



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:25 PM EDT

PDB ID : 1OYD / pdb_00001oyd
Title : Structural Basis of Multiple Binding Capacity of the AcrB multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on : 2003-04-03
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

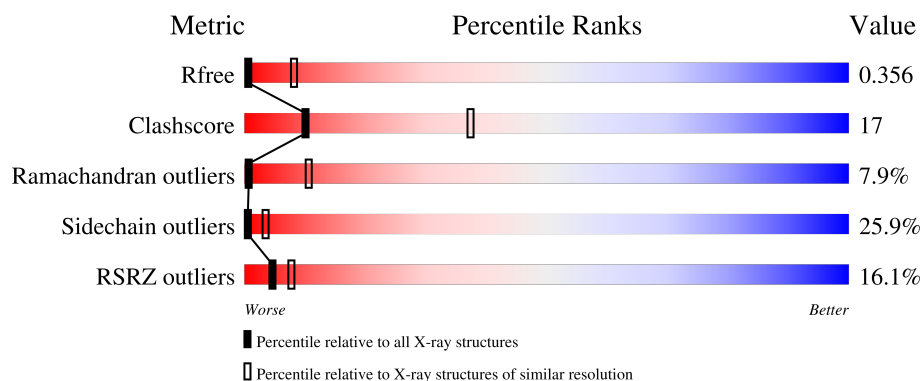
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1049	

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	DEQ	A	4001	-	X	-	-

2 Entry composition [i](#)

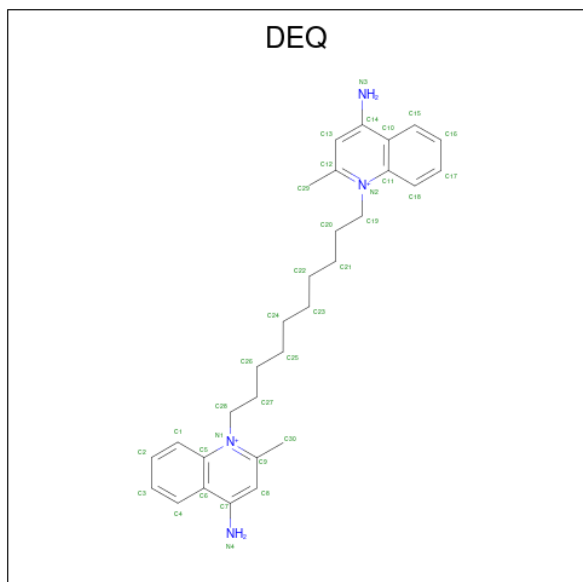
There are 2 unique types of molecules in this entry. The entry contains 7673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

- Molecule 2 is DEQUALINIUM (CCD ID: DEQ) (formula: C₃₀H₄₀N₄).

