



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 11:44 AM EDT

PDB ID : 4DDH
Title : Pantothenate synthetase in complex with 6-methoxy-1-benzofuran-3-yl acetic acid
Authors : Silvestre, H.L.
Deposited on : 2012-01-18
Resolution : 2.07 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

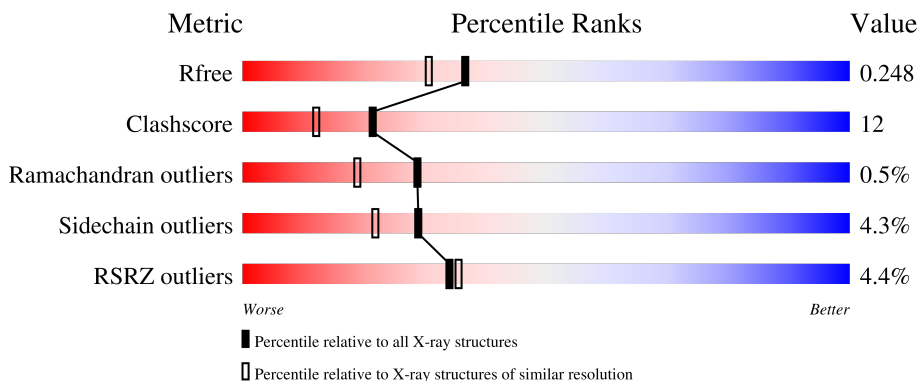
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	301	
1	B	301	

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	A	401	-	-	X	-
5	GOL	B	404	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4786 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.

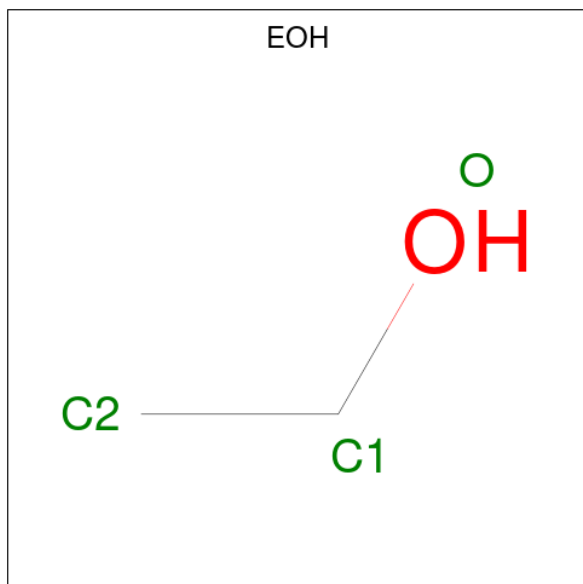
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2165	1369	390	400	6	0	7	0
1	B	279	2116	1340	383	387	6	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

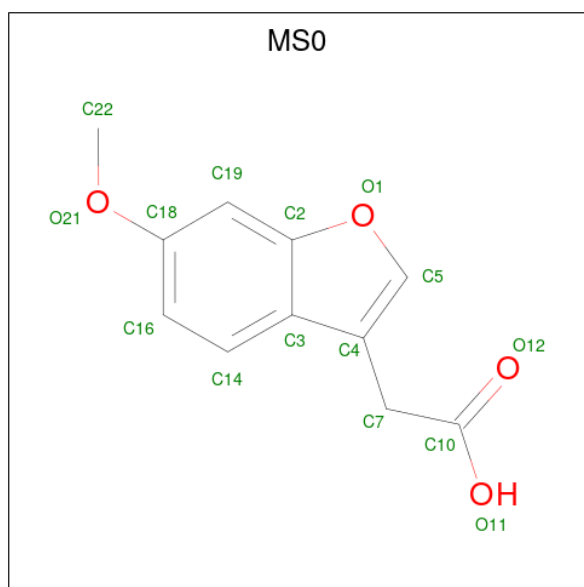
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is ETHANOL (three-letter code: EOH) (formula: 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 (6-methoxy-1-benzofuran-3-yl)acetic acid (three-letter code: MS0) (formula: $C_{11}H_{10}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		
3	B	1	Total	C	O	0	0
			15	11	4		

