



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:36 AM GMT

PDB ID : 1N0U
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

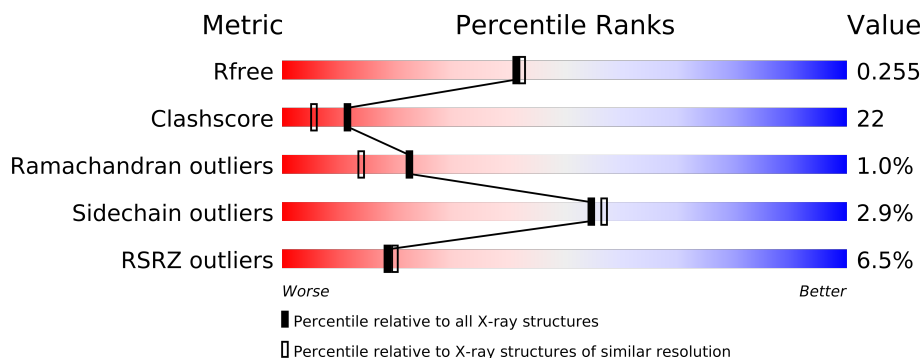
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition i

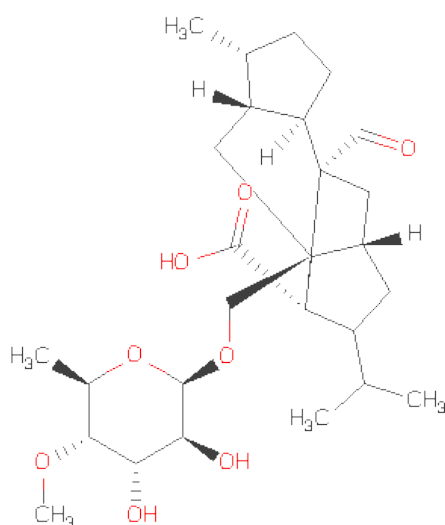
There are 3 unique types of molecules in this entry. The entry contains 6904 atoms, of which 0 are hydrogen and 0 are deuterium.

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.B.ETA.)]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)-CARBOXYLICACID (three-letter code: SO1) (formula: C₂₇H₄₂O₈).