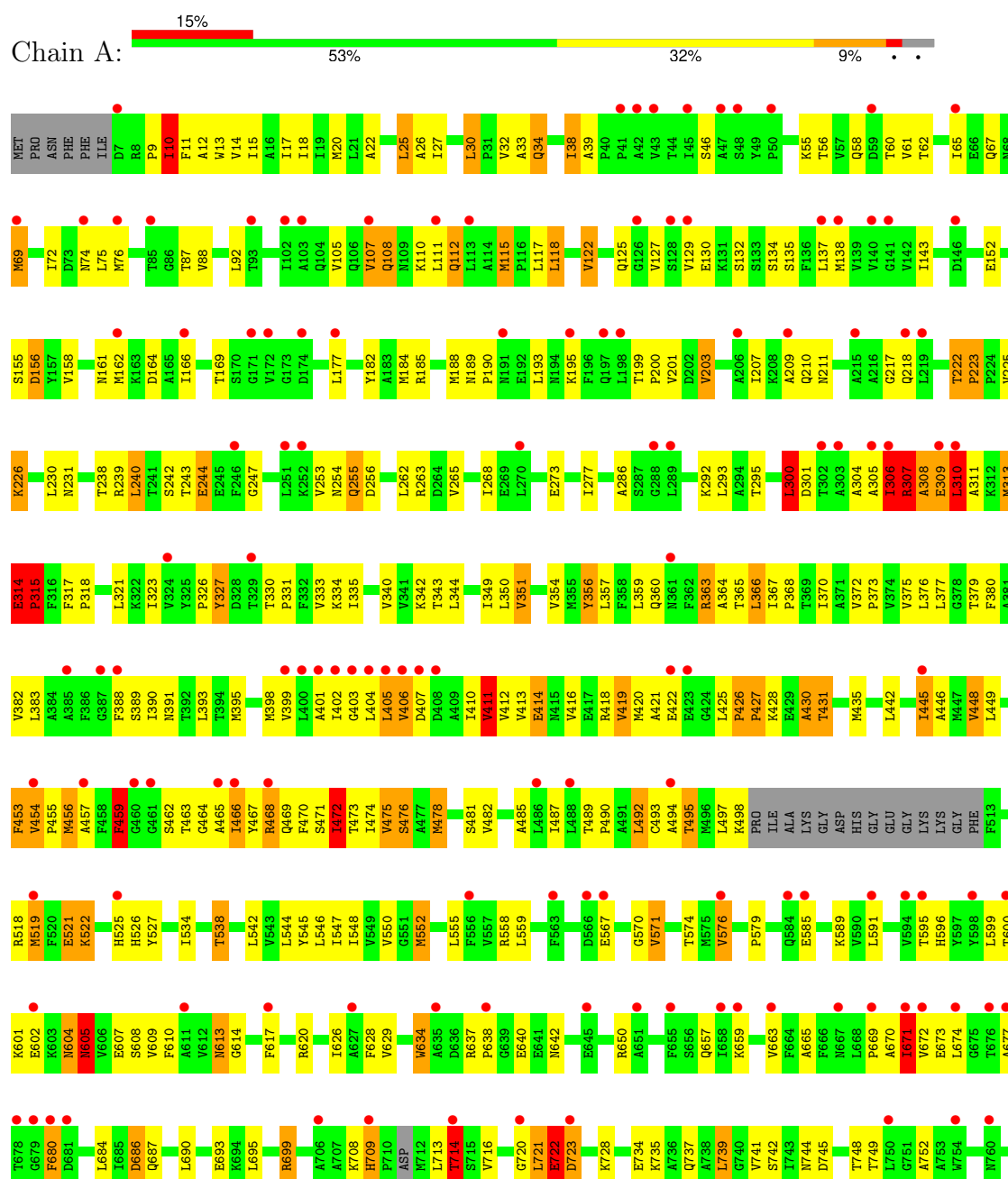


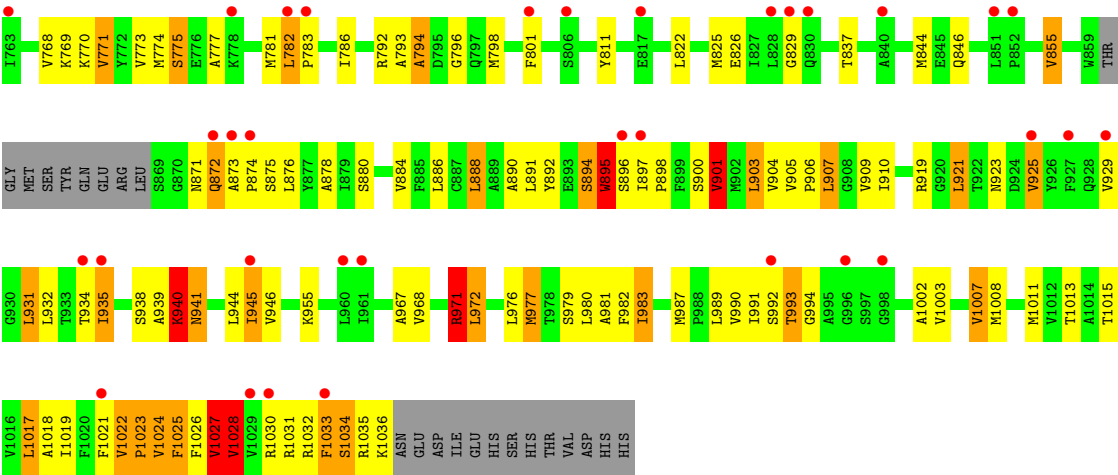
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			34	30	4		

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: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.77Å 144.77Å 517.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.80 46.60 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.80) 99.3 (46.60-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.284 , 0.338 0.362 , 0.356	Depositor DCC
R_{free} test set	1083 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: DEQ

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	0.54	0/7779	0.91	13/10563 (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	2	0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	680	PHE	N-CA-C	10.43	125.77	109.81
1	A	470	PHE	N-CA-C	9.49	127.03	111.37
1	A	315	PRO	N-CA-C	8.43	129.84	112.47
1	A	426	PRO	N-CA-C	7.76	120.17	110.70
1	A	315	PRO	CB-CA-C	-6.65	100.59	111.56
1	A	310	LEU	CA-CB-CG	5.65	136.09	116.30
1	A	307	ARG	CA-C-N	5.54	131.68	121.70
1	A	307	ARG	C-N-CA	5.54	131.68	121.70
1	A	309	GLU	CA-C-N	5.53	131.66	121.70
1	A	309	GLU	C-N-CA	5.53	131.66	121.70
1	A	454	VAL	N-CA-CB	5.34	113.87	110.50
1	A	454	VAL	CB-CA-C	-5.23	108.80	114.35
1	A	315	PRO	N-CA-CB	-5.07	97.93	103.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	PHE	CA
1	A	680	PHE	CA

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	7639	0	7800	249	1
2	A	34	0	36	20	0
All	All	7673	0	7836	269	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 17.

