Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2018 – 02:48 PM EST

PDB ID : 5Z4V

Title : Crystal structure of the sheep signalling glycoprotein (SPS-40) complex with 2-methyl-2-4-pentanediol at 1.65A resolution reveals specific binding characteristics of SPS-40

Authors : Sharma, P.; Singh, P.K.; Singh, N.; Sharma, S.; Kaur, P.; Betzel, C.; Singh, T.P.

Deposited on : 2018-01-15

Resolution : 1.65 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.
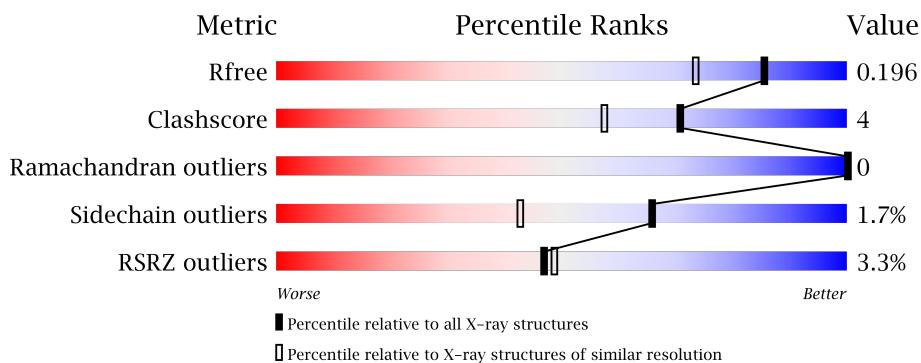
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
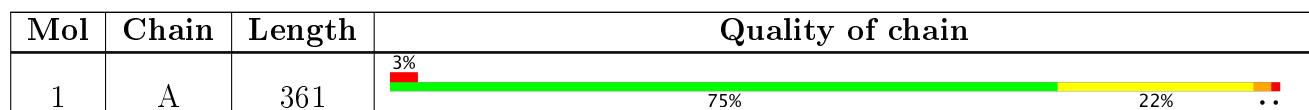
The reported resolution of this entry is 1.65 Å.

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		0.196
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.7%
RSRZ outliers		3.3%

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}	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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	361	3% 75% 22% ..

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	NAG	A	401	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3544 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.
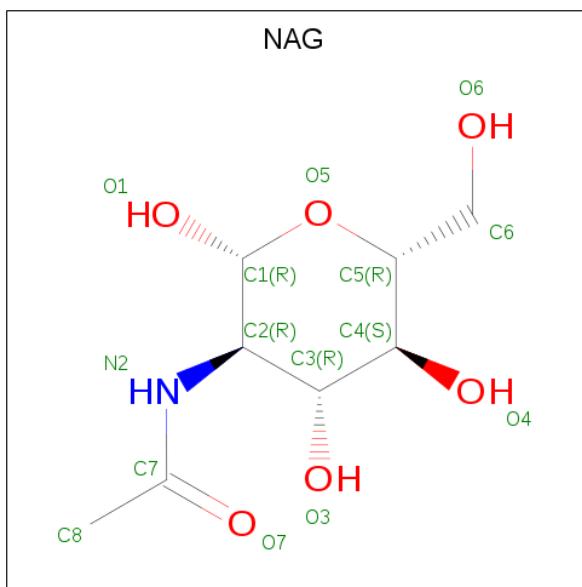
- Molecule 1 is a protein called Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	6	0
			2907	1853	511	534	9			

