



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:33 PM EDT

PDB ID : 4MUG / pdb_00004mug
Title : Crystal structure of pantothenate synthetase in complex with 2-(5-methoxy-2-(morpholinosulfonylcarbamoyl)-1H-indol-1-yl)acetic acid
Authors : Silvestre, H.L.; Blundell, T.L.
Deposited on : 2013-09-21
Resolution : 1.54 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

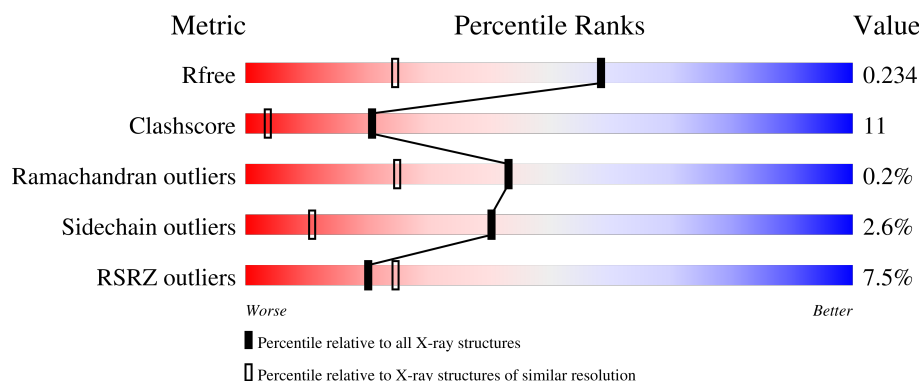
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	300	
1	B	300	

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	EOH	B	401	-	-	X	-
5	GOL	B	402	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4824 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.

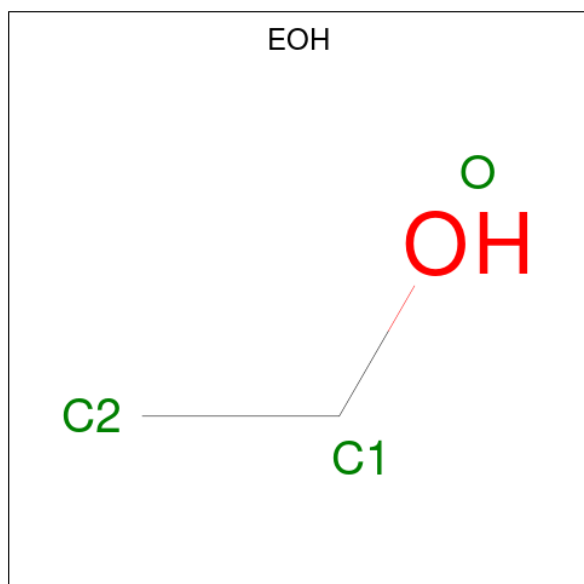
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	6	0
			2135	1350	382	396	7			
1	B	274	Total	C	N	O	S	0	7	0
			2061	1306	370	380	5			

There are 4 discrepancies between the modelled and reference sequences:

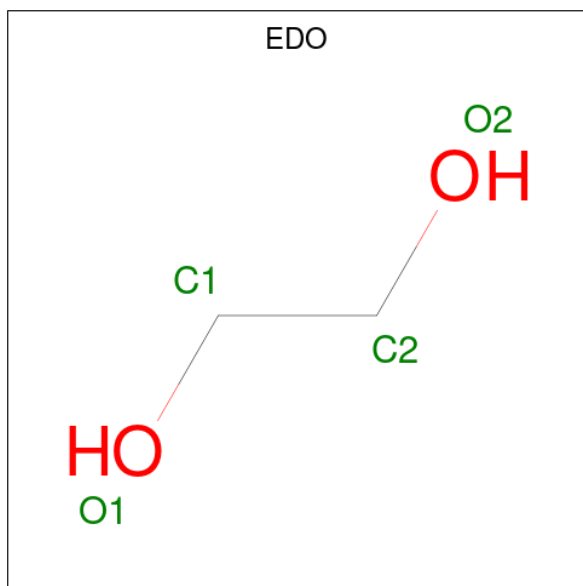
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



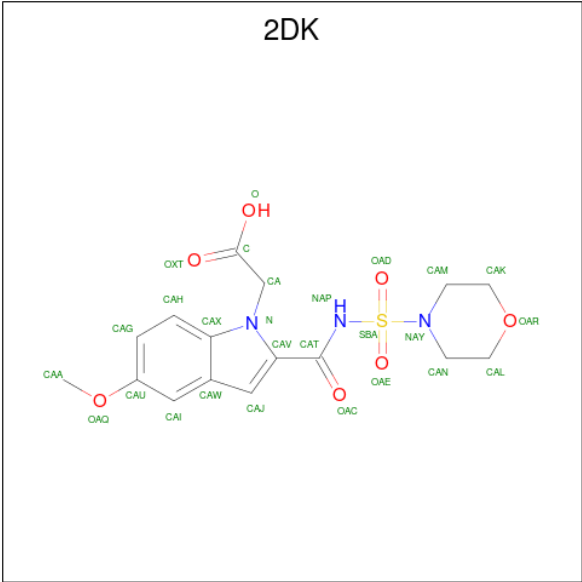
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	2	1		
2	A	1	Total	C	O	0	0
			3	2	1		
2	B	1	Total	C	O	0	0
			3	2	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



