:A:411:VAL:HG12	1:A:412:ARG:N	2.24	0.52
1:A:91:GLN:HE22	1:A:344:SER:N	2.04	0.52
1:A:167:LEU:HD12	1:A:167:LEU:N	2.24	0.52
1:A:693:LEU:HB3	1:A:700:ARG:CD	2.39	0.52
1:A:433:ARG:HB3	1:A:457:VAL:HG13	1.92	0.52
1:A:607:ASN:HB2	1:A:610:ASP:OD2	2.10	0.52
1:A:89:ILE:HG22	1:A:91:GLN:HB3	1.92	0.52
1:A:466:THR:HG22	3:A:968:HOH:O	2.09	0.52
1:A:193:ALA:CB	1:A:200:VAL:HG11	2.40	0.52
1:A:258:THR:HG21	3:A:1071:HOH:O	2.08	0.52
1:A:454:ILE:HG13	1:A:455:GLY:H	1.75	0.52
1:A:547:HIS:HD2	1:A:548:ASP:OD1	1.93	0.52
1:A:109:VAL:CG1	1:A:115:VAL:HG21	2.40	0.51
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.39	0.51
1:A:454:ILE:HG13	1:A:455:GLY:N	2.25	0.51
1:A:533:THR:N	1:A:537:HIS:HD2	2.03	0.51
1:A:569:SER:O	1:A:720:ALA:HB1	2.11	0.51
1:A:758:GLU:HG3	1:A:767:THR:OG1	2.10	0.51
1:A:457:VAL:HG23	3:A:973:HOH:O	2.09	0.51
1:A:120:ARG:NH1	1:A:481:MET:CE	2.74	0.51
1:A:806:SER:HB2	1:A:813:SER:HB2	1.92	0.50
1:A:360:PRO:HD2	3:A:1019:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HH12	1:A:481:MET:HE2	1.77	0.50
1:A:736:PRO:HB2	1:A:738:GLN:OE1	2.11	0.49
1:A:120:ARG:HH12	1:A:481:MET:CE	2.25	0.49
1:A:576:LEU:HD21	1:A:585:ARG:HH11	1.77	0.49
1:A:202:VAL:CG1	1:A:209:VAL:CG2	2.90	0.49
1:A:107:GLY:O	1:A:109:VAL:HG13	2.13	0.49
1:A:605:ILE:N	1:A:605:ILE:HD12	2.28	0.49
1:A:216:HIS:HB3	1:A:218:TRP:CD1	2.48	0.49
1:A:644:ASN:ND2	1:A:684:VAL:H	2.09	0.49
1:A:433:ARG:HB3	1:A:457:VAL:HG11	1.93	0.49
1:A:400:VAL:HG12	1:A:450:ALA:HA	1.95	0.48
1:A:433:ARG:HD2	3:A:942:HOH:O	2.13	0.48
1:A:533:THR:HG22	3:A:1182:HOH:O	2.14	0.48
1:A:785:ARG:HG3	1:A:785:ARG:NH1	2.27	0.48
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.95	0.48
1:A:559:PRO:HG2	1:A:778:PHE:CE1	2.48	0.48
1:A:737:GLU:HB2	1:A:766:PHE:CE2	2.49	0.48
1:A:37:ASP:O	1:A:41:GLN:HG3	2.13	0.48
1:A:419:VAL:HG12	3:A:1063:HOH:O	2.14	0.48
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.48	0.48
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.48	0.48
1:A:202:VAL:CG1	1:A:209:VAL:HG22	2.42	0.48
1:A:16:VAL:O	1:A:345:PRO:HD2	2.13	0.48