- 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 C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

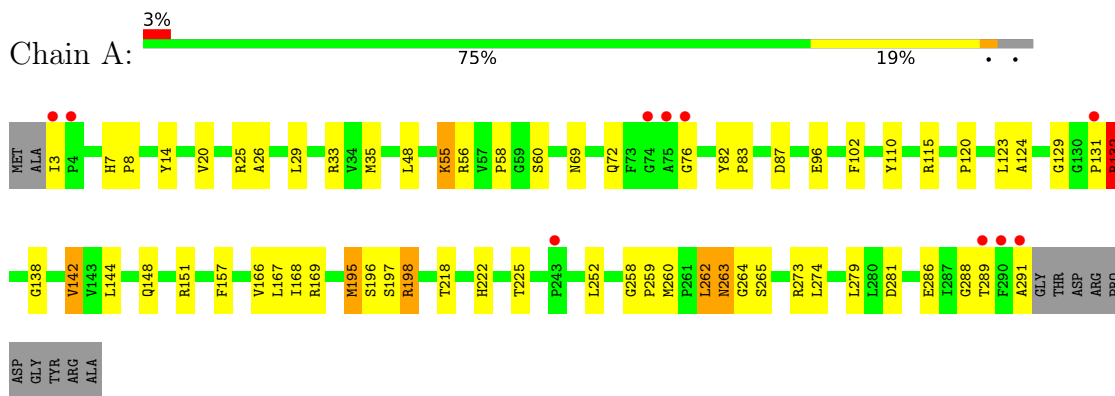
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	228	Total O 228 228	0	0
6	B	202	Total O 202 202	0	0

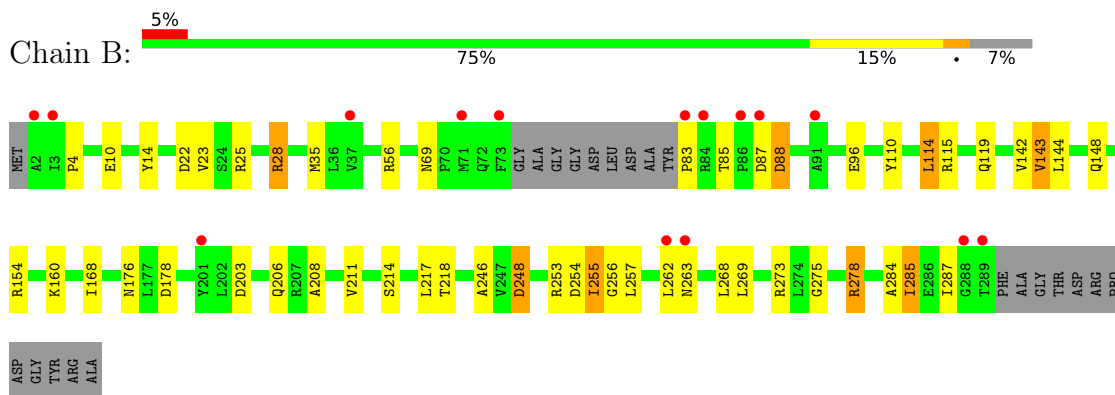
3 Residue-property plots [i](#)

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	48.58Å 70.93Å 82.01Å 90.00° 99.40° 90.00°	Depositor
Resolution (Å)	53.38 – 2.07 28.69 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (53.38-2.07) 99.3 (28.69-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.06Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.250 0.186 , 0.248	Depositor DCC
R_{free} test set	1693 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, EOH, MS0, GOL

