



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:24 PM UTC

PDB ID : 9R6H / pdb_00009r6h
Title : Crystal Structure of the M18BP1 SANTA domain as a EGFP-SANTA-nanobody fusion
Authors : Pan, D.; Vetter, I.R.; Musacchio, A.
Deposited on : 2025-05-12
Resolution : 2.42 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

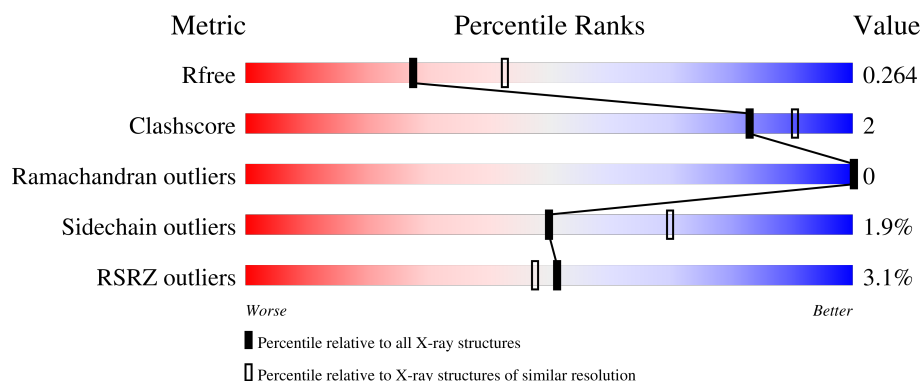
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

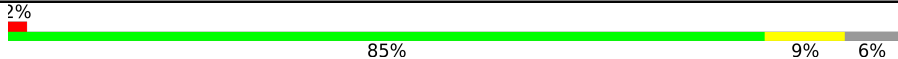
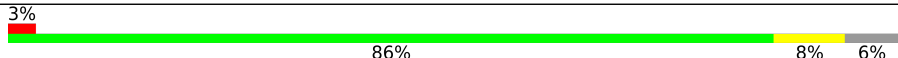
The reported resolution of this entry is 2.42 Å.

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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	487	
1	B	487	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7601 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 Genome polyprotein,Mis18-binding protein 1,Chains: A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3685	2331	637	700	17			
1	B	459	Total	C	N	O	S	0	0	0
			3679	2327	637	699	16			

There are 38 discrepancies between the modelled and reference sequences:

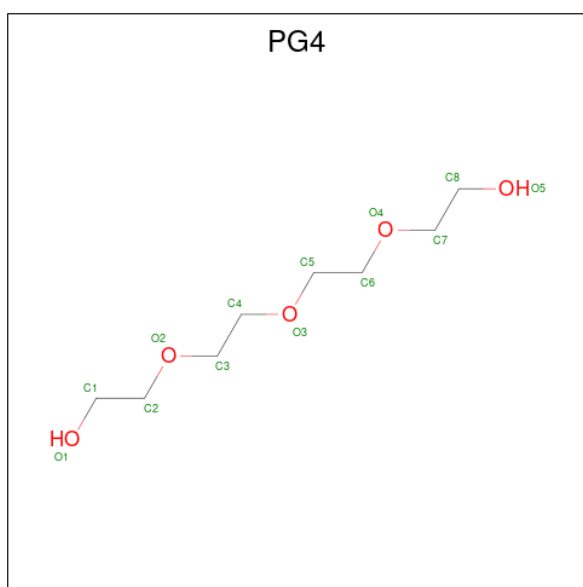
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP B6F2F5
A	65	C12	THR	chromophore	UNP B6F2F5
A	65	C12	TYR	chromophore	UNP B6F2F5
A	65	C12	GLY	chromophore	UNP B6F2F5
A	224	ALA	-	linker	UNP B6F2F5
A	225	ALA	-	linker	UNP B6F2F5
A	226	GLY	-	linker	UNP B6F2F5
A	227	ILE	-	linker	UNP B6F2F5
A	228	THR	-	linker	UNP B6F2F5
A	229	LEU	-	linker	UNP B6F2F5
A	230	GLY	-	linker	UNP B6F2F5
A	231	MET	-	linker	UNP B6F2F5
A	232	ASP	-	linker	UNP B6F2F5
A	233	GLU	-	linker	UNP B6F2F5
A	234	LEU	-	linker	UNP B6F2F5
A	235	TYR	-	linker	UNP B6F2F5
A	236	LYS	-	linker	UNP B6F2F5
A	237	ALA	-	linker	UNP B6F2F5
A	238	SER	-	linker	UNP B6F2F5
B	0	MET	-	initiating methionine	UNP B6F2F5
B	65	C12	THR	chromophore	UNP B6F2F5
B	65	C12	TYR	chromophore	UNP B6F2F5
B	65	C12	GLY	chromophore	UNP B6F2F5
B	224	ALA	-	linker	UNP B6F2F5
B	225	ALA	-	linker	UNP B6F2F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	GLY	-	linker	UNP B6F2F5
B	227	ILE	-	linker	UNP B6F2F5
B	228	THR	-	linker	UNP B6F2F5
B	229	LEU	-	linker	UNP B6F2F5
B	230	GLY	-	linker	UNP B6F2F5
B	231	MET	-	linker	UNP B6F2F5
B	232	ASP	-	linker	UNP B6F2F5
B	233	GLU	-	linker	UNP B6F2F5
B	234	LEU	-	linker	UNP B6F2F5
B	235	TYR	-	linker	UNP B6F2F5
B	236	LYS	-	linker	UNP B6F2F5
B	237	ALA	-	linker	UNP B6F2F5
B	238	SER	-	linker	UNP B6F2F5

