WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2016 – 05:34 AM EST

PDB ID	:	4MUH
Title	:	Crystal structure of pantothenate synthetase in complex with 2-(2-(5-acetamido-1,3,4-thiadiazol-2-ylsulfonylcarbamoyl)-5-methoxy-1H-indol-1-yl)acetic acid
Authors	:	Silvestre, H.L.; Blundell, T.L.
Deposited on	:	2013-09-21
Resolution	:	1.72 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	Percentile Ranks	Value
Rfree		0.213
Clashscore		8
Ramachandran outliers		0.2%
Sidechain outliers		2.6%
RSRZ outliers		5.2%

Worse								*Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
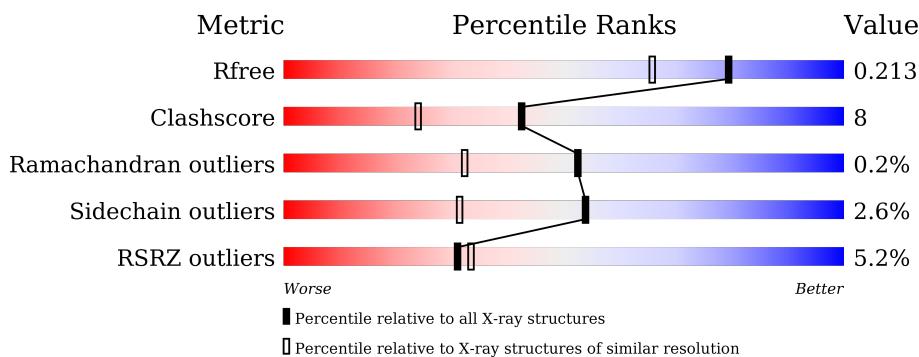
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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 <=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	3% · 81% · 13% · 5%
1	B	300	7% · 79% · 11% · 9%
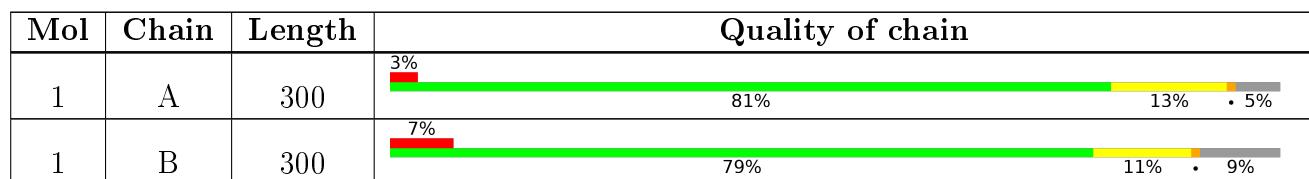
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Full wwPDB X-ray Structure Validation Report

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EOH	A	401	-	-	X	X
2	EOH	A	402	-	-	-	X
2	EOH	B	407	-	-	X	-
3	2DN	B	401	-	-	X	-
3	2DN	B	406	-	-	-	X
4	EDO	A	406	-	-	-	X
4	EDO	B	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4737 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	286	Total 2143	C 1351	N 386	O 400	S 6	0	7	0
1	B	274	Total 2083	C 1316	N 375	O 385	S 7	0	9	0

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 (three-letter code: EOH) (formula: C_2H_6O).