1:A:107:GLY:O	1:A:109:VAL:N	2.46	0.48
1:A:306:VAL:HG22	3:A:1111:HOH:O	2.14	0.48
1:A:500:ASP:CG	1:A:552:VAL:HG11	2.38	0.48
1:A:520:THR:HA	1:A:529:ILE:O	2.13	0.48
1:A:129:VAL:HG13	1:A:134:GLY:O	2.14	0.47
1:A:200:VAL:O	1:A:200:VAL:HG22	2.13	0.47
1:A:380:LEU:C	1:A:380:LEU:HD23	2.39	0.47
1:A:564:ARG:HG3	1:A:682:ARG:HB2	1.95	0.47
1:A:820:LEU:CB	3:A:1118:HOH:O	2.61	0.47
1:A:820:LEU:HB3	3:A:1118:HOH:O	2.13	0.47
1:A:440:ARG:HD2	3:A:1056:HOH:O	2.14	0.47
1:A:833:PRO:HA	3:A:1095:HOH:O	2.13	0.47
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.97	0.47
1:A:110:ASP:O	1:A:111:PHE:HB2	2.14	0.47
1:A:258:THR:HB	3:A:1028:HOH:O	2.14	0.47
1:A:110:ASP:HB3	1:A:785:ARG:NH1	2.30	0.47
1:A:111:PHE:CD2	1:A:789:GLY:HA2	2.49	0.47
1:A:292:LYS:HD3	1:A:295:GLU:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PHE:N	1:A:394:PHE:CD2	2.83	0.47
1:A:394:PHE:N	1:A:394:PHE:HD2	2.13	0.47
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.80	0.47
1:A:84:GLU:HG3	1:A:85:ASP:N	2.30	0.47
1:A:117:ALA:N	3:A:1057:HOH:O	2.48	0.47
1:A:279:ASP:OD2	1:A:283:ARG:CZ	2.63	0.47
1:A:386:VAL:HG11	1:A:437:MET:CE	2.43	0.47
1:A:633:ILE:C	1:A:633:ILE:HD12	2.40	0.46
1:A:718:LEU:HA	1:A:722:PRO:HG3	1.96	0.46
1:A:162:ARG:HG3	1:A:166:GLU:OE2	2.14	0.46
1:A:817:GLU:HA	3:A:1118:HOH:O	2.16	0.46
1:A:515:ASP:O	1:A:518:VAL:HG12	2.15	0.46
1:A:108:HIS:O	1:A:108:HIS:CG	2.69	0.46
1:A:584:ASN:HD21	1:A:700:ARG:HG2	1.79	0.46
1:A:357:TYR:CZ	1:A:476:HIS:HB3	2.50	0.46
1:A:633:ILE:HG13	1:A:633:ILE:O	2.16	0.45
1:A:737:GLU:HB2	1:A:766:PHE:HE2	1.80	0.45
1:A:774:VAL:HG11	2:A:843:SO1:H121	1.98	0.45
1:A:825:ARG:NE	3:A:1032:HOH:O	2.30	0.45
1:A:109:VAL:HG21	1:A:142:VAL:CG2	2.43	0.45
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.98	0.45
1:A:552:VAL:CG1	1:A:553:PRO:HD2	2.46	0.45
1:A:381:TYR:CZ	3:A:943:HOH:O	2.63	0.45
1:A:491:VAL:HA	1:A:559:PRO:HD3	1.98	0.45
1:A:197:LEU:N	1:A:197:LEU:HD12	2.31	0.45
1:A:108:HIS:CE1	3:A:1037:HOH:O	2.69	0.45
1:A:539:GLU:O	1:A:543:GLN:HG3	2.16	0.45
1:A:420:PRO:HB2	3:A:1063:HOH:O	2.16	0.45
1:A:129:VAL:HG11	1:A:181:THR:HG23	2.00	0.44