There are 5 discrepancies between the modelled and reference sequences:
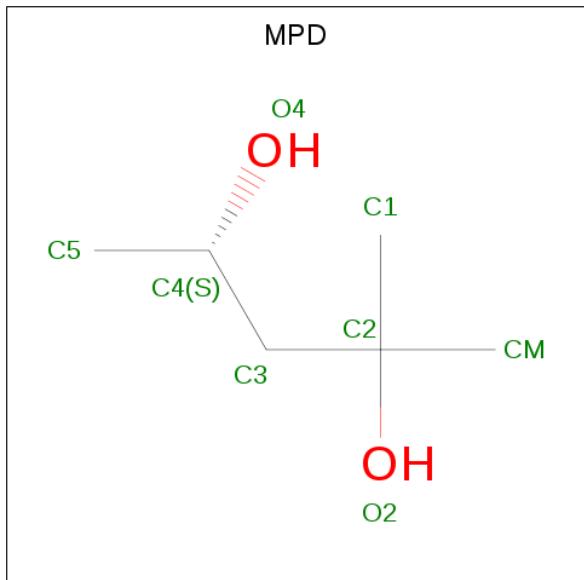
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	THR	SER	conflict	UNP Q6TMG6
A	87	LYS	ALA	conflict	UNP Q6TMG6
A	203	ARG	ALA	conflict	UNP Q6TMG6
A	262	ILE	VAL	conflict	UNP Q6TMG6
A	362	ALA	VAL	conflict	UNP Q6TMG6

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0
3	A	1	Total 16	C 12	O 4	0	1
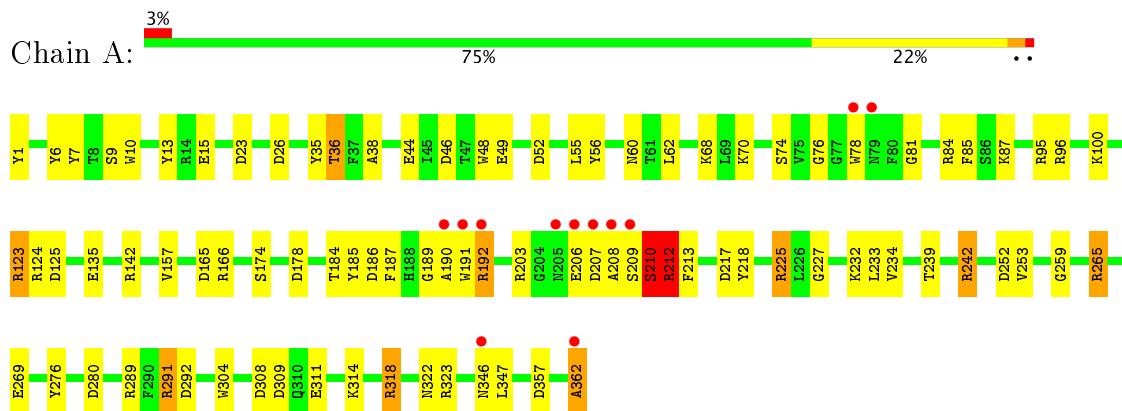
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	599	Total 599	O 599	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 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: Chitinase-3-like protein 1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.87Å 66.42Å 105.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.71 – 1.65 27.71 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.71-1.65) 99.9 (27.71-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	3.55 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.138 , 0.188 0.151 , 0.196	Depositor DCC
R_{free} test set	1075 reflections (2.11%)	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: MPD, NAG

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	1.75	47/2999 (1.6%)	1.90	74/4066 (1.8%)