All (269) 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)
2:A:4001:DEQ:C20	2:A:4001:DEQ:C21	1.80	1.57
2:A:4001:DEQ:C22	2:A:4001:DEQ:C23	1.83	1.52
2:A:4001:DEQ:C27	2:A:4001:DEQ:C28	1.84	1.51
1:A:313:MET:C	1:A:315:PRO:HD3	1.82	1.04
2:A:4001:DEQ:C20	2:A:4001:DEQ:C22	2.51	0.89
1:A:314:GLU:N	1:A:315:PRO:HD3	1.93	0.81
1:A:880:SER:O	1:A:884:VAL:HG23	1.80	0.81
1:A:300:LEU:HD22	1:A:333:VAL:HG11	1.62	0.80
1:A:613:ASN:C	1:A:613:ASN:HD22	1.89	0.79
2:A:4001:DEQ:C28	2:A:4001:DEQ:C26	2.61	0.78
2:A:4001:DEQ:C22	2:A:4001:DEQ:C24	2.67	0.72
1:A:941:ASN:HD21	1:A:1015:THR:HG22	1.51	0.72
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.71	0.72
1:A:721:LEU:HD22	1:A:825:MET:HE3	1.72	0.72
1:A:613:ASN:HD22	1:A:614:GLY:N	1.89	0.71
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.72	0.70
1:A:670:ALA:O	1:A:671:ILE:O	2.10	0.70
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HG	1:A:300:LEU:O	1.93	0.68
1:A:306:ILE:HA	1:A:308:ALA:C	2.17	0.68
1:A:613:ASN:C	1:A:613:ASN:ND2	2.49	0.67
1:A:112:GLN:O	1:A:112:GLN:HG2	1.95	0.67
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.78	0.66
1:A:359:LEU:HD21	1:A:977:MET:HE1	1.78	0.65
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.79	0.65
2:A:4001:DEQ:C1	2:A:4001:DEQ:H272	2.26	0.65
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.80	0.64
1:A:709:HIS:CG	1:A:709:HIS:O	2.51	0.64
2:A:4001:DEQ:H272	2:A:4001:DEQ:H11	1.78	0.64
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.81	0.63
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.81	0.63
1:A:407:ASP:OD1	1:A:940:LYS:HG2	1.98	0.63
1:A:308:ALA:O	1:A:311:ALA:HB2	1.99	0.62
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.82	0.62
2:A:4001:DEQ:C27	2:A:4001:DEQ:H11	2.30	0.62
1:A:309:GLU:CG	1:A:310:LEU:HD13	2.30	0.62
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.35	0.61
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.83	0.61
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.36	0.60
1:A:305:ALA:HA	1:A:306:ILE:HB	1.84	0.60
1:A:370:ILE:O	1:A:370:ILE:HG22	2.01	0.60
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.67	0.60
1:A:344:LEU:HD21	1:A:376:LEU:HD11	1.84	0.59
1:A:359:LEU:HD13	1:A:364:ALA:HB1	1.83	0.59
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.84	0.59
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.66	0.59
1:A:721:LEU:O	1:A:723:ASP:N	2.36	0.59
1:A:1026:PHE:O	1:A:1030:ARG:HG2	2.03	0.59
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.38	0.59
1:A:309:GLU:HG2	1:A:310:LEU:HD13	1.84	0.59
1:A:310:LEU:HB2	1:A:313:MET:HB2	1.85	0.58
1:A:308:ALA:HB1	1:A:309:GLU:C	2.28	0.58
1:A:454:VAL:N	1:A:455:PRO:HD2	2.18	0.58
1:A:306:ILE:C	1:A:308:ALA:HB3	2.28	0.58
1:A:448:VAL:HG11	1:A:888:LEU:HD23	1.84	0.58
1:A:308:ALA:HB1	1:A:309:GLU:HA	1.85	0.58
1:A:457:ALA:HB2	1:A:471:SER:CB	2.34	0.58
1:A:306:ILE:HG23	1:A:308:ALA:O	2.05	0.57
1:A:306:ILE:CG2	1:A:307:ARG:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:CA	1:A:308:ALA:HB3	2.35	0.57
1:A:314:GLU:N	1:A:315:PRO:CD	2.67	0.56
1:A:425:LEU:C	1:A:427:PRO:HD2	2.30	0.56
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.88	0.56
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.87	0.56
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.88	0.56
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.88	0.55
1:A:454:VAL:HG22	1:A:475:VAL:HG21	1.89	0.55
1:A:326:PRO:O	1:A:327:TYR:C	2.48	0.55
1:A:967:ALA:O	1:A:971:ARG:HG3	2.06	0.55
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.60	0.55
1:A:709:HIS:O	1:A:709:HIS:CD2	2.60	0.55
1:A:304:ALA:O	1:A:306:ILE:HB	2.07	0.55
1:A:634:TRP:H	1:A:634:TRP:CD1	2.25	0.55
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.90	0.54
2:A:4001:DEQ:C21	2:A:4001:DEQ:H201	2.21	0.54
1:A:419:VAL:CG1	1:A:430:ALA:HB1	2.38	0.54
1:A:466:ILE:HG23	1:A:925:VAL:HG21	1.89	0.54
1:A:716:VAL:HG12	1:A:829:GLY:HA3	1.90	0.54
2:A:4001:DEQ:C22	2:A:4001:DEQ:H202	2.38	0.54
1:A:372:VAL:N	1:A:373:PRO:HD2	2.23	0.54
1:A:468:ARG:O	1:A:472:ILE:HG22	2.08	0.54
1:A:576:VAL:HG13	1:A:663:VAL:HG22	1.88	0.53
1:A:907:LEU:O	1:A:1013:THR:HG22	2.09	0.53
2:A:4001:DEQ:H201	2:A:4001:DEQ:C18	2.38	0.53
1:A:201:VAL:HG22	1:A:748:THR:HG23	1.89	0.53
1:A:309:GLU:HB3	1:A:310:LEU:HD22	1.90	0.53
1:A:901:VAL:O	1:A:904:VAL:HG22	2.09	0.53
1:A:745:ASP:O	1:A:749:THR:OG1	2.24	0.53
1:A:25:LEU:C	1:A:25:LEU:HD13	2.34	0.53
1:A:752:ALA:O	1:A:774:MET:HA	2.09	0.52
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.09	0.52
1:A:92:LEU:HD13	1:A:107:VAL:HG21	1.92	0.52
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.92	0.52
2:A:4001:DEQ:C27	2:A:4001:DEQ:N1	2.68	0.52
1:A:308:ALA:HB1	1:A:309:GLU:CA	2.40	0.52
1:A:475:VAL:HA	1:A:478:MET:HE2	1.92	0.52
1:A:39:ALA:HB2	1:A:672:VAL:HG11	1.92	0.52
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.91	0.52
1:A:380:PHE:CE2	1:A:398:MET:HE2	2.45	0.51
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HA	1:A:445:ILE:HD11	1.92	0.51
1:A:534:ILE:HD12	1:A:1026:PHE:HE1	1.75	0.51
1:A:401:ALA:HB2	1:A:474:ILE:HG23	1.92	0.51
1:A:570:GLY:O	1:A:571:VAL:HG23	2.11	0.51
1:A:774:MET:O	1:A:775:SER:CB	2.58	0.51
1:A:972:LEU:HD13	1:A:972:LEU:C	2.35	0.51
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.50
1:A:310:LEU:O	1:A:310:LEU:CD2	2.59	0.50
1:A:356:TYR:CD1	1:A:365:THR:HG21	2.46	0.50
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.93	0.50
1:A:10:ILE:N	1:A:10:ILE:HD13	2.27	0.50
1:A:405:LEU:HD23	1:A:481:SER:HB3	1.92	0.50
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.93	0.50
1:A:313:MET:CA	1:A:315:PRO:HD3	2.41	0.50
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.40	0.50
1:A:306:ILE:HG22	1:A:307:ARG:HA	1.93	0.49
2:A:4001:DEQ:H202	2:A:4001:DEQ:H222	1.93	0.49
1:A:38:ILE:HG23	1:A:466:ILE:HD11	1.93	0.49
1:A:111:LEU:HD23	1:A:111:LEU:C	2.37	0.49
1:A:774:MET:O	1:A:775:SER:HB3	2.12	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:A:308:ALA:HA	1:A:311:ALA:H	1.77	0.49
1:A:427:PRO:O	1:A:430:ALA:HB3	2.13	0.49
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.92	0.49
1:A:684:LEU:HD23	1:A:699:ARG:HB2	1.95	0.49
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.94	0.49
2:A:4001:DEQ:C26	2:A:4001:DEQ:H11	2.43	0.49
1:A:118:LEU:HD13	1:A:122:VAL:CG1	2.42	0.49
2:A:4001:DEQ:C20	2:A:4001:DEQ:H222	2.43	0.49
1:A:38:ILE:HB	1:A:672:VAL:HG21	1.95	0.48
1:A:905:VAL:HG13	1:A:935:ILE:HG12	1.94	0.48