1:A:379:MET:HB2	1:A:402:ALA:HB3	2.00	0.44
1:A:321:LYS:HE2	3:A:1026:HOH:O	2.17	0.44
1:A:325:ARG:O	1:A:329:PRO:HG3	2.18	0.44
1:A:740:VAL:HG12	1:A:744:TYR:CE2	2.53	0.44
1:A:669:TRP:CD1	1:A:710:ARG:NH1	2.85	0.44
1:A:21:ASN:ND2	1:A:345:PRO:HG3	2.33	0.44
1:A:306:VAL:HG23	1:A:306:VAL:O	2.17	0.44
1:A:633:ILE:HD12	1:A:635:CYS:N	2.32	0.44
1:A:722:PRO:O	1:A:723:LYS:HD2	2.18	0.44
1:A:524:GLU:HG3	3:A:1156:HOH:O	2.17	0.43
1:A:114:GLU:CG	3:A:1037:HOH:O	2.66	0.43
1:A:216:HIS:HB3	1:A:218:TRP:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:O	1:A:36:THR:HG23	2.18	0.43
1:A:459:ILE:HG22	1:A:459:ILE:O	2.18	0.43
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.19	0.43
1:A:289:MET:HE1	1:A:317:LYS:HG3	2.01	0.43
1:A:647:ILE:HD12	1:A:647:ILE:N	2.34	0.43
1:A:81:MET:O	1:A:96:ASN:HB3	2.19	0.43
1:A:261:ASP:OD1	1:A:262:THR:HG23	2.18	0.43
1:A:223:ARG:HG3	1:A:241:MET:HE1	1.99	0.43
1:A:559:PRO:HB2	2:A:843:SO1:H201	2.01	0.43
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.34	0.43
1:A:18:ASN:N	1:A:18:ASN:HD22	2.17	0.43
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.84	0.42
1:A:478:MET:O	1:A:479:LYS:C	2.62	0.42
1:A:16:VAL:HG11	1:A:450:ALA:O	2.19	0.42
1:A:462:PHE:HE2	3:A:1286:HOH:O	2.02	0.42
1:A:484:SER:O	1:A:533:THR:HG21	2.19	0.42
1:A:738:GLN:OE1	1:A:738:GLN:N	2.51	0.42
1:A:22:MET:SD	1:A:102:LEU:HD12	2.59	0.42
1:A:108:HIS:O	1:A:108:HIS:CD2	2.72	0.42
1:A:763:THR:N	1:A:764:PRO:CD	2.78	0.42
1:A:126:LEU:CD1	1:A:156:VAL:HG23	2.36	0.42
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.49	0.42
1:A:241:MET:HE1	3:A:1290:HOH:O	2.18	0.42
1:A:489:VAL:HG22	1:A:781:THR:HG21	2.02	0.42
1:A:515:ASP:OD2	1:A:537:HIS:HE1	2.02	0.42
1:A:26:ALA:CB	1:A:128:VAL:HB	2.50	0.42
1:A:470:THR:HG21	1:A:475:ALA:HB1	2.02	0.42
1:A:383:SER:O	1:A:384:LYS:HB3	2.20	0.42
1:A:718:LEU:HA	1:A:718:LEU:HD12	1.92	0.42
1:A:448:CYS:SG	1:A:452:ASN:HB2	2.60	0.42
1:A:659:ILE:CG2	1:A:705:ILE:HD13	2.50	0.42
1:A:162:ARG:HG3	1:A:166:GLU:CD	2.45	0.41
1:A:785:ARG:HB2	1:A:790:GLY:HA2	2.01	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.86	0.41