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

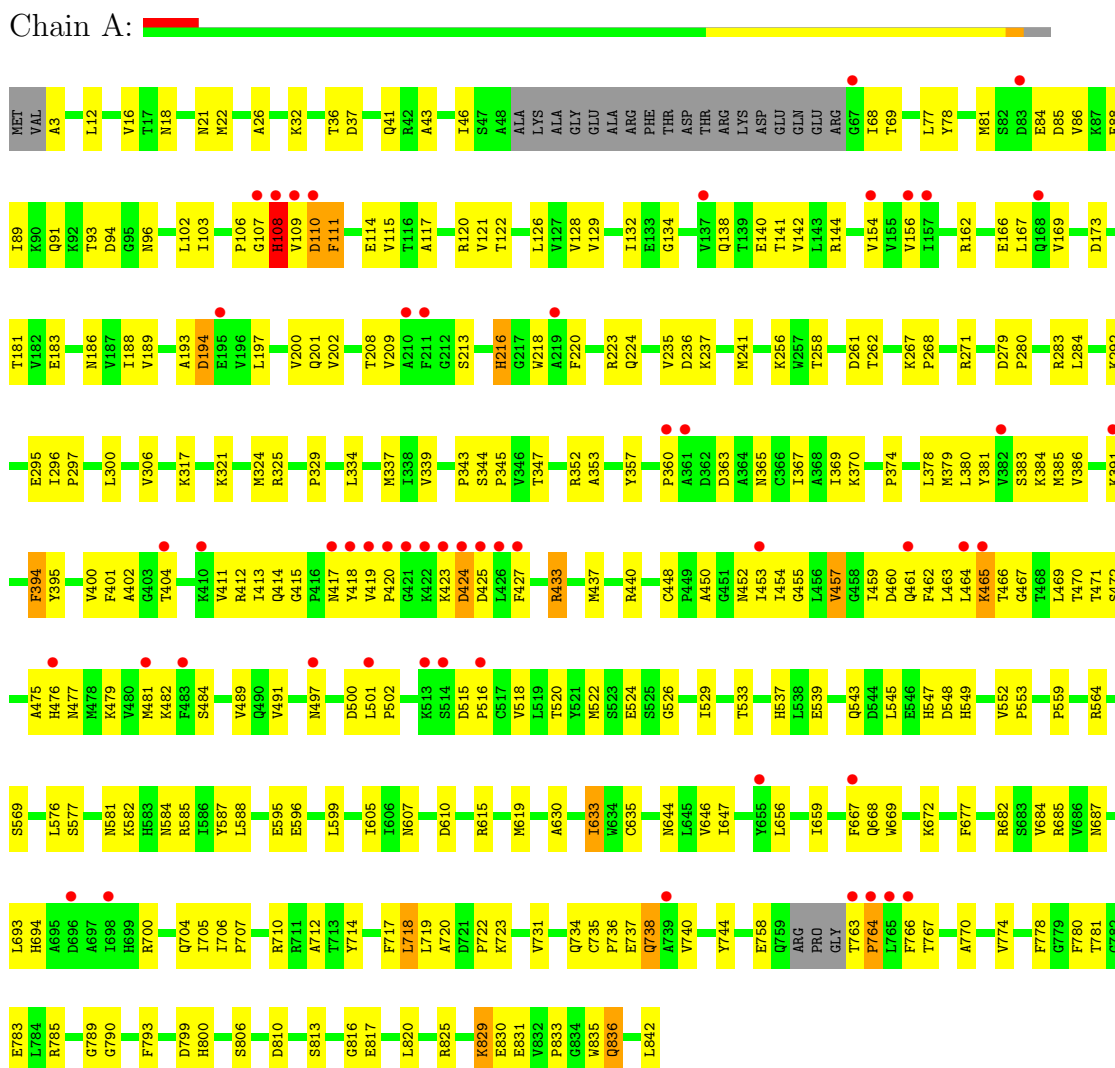
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 29.99 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.0 (31.00-2.12) 98.0 (29.99-2.12)	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 , 0.255	Depositor DCC
R_{free} test set	1953 reflections (2.94%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 66839 reflections (0.003%)	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.