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		

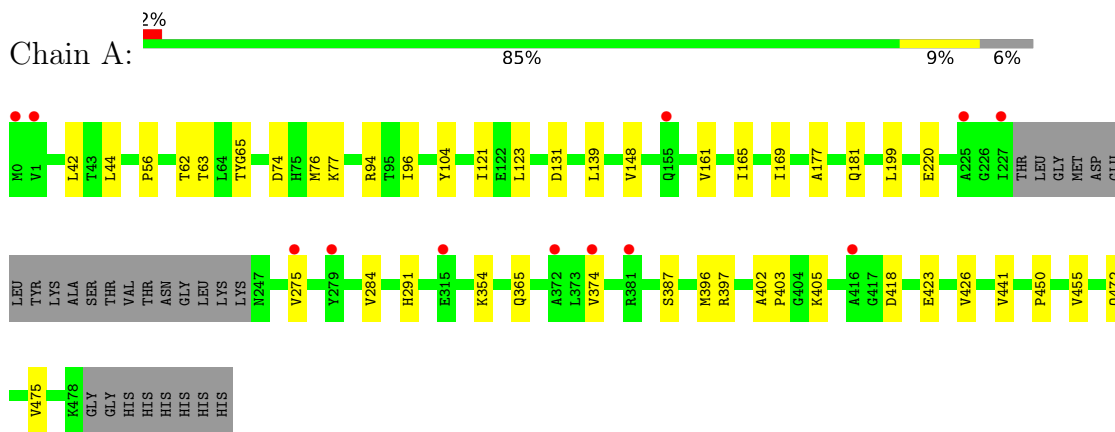
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	47	Total	O	0	0
			47	47		

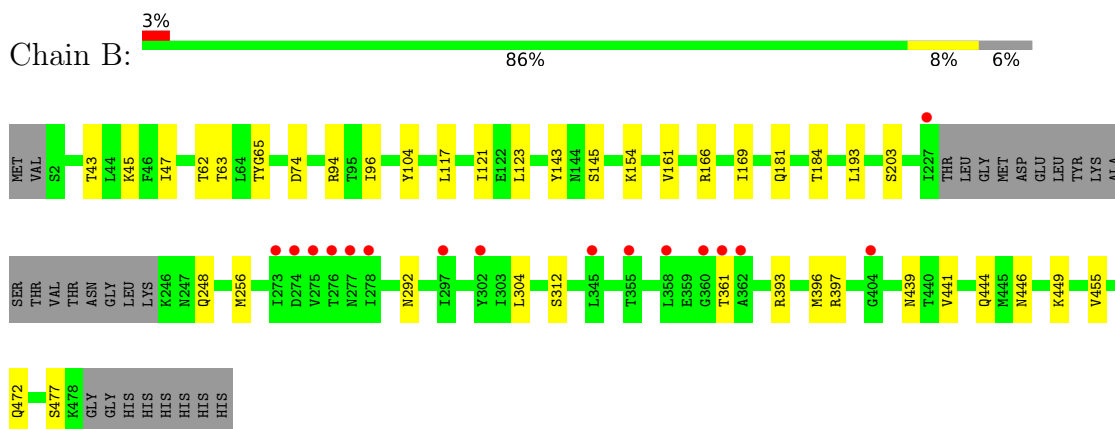
3 Residue-property plots [i](#)