1:A:202:VAL:CG1	1:A:208:THR:O	2.67	0.41
1:A:91:GLN:HG3	1:A:347:THR:OG1	2.21	0.41
1:A:522:MET:CE	1:A:526:GLY:C	2.89	0.41
1:A:717:PHE:HD2	1:A:718:LEU:HD13	1.86	0.41
1:A:734:GLN:O	1:A:735:CYS:HB3	2.21	0.41
1:A:785:ARG:O	1:A:790:GLY:N	2.46	0.41
1:A:577:SER:HB2	1:A:712:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:O	1:A:321:LYS:HG3	2.21	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.87	0.41
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.56	0.41
1:A:829:LYS:HE3	1:A:829:LYS:CA	2.51	0.41
1:A:169:VAL:HG12	1:A:173:ASP:HB2	2.02	0.41
1:A:256:LYS:NZ	3:A:1120:HOH:O	2.53	0.41
1:A:401:PHE:CD2	1:A:478:MET:HE1	2.56	0.41
1:A:656:LEU:O	1:A:659:ILE:HG12	2.20	0.41
1:A:68:ILE:HG22	1:A:69:THR:N	2.36	0.40
1:A:235:VAL:HG21	3:A:1045:HOH:O	2.21	0.40
1:A:360:PRO:HB2	1:A:363:ASP:HB2	2.03	0.40
1:A:419:VAL:HG13	1:A:420:PRO:HD2	2.02	0.40
1:A:43:ALA:HB1	1:A:78:TYR:O	2.21	0.40
1:A:202:VAL:HG11	1:A:209:VAL:HG22	2.03	0.40
1:A:235:VAL:HG12	1:A:236:ASP:N	2.36	0.40
1:A:370:LYS:HD3	3:A:1291:HOH:O	2.21	0.40
1:A:672:LYS:NZ	3:A:1226:HOH:O	2.52	0.40
1:A:268:PRO:HG3	3:A:1335:HOH:O	2.21	0.40
1:A:111:PHE:CE1	1:A:141:THR:HG23	2.56	0.40
1:A:271:ARG:HB2	3:A:926:HOH:O	2.22	0.40
1:A:363:ASP:O	1:A:367:ILE:HG12	2.21	0.40
1:A:547:HIS:CD2	1:A:548:ASP:OD1	2.73	0.40
1:A:111:PHE:CE2	1:A:144:ARG:HD3	2.57	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	813/842 (97%)	780 (96%)	25 (3%)	8 (1%)	12 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	108	HIS
1	A	460	ASP
1	A	111	PHE
1	A	391	LYS
1	A	465	LYS
1	A	764	PRO
1	A	479	LYS

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	697/715 (98%)	680 (98%)	17 (2%)	43	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	77	LEU
1	A	154	VAL
1	A	183	GLU
1	A	216	HIS
1	A	394	PHE
1	A	457	VAL
1	A	595	GLU
1	A	596	GLU
1	A	599	LEU
1	A	633	ILE
1	A	677	PHE
1	A	718	LEU
1	A	738	GLN
1	A	758	GLU
1	A	829	LYS
1	A	836	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	41	GLN
1	A	91	GLN
1	A	101	ASN
1	A	108	HIS