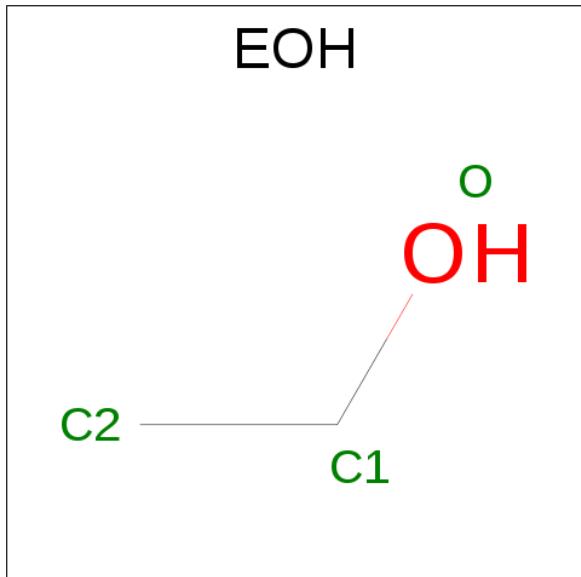
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 3	C 2	O 1	0	0
2	A	1	Total 3	C 2	O 1	0	0
2	A	1	Total 3	C 2	O 1	0	0
2	B	1	Total 3	C 2	O 1	0	0

- Molecule 3 is [2-({[5-(ACETYLAMINO)-1,3,4-THIADIAZOL-2-YL]SULFONYL}CARBA MOYL)-5-METHOXY-1H-INDOL-1-YL]ACETIC ACID (three-letter code: 2DN) (formula: $C_{16}H_{15}N_5O_7S_2$).
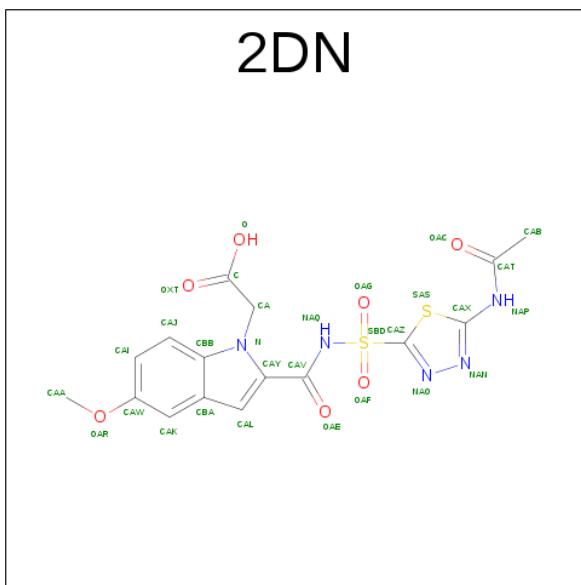
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 16	N 5	O 7	S 2	0	0
3	B	1	Total 30	C 16	N 5	O 7	S 2	0	0
3	B	1	Total 30	C 16	N 5	O 7	S 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
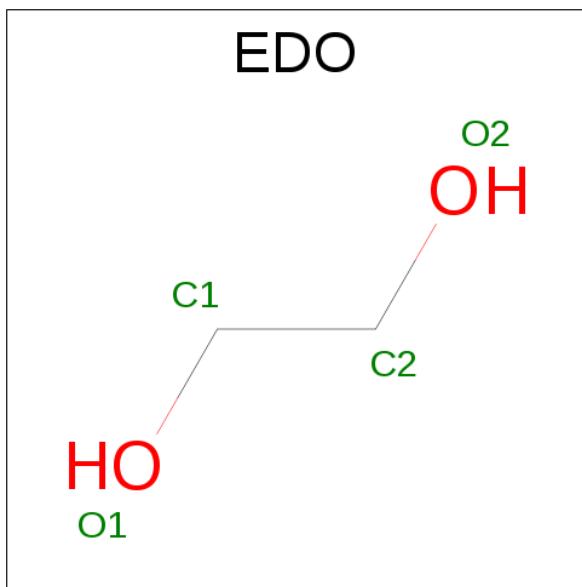
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total 197	O 197	0	0
5	B	180	Total 180	O 180	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: Pantothenate synthetase
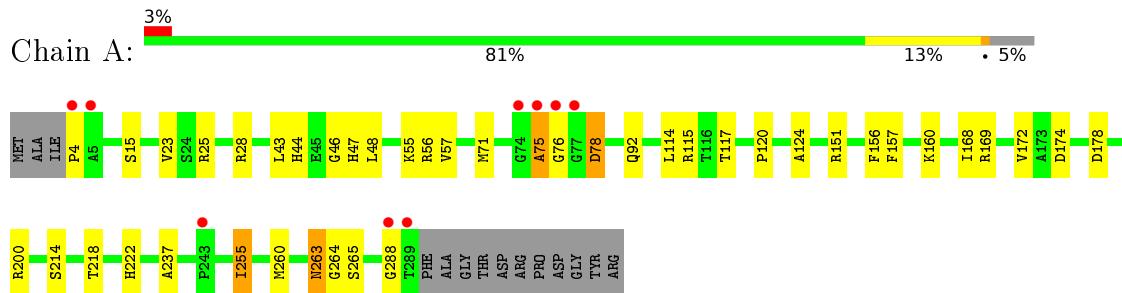
- Molecule 1: Pantothenate synthetase
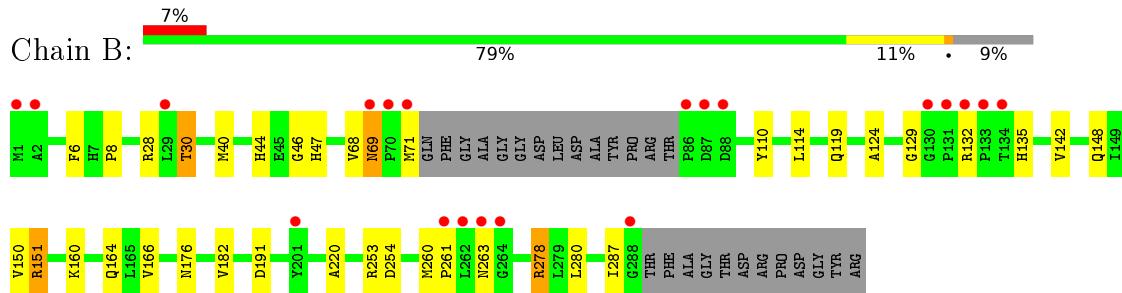
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.41Å 71.07Å 81.64Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	28.00 – 1.72	Depositor
	27.71 – 1.72	EDS
% Data completeness	100.0 (28.00-1.72)	Depositor
(in resolution range)	100.0 (27.71-1.72)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.168 , 0.213	Depositor
	0.168 , 0.213	DCC
R_{free} test set	2949 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4737	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, 2DN, 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	1.22	3/2181 (0.1%)	1.04	3/2978 (0.1%)
1	B	1.19	4/2123 (0.2%)	1.01	4/2898 (0.1%)
All	All	1.20	7/4304 (0.2%)	1.02	7/5876 (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	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	VAL	CB-CG1	7.07	1.67	1.52
1	A	214	SER	CB-OG	5.95	1.50	1.42
1	B	220	ALA	CA-CB	5.91	1.64	1.52
1	B	182	VAL	CB-CG2	5.46	1.64	1.52
1	B	166	VAL	CB-CG2	5.42	1.64	1.52
1	A	237	ALA	CA-CB	5.34	1.63	1.52