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	1.11	0/2207	0.99	4/3014 (0.1%)
1	B	1.06	2/2157 (0.1%)	0.97	3/2946 (0.1%)
All	All	1.08	2/4364 (0.0%)	0.98	7/5960 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	ASP	CB-CG	5.39	1.63	1.51
1	B	143	VAL	CB-CG2	5.02	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	B	115	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	281	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	132	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	B	248	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	56	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	169	ARG	NE-CZ-NH2	-5.23	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2165	0	2207	56	0
1	B	2116	0	2177	48	0
2	A	6	0	12	3	0
2	B	3	0	6	0	0
3	A	15	0	9	0	0
3	B	15	0	9	1	0
4	A	12	0	18	5	0
4	B	12	0	18	3	0
5	B	12	0	16	5	0
6	A	228	0	0	13	0
6	B	202	0	0	9	0
All	All	4786	0	4472	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (106) 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:273[A]:ARG:HD2	1:B:275:GLY:O	1.54	1.07
1:B:4:PRO:HB3	4:B:407:EDO:H12	1.41	1.03
1:A:195:MET:HE2	6:A:725:HOH:O	1.67	0.94
1:A:263:ASN:CG	1:A:264:GLY:H	1.70	0.93
1:A:197[A]:SER:OG	1:A:198[A]:ARG:HD3	1.68	0.92
1:A:69:ASN:ND2	1:A:142:VAL:HG21	1.86	0.90
1:A:69:ASN:HD22	1:A:72:GLN:HE21	1.22	0.87
1:B:246:ALA:HB2	5:B:404:GOL:O1	1.78	0.84
1:B:273[A]:ARG:CD	1:B:275:GLY:O	2.27	0.83
1:B:218[B]:THR:HG21	6:B:506:HOH:O	1.76	0.82
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.44	0.82
1:A:69:ASN:ND2	1:A:142:VAL:CG2	2.42	0.81
1:A:69:ASN:CG	1:A:142:VAL:HG21	2.01	0.81
1:A:14:TYR:HB2	1:A:20[B]:VAL:HG23	1.66	0.78
1:B:83:PRO:HG2	6:B:676:HOH:O	1.84	0.77
1:A:263:ASN:CG	1:A:264:GLY:N	2.38	0.75
1:B:22:ASP:OD1	1:B:25[A]:ARG:NH1	2.16	0.73
1:A:286:GLU:OE1	6:A:650:HOH:O	2.07	0.72
1:A:115:ARG:O	2:A:401:EOH:H22	1.90	0.71
1:A:263:ASN:ND2	1:A:265:SER:H	1.87	0.71
1:A:274:LEU:HD13	1:A:279:LEU:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197[A]:SER:OG	1:A:198[A]:ARG:CD	2.39	0.71
1:A:258:GLY:HA3	6:A:726:HOH:O	1.90	0.70
1:A:110:TYR:HD1	4:A:404:EDO:H21	1.58	0.69
1:A:263:ASN:ND2	6:A:618:HOH:O	2.19	0.69
1:A:25:ARG:NH1	6:A:517:HOH:O	2.28	0.67
1:B:246:ALA:CB	5:B:404:GOL:O1	2.44	0.66
1:A:198[B]:ARG:HD2	6:A:640:HOH:O	1.95	0.66
2:A:401:EOH:H21	1:B:119:GLN:HG2	1.78	0.66
1:B:28:ARG:HH11	1:B:28:ARG:CG	2.09	0.66
1:A:198[A]:ARG:HG2	1:A:198[A]:ARG:HH21	1.62	0.65
1:B:214:SER:O	1:B:218[B]:THR:HG22	1.96	0.65
1:A:258:GLY:CA	6:A:726:HOH:O	2.45	0.64
1:B:248:ASP:HB3	6:B:531:HOH:O	1.97	0.63
1:A:33:ARG:NH2	1:A:58:PRO:O	2.32	0.62
1:A:3:ILE:HG21	1:A:26:ALA:HB2	1.83	0.60
1:B:10:GLU:HB2	6:B:631:HOH:O	2.03	0.59
1:B:85:THR:HB	1:B:88:ASP:CG	2.22	0.59
1:B:143:VAL:HG11	1:B:168[A]:ILE:HD12	1.84	0.58
1:B:96:GLU:HB3	6:B:530:HOH:O	2.03	0.58
1:A:196:SER:OG	1:A:198[B]:ARG:HB2	2.04	0.57
1:A:291:ALA:HB1	6:A:655:HOH:O	2.04	0.56
1:A:33:ARG:HH22	1:A:58:PRO:HG2	1.70	0.56
1:A:218:THR:O	1:A:222:HIS:HD2	1.89	0.55
1:B:269:LEU:N	1:B:269:LEU:HD12	2.21	0.55
1:A:262:LEU:HB2	4:A:406:EDO:H22	1.90	0.54