1:A:367:ILE:HG23	1:A:492:LEU:CD1	2.44	0.48
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.14	0.48
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.94	0.48
1:A:637:ARG:HG2	1:A:642:ASN:HB3	1.95	0.48
1:A:903:LEU:O	1:A:906:PRO:HD2	2.13	0.48
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.48
1:A:445:ILE:O	1:A:449:LEU:HG	2.13	0.48
1:A:118:LEU:HD13	1:A:122:VAL:HG11	1.94	0.48
1:A:310:LEU:O	1:A:310:LEU:HD23	2.13	0.48
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:HD12	1:A:466:ILE:H	1.78	0.48
1:A:713:LEU:O	1:A:714:THR:HG23	2.13	0.48
1:A:112:GLN:O	1:A:112:GLN:CG	2.62	0.48
1:A:979:SER:O	1:A:983:ILE:HG13	2.13	0.48
1:A:475:VAL:HG22	1:A:478:MET:CE	2.44	0.48
1:A:744:ASN:O	1:A:748:THR:HG22	2.14	0.48
2:A:4001:DEQ:C25	2:A:4001:DEQ:H282	2.44	0.47
1:A:34:GLN:O	1:A:391:ASN:HA	2.13	0.47
1:A:390:ILE:HG22	1:A:390:ILE:O	2.14	0.47
1:A:200:PRO:CD	1:A:749:THR:HG23	2.45	0.47
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.49	0.47
1:A:407:ASP:O	1:A:411:VAL:HG23	2.15	0.47
1:A:604:ASN:O	1:A:605:ASN:ND2	2.47	0.47
2:A:4001:DEQ:C28	2:A:4001:DEQ:C25	2.93	0.47
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.78	0.47
1:A:465:ALA:O	1:A:466:ILE:C	2.58	0.47
1:A:695:LEU:HD22	1:A:825:MET:SD	2.55	0.47
1:A:115:MET:O	1:A:118:LEU:HB2	2.15	0.46
1:A:792:ARG:HA	1:A:798:MET:HE3	1.97	0.46
1:A:449:LEU:HB2	1:A:478:MET:SD	2.55	0.46
1:A:158:VAL:HG22	1:A:162:MET:CE	2.46	0.46
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.98	0.46
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.97	0.46
1:A:875:SER:O	1:A:878:ALA:HB3	2.16	0.46
1:A:485:ALA:HA	1:A:489:THR:HB	1.98	0.46
1:A:494:ALA:O	1:A:495:THR:C	2.59	0.46
1:A:637:ARG:HG2	1:A:642:ASN:HD22	1.81	0.46
1:A:390:ILE:HG23	1:A:395:MET:CG	2.46	0.46
1:A:525:HIS:O	1:A:527:TYR:N	2.49	0.46
1:A:931:LEU:O	1:A:935:ILE:HD12	2.15	0.45
1:A:739:LEU:N	1:A:739:LEU:HD23	2.31	0.45
1:A:313:MET:O	1:A:317:PHE:CZ	2.69	0.45
1:A:383:LEU:HB3	1:A:388:PHE:HB2	1.98	0.45
1:A:414:GLU:CD	1:A:414:GLU:C	2.85	0.45
1:A:493:CYS:SG	1:A:497:LEU:HD22	2.56	0.45
1:A:855:VAL:HG12	1:A:855:VAL:O	2.16	0.45
1:A:188:MET:N	1:A:775:SER:HA	2.32	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.98	0.45
1:A:390:ILE:HG23	1:A:395:MET:SD	2.56	0.45
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.45
1:A:343:THR:CG2	1:A:989:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:HB3	1:A:310:LEU:HD13	1.99	0.45
1:A:398:MET:O	1:A:402:ILE:HG13	2.17	0.45
1:A:38:ILE:HD13	1:A:672:VAL:HG22	1.99	0.44
1:A:300:LEU:CD2	1:A:333:VAL:HG11	2.39	0.44
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.99	0.44
1:A:401:ALA:O	1:A:402:ILE:C	2.60	0.44
1:A:25:LEU:HD13	1:A:26:ALA:N	2.33	0.44
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.49	0.44
1:A:410:ILE:O	1:A:411:VAL:C	2.60	0.44
1:A:993:THR:HB	1:A:994:GLY:CA	2.47	0.44
1:A:367:ILE:HG12	1:A:492:LEU:HD13	1.98	0.44
1:A:412:VAL:HG13	1:A:435:MET:HE1	1.99	0.44
1:A:892:TYR:HB3	1:A:897:ILE:HG21	2.00	0.44
1:A:343:THR:OG1	1:A:989:LEU:HD21	2.18	0.44
1:A:465:ALA:HB1	1:A:469:GLN:CG	2.48	0.44
1:A:65:ILE:O	1:A:69:MET:HB2	2.17	0.43
1:A:472:ILE:O	1:A:473:THR:C	2.61	0.43
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	2.00	0.43
1:A:1033:PHE:C	1:A:1034:SER:HG	2.23	0.43
1:A:10:ILE:N	1:A:10:ILE:CD1	2.81	0.43
1:A:10:ILE:O	1:A:14:VAL:HG23	2.18	0.43
1:A:905:VAL:O	1:A:909:VAL:HG23	2.18	0.43
1:A:721:LEU:O	1:A:722:GLU:C	2.61	0.43
1:A:465:ALA:HB1	1:A:469:GLN:HG3	2.00	0.43
1:A:894:SER:O	1:A:895:TRP:HB2	2.18	0.43
1:A:793:ALA:O	1:A:794:ALA:C	2.62	0.43
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.99	0.43
2:A:4001:DEQ:C27	2:A:4001:DEQ:C1	2.93	0.43
1:A:60:THR:HG23	1:A:61:VAL:HG23	2.01	0.43
1:A:686:ASP:CB	1:A:695:LEU:HD12	2.49	0.43
1:A:373:PRO:O	1:A:377:LEU:HG	2.18	0.43
1:A:777:ALA:O	1:A:781:MET:HG2	2.19	0.43
1:A:1027:VAL:O	1:A:1030:ARG:N	2.51	0.43
1:A:426:PRO:N	1:A:427:PRO:HD2	2.34	0.43
1:A:367:ILE:HG21	1:A:413:VAL:HG22	2.00	0.43
1:A:399:VAL:O	1:A:402:ILE:HB	2.19	0.43
1:A:453:PHE:HE1	1:A:932:LEU:HB2	1.83	0.43
1:A:468:ARG:HG2	1:A:469:GLN:N	2.34	0.43
1:A:672:VAL:HG12	1:A:673:GLU:N	2.34	0.43
1:A:306:ILE:HG22	1:A:307:ARG:HD3	2.00	0.42
1:A:521:GLU:O	1:A:522:LYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:CG1	1:A:262:LEU:HD13	2.48	0.42
1:A:466:ILE:HD12	1:A:466:ILE:N	2.35	0.42
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.49	0.42
1:A:1027:VAL:O	1:A:1028:VAL:C	2.63	0.42
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.02	0.42
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.68	0.42
1:A:890:ALA:C	1:A:891:LEU:HD22	2.45	0.42
1:A:410:ILE:HG22	1:A:411:VAL:N	2.35	0.42
1:A:684:LEU:CD1	1:A:855:VAL:HG13	2.50	0.42
1:A:33:ALA:O	1:A:34:GLN:O	2.38	0.41
1:A:211:ASN:HA	1:A:240:LEU:HD23	2.02	0.41
1:A:463:THR:HG23	1:A:466:ILE:HG21	2.02	0.41
1:A:929:VAL:HA	1:A:932:LEU:HD12	2.02	0.41
1:A:379:THR:HB	1:A:398:MET:HE1	2.02	0.41
1:A:940:LYS:O	1:A:941:ASN:C	2.62	0.41
1:A:12:ALA:HB1	1:A:487:ILE:HG22	2.02	0.41
1:A:456:MET:HA	1:A:876:LEU:HB3	2.02	0.41
1:A:468:ARG:CG	1:A:469:GLN:N	2.83	0.41
1:A:367:ILE:HG23	1:A:492:LEU:HD12	2.02	0.41
1:A:416:VAL:O	1:A:420:MET:HG3	2.21	0.41
1:A:344:LEU:HD21	1:A:376:LEU:CD1	2.49	0.41
1:A:1033:PHE:O	1:A:1034:SER:OG	2.27	0.41
1:A:247:GLY:HA2	1:A:268:ILE:HD12	2.02	0.41
1:A:459:PHE:CD1	1:A:459:PHE:N	2.88	0.41
1:A:559:LEU:HD22	1:A:923:ASN:HB2	2.02	0.41
1:A:38:ILE:HD13	1:A:672:VAL:CG2	2.51	0.41
1:A:921:LEU:CD1	1:A:1002:ALA:HA	2.50	0.41
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.41
1:A:453:PHE:CD2	1:A:471:SER:HA	2.56	0.41
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.41
1:A:713:LEU:C	1:A:714:THR:HG1	2.29	0.41
1:A:782:LEU:CB	1:A:783:PRO:HD2	2.51	0.41
1:A:545:TYR:HA	1:A:548:ILE:HD12	2.03	0.41
1:A:354:VAL:HG13	1:A:980:LEU:HD23	2.03	0.40
1:A:370:ILE:O	1:A:370:ILE:CG2	2.69	0.40
1:A:30:LEU:CD2	1:A:390:ILE:HG13	2.51	0.40
1:A:330:THR:HB	1:A:331:PRO:HD3	2.03	0.40
1:A:467:TYR:CE2	1:A:925:VAL:HG22	2.56	0.40
2:A:4001:DEQ:C21	2:A:4001:DEQ:H202	2.21	0.40
1:A:873:ALA:O	1:A:874:PRO:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:SER:N	1:A:898:PRO:HD2	2.37	0.40
1:A:534:ILE:HD12	1:A:1026:PHE:CE1	2.56	0.40
1:A:939:ALA:O	1:A:940:LYS:C	2.63	0.40
1:A:111:LEU:HD23	1:A:111:LEU:O	2.20	0.40
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.92	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:226:LYS:O	1:A:596:HIS:NE2[16_445]	1.90	0.30