1	A	172	VAL	CB-CG1	5.01	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	191	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	169	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	160[A]	LYS	CD-CE-NZ	-6.15	97.56	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	B	280	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	56	ARG	NE-CZ-NH2	5.31	122.95	120.30

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	2143	0	2176	38	0
1	B	2083	0	2140	35	0
2	A	9	0	18	4	0
2	B	3	0	6	2	0
3	A	30	0	14	1	0
3	B	60	0	28	9	0
4	A	16	0	24	3	0
4	B	16	0	24	3	0
5	A	197	0	0	5	1
5	B	180	0	0	4	0
All	All	4737	0	4430	73	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (73) 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:151:ARG:CG	1:B:151:ARG:HH21	1.60	1.12
1:A:75:ALA:HB1	1:A:76:GLY:HA3	1.10	1.09
1:A:75:ALA:CB	1:A:76:GLY:HA3	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:NH2	1:B:151:ARG:HG2	1.46	1.02
3:B:401:2DN:H14	5:B:671:HOH:O	1.63	0.98
1:A:255:ILE:HD13	1:A:255:ILE:H	1.38	0.89
1:A:263:ASN:CG	1:A:264:GLY:H	1.77	0.87
1:B:164:GLN:HE22	3:B:401:2DN:H12	1.18	0.85
1:A:75:ALA:HB1	1:A:76:GLY:CA	2.03	0.82
1:A:92[A]:GLN:NE2	5:A:660:HOH:O	2.12	0.81
1:B:44:HIS:HE1	3:B:401:2DN:OXT	1.63	0.79
1:A:263:ASN:CG	1:A:264:GLY:N	2.38	0.75
1:B:160:LYS:HG2	5:B:653:HOH:O	1.88	0.72
1:A:151:ARG:HH22	1:B:151:ARG:NH2	1.86	0.72
1:A:55:LYS:HE3	5:A:641:HOH:O	1.92	0.68
1:B:44:HIS:HD2	1:B:46:GLY:H	1.41	0.67
1:A:151:ARG:HH22	1:B:151:ARG:CZ	2.08	0.66
1:A:44:HIS:HD2	1:A:46:GLY:H	1.43	0.65
1:A:75:ALA:CB	1:A:76:GLY:CA	2.69	0.65
1:A:218[B]:THR:HG21	2:A:402:EOH:H23	1.78	0.65
1:A:115:ARG:O	2:A:401:EOH:H22	1.97	0.64
1:B:151:ARG:HH21	1:B:151:ARG:HG2	0.67	0.62
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.80	0.61
1:A:117:THR:OG1	2:A:401:EOH:H21	2.01	0.61
1:B:135:HIS:NE2	3:B:401:2DN:CAB	2.65	0.59
1:B:124:ALA:O	1:B:129:GLY:HA3	2.04	0.58
1:B:40:MET:HE3	1:B:68:VAL:HA	1.86	0.57
1:B:44:HIS:HD2	1:B:46:GLY:N	2.03	0.56