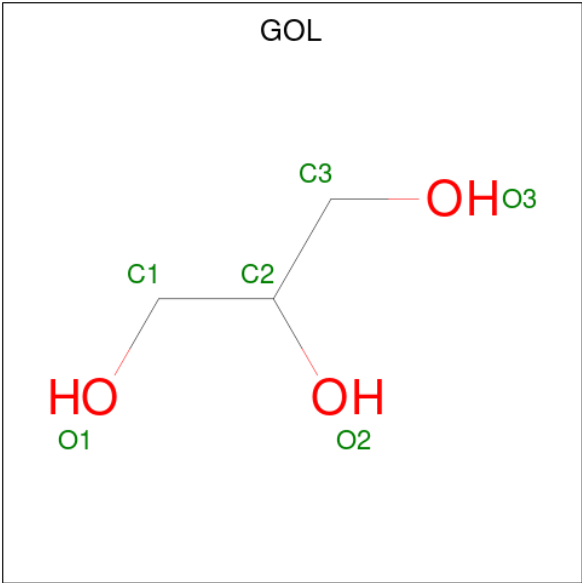
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is {5-methoxy-2-[(morpholin-4-ylsulfonyl)carbamoyl]-1H-indol-1-yl}acetic acid (CCD ID: 2DK) (formula: C₁₆H₁₉N₃O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	16	3	7	1		
4	B	1	Total	C	N	O	S	0	0
			27	16	3	7	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

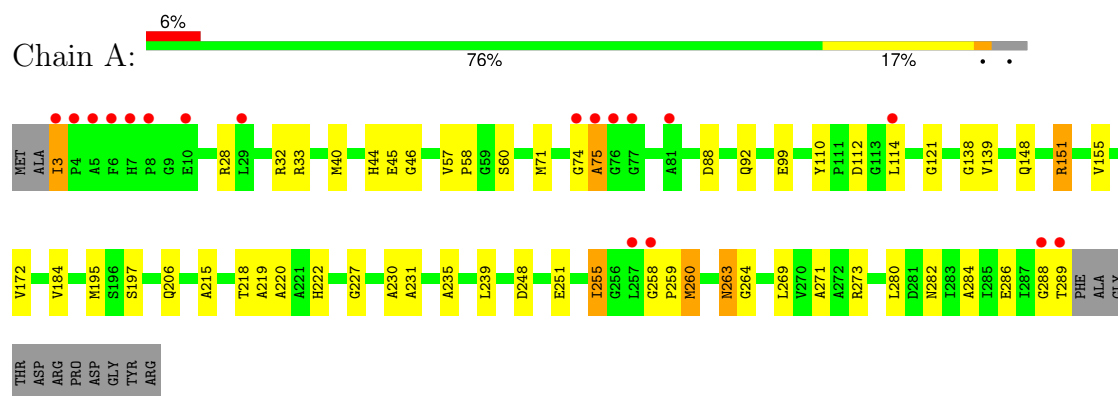
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	285	Total 285	O 285	0	0
6	B	248	Total 248	O 248	0	0

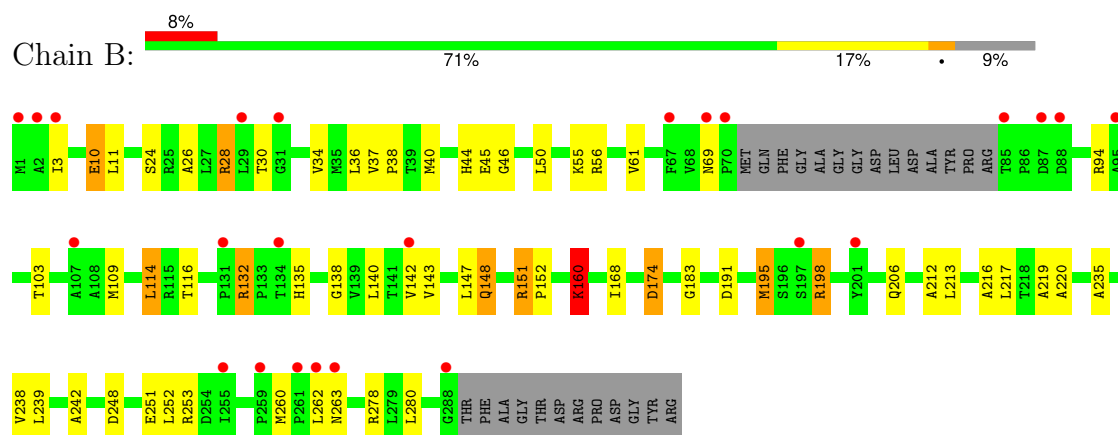
3 Residue-property plots [i](#)

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: Pantothenate synthetase



• Molecule 1: Pantothenate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.27Å 70.88Å 81.59Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	21.96 – 1.54 21.96 – 1.54	Depositor EDS
% Data completeness (in resolution range)	98.2 (21.96-1.54) 98.2 (21.96-1.54)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.237 0.191 , 0.234	Depositor DCC
R_{free} test set	3956 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4824	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: GOL, EOH, 2DK, EDO