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	4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLY	N-CA	10.62	1.61	1.46
1	A	49	GLU	CD-OE2	-9.98	1.14	1.25
1	A	60[A]	ASN	CG-ND2	8.54	1.54	1.32
1	A	60[B]	ASN	CG-ND2	8.54	1.54	1.32
1	A	210	SER	C-N	7.94	1.52	1.34
1	A	234	VAL	CB-CG1	-7.79	1.36	1.52
1	A	174	SER	CA-CB	7.73	1.64	1.52
1	A	259	GLY	N-CA	-7.61	1.34	1.46
1	A	9	SER	CB-OG	-7.44	1.32	1.42
1	A	208	ALA	C-O	6.99	1.36	1.23
1	A	174	SER	CB-OG	-6.94	1.33	1.42
1	A	210	SER	CB-OG	6.83	1.51	1.42
1	A	10	TRP	CB-CG	-6.76	1.38	1.50
1	A	166	ARG	CZ-NH1	6.70	1.41	1.33
1	A	362	ALA	N-CA	6.69	1.59	1.46
1	A	227	GLY	CA-C	-6.55	1.41	1.51
1	A	311	GLU	CD-OE1	6.54	1.32	1.25
1	A	36	THR	CB-CG2	-6.54	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ARG	CD-NE	-6.50	1.35	1.46
1	A	49	GLU	CD-OE1	-6.18	1.18	1.25
1	A	225	ARG	CZ-NH1	6.12	1.41	1.33
1	A	218	TYR	CG-CD1	-6.06	1.31	1.39
1	A	48	TRP	CE3-CZ3	6.06	1.48	1.38
1	A	56	TYR	CE1-CZ	-5.97	1.30	1.38
1	A	311	GLU	CG-CD	5.92	1.60	1.51
1	A	36	THR	CB-OG1	-5.90	1.31	1.43
1	A	76	GLY	N-CA	-5.88	1.37	1.46
1	A	85	PHE	CG-CD2	-5.87	1.29	1.38
1	A	85	PHE	CD2-CE2	-5.87	1.27	1.39
1	A	304	TRP	CE3-CZ3	5.80	1.48	1.38
1	A	242[A]	ARG	CD-NE	-5.75	1.36	1.46
1	A	242[B]	ARG	CD-NE	-5.75	1.36	1.46
1	A	191	TRP	CE3-CZ3	5.74	1.48	1.38
1	A	311	GLU	CD-OE2	5.68	1.31	1.25
1	A	84	ARG	CZ-NH1	5.60	1.40	1.33
1	A	322	ASN	CG-OD1	-5.59	1.11	1.24
1	A	323	ARG	CG-CD	-5.43	1.38	1.51
1	A	81	GLY	C-N	5.40	1.44	1.34
1	A	15	GLU	CD-OE1	5.27	1.31	1.25
1	A	38	ALA	C-O	5.25	1.33	1.23
1	A	13	TYR	CE1-CZ	-5.20	1.31	1.38
1	A	15	GLU	CG-CD	5.19	1.59	1.51
1	A	135	GLU	CD-OE2	5.19	1.31	1.25
1	A	276	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	48	TRP	CE2-CZ2	5.03	1.48	1.39
1	A	1	TYR	CB-CG	5.00	1.59	1.51
1	A	7	TYR	CE1-CZ	-5.00	1.32	1.38