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: Genome polyprotein,Mis18-binding protein 1,Chains: A



- Molecule 1: Genome polyprotein,Mis18-binding protein 1,Chains: A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.20Å 120.28Å 77.36Å 90.00° 121.28° 90.00°	Depositor
Resolution (Å)	45.04 – 2.42 45.04 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.04-2.42) 98.9 (45.04-2.42)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.229 , 0.262 0.229 , 0.264	Depositor DCC
R_{free} test set	2115 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.024 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7601	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: PG4, C12

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	0.30	0/3741	0.57	0/5051
1	B	0.32	1/3735 (0.0%)	0.59	0/5042
All	All	0.31	1/7476 (0.0%)	0.58	0/10093

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	LYS	C-N	5.08	1.40	1.33

There are no bond angle outliers.

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	3685	0	3602	20	0
1	B	3679	0	3594	15	0
2	A	78	0	108	1	0
2	B	65	0	90	1	0
3	A	47	0	0	0	0
3	B	47	0	0	0	0
All	All	7601	0	7394	36	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 2.

All (36) 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:96:ILE:HB	1:A:104:TYR:HB2	1.85	0.59
1:B:96:ILE:HB	1:B:104:TYR:HB2	1.87	0.57
1:A:42:LEU:HB2	1:A:220:GLU:HB3	1.87	0.55
1:A:455:VAL:HG22	1:A:472:GLN:HG2	1.89	0.54
1:A:74:ASP:HA	1:A:77:LYS:HD2	1.91	0.53
1:A:131:ASP:OD1	1:A:131:ASP:N	2.41	0.53
1:A:284:VAL:HG11	1:A:403:PRO:HB3	1.93	0.51
1:A:354:LYS:HE3	1:A:365:GLN:HG2	1.91	0.51
1:A:450:PRO:HA	1:A:475:VAL:HG13	1.93	0.50
1:A:165:ILE:HB	1:A:177:ALA:HB3	1.93	0.49
1:A:161:VAL:HB	1:A:181:GLN:HB3	1.93	0.49
1:B:62:THR:O	1:B:94:ARG:NH1	2.43	0.49
1:B:256:MET:SD	1:B:312:SER:OG	2.70	0.49
1:B:444:GLN:NE2	1:B:446:ASN:OD1	2.46	0.46
1:A:76:MET:HE3	1:A:76:MET:HB3	1.91	0.45
1:B:161:VAL:HB	1:B:181:GLN:HB3	1.99	0.45
1:A:169:ILE:O	1:A:397:ARG:NH2	2.49	0.45
1:A:63:THR:HG21	1:A:123:LEU:HD12	2.00	0.44
1:A:396:MET:HE2	1:A:441:VAL:HG21	2.00	0.44
1:B:169:ILE:O	1:B:397:ARG:NH2	2.51	0.44
1:A:62:THR:O	1:A:94:ARG:NH1	2.46	0.44
1:B:63:THR:HG21	1:B:123:LEU:HD12	2.00	0.43
1:B:396:MET:HE2	1:B:441:VAL:HG21	2.00	0.43
1:A:56:PRO:HG2	1:A:139:LEU:HD13	2.00	0.43
1:B:154:LYS:HG2	1:B:193:LEU:HD23	2.01	0.42
1:A:402:ALA:HB3	1:A:405:LYS:HB2	2.02	0.42
1:A:418:ASP:OD1	1:A:418:ASP:N	2.52	0.41
1:B:43:THR:HG21	2:B:501:PG4:H21	2.01	0.41
1:B:292:ASN:HB2	1:B:304:LEU:HB2	2.03	0.41
1:A:148:VAL:HB	1:A:199:LEU:HB2	2.02	0.41
1:B:143:TYR:HB3	1:B:203:SER:HB2	2.01	0.41
1:B:145:SER:O	1:B:166:ARG:NH2	2.53	0.41
1:A:423:GLU:HG3	1:A:426:VAL:HG22	2.03	0.41
2:A:501:PG4:H81	2:A:501:PG4:H61	1.94	0.41
1:B:455:VAL:HG22	1:B:472:GLN:HG2	2.01	0.41
1:B:45:LYS:HE2	1:B:47:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	453/487 (93%)	442 (98%)	11 (2%)	0	100	100
1	B	452/487 (93%)	442 (98%)	10 (2%)	0	100	100
All	All	905/974 (93%)	884 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	400/422 (95%)	394 (98%)	6 (2%)	57	75
1	B	399/422 (94%)	390 (98%)	9 (2%)	44	64
All	All	799/844 (95%)	784 (98%)	15 (2%)	50	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	121	ILE
1	A	275	VAL
1	A	291	HIS
1	A	374	VAL
1	A	387	SER
1	B	74	ASP
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	121	ILE
1	B	184	THR
1	B	248	GLN
1	B	361	THR
1	B	393	ARG
1	B	439	ASN
1	B	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	157	ASN
1	A	202	GLN
1	A	247	ASN
1	A	340	ASN
1	A	357	GLN
1	A	363	GLN
1	B	157	ASN
1	B	253	GLN
1	B	340	ASN
1	B	357	GLN
1	B	461	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	C12	B	65	1	21,23,24	1.51	2 (9%)	23,32,34	2.05	4 (17%)
1	C12	A	65	1	21,23,24	1.53	2 (9%)	23,32,34	2.03	4 (17%)