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	1.59	17/2173 (0.8%)	1.50	14/2968 (0.5%)
1	B	1.54	21/2098 (1.0%)	1.53	23/2868 (0.8%)
All	All	1.57	38/4271 (0.9%)	1.52	37/5836 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	ARG	N-CA	8.65	1.52	1.46
1	A	155	VAL	N-CA	7.12	1.54	1.46
1	B	239	LEU	C-O	7.03	1.32	1.24
1	A	151	ARG	C-O	6.97	1.27	1.23
1	B	152	PRO	CA-C	-6.78	1.44	1.52
1	A	235	ALA	N-CA	6.72	1.54	1.46
1	B	34	VAL	N-CA	6.58	1.53	1.46
1	A	206	GLN	N-CA	6.51	1.54	1.46
1	A	231	ALA	N-CA	6.43	1.54	1.46
1	B	36	LEU	N-CA	6.35	1.53	1.46
1	A	239	LEU	N-CA	6.16	1.53	1.46
1	B	103	THR	CA-CB	6.02	1.60	1.53
1	A	269	LEU	CA-C	-6.00	1.45	1.52
1	B	239	LEU	N-CA	5.96	1.53	1.46
1	B	116	THR	N-CA	5.93	1.53	1.46
1	B	38	PRO	CA-C	5.90	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	GLU	CA-C	-5.89	1.45	1.52
1	B	217	LEU	N-CA	5.89	1.53	1.46
1	A	258	GLY	N-CA	5.85	1.52	1.44
1	B	151	ARG	CA-CB	5.79	1.56	1.52
1	A	282	ASN	C-O	5.76	1.30	1.23
1	B	212	ALA	N-CA	5.74	1.53	1.46
1	A	284	ALA	N-CA	5.59	1.52	1.46
1	A	138	GLY	N-CA	5.58	1.52	1.45
1	A	206	GLN	C-O	5.58	1.30	1.24
1	B	50	LEU	N-CA	5.46	1.52	1.46
1	B	160	LYS	C-O	-5.40	1.17	1.24
1	B	183	GLY	C-O	5.37	1.29	1.23
1	B	213	LEU	N-CA	5.32	1.52	1.46
1	A	110	TYR	CA-C	5.28	1.59	1.52
1	B	148	GLN	CD-NE2	-5.28	1.22	1.33
1	B	219	ALA	N-CA	5.27	1.52	1.46
1	B	280	LEU	N-CA	5.24	1.52	1.45
1	B	109	MET	N-CA	5.16	1.52	1.46
1	A	112	ASP	C-O	5.14	1.30	1.24
1	B	198	ARG	N-CA	5.11	1.52	1.46
1	A	227	GLY	N-CA	5.05	1.51	1.45
1	A	32	ARG	CA-C	5.01	1.59	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ALA	CA-C-O	-9.21	111.21	120.70
1	B	220	ALA	CA-C-O	-8.98	111.03	120.55
1	B	132	ARG	CA-C-N	8.88	129.77	119.47
1	B	132	ARG	C-N-CA	8.88	129.77	119.47
1	B	216	ALA	N-CA-C	-8.35	102.13	111.14
1	B	242	ALA	CA-C-N	-8.24	111.68	120.66
1	B	242	ALA	C-N-CA	-8.24	111.68	120.66
1	A	215	ALA	N-CA-C	-8.03	102.61	111.36
1	B	37	VAL	CA-C-O	-6.75	116.29	120.88
1	A	57	VAL	CA-C-N	-6.74	112.82	119.76
1	A	57	VAL	C-N-CA	-6.74	112.82	119.76
1	A	230	ALA	N-CA-C	-6.69	104.07	111.36
1	A	121	GLY	CA-C-N	6.68	126.37	119.56
1	A	121	GLY	C-N-CA	6.68	126.37	119.56
1	B	206	GLN	N-CA-C	-6.58	104.19	111.36
1	A	219	ALA	N-CA-C	-6.29	104.50	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ALA	O-C-N	6.26	128.75	122.12
1	A	99	GLU	N-CA-C	6.00	120.67	113.23
1	B	61	VAL	N-CA-C	-5.98	99.52	108.12
1	B	239	LEU	CA-C-O	-5.90	114.30	120.55
1	A	220	ALA	N-CA-C	-5.87	104.88	111.28
1	B	195	MET	CB-CG-SD	-5.78	95.35	112.70
1	A	148	GLN	N-CA-C	5.74	117.62	111.36
1	B	238	VAL	CA-C-O	-5.71	115.12	121.17
1	A	219	ALA	CA-C-O	-5.63	114.45	120.42
1	B	212	ALA	CA-C-O	-5.56	113.69	120.09
1	A	139	VAL	CB-CA-C	-5.50	104.82	112.02
1	B	238	VAL	O-C-N	5.45	127.25	121.91
1	B	174	ASP	N-CA-C	5.44	118.13	111.82
1	B	183	GLY	O-C-N	-5.41	119.34	123.35
1	B	24	SER	N-CA-C	-5.38	105.31	111.07
1	A	172	VAL	O-C-N	5.37	127.08	121.87
1	B	37	VAL	O-C-N	5.30	126.05	120.96
1	B	235	ALA	CA-C-O	-5.18	114.93	120.42
1	B	138	GLY	N-CA-C	5.08	118.39	112.50
1	A	184	VAL	N-CA-CB	-5.04	106.21	111.61
1	B	216	ALA	O-C-N	5.03	127.53	122.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288	GLY	Peptide

5.2 Too-close contacts [i](#)

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	2135	0	2170	32	0
1	B	2061	0	2121	60	0
2	A	6	0	12	0	0
2	B	3	0	6	6	0
3	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	0	0
4	A	27	0	18	3	0
4	B	27	0	18	3	0
5	A	6	0	8	3	0
5	B	6	0	8	5	0
6	A	285	0	0	9	1
6	B	248	0	0	17	0
All	All	4824	0	4391	97	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 11.