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	32.59	136.60	120.30
1	A	225	ARG	NE-CZ-NH2	-25.50	107.55	120.30
1	A	212	ARG	NE-CZ-NH2	-21.64	109.48	120.30
1	A	166	ARG	NE-CZ-NH1	-18.03	111.28	120.30
1	A	210	SER	O-C-N	-15.34	98.16	122.70
1	A	265	ARG	NE-CZ-NH2	15.33	127.97	120.30
1	A	178	ASP	CB-CG-OD2	14.34	131.21	118.30
1	A	212	ARG	NE-CZ-NH1	13.01	126.81	120.30
1	A	265	ARG	NE-CZ-NH1	-12.02	114.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ARG	CD-NE-CZ	11.52	139.73	123.60
1	A	323	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	A	242[A]	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	242[B]	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	26	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	166	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	A	318	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	A	26	ASP	CB-CG-OD2	-9.55	109.71	118.30
1	A	85	PHE	CB-CG-CD2	-9.49	114.16	120.80
1	A	55	LEU	CB-CG-CD1	9.47	127.10	111.00
1	A	291	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	357	ASP	CB-CG-OD2	-9.23	110.00	118.30
1	A	56	TYR	CB-CG-CD1	9.15	126.49	121.00
1	A	242[A]	ARG	NE-CZ-NH1	-9.01	115.79	120.30
1	A	242[B]	ARG	NE-CZ-NH1	-9.01	115.79	120.30
1	A	124	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	A	242[A]	ARG	NH1-CZ-NH2	8.95	129.25	119.40
1	A	242[B]	ARG	NH1-CZ-NH2	8.95	129.25	119.40
1	A	323	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	252	ASP	CB-CG-OD1	8.78	126.20	118.30
1	A	84	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	185	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	96	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	52	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	85	PHE	CB-CG-CD1	8.04	126.43	120.80
1	A	289	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	46	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	174	SER	CA-CB-OG	-7.62	90.62	111.20
1	A	84	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	232	LYS	CD-CE-NZ	6.77	127.28	111.70
1	A	124	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	56	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	36	THR	OG1-CB-CG2	-6.51	95.03	110.00
1	A	347	LEU	CB-CG-CD1	-6.46	100.01	111.00
1	A	212	ARG	CG-CD-NE	-6.46	98.24	111.80
1	A	62	LEU	CB-CG-CD1	-6.31	100.27	111.00
1	A	46	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	A	233	LEU	CB-CG-CD1	6.16	121.48	111.00
1	A	207	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	44	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	A	157	VAL	CA-CB-CG1	6.04	119.95	110.90
1	A	217	ASP	CB-CG-OD1	5.99	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ALA	CB-CA-C	5.97	119.06	110.10
1	A	125	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	A	323	ARG	CA-CB-CG	-5.97	100.27	113.40
1	A	289	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	35	TYR	CG-CD1-CE1	-5.87	116.60	121.30
1	A	142	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	280	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	178	ASP	OD1-CG-OD2	-5.75	112.37	123.30
1	A	210	SER	C-N-CA	5.59	135.69	121.70
1	A	123	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	192	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	309	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	314	LYS	CD-CE-NZ	5.45	124.24	111.70
1	A	165	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	60[A]	ASN	CB-CA-C	5.31	121.02	110.40
1	A	60[B]	ASN	CB-CA-C	5.31	121.02	110.40
1	A	233	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	207	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	252	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	208	ALA	N-CA-CB	5.27	117.47	110.10
1	A	187	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	A	308	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	23	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	SER	Mainchain,Peptide
1	A	212	ARG	Sidechain
1	A	239	THR	Mainchain

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	2907	0	2839	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	12	0	0
3	A	24	0	42	2	0
4	A	599	0	0	14	1
All	All	3544	0	2893	24	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 4.

All (24) 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:A:291:ARG:NH1	1:A:292[A]:ASP:OD1	2.17	0.78
1:A:242[B]:ARG:NH1	4:A:503:HOH:O	2.17	0.78
1:A:206:GLU:HB2	4:A:878:HOH:O	1.84	0.75
1:A:346:ASN:ND2	4:A:506:HOH:O	2.24	0.70
1:A:78:TRP:HA	4:A:516:HOH:O	1.93	0.69
1:A:70:LYS:HE2	4:A:783:HOH:O	1.94	0.68
1:A:269:GLU:OE2	4:A:501:HOH:O	2.13	0.66
1:A:186:ASP:HA	1:A:242[B]:ARG:HH12	1.63	0.63
1:A:78:TRP:HZ3	3:A:403[B]:MPD:C1	2.13	0.62
1:A:36:THR:HG22	1:A:74:SER:HB3	1.83	0.60
1:A:189:GLY:O	1:A:192:ARG:HG3	2.02	0.59
1:A:190:ALA:HA	4:A:512:HOH:O	2.02	0.59
1:A:100:LYS:HE2	4:A:835:HOH:O	2.02	0.59
1:A:210:SER:HB3	1:A:213:PHE:H	1.69	0.57
1:A:210:SER:CB	1:A:213:PHE:H	2.22	0.51
1:A:362:ALA:HA	4:A:868:HOH:O	2.11	0.51
1:A:318:ARG:NH1	4:A:505:HOH:O	2.24	0.47
1:A:203:ARG:HD3	4:A:754:HOH:O	2.15	0.47
1:A:123:ARG:NH2	4:A:509:HOH:O	2.32	0.45
1:A:78:TRP:CZ3	3:A:403[B]:MPD:C1	2.96	0.45
1:A:253:VAL:HG12	4:A:960:HOH:O	2.20	0.42
1:A:6:TYR:HD2	1:A:36:THR:HG23	1.85	0.42
1:A:87:LYS:HD3	4:A:1032:HOH:O	2.21	0.41
1:A:68:LYS:HE3	1:A:68:LYS:HB3	1.96	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)
4:A:857:HOH:O	4:A:880:HOH:O[4_545]	1.89	0.31