1:B:88:ASP:OD2	1:B:88:ASP:N	2.30	0.52
1:B:35:MET:SD	1:B:154:ARG:HB2	2.50	0.52
1:A:72:GLN:HE22	4:A:405:EDO:C2	2.23	0.52
2:A:402:EOH:C2	6:A:719:HOH:O	2.59	0.52
1:A:198[A]:ARG:HG2	1:A:198[A]:ARG:NH2	2.23	0.51
1:B:85:THR:HB	1:B:88:ASP:OD1	2.10	0.51
1:A:110:TYR:CD1	4:A:404:EDO:H21	2.41	0.51
1:A:20[B]:VAL:HG21	1:A:102:PHE:HB2	1.94	0.50
1:B:176:ASN:HD22	4:B:406:EDO:H22	1.77	0.49
1:A:138:GLY:O	1:A:142:VAL:HG23	2.13	0.49
1:B:203:ASP:OD1	1:B:203:ASP:C	2.51	0.49
1:B:206:GLN:HG2	6:B:701:HOH:O	2.13	0.48
1:A:151:ARG:HD2	1:B:178[B]:ASP:OD2	2.13	0.48
1:A:273:ARG:HD2	6:A:680:HOH:O	2.13	0.48
1:A:131:PRO:HG2	1:A:132:ARG:NH2	2.29	0.47
1:A:124:ALA:O	1:A:129:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:MET:HG2	1:A:60:SER:HB2	1.96	0.46
1:B:69:ASN:CG	1:B:142[B]:VAL:HG21	2.35	0.46
1:A:252:LEU:HG	1:A:262:LEU:HD23	1.97	0.46
1:B:28:ARG:CG	1:B:28:ARG:NH1	2.78	0.46
1:A:72:GLN:HE22	4:A:405:EDO:H21	1.79	0.46
1:A:157:PHE:CZ	1:A:168:ILE:HD13	2.52	0.45
1:B:4:PRO:CB	4:B:407:EDO:H12	2.28	0.45
1:B:114:LEU:HD22	1:B:114:LEU:HA	1.77	0.45
1:B:217:LEU:HD23	1:B:268:LEU:HD23	1.99	0.45
1:A:120:PRO:HB2	1:A:124:ALA:CB	2.46	0.45
1:A:263:ASN:ND2	1:A:264:GLY:N	2.64	0.45
1:B:160:LYS:HE3	6:B:615:HOH:O	2.16	0.45
1:A:262:LEU:HD12	1:A:263:ASN:N	2.33	0.44
1:B:246:ALA:HB3	1:B:273[B]:ARG:HG2	1.99	0.44
1:B:56:ARG:NH1	6:B:669:HOH:O	2.51	0.44
1:B:256:GLY:O	1:B:257:LEU:HB2	2.18	0.44
1:A:87:ASP:HB3	6:A:653:HOH:O	2.17	0.44
1:B:28:ARG:HG3	1:B:28:ARG:NH1	2.23	0.44
1:B:110:TYR:OH	1:B:142[B]:VAL:CG2	2.67	0.43
1:B:273[B]:ARG:O	5:B:404:GOL:H31	2.18	0.43
1:A:225:THR:HA	1:A:288:GLY:HA3	2.01	0.42
1:B:14:TYR:CZ	1:B:23:VAL:HG21	2.54	0.42
1:A:144:LEU:O	1:A:148:GLN:HG2	2.19	0.42
1:A:166:VAL:HG13	6:A:687:HOH:O	2.18	0.42
1:B:284:ALA:O	1:B:285:ILE:HG12	2.20	0.42
1:B:246:ALA:CB	5:B:404:GOL:HO1	2.33	0.42
1:B:253:ARG:HB3	1:B:257:LEU:HA	2.02	0.41
1:A:274:LEU:CD1	1:A:279:LEU:HD12	2.47	0.41
1:B:208:ALA:O	1:B:211[A]:VAL:HG12	2.20	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.95	0.41
1:A:55:LYS:HD2	6:A:654:HOH:O	2.20	0.41
1:A:263:ASN:HD21	1:A:265:SER:H	1.64	0.41
1:A:123:LEU:HD23	1:A:167:LEU:HG	2.03	0.41
1:A:48:LEU:HD22	1:A:96:GLU:HG3	2.03	0.41
1:B:144:LEU:O	1:B:148:GLN:HG2	2.20	0.41
1:A:33:ARG:O	1:A:60:SER:HA	2.20	0.41
1:B:255:ILE:HD12	1:B:255:ILE:HA	1.77	0.41
3:B:401:MS0:H22A	3:B:401:MS0:H19	1.80	0.41
5:B:405:GOL:H2	6:B:516:HOH:O	2.20	0.41
1:B:248:ASP:OD1	1:B:273[B]:ARG:NH2	2.54	0.41
1:A:7:HIS:HA	1:A:8:PRO:HD2	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CG	1:A:83:PRO:HD2	2.57	0.40
1:B:110:TYR:OH	1:B:142[B]:VAL:HG22	2.22	0.40
1:B:287:ILE:HA	1:B:287:ILE:HD13	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/301 (97%)	277 (95%)	12 (4%)	3 (1%)	15	6
1	B	284/301 (94%)	273 (96%)	11 (4%)	0	100	100
All	All	576/602 (96%)	550 (96%)	23 (4%)	3 (0%)	29	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLY
1	A	289	THR
1	A	259	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/223 (99%)	210 (96%)	10 (4%)	27	20
1	B	216/223 (97%)	207 (96%)	9 (4%)	30	23
All	All	436/446 (98%)	417 (96%)	19 (4%)	29	21

