



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 PM UTC

PDB ID : 5Z4V / pdb_00005z4v
Title : Crystal structure of the sheep signalling glycoprotein (SPS-40) complex with 2-methyl-2,4-pentanediol at 1.65Å 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

<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
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

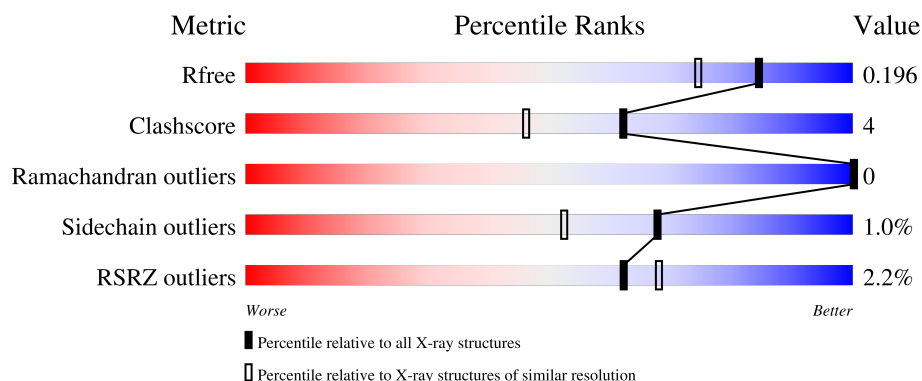
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

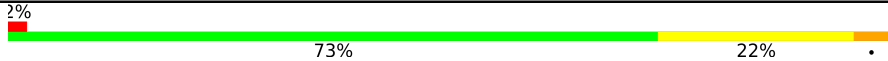
The reported resolution of this entry is 1.65 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	361	

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.

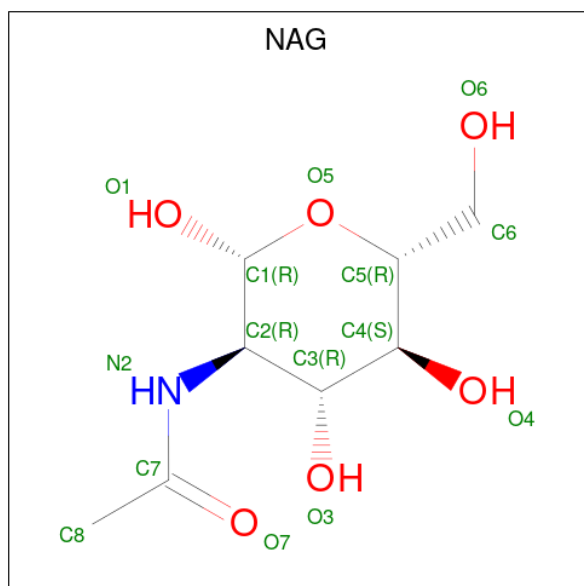
- Molecule 1 is a protein called Chitinase-3-like protein 1.

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

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	1
			16	12	4		

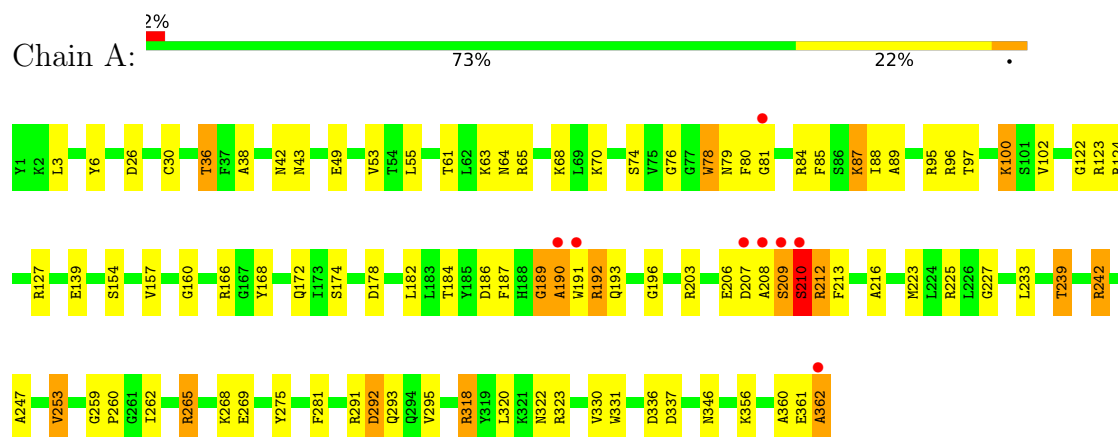
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	599	Total	O	0	0
			599	599		