1:A:157:PHE:CZ	1:A:168:ILE:HD13	2.41	0.55
1:A:255:ILE:CD1	1:A:255:ILE:H	2.15	0.55
1:B:151:ARG:CG	1:B:151:ARG:NH2	2.31	0.55
1:A:178[A]:ASP:HB3	1:B:151:ARG:HH11	1.71	0.55
1:A:15[B]:SER:O	5:A:532:HOH:O	2.14	0.54
1:A:151:ARG:NH2	1:B:151:ARG:NH2	2.55	0.53
1:A:44:HIS:HD2	1:A:46:GLY:N	2.07	0.53
1:B:260:MET:SD	1:B:261:PRO:HD2	2.49	0.52
1:A:71:MET:SD	1:A:114:LEU:HD21	2.50	0.52
1:B:176:ASN:HD22	2:B:407:EOH:H21	1.75	0.52
1:B:44:HIS:CE1	3:B:401:2DN:OXT	2.54	0.51
4:B:404:EDO:H22	5:B:592:HOH:O	2.10	0.51
1:B:47:HIS:HE2	3:B:401:2DN:H11	1.58	0.50
1:A:174:ASP:HB3	4:B:402:EDO:H22	1.93	0.50
1:B:30:THR:CG2	1:B:30:THR:O	2.60	0.49
1:B:278:ARG:HG2	1:B:278:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:EOH:H21	1:B:119:GLN:HG2	1.95	0.49
1:B:71:MET:CE	1:B:110:TYR:OH	2.62	0.48
1:A:75:ALA:HB3	1:A:78:ASP:HB2	1.95	0.47
1:A:57:VAL:HG22	4:A:406:EDO:H12	1.96	0.47
3:B:401:2DN:OAC	3:B:401:2DN:SAS	2.72	0.47
1:A:156:PHE:CE2	4:A:406:EDO:H11	2.49	0.47
1:B:148:GLN:O	1:B:151:ARG:CD	2.63	0.46
3:B:401:2DN:CAB	5:B:671:HOH:O	2.39	0.46
1:A:25:ARG:HA	1:A:28:ARG:NH1	2.31	0.45
1:B:44:HIS:CD2	1:B:46:GLY:H	2.29	0.45
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.81	0.45
1:A:4:PRO:HG2	1:A:23:VAL:HG23	1.99	0.45
1:A:218[B]:THR:O	1:A:222:HIS:HD2	2.00	0.44
1:A:156:PHE:CZ	4:A:406:EDO:H11	2.52	0.44
1:A:200:ARG:NH2	5:A:581:HOH:O	2.49	0.44
1:B:71:MET:SD	1:B:114:LEU:HD21	2.57	0.44
1:B:69[B]:ASN:CG	1:B:142[B]:VAL:HG21	2.38	0.44
1:A:92[B]:GLN:OE1	1:A:92[B]:GLN:HA	2.17	0.44
1:B:135:HIS:NE2	3:B:401:2DN:H13	2.34	0.43
1:A:43:LEU:HA	1:A:47:HIS:ND1	2.34	0.42
1:A:120:PRO:HB2	1:A:124:ALA:HB2	2.01	0.42
1:A:178[A]:ASP:HB3	1:B:151:ARG:NH1	2.33	0.42
1:A:255:ILE:HD12	1:A:265:SER:HB2	2.01	0.42
1:B:176:ASN:HD22	2:B:407:EOH:C2	2.33	0.41
3:A:403:2DN:C	3:A:403:2DN:OAE	2.68	0.41
1:B:287:ILE:HA	1:B:287:ILE:HD13	1.84	0.41
1:B:110:TYR:CD1	4:B:402:EDO:H12	2.56	0.41
1:A:151:ARG:NH1	5:A:690:HOH:O	2.23	0.41