All (97) 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:B:160:LYS:HG2	6:B:737:HOH:O	1.27	1.34
1:B:252[B]:LEU:HD21	1:B:260:MET:SD	1.86	1.14
1:A:263:ASN:CG	1:A:264:GLY:H	1.55	1.13
1:A:248[B]:ASP:OD1	1:A:273:ARG:NH1	1.83	1.11
1:B:248:ASP:OD1	6:B:699:HOH:O	1.71	1.06
1:B:252[B]:LEU:HD23	1:B:252[B]:LEU:C	1.86	0.98
1:B:3:ILE:HD13	1:B:26:ALA:HB2	1.49	0.92
1:B:44:HIS:HD2	1:B:46:GLY:H	1.16	0.92
1:B:28:ARG:HG2	2:B:401:EOH:H23	1.53	0.90
1:A:263:ASN:CG	1:A:264:GLY:N	2.24	0.87
1:B:44:HIS:HE1	4:B:403:2DK:OXT	1.58	0.84
1:B:252[B]:LEU:C	1:B:252[B]:LEU:CD2	2.53	0.82
1:B:248:ASP:HB3	6:B:537:HOH:O	1.79	0.82
1:A:40:MET:HG2	5:A:406:GOL:H32	1.66	0.77
1:A:255:ILE:H	1:A:255:ILE:HD13	1.48	0.77
1:A:71:MET:SD	1:A:114:LEU:HD21	2.25	0.77
1:A:44:HIS:HD2	1:A:46:GLY:H	1.33	0.74
1:B:252[B]:LEU:CD2	1:B:260:MET:SD	2.73	0.73
1:B:252[B]:LEU:HD23	1:B:253:ARG:N	2.04	0.72
1:B:3:ILE:CD1	1:B:26:ALA:HB2	2.19	0.71
1:B:44:HIS:HD2	1:B:46:GLY:N	1.86	0.71
1:B:151:ARG:HE	2:B:401:EOH:H22	1.56	0.70
4:A:405:2DK:H11	4:A:405:2DK:H2	1.56	0.70
1:B:140:LEU:CD2	1:B:168[A]:ILE:HD13	2.24	0.68
1:B:151:ARG:HB3	2:B:401:EOH:H11	1.76	0.67
1:B:69:ASN:CG	1:B:142[B]:VAL:HG21	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:HIS:CD2	1:B:46:GLY:H	2.07	0.67
1:A:60:SER:OG	6:A:761:HOH:O	2.13	0.66
1:B:55:LYS:HD3	6:B:536:HOH:O	1.95	0.66
1:B:45:GLU:HG2	6:B:565:HOH:O	1.95	0.66
1:B:44:HIS:CE1	4:B:403:2DK:OXT	2.46	0.65
1:A:44:HIS:HD2	1:A:46:GLY:N	1.96	0.64
1:B:143:VAL:HG11	1:B:168[A]:ILE:HD12	1.79	0.63
1:A:45:GLU:HB3	1:A:195[B]:MET:SD	2.38	0.63
1:A:248[B]:ASP:CG	1:A:273:ARG:HH11	2.08	0.62
1:B:28:ARG:CG	2:B:401:EOH:H23	2.30	0.61
1:B:132:ARG:NH2	6:B:598:HOH:O	2.34	0.61
1:A:3:ILE:HD12	1:A:3:ILE:N	2.16	0.60
1:A:44:HIS:HE1	4:A:405:2DK:O	1.84	0.60
1:B:248:ASP:CG	6:B:699:HOH:O	2.35	0.58
1:B:56:ARG:NH1	6:B:701:HOH:O	2.32	0.58
1:B:252[B]:LEU:HD21	1:B:260:MET:CG	2.33	0.58
1:B:26:ALA:O	1:B:30:THR:HG23	2.04	0.57
1:B:278:ARG:HG2	1:B:278:ARG:HH11	1.69	0.57
1:B:10:GLU:CD	1:B:11:LEU:H	2.13	0.56
1:B:252[B]:LEU:HD22	1:B:260:MET:HB2	1.88	0.56
1:B:147:LEU:HB3	5:B:402:GOL:H12	1.89	0.55
1:B:278:ARG:HG2	1:B:278:ARG:NH1	2.21	0.55
1:B:148:GLN:OE1	5:B:402:GOL:H31	2.08	0.54
1:B:252[B]:LEU:CD2	1:B:260:MET:CG	2.87	0.53
1:B:160:LYS:HE3	6:B:627:HOH:O	2.08	0.53
1:A:75:ALA:HA	6:A:597:HOH:O	2.09	0.52
1:B:252[B]:LEU:CD2	1:B:260:MET:HB2	2.40	0.51
1:B:3:ILE:HD13	1:B:26:ALA:CB	2.30	0.51
1:B:262:LEU:HD13	6:B:702:HOH:O	2.11	0.50
3:A:404:EDO:H12	1:B:174:ASP:HB3	1.95	0.49
1:B:69:ASN:ND2	1:B:142[B]:VAL:HG21	2.27	0.49
1:B:10:GLU:OE1	1:B:94:ARG:HD3	2.13	0.48
1:A:286:GLU:CD	6:A:758:HOH:O	2.55	0.48
1:A:33:ARG:HD2	6:A:688:HOH:O	2.12	0.48
1:A:88:ASP:O	1:A:92:GLN:HG3	2.16	0.46
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.82	0.45
5:B:402:GOL:H11	6:B:547:HOH:O	2.16	0.45
1:B:94:ARG:NH2	6:B:691:HOH:O	2.49	0.45
1:A:74:GLY:O	1:A:75:ALA:CB	2.65	0.44
1:B:69:ASN:HB2	6:B:745:HOH:O	2.17	0.44
1:B:114:LEU:CD2	6:B:738:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:402:GOL:O3	6:B:506:HOH:O	2.19	0.44
1:B:132:ARG:HB3	1:B:135:HIS:HB2	2.00	0.44
4:A:405:2DK:H11	4:A:405:2DK:CA	2.27	0.44
1:B:252[B]:LEU:HD22	1:B:260:MET:CB	2.47	0.44
1:B:151:ARG:HE	2:B:401:EOH:C2	2.26	0.44
1:A:273:ARG:HD3	6:A:695:HOH:O	2.17	0.43
1:B:28:ARG:HG2	2:B:401:EOH:C2	2.36	0.43
1:A:40:MET:CG	5:A:406:GOL:H32	2.44	0.43
1:B:45:GLU:HB2	1:B:195:MET:CE	2.49	0.43
1:B:40:MET:HE3	4:B:403:2DK:CAN	2.49	0.42
1:B:114:LEU:HD13	1:B:114:LEU:HA	1.87	0.42
5:B:402:GOL:C1	6:B:547:HOH:O	2.68	0.42
5:A:406:GOL:H31	6:A:506:HOH:O	2.19	0.42
1:A:263:ASN:HB3	6:A:705:HOH:O	2.19	0.42
1:B:44:HIS:CD2	1:B:46:GLY:N	2.77	0.42
1:B:191:ASP:N	6:B:705:HOH:O	2.44	0.42
1:A:33:ARG:NH2	1:A:58:PRO:O	2.45	0.42
1:A:197[A]:SER:HA	6:A:558:HOH:O	2.19	0.41
1:B:3:ILE:CD1	1:B:26:ALA:CB	2.95	0.41
1:A:259:PRO:HD2	1:A:260:MET:CE	2.51	0.41
1:A:271:ALA:HB2	1:A:280:LEU:HD22	2.03	0.41
1:A:151:ARG:CZ	1:B:151:ARG:HD2	2.51	0.41
1:A:218:THR:O	1:A:222:HIS:HD2	2.04	0.41
1:A:44:HIS:HB2	1:A:195[A]:MET:HE3	2.03	0.40
1:B:140:LEU:HD22	1:B:168[A]:ILE:HD13	2.01	0.40
1:B:262:LEU:HD13	1:B:262:LEU:HA	1.96	0.40
1:A:259:PRO:HD2	1:A:260:MET:HE2	2.02	0.40
1:B:198:ARG:NH1	1:B:278:ARG:HB3	2.35	0.40
1:A:28:ARG:O	1:A:28:ARG:NH1	2.54	0.40
1:A:195[A]:MET:CE	6:A:596:HOH:O	2.70	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)
6:A:664:HOH:O	6:A:709:HOH:O[2_645]	2.10	0.10

