Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2025 – 08:34 AM EDT

PDB ID	:	9NN3 / pdb_00009nn3
Title	:	BET BRD2-BD1 in complex with peptide 6.2
Deposited on	:	2025-03-05
Resolution	:	1.60 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

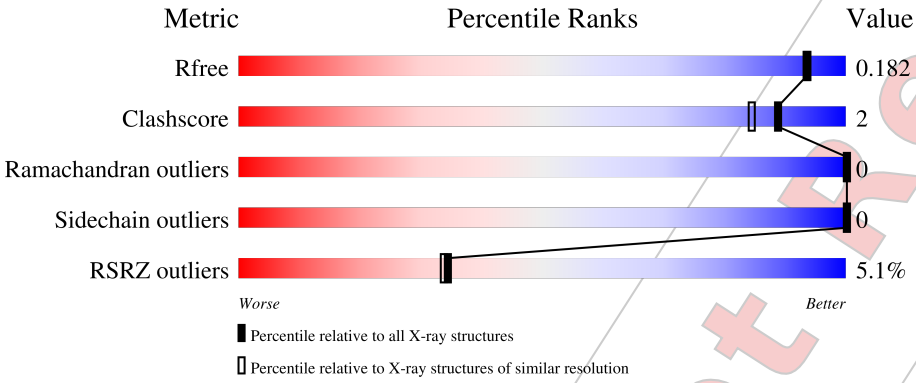
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

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 1.60 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 <=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	111	5% 96%
1	B	111	2% 92% 6%
2	C	11	18% 100%
2	D	11	18% 91% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4286 atoms, of which 1912 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 Bromodomain-containing protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	111	Total	C	H	N	O	S	0	0	0
			1853	602	924	155	163	9			
1	B	109	Total	C	H	N	O	S	0	0	0
			1781	592	870	152	158	9			

- Molecule 2 is a protein called peptide 6.2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	11	Total	C	H	N	O	S	0	0	1
			145	60	58	14	12	1			
2	D	11	Total	C	H	N	O	S	0	0	1
			147	60	60	14	12	1			

- Molecule 3 is water.

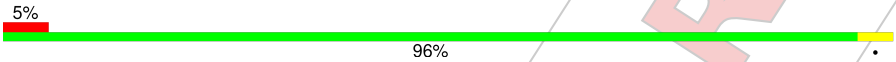
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	161	Total	O	0	0
			161	161		
3	C	19	Total	O	0	0
			19	19		
3	D	9	Total	O	0	0
			9	9		

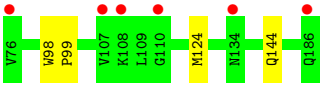
3 Residue-property plots (i)

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: Bromodomain-containing protein 2

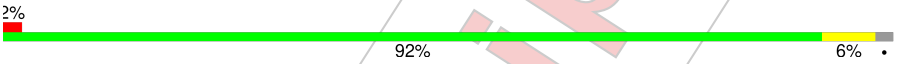
Chain A:

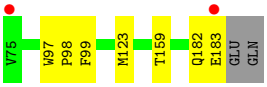




• Molecule 1: Bromodomain-containing protein 2

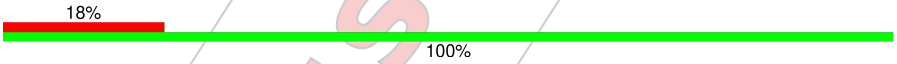
Chain B:





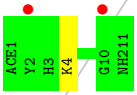
• Molecule 2: peptide 6.2

Chain C:



• Molecule 2: peptide 6.2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.73Å 66.93Å 90.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 1.60 45.08 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.08-1.60) 100.0 (45.08-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.77 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.182 0.157 , 0.182	Depositor DCC
R_{free} test set	2131 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4286	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ALY, NH2

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	0.43	1/954 (0.1%)	0.54	0/1291
1	B	0.41	0/936	0.57	0/1267
2	C	0.55	0/77	0.67	0/104
2	D	0.41	0/77	0.72	0/104
All	All	0.42	1/2044 (0.0%)	0.57	0/2766

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MET	SD-CE	-5.51	1.65	1.79

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	929	924	924	2	0
1	B	911	870	910	6	0
2	C	87	58	72	0	0
2	D	87	60	72	0	0
3	A	171	0	0	0	1
3	B	161	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	19	0	0	0	1
3	D	9	0	0	0	0
All	All	2374	1912	1978	7	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 2.

All (7) 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:182:GLN:O	1:B:183:GLU:HG2	2.10	0.52
1:A:98:TRP:CD2	1:A:99:PRO:HD3	2.50	0.47
1:B:99:PHE:HB2	1:B:123:MET:HE3	1.99	0.45
1:B:97:TRP:CD2	1:B:98:PRO:HD3	2.52	0.44
1:B:182:GLN:HE21	1:B:182:GLN:HA	1.83	0.43
1:A:144:GLN:CG	1:B:159:THR:HG21	2.51	0.41
1:B:182:GLN:HA	1:B:182:GLN:NE2	2.35	0.41

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)
3:A:299:HOH:O	3:C:109:HOH:O[4_455]	2.14	0.06

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	109/111 (98%)	108 (99%)	1 (1%)	0	100	100
1	B	107/111 (96%)	107 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
2	D	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	232/244 (95%)	228 (98%)	4 (2%)	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	102/102 (100%)	102 (100%)	0	100	100
1	B	100/102 (98%)	100 (100%)	0	100	100
2	C	7/7 (100%)	7 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	216/218 (99%)	216 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	B	78	GLN
1	B	94	GLN
1	B	182	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)