1:B:6:PHE:O	1:B:8:PRO:HD3	2.20	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)
5:A:637:HOH:O	5:A:685:HOH:O[2_645]	1.96	0.24

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%)	285 (99%)	3 (1%)	1 (0%)	46	26
1	B	279/300 (93%)	275 (99%)	4 (1%)	0	100	100
All	All	568/600 (95%)	560 (99%)	7 (1%)	1 (0%)	52	32

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	218/223 (98%)	213 (98%)	5 (2%)	58	37
1	B	214/223 (96%)	207 (97%)	7 (3%)	45	21
All	All	432/446 (97%)	420 (97%)	12 (3%)	54	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	78	ASP
1	A	255	ILE
1	A	260	MET
1	A	263	ASN

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Mol	Chain	Res	Type
1	B	28	ARG
1	B	30	THR
1	B	69[A]	ASN
1	B	69[B]	ASN
1	B	132	ARG
1	B	151	ARG
1	B	263	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	119	GLN
1	A	222	HIS
1	B	44	HIS
1	B	164	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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
2	EOH	A	401	-	2,2,2	0.61	0	1,1,1	0.21	0
2	EOH	A	402	-	2,2,2	0.58	0	1,1,1	0.37	0
3	2DN	A	403	-	23,32,32	2.90	7 (30%)	26,47,47	3.03	4 (15%)
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.65	0
4	EDO	A	405	-	3,3,3	0.57	0	2,2,2	1.06	0
4	EDO	A	406	-	3,3,3	0.34	0	2,2,2	1.07	0
2	EOH	A	407	-	2,2,2	0.38	0	1,1,1	0.15	0
4	EDO	A	408	-	3,3,3	0.44	0	2,2,2	0.89	0
3	2DN	B	401	-	23,32,32	3.54	8 (34%)	26,47,47	2.73	10 (38%)
4	EDO	B	402	-	3,3,3	0.18	0	2,2,2	1.16	0
4	EDO	B	403	-	3,3,3	0.53	0	2,2,2	0.60	0
4	EDO	B	404	-	3,3,3	0.37	0	2,2,2	0.93	0
4	EDO	B	405	-	3,3,3	0.75	0	2,2,2	0.64	0
3	2DN	B	406	-	23,32,32	3.58	12 (52%)	26,47,47	2.04	5 (19%)
2	EOH	B	407	-	2,2,2	0.42	0	1,1,1	0.25	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
2	EOH	A	401	-	-	0/0/0/0	0/0/0/0
2	EOH	A	402	-	-	0/0/0/0	0/0/0/0
3	2DN	A	403	-	-	0/12/25/25	0/2/3/3
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	EDO	A	405	-	-	0/1/1/1	0/0/0/0
4	EDO	A	406	-	-	0/1/1/1	0/0/0/0
2	EOH	A	407	-	-	0/0/0/0	0/0/0/0