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	289/300 (96%)	283 (98%)	5 (2%)	1 (0%)	36	19
1	B	277/300 (92%)	273 (99%)	4 (1%)	0	100	100
All	All	566/600 (94%)	556 (98%)	9 (2%)	1 (0%)	43	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/223 (97%)	211 (98%)	5 (2%)	44	14
1	B	211/223 (95%)	205 (97%)	6 (3%)	38	9
All	All	427/446 (96%)	416 (97%)	11 (3%)	40	11

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	255	ILE
1	A	260	MET
1	A	263	ASN
1	A	289	THR

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Mol	Chain	Res	Type
1	B	10	GLU
1	B	28	ARG
1	B	114	LEU
1	B	160	LYS
1	B	251	GLU
1	B	263	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	164	GLN
1	A	222	HIS
1	B	44	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2DK	B	403	-	27,29,29	3.17	11 (40%)	37,42,42	2.47	13 (35%)
3	EDO	B	405	-	3,3,3	0.53	0	2,2,2	0.44	0
2	EOH	A	402	-	2,2,2	0.32	0	1,1,1	0.36	0
3	EDO	B	404	-	3,3,3	0.63	0	2,2,2	0.77	0
3	EDO	A	404	-	3,3,3	0.38	0	2,2,2	0.62	0
3	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.74	0
2	EOH	B	401	-	2,2,2	0.84	0	1,1,1	0.21	0
4	2DK	A	405	-	27,29,29	3.09	9 (33%)	37,42,42	2.69	17 (45%)
5	GOL	B	402	-	5,5,5	0.46	0	5,5,5	1.24	0
5	GOL	A	406	-	5,5,5	0.49	0	5,5,5	0.72	0
2	EOH	A	401	-	2,2,2	0.47	0	1,1,1	0.16	0
3	EDO	A	403	-	3,3,3	0.14	0	2,2,2	1.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2DK	B	403	-	-	1/19/29/29	0/3/3/3
3	EDO	B	405	-	-	0/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-
4	2DK	A	405	-	-	7/19/29/29	0/3/3/3
5	GOL	B	402	-	-	2/4/4/4	-
5	GOL	A	406	-	-	2/4/4/4	-
3	EDO	A	403	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	2DK	OAE-SBA	9.83	1.54	1.43
4	A	405	2DK	OAD-SBA	9.06	1.53	1.43
4	B	403	2DK	OAD-SBA	9.00	1.53	1.43
4	B	403	2DK	CA-N	7.12	1.60	1.46
4	B	403	2DK	CAT-NAP	-5.60	1.32	1.38
4	B	403	2DK	CAV-CAT	-4.70	1.40	1.49
4	A	405	2DK	CAI-CAU	4.40	1.46	1.39
4	B	403	2DK	OAE-SBA	4.06	1.47	1.43
4	A	405	2DK	CAV-CAT	-3.78	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	2DK	CAH-CAX	-3.74	1.33	1.39
4	B	403	2DK	CAX-N	-3.56	1.33	1.39
4	B	403	2DK	CAM-NAY	3.42	1.51	1.47
4	A	405	2DK	CAG-CAU	3.19	1.44	1.38
4	B	403	2DK	CAW-CAX	-2.73	1.37	1.41
4	A	405	2DK	CAN-NAY	2.42	1.50	1.47
4	B	403	2DK	CAI-CAW	-2.35	1.36	1.40
4	A	405	2DK	CAW-CAX	-2.21	1.38	1.41
4	A	405	2DK	CAG-CAH	-2.15	1.35	1.38
4	A	405	2DK	OAR-CAL	2.13	1.50	1.42
4	B	403	2DK	CAW-CAJ	-2.02	1.37	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	2DK	OAE-SBA-OAD	-8.77	104.15	119.80
4	B	403	2DK	CAN-NAY-CAM	-7.74	103.22	112.12
4	A	405	2DK	CAJ-CAV-N	-6.19	105.92	109.42
4	B	403	2DK	CAK-CAM-NAY	5.85	112.44	108.27
4	A	405	2DK	OAR-CAK-CAM	-4.29	102.53	111.77
4	A	405	2DK	OAC-CAT-NAP	-4.21	115.84	121.94
4	B	403	2DK	CAW-CAX-N	-3.73	105.54	107.85
4	A	405	2DK	CAK-CAM-NAY	-3.69	105.63	108.27
4	B	403	2DK	CAH-CAG-CAU	-3.60	115.62	119.73
4	B	403	2DK	CAI-CAW-CAX	-3.59	115.92	119.56
4	B	403	2DK	CAJ-CAV-N	-3.59	107.39	109.42
4	A	405	2DK	C-CA-N	3.09	121.09	113.08
4	B	403	2DK	CA-N-CAV	-3.05	122.80	127.43
4	A	405	2DK	O-C-OXT	3.04	131.16	123.33
4	B	403	2DK	CAW-CAI-CAU	3.00	123.86	120.46
4	A	405	2DK	CAG-CAU-CAI	-2.80	116.74	120.50
4	B	403	2DK	CAX-N-CAV	2.78	110.48	108.44
4	A	405	2DK	CAW-CAJ-CAV	2.74	111.40	107.31
4	A	405	2DK	CAV-CAT-NAP	2.74	118.77	114.26
4	A	405	2DK	CAI-CAW-CAX	2.72	122.31	119.56
4	B	403	2DK	CAX-CAW-CAJ	2.70	109.73	107.05
4	A	405	2DK	OXT-C-CA	-2.64	111.34	122.38
4	A	405	2DK	OAE-SBA-NAP	2.59	112.77	105.80
4	B	403	2DK	C-CA-N	2.55	119.69	113.08
4	A	405	2DK	CAW-CAX-N	2.54	109.43	107.85
4	A	405	2DK	CAJ-CAV-CAT	-2.53	123.17	129.48
4	A	405	2DK	CAX-CAW-CAJ	-2.44	104.63	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	2DK	CAL-OAR-CAK	2.22	117.05	109.88
4	B	403	2DK	OAR-CAK-CAM	-2.19	107.05	111.77
4	A	405	2DK	OAD-SBA-NAP	2.18	111.69	105.80