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	0.37	0/6497	0.62	1/8797 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	N-CA-C	-5.38	96.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6375	0	6441	284	0
2	A	35	0	40	2	0
3	A	494	0	0	48	0
All	All	6904	0	6481	284	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (284) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:284:LEU:HD13	1:A:324:MET:HE3	1.64	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
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: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:202:VAL:HG12	1:A:209:VAL:CG2	2.23	0.68
1:A:189:VAL:CG1	1:A:200:VAL:HG13	2.24	0.68
1:A:103:ILE:HD11	1:A:453:ILE:HD11	1.76	0.68
1:A:836:GLN:H	1:A:836:GLN:NE2	1.90	0.67
1:A:482:LYS:HB2	1:A:793:PHE:CZ	2.29	0.67
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.59	0.67
1:A:424:ASP:O	1:A:425:ASP:HB2	1.92	0.67
1:A:386:VAL:HG12	1:A:395:TYR:O	1.94	0.67
1:A:417:ASN:HB2	1:A:425:ASP:OD2	1.94	0.67
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:497:ASN:HB3	1:A:500:ASP:OD2	1.97	0.64
1:A:385:MET:HG2	3:A:1102:HOH:O	1.97	0.64
1:A:284:LEU:HD13	1:A:324:MET:CE	2.27	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: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
1:A:186:ASN:HB3	1:A:201:GLN:NE2	2.14	0.63
1:A:103:ILE:HD11	1:A:453:ILE:CD1	2.29	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:644:ASN:HD22	1:A:684:VAL:H	1.45	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: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: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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:482:LYS:HB2	1:A:793:PHE:HZ	1.70	0.55
1:A:237:LYS:O	1:A:241:MET:HG2	2.06	0.55
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.89	0.55
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:O	1:A:423:LYS:HG2	2.08	0.54
1:A:501:LEU:HB2	1:A:502:PRO:HD3	1.90	0.54
1:A:552:VAL:HG13	1:A:553:PRO:HD2	1.89	0.54
1:A:88:GLU:CD	1:A:223:ARG:HH21	2.12	0.54
1:A:200:VAL:HG12	3:A:1237:HOH:O	2.06	0.54
1:A:114:GLU:HB2	3:A:1037:HOH:O	2.07	0.54
1:A:88:GLU:OE2	1:A:223:ARG:NH2	2.42	0.53
1:A:829:LYS:HA	1:A:829:LYS:HE3	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:615:ARG:HG2	1:A:619:MET:CE	2.39	0.53
1:A:646:VAL:C	1:A:647:ILE:HD12	2.29	0.53
1:A:461:GLN:HG2	3:A:904:HOH:O	2.09	0.53
1:A:3:ALA:HA	1:A:46:ILE:O	2.09	0.53
1:A:103:ILE:HD13	1:A:121:VAL:HG23	1.91	0.52
1:A:411:VAL:HG12	1:A:412:ARG:N	2.24	0.52
1:A:169:VAL:CG1	1:A:173:ASP:HB2	2.39	0.52
1:A:693:LEU:HB3	1:A:700:ARG:CD	2.39	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:547:HIS:HD2	1:A:548:ASP:OD1	1.93	0.52
1:A:454:ILE:HG13	1:A:455:GLY:H	1.75	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:615:ARG:HG2	1:A:619:MET:HE1	1.92	0.50
1:A:241:MET:HE1	3:A:1290:HOH:O	2.10	0.50
1:A:360:PRO:HD2	3:A:1019:HOH:O	2.11	0.50
1:A:736:PRO:HB2	1:A:738:GLN:OE1	2.11	0.49
1:A:576:LEU:HD21	1:A:585:ARG:HH11	1.77	0.49
1:A:120:ARG:HH12	1:A:481:MET:CE	2.25	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:588:LEU:HD12	1:A:588:LEU:C	2.33	0.48
1:A:400:VAL:HG12	1:A:450:ALA:HA	1.95	0.48
1:A:533:THR:HG22	3:A:1182:HOH:O	2.14	0.48
1:A:433:ARG:HD2	3:A:942:HOH:O	2.13	0.48
1:A:785:ARG:HG3	1:A:785:ARG:NH1	2.27	0.48
1:A:386:VAL:HG11	1:A:437:MET:CE	2.43	0.48
1:A:737:GLU:HB2	1:A:766:PHE:CE2	2.49	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:576:LEU:HD13	1:A:587:TYR:CE1	2.48	0.48
1:A:419:VAL:HG12	3:A:1063:HOH:O	2.14	0.48
1:A:37:ASP:O	1:A:41:GLN:HG3	2.13	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:107:GLY:O	1:A:109:VAL:N	2.46	0.48
1:A:16:VAL:O	1:A:345:PRO:HD2	2.13	0.48
1:A:306:VAL:HG22	3:A:1111:HOH:O	2.14	0.48
1:A:520:THR:HA	1:A:529:ILE:O	2.13	0.48