1	A	138	GLN
1	A	201	GLN
1	A	355	GLN
1	A	365	ASN
1	A	414	GLN
1	A	452	ASN
1	A	476	HIS
1	A	528	HIS
1	A	537	HIS
1	A	547	HIS
1	A	584	ASN
1	A	644	ASN
1	A	687	ASN
1	A	699	HIS
1	A	734	GLN
1	A	748	ASN
1	A	753	GLN
1	A	759	GLN
1	A	791	GLN
1	A	800	HIS
1	A	836	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

1 ligand is 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	SO1	A	843	-	34,39,39	1.84	5 (14%)	38,64,64	2.00	6 (15%)

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	SO1	A	843	-	1/1/15/16	6/21/104/104	0/7/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	843	SO1	C12-C4	-7.28	1.38	1.54
2	A	843	SO1	C7-C2	4.33	1.60	1.54
2	A	843	SO1	C1-C5	2.90	1.57	1.50
2	A	843	SO1	C55-C56	2.44	1.56	1.52
2	A	843	SO1	C8-C2	2.24	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	843	SO1	C1-C4-C13	8.21	127.15	118.36
2	A	843	SO1	C18-C9-C16	-4.21	97.96	103.72
2	A	843	SO1	C7-C2-C6	3.76	119.24	112.05
2	A	843	SO1	C10-C6-C2	3.66	108.46	104.12
2	A	843	SO1	O17-C52-C53	3.55	113.67	108.27
2	A	843	SO1	C12-C6-C10	-2.16	106.23	107.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	843	SO1	C4

All (6) torsion outliers are listed below:

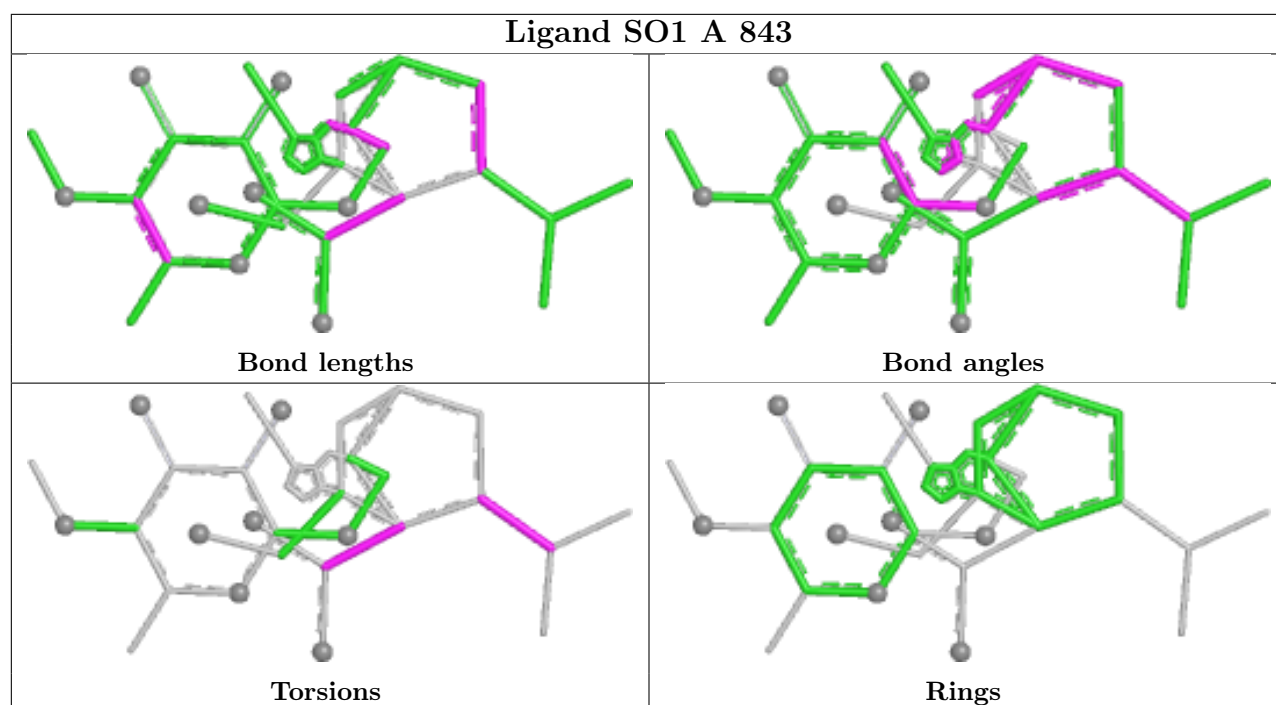
Mol	Chain	Res	Type	Atoms
2	A	843	SO1	C2-C1-C5-O14
2	A	843	SO1	C2-C1-C5-O15
2	A	843	SO1	C21-C13-C4-C12
2	A	843	SO1	C20-C13-C4-C1
2	A	843	SO1	C21-C13-C4-C1
2	A	843	SO1	C20-C13-C4-C12

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	843	SO1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	819/842 (97%)	0.78	119 (14%) 6 6	19, 37, 64, 82	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	VAL	6.8
1	A	464	LEU	6.6
1	A	107	GLY	6.0
1	A	427	PHE	5.5
1	A	110	ASP	5.3
1	A	483	PHE	5.1
1	A	463	LEU	5.0
1	A	501	LEU	4.6
1	A	404	THR	4.5
1	A	471	THR	4.4
1	A	462	PHE	4.3
1	A	108	HIS	4.2
1	A	765	LEU	4.2
1	A	426	LEU	4.2
1	A	476	HIS	4.2
1	A	428	ILE	4.1
1	A	418	TYR	4.0
1	A	419	VAL	3.9
1	A	764	PRO	3.9
1	A	481	MET	3.8
1	A	216	HIS	3.8
1	A	111	PHE	3.8
1	A	763	THR	3.8
1	A	424	ASP	3.8
1	A	581	ASN	3.7
1	A	360	PRO	3.6