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	2DK	CAT-NAP-SBA-NAY
4	B	403	2DK	C-CA-N-CAX
5	A	406	GOL	O1-C1-C2-C3
5	B	402	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
4	A	405	2DK	CAI-CAU-OAQ-CAA
3	B	406	EDO	O1-C1-C2-O2
4	A	405	2DK	OAC-CAT-CAV-N
4	A	405	2DK	NAP-CAT-CAV-N
3	A	404	EDO	O1-C1-C2-O2
4	A	405	2DK	CAG-CAU-OAQ-CAA
4	A	405	2DK	CAM-NAY-SBA-OAE
5	B	402	GOL	O2-C2-C3-O3
4	A	405	2DK	NAP-CAT-CAV-CAJ

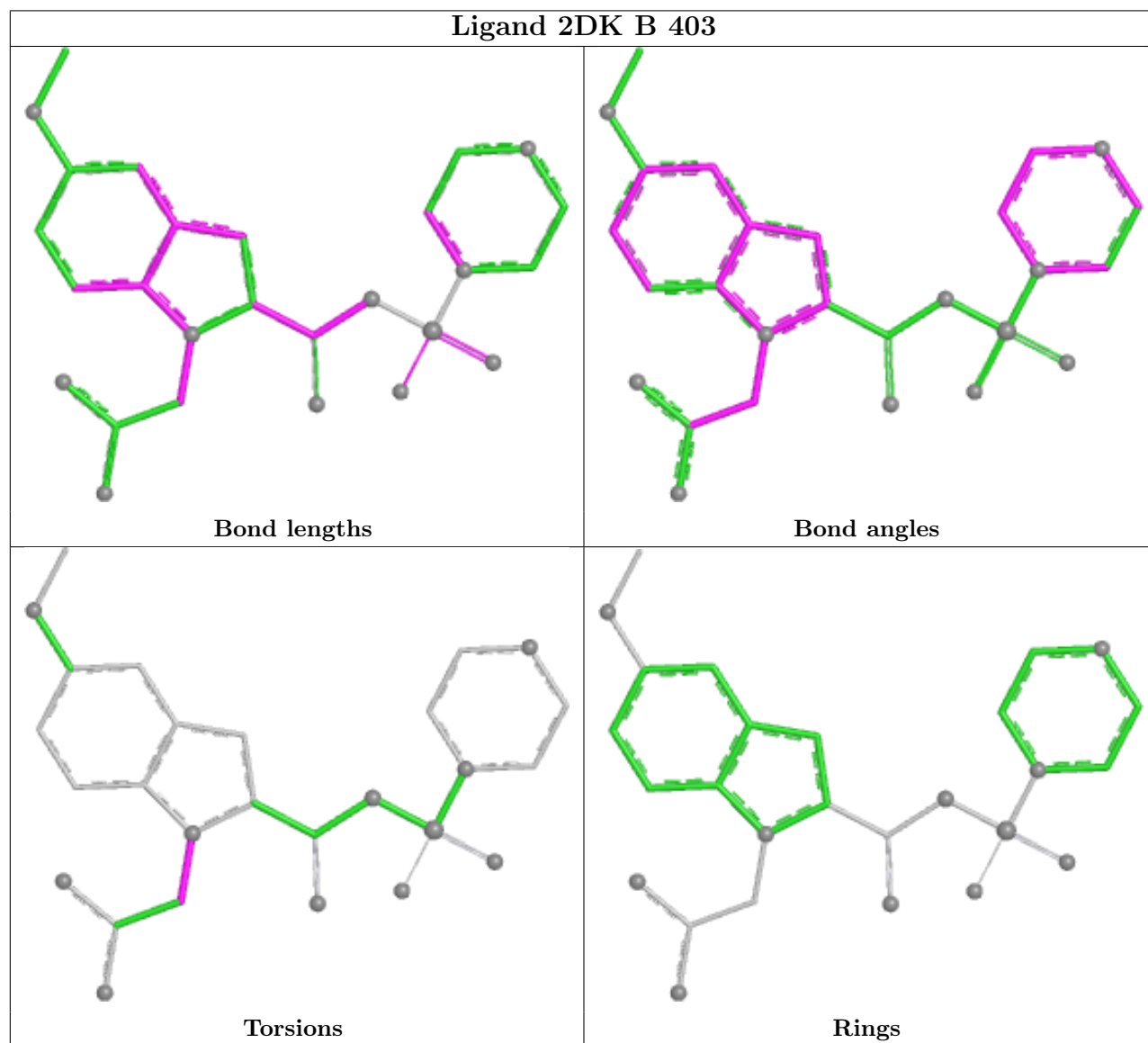
There are no ring outliers.