3 Residue-property plots

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: Chitinase-3-like protein 1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (2.06%)	wwPDB-VP
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 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: NAG, MPD

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	2.09	81/2999 (2.7%)	1.76	54/4066 (1.3%)

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 (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	SER	C-N	13.84	1.52	1.33
1	A	81	GLY	N-CA	12.61	1.61	1.44
1	A	208	ALA	C-O	10.62	1.36	1.23
1	A	223	MET	SD-CE	-9.97	1.54	1.79
1	A	208	ALA	CA-C	9.40	1.65	1.52
1	A	190	ALA	N-CA	7.82	1.56	1.46
1	A	95	ARG	CD-NE	-7.75	1.35	1.46
1	A	207	ASP	CA-C	7.72	1.63	1.53
1	A	36	THR	CB-OG1	-7.69	1.31	1.43
1	A	85	PHE	CA-C	-7.36	1.43	1.52
1	A	259	GLY	N-CA	-7.35	1.34	1.44
1	A	260	PRO	CA-C	7.26	1.61	1.52
1	A	227	GLY	CA-C	-7.17	1.41	1.51
1	A	38	ALA	C-O	7.11	1.33	1.23
1	A	362	ALA	N-CA	7.09	1.59	1.46
1	A	166	ARG	N-CA	6.99	1.55	1.46
1	A	174	SER	CA-CB	6.84	1.64	1.53
1	A	260	PRO	N-CA	-6.79	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ARG	C-N	-6.70	1.24	1.33
1	A	36	THR	CB-CG2	-6.60	1.30	1.52
1	A	80	PHE	C-O	-6.54	1.16	1.24
1	A	361	GLU	CA-C	6.50	1.61	1.52
1	A	207	ASP	C-O	6.46	1.32	1.23
1	A	166	ARG	CZ-NH1	6.43	1.41	1.32
1	A	61	THR	CA-C	6.39	1.61	1.52
1	A	53	VAL	N-CA	6.33	1.54	1.46
1	A	322	ASN	CG-OD1	-6.26	1.11	1.23
1	A	64	ASN	C-O	6.19	1.31	1.24
1	A	209	SER	N-CA	6.07	1.54	1.46
1	A	225	ARG	N-CA	-6.06	1.38	1.46
1	A	80	PHE	CA-CB	6.01	1.62	1.53
1	A	182	LEU	CB-CG	-5.93	1.41	1.53
1	A	225	ARG	CZ-NH1	5.90	1.41	1.32
1	A	78	TRP	C-O	5.84	1.31	1.24
1	A	239	THR	C-N	-5.83	1.25	1.33
1	A	292[A]	ASP	C-O	5.81	1.30	1.24
1	A	292[B]	ASP	C-O	5.81	1.30	1.24
1	A	97	THR	N-CA	-5.79	1.39	1.46
1	A	207	ASP	CA-CB	5.77	1.62	1.53
1	A	87	LYS	N-CA	-5.76	1.39	1.46
1	A	323	ARG	CD-NE	-5.76	1.38	1.46
1	A	275	TYR	CA-C	-5.72	1.45	1.52
1	A	49	GLU	CD-OE2	-5.62	1.14	1.25
1	A	76	GLY	N-CA	-5.62	1.37	1.45
1	A	233	LEU	CB-CG	-5.59	1.42	1.53
1	A	65	ARG	NE-CZ	5.59	1.39	1.33
1	A	154	SER	CA-C	-5.56	1.45	1.52
1	A	88	ILE	C-O	-5.55	1.17	1.24
1	A	295	VAL	CA-C	5.51	1.58	1.52
1	A	268	LYS	C-O	5.49	1.30	1.23
1	A	212	ARG	CD-NE	-5.48	1.38	1.46
1	A	30	CYS	N-CA	5.47	1.52	1.45
1	A	242[A]	ARG	CD-NE	5.44	1.53	1.46
1	A	242[B]	ARG	CD-NE	5.44	1.53	1.46
1	A	84	ARG	CZ-NH1	5.41	1.40	1.32
1	A	330	VAL	CA-CB	-5.41	1.48	1.54
1	A	247	ALA	N-CA	-5.40	1.38	1.46
1	A	63	LYS	N-CA	5.36	1.53	1.46
1	A	182	LEU	N-CA	-5.36	1.39	1.46
1	A	43	ASN	CG-ND2	-5.34	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	ASN	C-O	-5.32	1.16	1.23
1	A	160	GLY	C-O	-5.29	1.18	1.23
1	A	356	LYS	CA-C	-5.29	1.45	1.52
1	A	318	ARG	CA-C	5.27	1.59	1.52
1	A	331	TRP	CA-C	-5.26	1.46	1.53
1	A	196	GLY	CA-C	-5.26	1.45	1.51
1	A	281	PHE	C-O	-5.24	1.17	1.24
1	A	168	TYR	C-O	5.20	1.29	1.24
1	A	337	ASP	N-CA	5.18	1.53	1.46