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	365/361 (101%)	354 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	308/303 (102%)	303 (98%)	5 (2%)	68	45

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	THR
1	A	209	SER
1	A	212	ARG
1	A	225	ARG
1	A	265	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	NAG	A	401	1	14,14,15	1.83	4 (28%)	15,19,21	3.13	9 (60%)
3	MPD	A	402	-	7,7,7	1.40	2 (28%)	9,10,10	1.51	1 (11%)
3	MPD	A	403[A]	-	7,7,7	0.40	0	9,10,10	0.89	0
3	MPD	A	403[B]	-	7,7,7	0.80	0	9,10,10	0.95	1 (11%)

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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	MPD	A	402	-	-	0/5/5/5	0/0/0/0
3	MPD	A	403[A]	-	-	0/5/5/5	0/0/0/0
3	MPD	A	403[B]	-	-	0/5/5/5	0/0/0/0

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All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAG	C1-C2	-2.73	1.48	1.52
2	A	401	NAG	O5-C1	-2.43	1.39	1.43
3	A	402	MPD	C3-C2	-2.18	1.47	1.53
2	A	401	NAG	O5-C5	2.18	1.48	1.43
3	A	402	MPD	C1-C2	2.42	1.60	1.52
2	A	401	NAG	O3-C3	2.91	1.49	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	O6-C6-C5	-5.00	94.52	111.34
2	A	401	NAG	C1-O5-C5	-4.30	106.25	112.17
3	A	402	MPD	CM-C2-C1	-3.56	102.48	110.42
2	A	401	NAG	O7-C7-N2	-2.99	116.16	121.92
2	A	401	NAG	C4-C3-C2	-2.95	106.69	111.02
2	A	401	NAG	C1-C2-N2	-2.58	106.08	110.49
3	A	403[B]	MPD	CM-C2-C3	2.03	120.19	110.08
2	A	401	NAG	C3-C4-C5	2.47	114.57	110.22
2	A	401	NAG	O5-C1-C2	3.16	115.87	111.47
2	A	401	NAG	O7-C7-C8	3.83	129.03	122.06
2	A	401	NAG	C6-C5-C4	6.65	128.57	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403[B]	MPD	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	361/361 (100%)	-0.19	12 (3%)	47	49	13, 20, 38, 90	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	SER	10.7
1	A	208	ALA	7.8
1	A	191	TRP	5.6
1	A	206	GLU	5.4
1	A	207	ASP	4.9
1	A	205	ASN	4.6
1	A	190	ALA	3.5
1	A	78	TRP	3.4
1	A	362	ALA	3.3
1	A	79	ASN	3.1
1	A	346	ASN	2.7
1	A	192	ARG	2.3

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

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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	NAG	A	401	14/15	0.91	0.16	2.66	23,32,38,40	0
3	MPD	A	403[B]	8/8	0.90	0.16	1.44	23,25,28,29	8
3	MPD	A	403[A]	8/8	0.90	0.16	1.43	27,28,31,35	8
3	MPD	A	402	8/8	0.95	0.08	-0.50	19,21,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.