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
1	C12	B	65	1	-	2/12/15/16	0/2/2/2
1	C12	A	65	1	-	2/12/15/16	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	C12	CA2-C2	5.36	1.47	1.36
1	B	65	C12	CA2-C2	5.31	1.46	1.36
1	B	65	C12	C1-N2	3.46	1.37	1.32
1	A	65	C12	C1-N2	3.45	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	C12	CG2-CB2-CA2	7.79	131.47	113.53
1	A	65	C12	CG2-CB2-CA2	7.70	131.28	113.53
1	B	65	C12	C2-CA2-N2	-3.41	104.59	109.85
1	A	65	C12	C2-CA2-N2	-3.36	104.66	109.85
1	A	65	C12	CB2-CG2-CD2	-3.26	116.10	120.89
1	B	65	C12	CB2-CG2-CD2	-3.23	116.14	120.89
1	A	65	C12	CB2-CG2-CD1	2.52	124.59	120.89
1	B	65	C12	CB2-CG2-CD1	2.50	124.56	120.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	C12	N2-CA2-CB2-CG2
1	A	65	C12	C2-CA2-CB2-CG2
1	B	65	C12	N2-CA2-CB2-CG2
1	B	65	C12	C2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	PG4	B	501	-	12,12,12	0.11	0	11,11,11	0.56	0
2	PG4	B	504	-	12,12,12	0.10	0	11,11,11	0.68	0
2	PG4	A	503	-	12,12,12	0.18	0	11,11,11	0.51	0
2	PG4	A	501	-	12,12,12	0.18	0	11,11,11	0.49	0
2	PG4	A	504	-	12,12,12	0.11	0	11,11,11	0.64	0
2	PG4	A	506	-	12,12,12	0.11	0	11,11,11	0.65	0
2	PG4	B	502	-	12,12,12	0.11	0	11,11,11	0.64	0
2	PG4	A	502	-	12,12,12	0.12	0	11,11,11	0.57	0
2	PG4	B	505	-	12,12,12	0.14	0	11,11,11	0.56	0
2	PG4	B	503	-	12,12,12	0.11	0	11,11,11	0.65	0
2	PG4	A	505	-	12,12,12	0.13	0	11,11,11	0.58	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	PG4	B	501	-	-	1/10/10/10	-
2	PG4	B	504	-	-	3/10/10/10	-
2	PG4	A	503	-	-	4/10/10/10	-
2	PG4	A	501	-	-	2/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	A	504	-	-	4/10/10/10	-
2	PG4	A	506	-	-	2/10/10/10	-
2	PG4	B	502	-	-	6/10/10/10	-
2	PG4	A	502	-	-	3/10/10/10	-
2	PG4	B	505	-	-	4/10/10/10	-
2	PG4	B	503	-	-	6/10/10/10	-
2	PG4	A	505	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	PG4	O2-C3-C4-O3
2	B	502	PG4	O2-C3-C4-O3
2	A	503	PG4	O3-C5-C6-O4
2	A	504	PG4	O4-C7-C8-O5
2	A	502	PG4	O2-C3-C4-O3
2	B	505	PG4	O2-C3-C4-O3
2	B	502	PG4	O4-C7-C8-O5
2	A	505	PG4	O3-C5-C6-O4
2	A	502	PG4	O3-C5-C6-O4
2	A	503	PG4	O1-C1-C2-O2
2	B	501	PG4	O4-C7-C8-O5
2	B	503	PG4	O2-C3-C4-O3
2	A	506	PG4	O1-C1-C2-O2
2	B	502	PG4	C5-C6-O4-C7
2	A	504	PG4	C3-C4-O3-C5