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	55	LYS
1	A	132	ARG
1	A	142	VAL
1	A	195	MET
1	A	198[A]	ARG
1	A	198[B]	ARG
1	A	260	MET
1	A	262	LEU
1	A	263	ASN
1	B	28	ARG
1	B	87	ASP
1	B	88	ASP
1	B	114	LEU
1	B	254	ASP
1	B	255	ILE
1	B	263	ASN
1	B	278	ARG
1	B	285	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	222	HIS
1	A	263	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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
3	MSO	A	403	-	12,16,16	1.97	4 (33%)	15,22,22	1.14	0
4	EDO	A	405	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	A	406	-	3,3,3	0.57	0	2,2,2	0.04	0
4	EDO	B	402	-	3,3,3	0.35	0	2,2,2	1.04	0
4	EDO	B	406	-	3,3,3	0.47	0	2,2,2	0.40	0
5	GOL	B	405	-	5,5,5	0.32	0	5,5,5	0.67	0
4	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.56	0
4	EDO	A	404	-	3,3,3	0.26	0	2,2,2	0.76	0
5	GOL	B	404	-	5,5,5	0.55	0	5,5,5	0.84	0
3	MSO	B	401	-	12,16,16	2.00	4 (33%)	15,22,22	2.11	6 (40%)
2	EOH	A	402	-	2,2,2	0.63	0	1,1,1	0.21	0
2	EOH	B	403	-	2,2,2	0.52	0	1,1,1	0.22	0
2	EOH	A	401	-	2,2,2	0.47	0	1,1,1	0.06	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
3	MSO	A	403	-	-	2/6/6/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
5	GOL	B	405	-	-	4/4/4/4	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
5	GOL	B	404	-	-	0/4/4/4	-
3	MS0	B	401	-	-	1/6/6/6	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	MS0	C3-C2	-3.50	1.35	1.43
3	B	401	MS0	C3-C2	-3.22	1.36	1.43
3	B	401	MS0	C14-C3	-3.18	1.35	1.42
3	A	403	MS0	C14-C3	-3.12	1.35	1.42
3	A	403	MS0	C19-C18	2.95	1.42	1.37
3	B	401	MS0	C19-C18	2.87	1.42	1.37
3	B	401	MS0	C14-C16	2.59	1.42	1.36
3	A	403	MS0	C7-C10	-2.12	1.46	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	MS0	C22-O21-C18	-4.90	106.87	117.51
3	B	401	MS0	C7-C4-C3	2.86	132.10	126.50
3	B	401	MS0	C14-C16-C18	-2.73	116.50	120.17
3	B	401	MS0	C14-C3-C2	-2.45	118.83	120.38
3	B	401	MS0	C18-C19-C2	2.39	121.83	119.13
3	B	401	MS0	C16-C18-C19	-2.02	118.09	120.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	405	GOL	O1-C1-C2-C3
5	B	405	GOL	C1-C2-C3-O3
4	A	404	EDO	O1-C1-C2-O2
5	B	405	GOL	O2-C2-C3-O3
5	B	405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	401	MSO	C3-C4-C7-C10
4	A	406	EDO	O1-C1-C2-O2
3	A	403	MSO	O12-C10-C7-C4
3	A	403	MSO	O11-C10-C7-C4