1	A	842	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	381	TYR	3.6
1	A	461	GLN	3.6
1	A	785	ARG	3.5
1	A	698	ILE	3.4
1	A	112	SER	3.4
1	A	465	LYS	3.4
1	A	430	ALA	3.4
1	A	429	LYS	3.3
1	A	417	ASN	3.3
1	A	431	ILE	3.2
1	A	425	ASP	3.2
1	A	767	THR	3.2
1	A	410	LYS	3.2
1	A	497	ASN	3.2
1	A	197	LEU	3.1
1	A	196	VAL	3.1
1	A	411	VAL	3.1
1	A	466	THR	3.0
1	A	361	ALA	3.0
1	A	744	TYR	3.0
1	A	420	PRO	3.0
1	A	168	GLN	3.0
1	A	477	ASN	3.0
1	A	423	LYS	3.0
1	A	3	ALA	2.9
1	A	165	LEU	2.9
1	A	28	VAL	2.9
1	A	358	GLU	2.9
1	A	474	THR	2.9
1	A	766	PHE	2.9
1	A	475	ALA	2.9
1	A	293	LYS	2.8
1	A	748	ASN	2.8
1	A	229	TYR	2.8
1	A	460	ASP	2.8
1	A	755	VAL	2.8
1	A	68	ILE	2.8
1	A	394	PHE	2.8
1	A	446	ASP	2.7
1	A	655	TYR	2.7
1	A	391	LYS	2.7
1	A	457	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	516	PRO	2.7
1	A	259	ASN	2.7
1	A	745	SER	2.7
1	A	416	PRO	2.6
1	A	759	GLN	2.6
1	A	48	ALA	2.6
1	A	470	THR	2.6
1	A	161	ASP	2.6
1	A	359	GLY	2.5
1	A	480	VAL	2.5
1	A	482	LYS	2.5
1	A	498	ALA	2.5
1	A	164	LEU	2.4
1	A	355	GLN	2.4
1	A	113	SER	2.4
1	A	422	LYS	2.4
1	A	651	LYS	2.4
1	A	258	THR	2.4
1	A	657	HIS	2.4
1	A	305	ILE	2.3
1	A	364	ALA	2.3
1	A	703	GLY	2.3
1	A	829	LYS	2.3
1	A	652	ALA	2.3
1	A	67	GLY	2.3
1	A	33	SER	2.2
1	A	46	ILE	2.2
1	A	167	LEU	2.2
1	A	415	GLY	2.2
1	A	467	GLY	2.2
1	A	412	ARG	2.2
1	A	363	ASP	2.2
1	A	654	GLN	2.1
1	A	633	ILE	2.1
1	A	793	PHE	2.1
1	A	505	VAL	2.1
1	A	653	VAL	2.1
1	A	292	LYS	2.1
1	A	609	ARG	2.1
1	A	115	VAL	2.1
1	A	768	VAL	2.1
1	A	749	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	738	GLN	2.1
1	A	552	VAL	2.1
1	A	195	GLU	2.0
1	A	132	ILE	2.0
1	A	514	SER	2.0
1	A	735	CYS	2.0
1	A	34	THR	2.0
1	A	502	PRO	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](#)

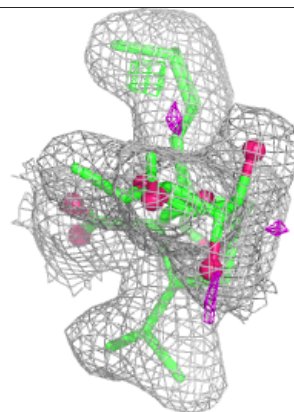
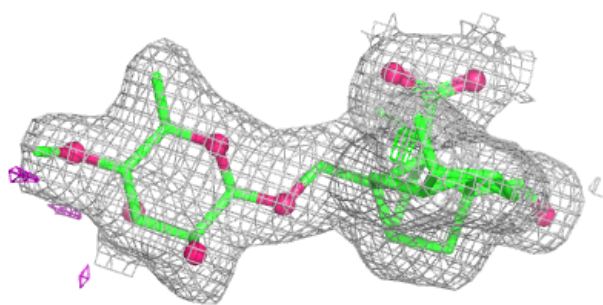
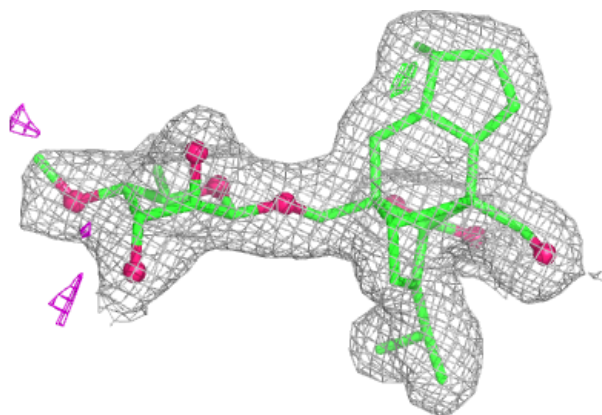
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO1	A	843	35/35	0.94	0.08	21,26,31,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SO1 A 843:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.