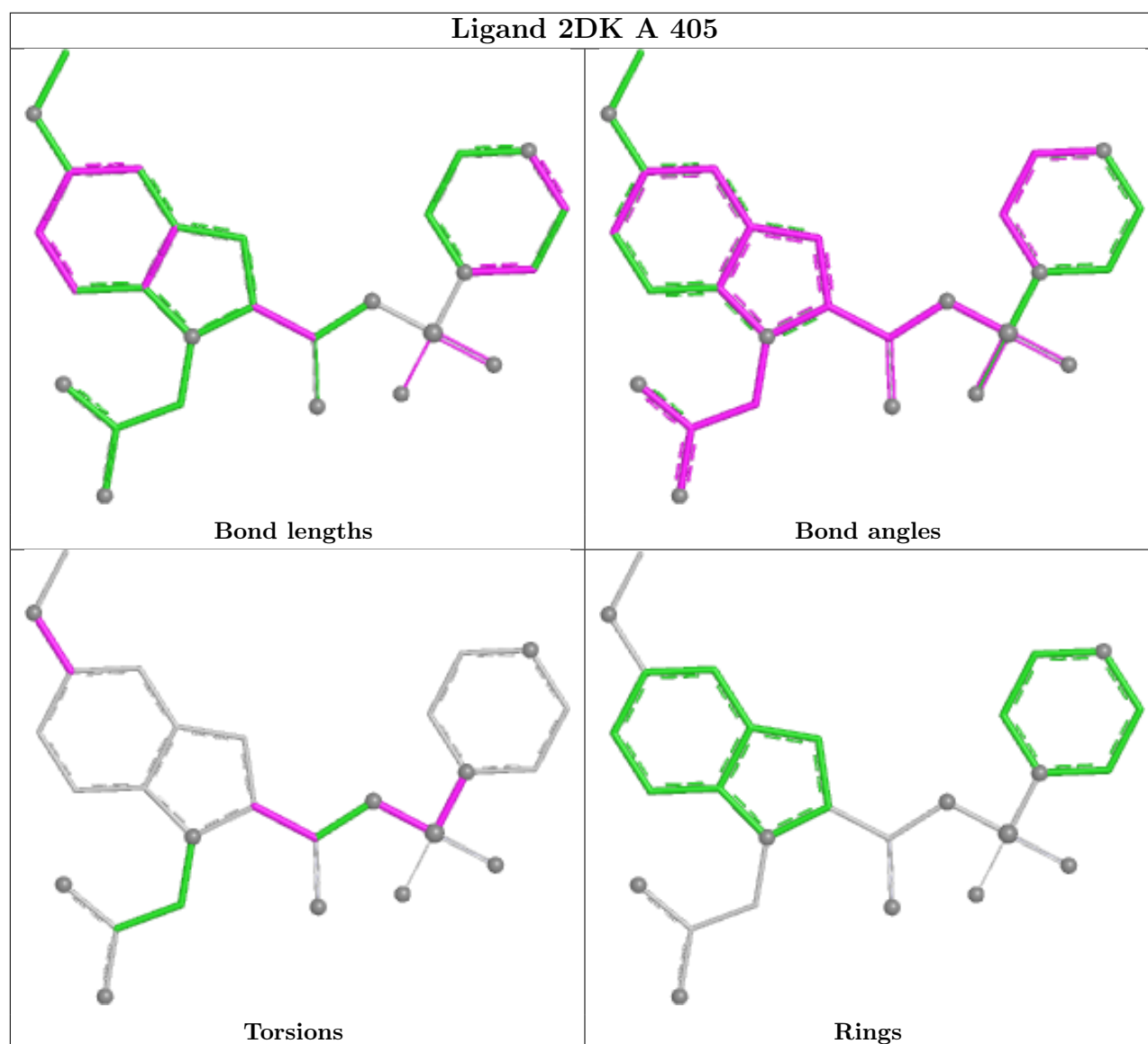
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	2DK	3	0
3	A	404	EDO	1	0
2	B	401	EOH	6	0
4	A	405	2DK	3	0
5	B	402	GOL	5	0
5	A	406	GOL	3	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	287/300 (95%)	0.44	18 (6%)	26 33	8, 16, 33, 62	6 (2%)
1	B	274/300 (91%)	0.62	24 (8%)	15 20	5, 19, 39, 70	8 (2%)
All	All	561/600 (93%)	0.53	42 (7%)	20 25	5, 17, 37, 70	14 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ILE	6.6
1	B	2	ALA	5.9
1	A	289	THR	5.0
1	B	31	GLY	4.8
1	B	85	THR	4.5
1	A	75	ALA	4.4
1	B	29	LEU	4.1
1	B	262	LEU	3.9
1	B	131	PRO	3.3
1	B	263	ASN	3.3
1	B	69	ASN	3.2
1	B	261	PRO	3.2
1	B	134	THR	3.1
1	A	4	PRO	2.9
1	A	74	GLY	2.9
1	B	201	TYR	2.9
1	A	288	GLY	2.8
1	A	81	ALA	2.7
1	B	87	ASP	2.7
1	A	8	PRO	2.7
1	B	70	PRO	2.6
1	B	288	GLY	2.5
1	B	1	MET	2.5
1	A	6	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	2.5
1	A	10	GLU	2.5
1	A	7	HIS	2.4
1	B	88	ASP	2.3
1	B	255	ILE	2.3
1	A	77	GLY	2.3
1	A	114	LEU	2.3
1	A	76	GLY	2.2
1	A	257	LEU	2.2
1	B	67	PHE	2.2
1	A	29	LEU	2.1
1	A	5	ALA	2.1
1	B	107	ALA	2.1
1	A	258	GLY	2.1
1	B	197[A]	SER	2.1
1	B	259	PRO	2.1
1	B	3	ILE	2.0
1	B	142[A]	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EOH	B	401	3/3	0.84	0.17	28,28,28,30	0
2	EOH	A	402	3/3	0.85	0.14	32,32,32,35	0
3	EDO	B	405	4/4	0.85	0.09	29,36,37,41	0
2	EOH	A	401	3/3	0.87	0.12	28,28,34,35	0
3	EDO	A	403	4/4	0.88	0.13	28,34,39,40	0