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	2	0
4	A	406	EDO	1	0
4	B	406	EDO	1	0
5	B	405	GOL	1	0
4	B	407	EDO	2	0
4	A	404	EDO	2	0
5	B	404	GOL	4	0
3	B	401	MSO	1	0
2	A	402	EOH	1	0
2	A	401	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

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	289/301 (96%)	-0.10	10 (3%) 44 46	12, 22, 42, 57	3 (1%)
1	B	279/301 (92%)	0.09	15 (5%) 25 26	13, 24, 47, 68	0
All	All	568/602 (94%)	-0.01	25 (4%) 34 35	12, 23, 43, 68	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	GLY	5.5
1	B	289	THR	4.6
1	B	86	PRO	4.3
1	B	73	PHE	4.1
1	B	2	ALA	4.0
1	B	83	PRO	4.0
1	A	3	ILE	3.9
1	A	291	ALA	3.7
1	B	84	ARG	3.6
1	B	262	LEU	3.6
1	B	3	ILE	3.4
1	B	263	ASN	3.3
1	A	290	PHE	3.2
1	A	289	THR	3.1
1	B	87	ASP	3.0
1	B	71	MET	2.9
1	B	201	TYR	2.8
1	A	4	PRO	2.6
1	A	74	GLY	2.5
1	A	243	PRO	2.4
1	A	131	PRO	2.1
1	B	37	VAL	2.1
1	B	288	GLY	2.1
1	B	91	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	2.1

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 monosaccharides 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
5	GOL	B	404	6/6	0.76	0.27	44,46,48,51	0
2	EOH	B	403	3/3	0.77	0.17	43,43,44,45	0
2	EOH	A	401	3/3	0.81	0.19	41,41,44,44	0
2	EOH	A	402	3/3	0.84	0.27	24,24,27,28	0
4	EDO	B	407	4/4	0.85	0.27	59,60,60,60	0
3	MS0	B	401	15/15	0.85	0.20	29,39,45,46	0
5	GOL	B	405	6/6	0.86	0.27	54,58,59,61	0
3	MS0	A	403	15/15	0.91	0.12	15,28,31,31	0
4	EDO	A	406	4/4	0.91	0.12	36,36,38,39	0
4	EDO	B	406	4/4	0.91	0.16	37,39,40,44	0
4	EDO	A	404	4/4	0.96	0.14	18,18,20,27	0
4	EDO	B	402	4/4	0.96	0.09	21,23,25,26	0
4	EDO	A	405	4/4	0.96	0.18	40,40,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.