1:A:200:VAL:HG22	1:A:200:VAL:O	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:VAL:HG13	1:A:134:GLY:O	2.14	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:564:ARG:HG3	1:A:682:ARG:HB2	1.95	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:110:ASP:O	1:A:111:PHE:HB2	2.14	0.47
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.97	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:394:PHE:N	1:A:394:PHE:HD2	2.13	0.47
1:A:394:PHE:N	1:A:394:PHE:CD2	2.83	0.47
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.80	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:84:GLU:HG3	1:A:85:ASP:N	2.30	0.47
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:584:ASN:HD21	1:A:700:ARG:HG2	1.79	0.46
1:A:108:HIS:O	1:A:108:HIS:CG	2.69	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:552:VAL:CG1	1:A:553:PRO:HD2	2.46	0.45
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.98	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:379:MET:HB2	1:A:402:ALA:HB3	2.00	0.44
1:A:129:VAL:HG11	1:A:181:THR:HG23	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:633:ILE:HD12	1:A:635:CYS:N	2.32	0.44
1:A:306:VAL:HG23	1:A:306:VAL:O	2.17	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:216:HIS:HB3	1:A:218:TRP:HD1	1.84	0.43
1:A:114:GLU:CG	3:A:1037:HOH:O	2.66	0.43
1:A:459:ILE:HG22	1:A:459:ILE:O	2.18	0.43
1:A:32:LYS:O	1:A:36:THR:HG23	2.18	0.43
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.19	0.43
1:A:500:ASP:CG	1:A:552:VAL:HG11	2.38	0.43
1:A:647:ILE:N	1:A:647:ILE:HD12	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:386:VAL:HG11	1:A:437:MET:HE3	2.01	0.43
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.34	0.43
1:A:559:PRO:HB2	2:A:843:SO1:H201	2.01	0.43
1:A:18:ASN:N	1:A:18:ASN:HD22	2.17	0.43
1:A:380:LEU:C	1:A:380:LEU:HD23	2.39	0.43
1:A:352:ARG:HH11	1:A:352:ARG:HG2	1.84	0.42
1:A:522:MET:HE2	1:A:526:GLY:O	2.18	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: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:763:THR:N	1:A:764:PRO:CD	2.78	0.42
1:A:292:LYS:HD3	1:A:295:GLU:CD	2.39	0.42
1:A:108:HIS:O	1:A:108:HIS:CD2	2.72	0.42
1:A:22:MET:SD	1:A:102:LEU:HD12	2.59	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:515:ASP:OD2	1:A:537:HIS:HE1	2.02	0.42
1:A:489:VAL:HG22	1:A:781:THR:HG21	2.02	0.42
1:A:633:ILE:HD12	1:A:633:ILE:C	2.40	0.42
1:A:470:THR:HG21	1:A:475:ALA:HB1	2.02	0.42
1:A:26:ALA:CB	1:A:128:VAL:HB	2.50	0.42
1:A:718:LEU:HD12	1:A:718:LEU:HA	1.92	0.42
1:A:383:SER:O	1:A:384:LYS:HB3	2.20	0.42
1:A:659:ILE:CG2	1:A:705:ILE:HD13	2.50	0.42
1:A:448:CYS:SG	1:A:452:ASN:HB2	2.60	0.42
1:A:785:ARG:HB2	1:A:790:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:734:GLN:O	1:A:735:CYS:HB3	2.21	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:717:PHE:HD2	1:A:718:LEU:HD13	1.86	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
1:A:672:LYS:NZ	3:A:1226:HOH:O	2.52	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.87	0.41
1:A:317:LYS:O	1:A:321:LYS:HG3	2.21	0.41
1:A:829:LYS:CA	1:A:829:LYS:HE3	2.51	0.41
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.56	0.41
1:A:656:LEU:O	1:A:659:ILE:HG12	2.20	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: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: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:202:VAL:HG11	1:A:209:VAL:HG22	2.03	0.40
1:A:370:LYS:HD3	3:A:1291:HOH:O	2.21	0.40
1:A:120:ARG:HH12	1:A:481:MET:HE1	1.86	0.40
1:A:235:VAL:HG12	1:A:236:ASP:N	2.36	0.40
1:A:43:ALA:HB1	1:A:78:TYR:O	2.21	0.40
1:A:522:MET:CE	1:A:526:GLY:C	2.89	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:547:HIS:CD2	1:A:548:ASP:OD1	2.73	0.40
1:A:363:ASP:O	1:A:367:ILE:HG12	2.21	0.40
1:A:271:ARG:HB2	3:A:926:HOH:O	2.22	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