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	998/1049 (95%)	759 (76%)	160 (16%)	79 (8%)	1	10

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	10	ILE
1	A	34	GLN
1	A	135	SER
1	A	255	GLN
1	A	306	ILE
1	A	308	ALA
1	A	315	PRO
1	A	411	VAL
1	A	431	THR
1	A	459	PHE

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Mol	Chain	Res	Type
1	A	466	ILE
1	A	495	THR
1	A	521	GLU
1	A	522	LYS
1	A	526	HIS
1	A	604	ASN
1	A	671	ILE
1	A	714	THR
1	A	722	GLU
1	A	723	ASP
1	A	775	SER
1	A	794	ALA
1	A	901	VAL
1	A	940	LYS
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	152	GLU
1	A	161	ASN
1	A	209	ALA
1	A	217	GLY
1	A	295	THR
1	A	301	ASP
1	A	327	TYR
1	A	421	ALA
1	A	464	GLY
1	A	552	MET
1	A	605	ASN
1	A	720	GLY
1	A	796	GLY
1	A	872	GLN
1	A	894	SER
1	A	900	SER
1	A	941	ASN
1	A	955	LYS
1	A	971	ARG
1	A	1027	VAL
1	A	74	ASN
1	A	105	VAL
1	A	134	SER
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	571	VAL
1	A	427	PRO
1	A	430	ALA
1	A	472	ILE
1	A	519	MET
1	A	538	THR
1	A	665	ALA
1	A	895	TRP
1	A	75	LEU
1	A	244	GLU
1	A	300	LEU
1	A	363	ARG
1	A	405	LEU
1	A	677	ALA
1	A	837	THR
1	A	22	ALA
1	A	223	PRO
1	A	1033	PHE
1	A	314	GLU
1	A	638	PRO
1	A	490	PRO
1	A	626	ILE
1	A	318	PRO
1	A	579	PRO
1	A	669	PRO
1	A	1028	VAL

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	818/855 (96%)	606 (74%)	212 (26%)	0 3