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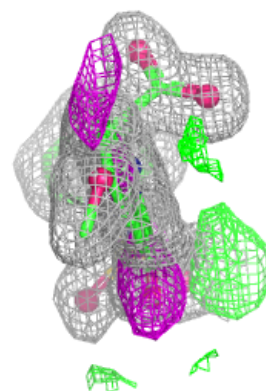
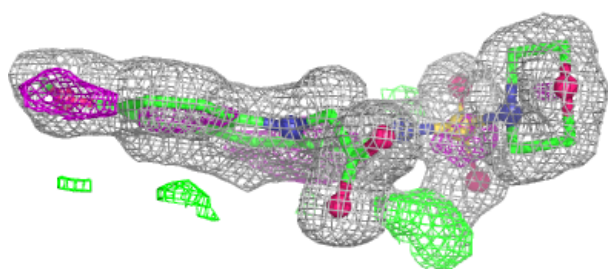
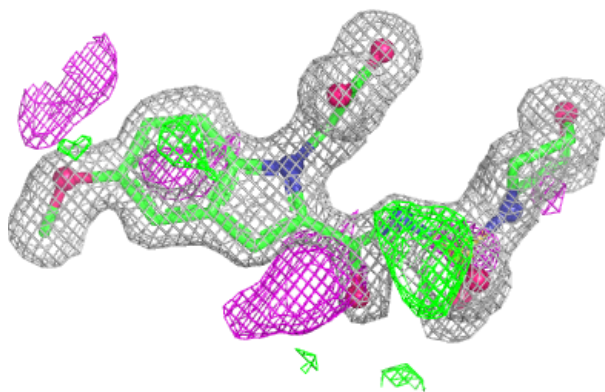
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	406	4/4	0.88	0.10	34,36,38,39	0
5	GOL	B	402	6/6	0.88	0.12	35,37,41,45	0
3	EDO	B	404	4/4	0.89	0.11	25,28,29,34	0
3	EDO	A	404	4/4	0.91	0.14	23,24,25,28	0
4	2DK	A	405	27/27	0.92	0.09	15,17,26,26	0
5	GOL	A	406	6/6	0.94	0.08	17,30,33,38	0
4	2DK	B	403	27/27	0.95	0.09	16,22,36,39	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.

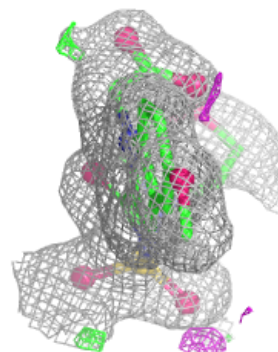
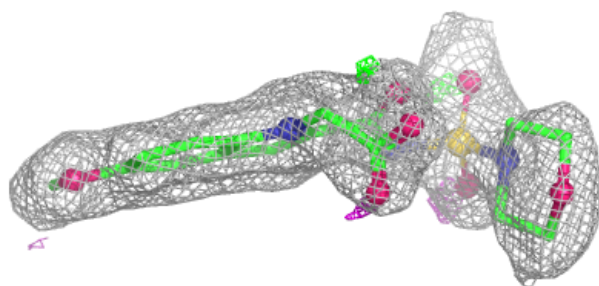
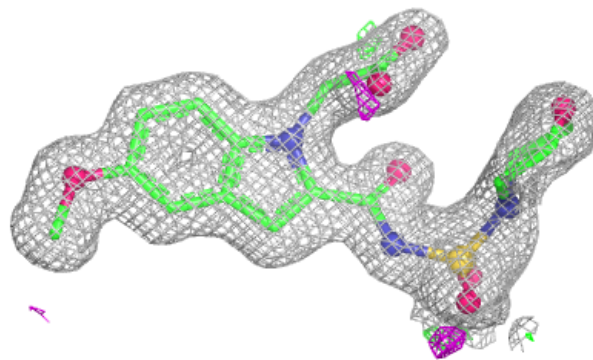
Electron density around 2DK A 405:

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



Electron density around 2DK B 403:

$2mF_o-DF_c$ (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.