4	EDO	A	408	-	-	0/1/1/1	0/0/0/0
3	2DN	B	401	-	-	0/12/25/25	0/2/3/3
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
3	2DN	B	406	-	-	0/12/25/25	0/2/3/3
2	EOH	B	407	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	2DN	CAZ-SBD	-9.66	1.65	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	2DN	CAL-CAY	-4.22	1.34	1.38
3	A	403	2DN	CAV-NAQ	-3.86	1.34	1.39
3	A	403	2DN	CAL-CAY	-3.60	1.35	1.38
3	B	406	2DN	CBA-CBB	-3.00	1.34	1.41
3	B	401	2DN	CAK-CBA	-2.67	1.35	1.42
3	A	403	2DN	CBA-CBB	-2.52	1.35	1.41
3	B	406	2DN	CAK-CBA	-2.35	1.36	1.42
3	B	406	2DN	CAJ-CBB	-2.28	1.36	1.41
3	B	406	2DN	CAY-CAV	-2.18	1.37	1.50
3	B	406	2DN	CAV-NAQ	-2.07	1.36	1.39
3	B	401	2DN	CAK-CAW	2.02	1.40	1.37
3	B	401	2DN	CAI-CAW	2.20	1.43	1.38
3	B	401	2DN	CA-N	2.45	1.53	1.49
3	B	401	2DN	SBD-NAQ	2.51	1.69	1.64
3	B	406	2DN	CAK-CAW	2.86	1.42	1.37
3	A	403	2DN	CAK-CAW	3.65	1.43	1.37
3	A	403	2DN	SBD-NAQ	4.08	1.72	1.64
3	B	406	2DN	SBD-NAQ	4.28	1.73	1.64
3	B	406	2DN	NAO-NAN	5.31	1.47	1.37
3	B	401	2DN	OAF-SBD	5.44	1.49	1.43
3	A	403	2DN	OAG-SBD	5.92	1.50	1.43
3	B	406	2DN	CAZ-SBD	7.35	1.88	1.78
3	B	406	2DN	OAF-SBD	7.57	1.51	1.43
3	B	406	2DN	OAG-SBD	8.59	1.53	1.43
3	A	403	2DN	OAF-SBD	8.69	1.53	1.43
3	B	401	2DN	OAG-SBD	10.69	1.55	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	2DN	OAG-SBD-OAF	-9.32	107.18	119.54
3	B	401	2DN	OAG-SBD-OAF	-8.58	108.16	119.54
3	B	401	2DN	CAV-NAQ-SBD	-3.47	119.38	123.34
3	B	401	2DN	CAJ-CAI-CAW	-2.60	116.70	120.19
3	B	406	2DN	OAG-SBD-OAF	-2.35	116.42	119.54
3	B	406	2DN	CAV-NAQ-SBD	-2.30	120.71	123.34
3	B	406	2DN	CAJ-CAI-CAW	-2.16	117.29	120.19
3	B	401	2DN	CAW-CAK-CBA	2.08	122.81	119.73
3	A	403	2DN	CAA-OAR-CAW	2.10	122.38	117.51
3	B	406	2DN	CAI-CAJ-CBB	2.25	123.21	119.42
3	A	403	2DN	OAC-CAT-NAP	2.45	126.07	123.08
3	B	401	2DN	OAG-SBD-NAQ	2.95	115.14	106.73

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	2DN	CAZ-SBD-NAQ	3.23	110.33	106.15
3	B	401	2DN	C-CA-N	3.24	118.47	114.11