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	13	TRP
1	A	15	ILE
1	A	17	ILE
1	A	18	ILE
1	A	20	MET
1	A	25	LEU
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	46	SER
1	A	55	LYS
1	A	58	GLN
1	A	67	GLN
1	A	69	MET
1	A	72	ILE
1	A	76	MET
1	A	87	THR
1	A	107	VAL
1	A	108	GLN
1	A	110	LYS
1	A	112	GLN
1	A	115	MET
1	A	117	LEU
1	A	118	LEU
1	A	122	VAL
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	155	SER
1	A	156	ASP
1	A	164	ASP
1	A	166	ILE
1	A	169	THR
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	193	LEU
1	A	195	LYS

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Mol	Chain	Res	Type
1	A	199	THR
1	A	203	VAL
1	A	207	ILE
1	A	210	GLN
1	A	222	THR
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	239	ARG
1	A	240	LEU
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	253	VAL
1	A	255	GLN
1	A	263	ARG
1	A	265	VAL
1	A	273	GLU
1	A	277	ILE
1	A	292	LYS
1	A	293	LEU
1	A	300	LEU
1	A	306	ILE
1	A	307	ARG
1	A	310	LEU
1	A	313	MET
1	A	314	GLU
1	A	321	LEU
1	A	323	ILE
1	A	334	LYS
1	A	335	ILE
1	A	340	VAL
1	A	342	LYS
1	A	349	ILE
1	A	350	LEU
1	A	351	VAL
1	A	356	TYR
1	A	357	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	411	VAL
1	A	414	GLU
1	A	418	ARG
1	A	419	VAL
1	A	422	GLU
1	A	428	LYS
1	A	431	THR
1	A	445	ILE
1	A	448	VAL
1	A	453	PHE
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	468	ARG
1	A	472	ILE
1	A	475	VAL
1	A	476	SER
1	A	478	MET
1	A	492	LEU
1	A	498	LYS
1	A	518	ARG
1	A	519	MET
1	A	538	THR
1	A	542	LEU
1	A	544	LEU
1	A	547	ILE
1	A	552	MET
1	A	555	LEU
1	A	558	ARG
1	A	567	GLU
1	A	574	THR
1	A	576	VAL
1	A	585	GLU
1	A	589	LYS
1	A	591	LEU
1	A	600	THR
1	A	601	LYS
1	A	602	GLU
1	A	605	ASN

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Mol	Chain	Res	Type
1	A	607	GLU
1	A	608	SER
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	629	VAL
1	A	634	TRP
1	A	640	GLU
1	A	650	ARG
1	A	657	GLN
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU
1	A	680	PHE
1	A	686	ASP
1	A	687	GLN
1	A	690	LEU
1	A	693	GLU
1	A	699	ARG
1	A	708	LYS
1	A	709	HIS
1	A	714	THR
1	A	721	LEU
1	A	722	GLU
1	A	728	LYS
1	A	734	GLU
1	A	735	LYS
1	A	737	GLN
1	A	739	LEU
1	A	741	VAL
1	A	742	SER
1	A	768	VAL
1	A	770	LYS
1	A	771	VAL
1	A	773	VAL
1	A	782	LEU
1	A	786	ILE
1	A	801	PHE
1	A	811	TYR
1	A	822	LEU
1	A	826	GLU

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Mol	Chain	Res	Type
1	A	844	MET
1	A	846	GLN
1	A	855	VAL
1	A	871	ASN
1	A	872	GLN
1	A	886	LEU
1	A	888	LEU
1	A	895	TRP
1	A	901	VAL
1	A	903	LEU
1	A	907	LEU
1	A	919	ARG
1	A	921	LEU
1	A	925	VAL
1	A	931	LEU
1	A	934	THR
1	A	935	ILE
1	A	938	SER
1	A	940	LYS
1	A	944	LEU
1	A	945	ILE
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	977	MET
1	A	983	ILE
1	A	987	MET
1	A	990	VAL
1	A	991	ILE
1	A	992	SER
1	A	993	THR
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1028	VAL
1	A	1031	ARG
1	A	1032	ARG
1	A	1034	SER
1	A	1035	ARG

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Mol	Chain	Res	Type
1	A	1036	LYS

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	58	GLN
1	A	68	ASN
1	A	123	GLN
1	A	125	GLN
1	A	161	ASN
1	A	194	ASN
1	A	231	ASN
1	A	254	ASN
1	A	255	GLN
1	A	284	GLN
1	A	338	HIS
1	A	391	ASN
1	A	469	GLN
1	A	569	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	623	ASN
1	A	642	ASN
1	A	667	ASN
1	A	700	ASN
1	A	701	GLN
1	A	760	ASN
1	A	872	GLN
1	A	941	ASN
1	A	1001	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	DEQ	A	4001	-	35,37,37	4.96	17 (48%)	46,50,50	3.90	28 (60%)