1	A	78	TRP	N-CA	5.17	1.52	1.46
1	A	139	GLU	CA-C	5.15	1.59	1.52
1	A	3	LEU	N-CA	-5.14	1.40	1.46
1	A	216	ALA	N-CA	5.11	1.52	1.46
1	A	253	VAL	CA-CB	5.09	1.61	1.54
1	A	127	ARG	N-CA	5.08	1.52	1.46
1	A	96	ARG	CD-NE	5.06	1.53	1.46
1	A	157	VAL	CA-C	5.04	1.58	1.52
1	A	122	GLY	C-O	5.04	1.29	1.23
1	A	293	GLN	CD-OE1	-5.04	1.14	1.23
1	A	172	GLN	CA-C	-5.02	1.46	1.52
1	A	233	LEU	CA-C	-5.02	1.46	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	SER	O-C-N	-17.81	98.16	122.74
1	A	225	ARG	NE-CZ-NH1	15.10	136.60	121.50
1	A	225	ARG	NE-CZ-NH2	-12.95	107.55	119.20
1	A	225	ARG	CD-NE-CZ	10.95	139.73	124.40
1	A	212	ARG	NE-CZ-NH2	-10.80	109.48	119.20
1	A	174	SER	CA-CB-OG	-10.24	90.62	111.10
1	A	166	ARG	NE-CZ-NH1	-10.22	111.28	121.50
1	A	85	PHE	N-CA-C	9.83	121.99	111.28
1	A	265	ARG	NE-CZ-NH2	9.74	127.97	119.20
1	A	191	TRP	N-CA-C	8.11	122.74	113.01
1	A	210	SER	CA-C-N	7.90	135.69	120.99
1	A	210	SER	C-N-CA	7.90	135.69	120.99
1	A	265	ARG	NE-CZ-NH1	-7.21	114.29	121.50
1	A	36	THR	OG1-CB-CG2	-7.13	95.03	109.30
1	A	323	ARG	CA-CB-CG	-6.91	100.27	114.10
1	A	166	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	A	322	ASN	O-C-N	6.38	129.68	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASN	N-CA-C	6.33	118.18	111.28
1	A	212	ARG	CG-CD-NE	-6.26	98.24	112.00
1	A	87	LYS	N-CA-C	-6.25	104.50	111.32
1	A	100	LYS	CG-CD-CE	6.04	125.18	111.30
1	A	318	ARG	NE-CZ-NH1	-6.04	115.47	121.50
1	A	262	ILE	CA-C-N	-6.03	113.57	119.78
1	A	262	ILE	C-N-CA	-6.03	113.57	119.78
1	A	102	VAL	CA-C-N	-5.98	114.22	120.38
1	A	102	VAL	C-N-CA	-5.98	114.22	120.38
1	A	89	ALA	N-CA-C	5.98	119.83	112.54
1	A	208	ALA	CB-CA-C	5.87	119.06	109.90
1	A	124	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	A	157	VAL	CA-CB-CG1	5.62	119.95	110.40
1	A	210	SER	N-CA-C	-5.58	101.25	109.18
1	A	178	ASP	CB-CG-OD2	5.57	131.21	118.40
1	A	336	ASP	N-CA-C	-5.49	103.66	110.41
1	A	55	LEU	CB-CG-CD1	5.47	127.10	110.70
1	A	193	GLN	N-CA-CB	-5.46	102.19	111.20
1	A	160	GLY	O-C-N	-5.38	119.37	123.35
1	A	212	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	A	189	GLY	CA-C-N	5.27	131.61	121.54
1	A	189	GLY	C-N-CA	5.27	131.61	121.54
1	A	207	ASP	CA-C-N	-5.18	113.52	120.82
1	A	207	ASP	C-N-CA	-5.18	113.52	120.82
1	A	320	LEU	N-CA-CB	5.16	118.27	110.28
1	A	166	ARG	N-CA-CB	-5.15	102.53	110.20
1	A	323	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	26	ASP	O-C-N	5.11	125.93	121.18
1	A	275	TYR	N-CA-C	5.11	117.51	111.33
1	A	166	ARG	N-CA-C	-5.09	105.42	111.69
1	A	208	ALA	N-CA-CB	5.09	117.47	109.69
1	A	360	ALA	N-CA-C	5.08	119.19	112.89
1	A	187	PHE	CA-C-N	-5.04	116.28	122.84
1	A	187	PHE	C-N-CA	-5.04	116.28	122.84
1	A	81	GLY	CA-C-O	-5.04	114.31	121.52
1	A	174	SER	CB-CA-C	-5.01	101.36	110.63
1	A	95	ARG	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2907	0	2839	24	0
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	305 (99%)	3 (1%)	68	52