2	B	504	PG4	C1-C2-O2-C3
2	B	504	PG4	C5-C6-O4-C7
2	B	505	PG4	C8-C7-O4-C6
2	B	503	PG4	C3-C4-O3-C5
2	B	505	PG4	C5-C6-O4-C7
2	A	502	PG4	O4-C7-C8-O5
2	A	504	PG4	O1-C1-C2-O2
2	B	502	PG4	C3-C4-O3-C5
2	B	503	PG4	C1-C2-O2-C3
2	B	503	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
2	A	504	PG4	C1-C2-O2-C3
2	A	501	PG4	O2-C3-C4-O3
2	A	505	PG4	C5-C6-O4-C7
2	B	502	PG4	O1-C1-C2-O2
2	A	505	PG4	C4-C3-O2-C2
2	A	503	PG4	C6-C5-O3-C4
2	A	503	PG4	C8-C7-O4-C6
2	A	506	PG4	O3-C5-C6-O4
2	A	505	PG4	C6-C5-O3-C4
2	B	504	PG4	C4-C3-O2-C2
2	B	503	PG4	O4-C7-C8-O5
2	B	503	PG4	C8-C7-O4-C6
2	B	502	PG4	O3-C5-C6-O4
2	B	505	PG4	O3-C5-C6-O4
2	A	501	PG4	O3-C5-C6-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PG4	1	0
2	A	501	PG4	1	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	459/487 (94%)	0.40	12 (2%) 57 54	40, 61, 92, 116	0
1	B	458/487 (94%)	0.37	16 (3%) 47 43	41, 59, 96, 133	0
All	All	917/974 (94%)	0.38	28 (3%) 51 48	40, 60, 94, 133	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	ILE	4.0
1	B	276	THR	3.8
1	B	273	ILE	3.6
1	B	277	ASN	3.6
1	B	345	LEU	3.4
1	A	275	VAL	3.0
1	B	275	VAL	3.0
1	B	362	ALA	3.0
1	A	372	ALA	2.9
1	B	227	ILE	2.8
1	A	1	VAL	2.6
1	A	279	TYR	2.6
1	B	358	LEU	2.6
1	B	355	THR	2.6
1	B	302	TYR	2.6
1	A	315	GLU	2.5
1	B	274	ASP	2.4
1	B	361	THR	2.4
1	B	404	GLY	2.2
1	A	227	ILE	2.2
1	A	0	MET	2.1
1	A	225	ALA	2.1
1	A	374	VAL	2.1
1	A	155	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	381	ARG	2.1
1	A	416	ALA	2.1
1	B	360	GLY	2.0
1	B	297	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	C12	A	65	22/23	0.93	0.08	37,43,48,50	0
1	C12	B	65	22/23	0.93	0.08	37,44,47,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PG4	B	503	13/13	0.63	0.17	82,87,92,95	0
2	PG4	A	505	13/13	0.77	0.14	66,70,80,80	0
2	PG4	B	505	13/13	0.77	0.17	69,83,93,97	0
2	PG4	A	506	13/13	0.79	0.16	69,79,83,87	0
2	PG4	B	504	13/13	0.80	0.14	56,67,74,75	0
2	PG4	A	503	13/13	0.80	0.14	52,61,72,76	0
2	PG4	A	504	13/13	0.81	0.17	59,69,85,90	0
2	PG4	A	502	13/13	0.84	0.14	64,72,79,79	0
2	PG4	A	501	13/13	0.87	0.13	51,60,64,66	0
2	PG4	B	502	13/13	0.89	0.11	51,57,65,66	0
2	PG4	B	501	13/13	0.90	0.10	53,60,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.