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	DEQ	A	4001	-	-	9/13/13/13	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	DEQ	C11-N2	14.85	1.58	1.40
2	A	4001	DEQ	C12-N2	12.63	1.53	1.36
2	A	4001	DEQ	C5-N1	12.36	1.55	1.40
2	A	4001	DEQ	C27-C28	9.03	1.84	1.51
2	A	4001	DEQ	C9-N1	7.68	1.46	1.36
2	A	4001	DEQ	C23-C22	6.28	1.83	1.51
2	A	4001	DEQ	C21-C20	5.70	1.80	1.51
2	A	4001	DEQ	C25-C24	-4.38	1.30	1.51
2	A	4001	DEQ	C24-C23	3.81	1.70	1.51
2	A	4001	DEQ	C20-C19	3.16	1.63	1.51
2	A	4001	DEQ	C10-C11	2.78	1.46	1.42
2	A	4001	DEQ	C17-C18	2.67	1.42	1.36
2	A	4001	DEQ	C2-C1	2.62	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	DEQ	C16-C15	2.35	1.41	1.36
2	A	4001	DEQ	C3-C4	2.32	1.41	1.36
2	A	4001	DEQ	C30-C9	2.27	1.54	1.49
2	A	4001	DEQ	C6-C5	2.15	1.45	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	DEQ	C12-N2-C11	-12.08	111.53	122.12
2	A	4001	DEQ	C19-N2-C11	10.63	133.07	118.98
2	A	4001	DEQ	C21-C20-C19	7.97	140.76	112.25
2	A	4001	DEQ	C20-C19-N2	-5.94	98.51	111.83
2	A	4001	DEQ	C25-C24-C23	5.90	144.18	114.37
2	A	4001	DEQ	C28-N1-C5	5.47	126.23	118.98
2	A	4001	DEQ	C14-C10-C11	5.27	121.54	118.32
2	A	4001	DEQ	C9-N1-C5	-4.81	117.90	122.12
2	A	4001	DEQ	C13-C14-N3	-4.19	110.59	120.20
2	A	4001	DEQ	C1-C5-N1	3.87	124.93	121.43
2	A	4001	DEQ	C18-C11-N2	3.79	124.86	121.43
2	A	4001	DEQ	C10-C14-N3	3.78	129.15	120.30
2	A	4001	DEQ	C30-C9-N1	3.73	125.43	119.72
2	A	4001	DEQ	C13-C12-N2	3.70	123.34	119.26
2	A	4001	DEQ	C27-C28-N1	-3.49	104.00	111.83
2	A	4001	DEQ	C22-C21-C20	-3.15	98.46	114.37
2	A	4001	DEQ	C24-C23-C22	-3.15	98.47	114.37
2	A	4001	DEQ	C29-C12-C13	-3.13	114.92	121.56
2	A	4001	DEQ	C27-C26-C25	3.11	130.10	114.37
2	A	4001	DEQ	C18-C11-C10	-3.11	115.60	119.43
2	A	4001	DEQ	C7-C6-C5	3.03	120.17	118.32
2	A	4001	DEQ	C30-C9-C8	-2.81	115.60	121.56
2	A	4001	DEQ	C26-C25-C24	2.54	127.18	114.37
2	A	4001	DEQ	C15-C10-C14	-2.53	118.83	122.74
2	A	4001	DEQ	C17-C18-C11	2.23	123.57	119.50
2	A	4001	DEQ	C8-C7-N4	-2.17	115.22	120.20
2	A	4001	DEQ	C1-C5-C6	-2.11	116.83	119.43
2	A	4001	DEQ	C6-C5-N1	-2.10	118.22	119.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4001	DEQ	C27-C28-N1-C5

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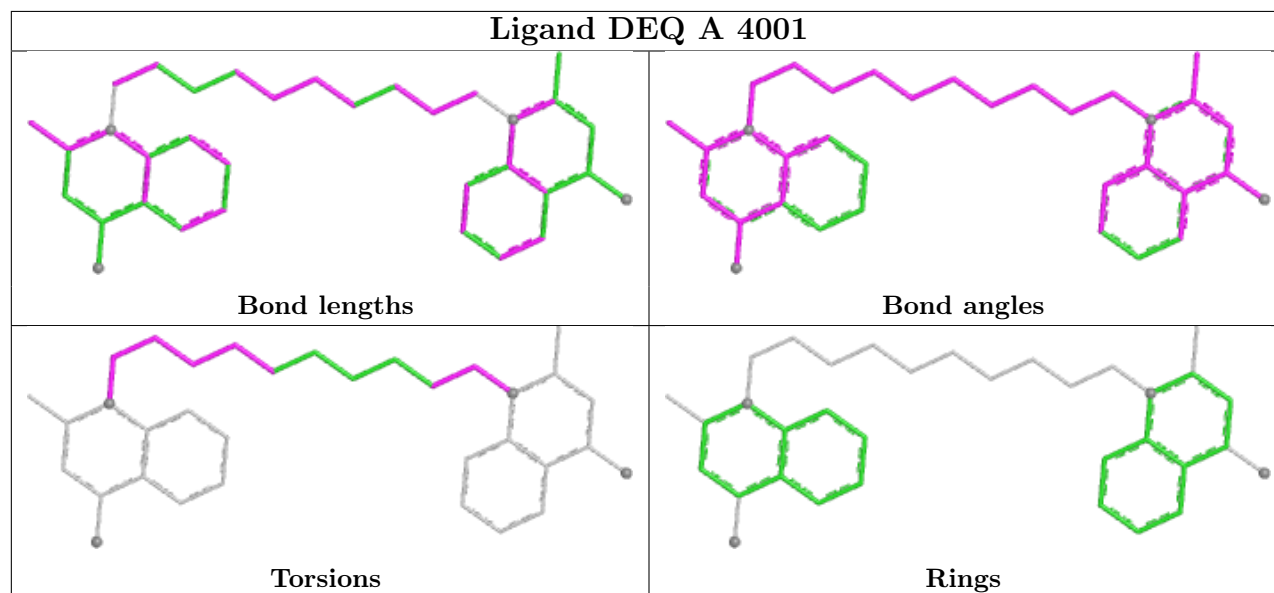
Mol	Chain	Res	Type	Atoms
2	A	4001	DEQ	C27-C28-N1-C9
2	A	4001	DEQ	C20-C19-N2-C11
2	A	4001	DEQ	C20-C19-N2-C12
2	A	4001	DEQ	C26-C27-C28-N1
2	A	4001	DEQ	N2-C19-C20-C21
2	A	4001	DEQ	C25-C26-C27-C28
2	A	4001	DEQ	C23-C24-C25-C26
2	A	4001	DEQ	C24-C25-C26-C27