All (3) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	288	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](#)

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	1.86	6 (42%)	17,19,21	3.22	10 (58%)
3	MPD	A	403[A]	-	7,7,7	0.42	0	9,10,10	0.94	0
3	MPD	A	403[B]	-	7,7,7	0.87	1 (14%)	9,10,10	1.03	1 (11%)
3	MPD	A	402	-	7,7,7	1.54	2 (28%)	9,10,10	1.61	2 (22%)

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	-	2/6/23/26	0/1/1/1
3	MPD	A	403[A]	-	-	3/5/5/5	-
3	MPD	A	403[B]	-	-	0/5/5/5	-
3	MPD	A	402	-	-	2/5/5/5	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	MPD	C1-C2	2.76	1.60	1.52
2	A	401	NAG	O3-C3	2.71	1.49	1.43
2	A	401	NAG	C1-C2	-2.71	1.48	1.52
2	A	401	NAG	O5-C5	2.36	1.48	1.43
2	A	401	NAG	O5-C1	-2.36	1.39	1.43
2	A	401	NAG	C7-N2	-2.22	1.27	1.34
3	A	402	MPD	C3-C2	-2.21	1.47	1.54
2	A	401	NAG	O7-C7	2.10	1.28	1.23
3	A	403[B]	MPD	O2-C2	-2.02	1.39	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	C6-C5-C4	6.33	128.57	113.02
2	A	401	NAG	O5-C5-C6	-5.25	97.45	107.66
2	A	401	NAG	O6-C6-C5	-4.94	94.52	111.33
2	A	401	NAG	C1-O5-C5	-4.43	106.25	112.19
2	A	401	NAG	O7-C7-C8	3.92	129.03	122.05
3	A	402	MPD	CM-C2-C1	-3.64	102.48	110.63
2	A	401	NAG	O7-C7-N2	-3.30	116.16	121.98
2	A	401	NAG	O5-C1-C2	2.96	115.87	111.29
2	A	401	NAG	C4-C3-C2	-2.95	106.69	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	C1-C2-N2	-2.76	106.08	110.43
2	A	401	NAG	C3-C4-C5	2.39	114.57	110.23
3	A	403[B]	MPD	CM-C2-C3	2.32	120.19	110.20
3	A	402	MPD	O2-C2-CM	-2.07	101.53	107.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	MPD	C2-C3-C4-O4
3	A	402	MPD	C2-C3-C4-C5
3	A	403[A]	MPD	C1-C2-C3-C4
3	A	403[A]	MPD	O2-C2-C3-C4
2	A	401	NAG	C4-C5-C6-O6
3	A	403[A]	MPD	CM-C2-C3-C4
2	A	401	NAG	O5-C5-C6-O6

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%)	-0.38	8 (2%) 62 68	9, 19, 38, 90	6 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	ALA	5.3
1	A	209	SER	3.7
1	A	190	ALA	3.1
1	A	81	GLY	2.6
1	A	191	TRP	2.5
1	A	210	SER	2.4
1	A	207	ASP	2.4
1	A	362	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	A	403[A]	8/8	0.73	0.14	27,28,31,35	8
3	MPD	A	403[B]	8/8	0.73	0.14	23,25,28,29	8
2	NAG	A	401	14/15	0.89	0.09	23,32,38,40	0
3	MPD	A	402	8/8	0.94	0.08	19,21,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.