3	B	401	2DN	OAC-CAT-NAP	3.33	127.16	123.08
3	B	401	2DN	CAL-CBA-CBB	3.59	109.40	106.27
3	B	401	2DN	CAA-OAR-CAW	5.30	129.79	117.51
3	B	406	2DN	CAZ-SBD-NAQ	7.98	116.46	106.15
3	A	403	2DN	C-CA-N	11.01	128.92	114.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EOH	3	0
2	A	402	EOH	1	0
3	A	403	2DN	1	0
4	A	406	EDO	3	0
3	B	401	2DN	9	0
4	B	402	EDO	2	0
4	B	404	EDO	1	0
2	B	407	EOH	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	286/300 (95%)	-0.05	9 (3%)	52	57	10, 19, 36, 48	4 (1%)
1	B	274/300 (91%)	0.21	20 (7%)	18	20	12, 20, 44, 63	1 (0%)
All	All	560/600 (93%)	0.07	29 (5%)	31	33	10, 20, 40, 63	5 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	8.5
1	B	1	MET	7.5
1	B	133	PRO	6.4
1	B	71	MET	6.2
1	B	261	PRO	5.8
1	A	76	GLY	5.2
1	B	86	PRO	4.8
1	A	75	ALA	4.7
1	A	74	GLY	4.5
1	B	131	PRO	4.5
1	B	132	ARG	4.4
1	A	4	PRO	4.4
1	B	2	ALA	4.3
1	B	87	ASP	4.1
1	A	289	THR	4.0
1	B	70	PRO	3.5
1	B	263	ASN	3.1
1	A	77	GLY	3.1
1	B	134	THR	3.0
1	B	69[A]	ASN	2.6
1	B	264	GLY	2.6
1	A	5	ALA	2.5
1	A	288	GLY	2.4
1	A	243	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLY	2.2
1	B	130	GLY	2.2
1	B	29	LEU	2.1
1	B	88	ASP	2.0
1	B	201	TYR	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EOH	A	402	3/3	0.90	0.23	11.71	33,33,34,36	0
2	EOH	A	401	3/3	0.81	0.18	11.35	27,27,35,36	0
3	2DN	B	406	30/30	0.84	0.27	2.84	25,45,59,61	30
4	EDO	A	406	4/4	0.93	0.20	2.15	35,38,39,39	0
4	EDO	B	402	4/4	0.94	0.14	2.10	25,27,32,33	0
4	EDO	B	404	4/4	0.90	0.22	1.91	42,44,44,45	0
4	EDO	A	408	4/4	0.91	0.15	1.78	34,34,39,40	0
4	EDO	A	404	4/4	0.97	0.10	1.60	21,23,24,27	0
3	2DN	A	403	30/30	0.92	0.12	1.04	18,27,53,55	0
2	EOH	A	407	3/3	0.98	0.11	1.02	27,27,28,29	0
4	EDO	A	405	4/4	0.94	0.13	0.81	28,33,36,42	0
4	EDO	B	405	4/4	0.92	0.09	0.12	27,30,32,32	0
4	EDO	B	403	4/4	0.86	0.11	-0.30	42,42,43,47	0
3	2DN	B	401	30/30	0.95	0.09	-0.34	15,23,46,49	0
2	EOH	B	407	3/3	0.95	0.10	-	39,39,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.