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	DEQ	20	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	1006/1049 (95%)	1.06	162 (16%) 4 8	131, 162, 176, 194	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	LYS	7.1
1	A	461	GLY	7.0
1	A	829	GLY	6.8
1	A	403	GLY	6.7
1	A	309	GLU	6.1
1	A	828	LEU	5.9
1	A	303	ALA	5.9
1	A	1021	PHE	5.7
1	A	401	ALA	5.5
1	A	782	LEU	5.4
1	A	556	PHE	5.3
1	A	146	ASP	5.1
1	A	402	ILE	5.1
1	A	591	LEU	5.1
1	A	563	PHE	4.8
1	A	754	TRP	4.7
1	A	594	VAL	4.7
1	A	830	GLN	4.6
1	A	219	LEU	4.6
1	A	387	GLY	4.5
1	A	935	ILE	4.5
1	A	107	VAL	4.4
1	A	488	LEU	4.3
1	A	663	VAL	4.1
1	A	111	LEU	4.0
1	A	1029	VAL	4.0
1	A	600	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	658	ILE	3.9
1	A	310	LEU	3.9
1	A	404	LEU	3.9
1	A	960	LEU	3.8
1	A	674	LEU	3.8
1	A	460	GLY	3.7
1	A	655	PHE	3.7
1	A	102	ILE	3.6
1	A	42	ALA	3.6
1	A	457	ALA	3.6
1	A	676	THR	3.6
1	A	709	HIS	3.6
1	A	206	ALA	3.5
1	A	251	LEU	3.5
1	A	302	THR	3.5
1	A	406	VAL	3.5
1	A	59	ASP	3.5
1	A	783	PRO	3.5
1	A	172	VAL	3.5
1	A	669	PRO	3.5
1	A	126	GLY	3.4
1	A	422	GLU	3.4
1	A	198	LEU	3.4
1	A	927	PHE	3.4
1	A	659	LYS	3.3
1	A	400	LEU	3.3
1	A	454	VAL	3.3
1	A	595	THR	3.2
1	A	945	ILE	3.2
1	A	929	VAL	3.2
1	A	329	THR	3.2
1	A	445	ILE	3.2
1	A	576	VAL	3.2
1	A	680	PHE	3.2
1	A	1033	PHE	3.1
1	A	585	GLU	3.1
1	A	215	ALA	3.1
1	A	405	LEU	3.1
1	A	681	ASP	3.1
1	A	48	SER	3.0
1	A	306	ILE	3.0
1	A	778	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	423	GLU	3.0
1	A	852	PRO	3.0
1	A	65	ILE	3.0
1	A	399	VAL	3.0
1	A	191	ASN	3.0
1	A	466	ILE	3.0
1	A	934	THR	3.0
1	A	85	THR	2.9
1	A	138	MET	2.8
1	A	714	THR	2.8
1	A	128	SER	2.8
1	A	47	ALA	2.8
1	A	677	ALA	2.8
1	A	611	ALA	2.8
1	A	961	ILE	2.7
1	A	566	ASP	2.7
1	A	925	VAL	2.7
1	A	598	TYR	2.7
1	A	998	GLY	2.6
1	A	525	HIS	2.6
1	A	288	GLY	2.6
1	A	7	ASP	2.6
1	A	289	LEU	2.6
1	A	519	MET	2.6
1	A	465	ALA	2.6
1	A	671	ILE	2.5
1	A	750	LEU	2.5
1	A	103	ALA	2.5
1	A	584	GLN	2.5
1	A	166	ILE	2.5
1	A	361	ASN	2.5
1	A	137	LEU	2.5
1	A	996	GLY	2.5
1	A	763	ILE	2.4
1	A	140	VAL	2.4
1	A	667	ASN	2.4
1	A	874	PRO	2.4
1	A	679	GLY	2.4
1	A	872	GLN	2.4
1	A	896	SER	2.4
1	A	897	ILE	2.4
1	A	113	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	567	GLU	2.4
1	A	385	ALA	2.4
1	A	840	ALA	2.4
1	A	76	MET	2.4
1	A	129	VAL	2.4
1	A	627	ALA	2.3
1	A	617	PHE	2.3
1	A	494	ALA	2.3
1	A	246	PHE	2.3
1	A	388	PHE	2.3
1	A	651	ALA	2.3
1	A	801	PHE	2.3
1	A	197	GLN	2.3
1	A	635	ALA	2.3
1	A	723	ASP	2.3
1	A	1030	ARG	2.3
1	A	74	ASN	2.2
1	A	195	LYS	2.2
1	A	171	GLY	2.2
1	A	720	GLY	2.2
1	A	486	LEU	2.2
1	A	851	LEU	2.2
1	A	41	PRO	2.2
1	A	69	MET	2.2
1	A	706	ALA	2.2
1	A	162	MET	2.2
1	A	177	LEU	2.2
1	A	93	THR	2.1
1	A	408	ASP	2.1
1	A	45	ILE	2.1
1	A	992	SER	2.1
1	A	218	GLN	2.1
1	A	50	PRO	2.1
1	A	645	GLU	2.1
1	A	817	GLU	2.1
1	A	43	VAL	2.1
1	A	672	VAL	2.1
1	A	141	GLY	2.1
1	A	760	ASN	2.1
1	A	324	VAL	2.0
1	A	468	ARG	2.0
1	A	678	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	174	ASP	2.0
1	A	407	ASP	2.0
1	A	270	LEU	2.0
1	A	638	PRO	2.0
1	A	602	GLU	2.0
1	A	209	ALA	2.0
1	A	305	ALA	2.0
1	A	806	SER	2.0
1	A	873	ALA	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](#)

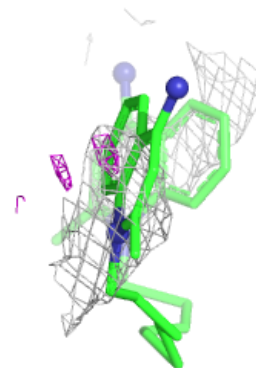
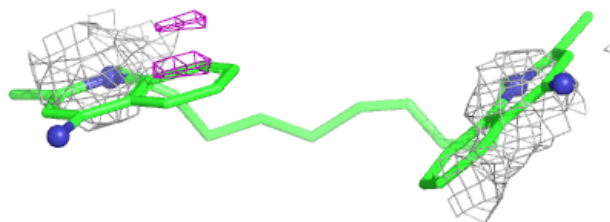
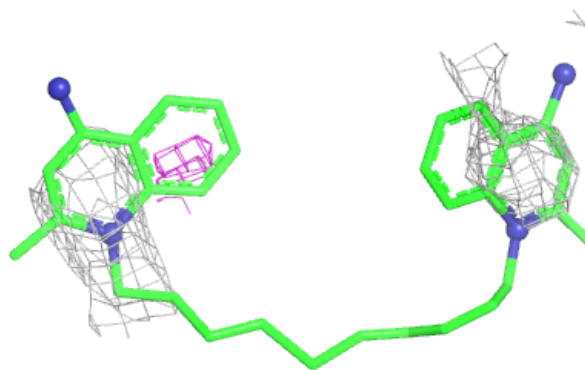
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	DEQ	A	4001	34/34	0.53	0.20	185,230,396,413	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 DEQ A 4001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.