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	813/842 (97%)	780 (96%)	25 (3%)	8 (1%)	22	14

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%)	677 (97%)	20 (3%)	55	57

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	77	LEU
1	A	108	HIS
1	A	183	GLU
1	A	194	ASP
1	A	216	HIS
1	A	394	PHE
1	A	424	ASP
1	A	433	ARG
1	A	457	VAL
1	A	477	ASN
1	A	595	GLU
1	A	596	GLU
1	A	599	LEU
1	A	633	ILE

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Mol	Chain	Res	Type
1	A	677	PHE
1	A	718	LEU
1	A	738	GLN
1	A	829	LYS
1	A	836	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	91	GLN
1	A	101	ASN
1	A	108	HIS
1	A	138	GLN
1	A	201	GLN
1	A	290	ASN
1	A	371	ASN
1	A	414	GLN
1	A	452	ASN
1	A	476	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	753	GLN
1	A	759	GLN
1	A	800	HIS
1	A	836	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	-	39,39,39	1.68	4 (10%)	64,64,64	1.94	11 (17%)

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	0/21/104/104	0/1/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	843	SO1	C12-C4	-6.51	1.38	1.54
2	A	843	SO1	C7-C2	4.12	1.60	1.54
2	A	843	SO1	C1-C5	3.15	1.57	1.50
2	A	843	SO1	C55-C56	2.30	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	843	SO1	C12-C4-C13	6.81	128.22	112.62
2	A	843	SO1	C1-C4-C13	5.48	127.15	118.65
2	A	843	SO1	C10-C6-C2	4.39	108.46	102.88
2	A	843	SO1	O17-C52-C53	4.31	113.67	108.18
2	A	843	SO1	C18-C9-C16	-3.91	97.96	103.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	843	SO1	C7-C2-C8	-3.47	102.42	109.89
2	A	843	SO1	C2-C1-C5	3.43	118.89	111.90
2	A	843	SO1	C7-C2-C6	3.34	119.24	112.25
2	A	843	SO1	C1-C3-C9	-3.06	107.57	109.31
2	A	843	SO1	C1-C2-C6	-2.98	89.13	100.88
2	A	843	SO1	C8-C2-C1	2.53	118.41	113.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	843	SO1	C4

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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%)	0.32	53 (6%) 18 20	19, 37, 64, 82	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	6.8
1	A	763	THR	6.3
1	A	109	VAL	5.8
1	A	698	ILE	5.3
1	A	424	ASP	5.1
1	A	420	PRO	5.1
1	A	422	LYS	5.0
1	A	107	GLY	5.0
1	A	483	PHE	4.6
1	A	426	LEU	3.9
1	A	427	PHE	3.8
1	A	418	TYR	3.7
1	A	168	GLN	3.7
1	A	108	HIS	3.7
1	A	764	PRO	3.6
1	A	195	GLU	3.6
1	A	421	GLY	3.6
1	A	417	ASN	3.5
1	A	67	GLY	3.4
1	A	391	LYS	3.3
1	A	765	LEU	3.2
1	A	360	PRO	3.2
1	A	419	VAL	3.1
1	A	655	TYR	3.0
1	A	739	ALA	3.0
1	A	423	LYS	2.8
1	A	156	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	513	LYS	2.7
1	A	461	GLN	2.6
1	A	476	HIS	2.6
1	A	514	SER	2.6
1	A	425	ASP	2.6
1	A	410	LYS	2.6
1	A	83	ASP	2.5
1	A	497	ASN	2.5
1	A	464	LEU	2.5
1	A	211	PHE	2.5
1	A	465	LYS	2.4
1	A	453	ILE	2.4
1	A	501	LEU	2.4
1	A	516	PRO	2.3
1	A	481	MET	2.3
1	A	210	ALA	2.3
1	A	361	ALA	2.3
1	A	157	ILE	2.3
1	A	219	ALA	2.2
1	A	766	PHE	2.1
1	A	382	VAL	2.1
1	A	137	VAL	2.1
1	A	696	ASP	2.1
1	A	154	VAL	2.0
1	A	404	THR	2.0
1	A	667	PHE	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO1	A	843	35/35	0.13	0.79	21,26,31,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.