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	$\#\|Z\| > 2$
2	ALY	D	4	2	10,11,12	0.76	0	7,12,14	1.95	3 (42%)
2	ALY	C	4	2	10,11,12	0.83	0	7,12,14	0.97	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	ALY	D	4	2	-	3/9/10/12	-
2	ALY	C	4	2	-	0/9/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	ALY	CE-NZ-CH	-3.27	117.73	122.56
2	D	4	ALY	CD-CE-NZ	2.89	120.30	112.20
2	D	4	ALY	CD-CG-CB	-2.70	103.43	113.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	ALY	C-CA-CB-CG
2	D	4	ALY	CG-CD-CE-NZ
2	D	4	ALY	N-CA-CB-CG

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)

There are no ligands in this entry.

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, 95^{th} 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	111/111 (100%)	-0.36	6 (5%) 32 31	10, 18, 39, 58	0
1	B	109/111 (98%)	-0.55	2 (1%) 67 69	9, 16, 32, 55	0
2	C	8/11 (72%)	0.33	2 (25%) 2 1	12, 18, 35, 43	0
2	D	8/11 (72%)	0.69	2 (25%) 2 1	12, 16, 32, 36	0
All	All	236/244 (96%)	-0.39	12 (5%) 34 34	9, 17, 36, 58	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	VAL	4.3
1	A	76	VAL	4.1
2	D	10	GLY	4.0
2	C	9	CYS	3.5
2	C	10	GLY	3.2
1	B	183	GLU	2.8
1	A	108	LYS	2.7
1	A	134	ASN	2.7
2	D	2	TYR	2.6
1	A	186	GLN	2.4
1	A	107	VAL	2.3
1	A	110	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	ALY	D	4	12/13	0.92	0.10	11,17,24,25	0
2	ALY	C	4	12/13	0.98	0.04	10,13,16,18	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2025 – 08:36 AM EDT

PDB ID	:	9NN5 / pdb_00009nn5
Title	:	BET BRD4-BD1 in complex with peptide 9.2
Deposited on	:	2025-03-05
Resolution	:	1.47 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

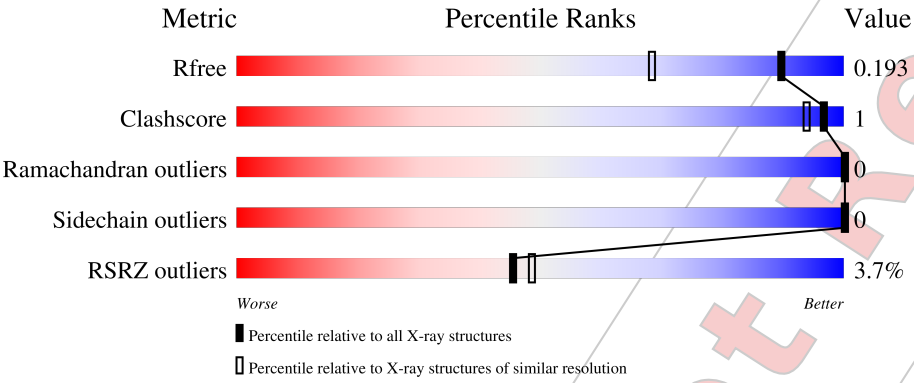
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

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 1.47 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}	164625	6131 (1.50-1.46)
Clashscore	180529	6623 (1.50-1.46)
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RSRZ outliers	164620	6132 (1.50-1.46)

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 <=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	130	3% 95%
2	B	14	7% 93% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2460 atoms, of which 1154 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	126	2099	681	1048	173	191	6	10	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP O60885
A	41	SER	-	expression tag	UNP O60885
A	169	GLU	-	expression tag	UNP O60885

- Molecule 2 is a protein called peptide 9.2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	14	213	73	106	17	16	1	0	0	1

- Molecule 3 is water.

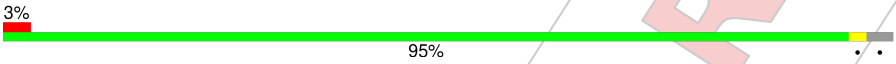
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	135	135	135	0	0
3	B	13	13	13	0	0

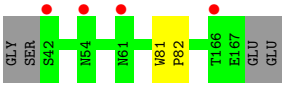
3 Residue-property plots (i)

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: Bromodomain-containing protein 4

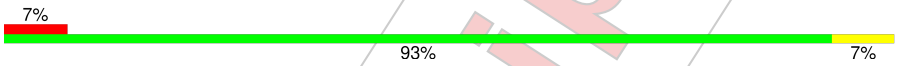
Chain A:

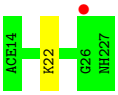




- Molecule 2: peptide 9.2

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.72Å 42.07Å 29.70Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	39.82 – 1.47 39.82 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.82-1.47) 99.6 (39.82-1.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.193 0.168 , 0.193	Depositor DCC
R_{free} test set	2004 reflections (7.69%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2460	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ALY, NH2

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	0.40	0/1081	0.58	0/1472
2	B	0.67	0/81	0.69	0/107
All	All	0.42	0/1162	0.59	0/1579

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1051	1048	1048	1	0
2	B	107	106	110	1	0
3	A	135	0	0	0	0
3	B	13	0	0	1	0
All	All	1306	1154	1158	2	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 1.

All (2) 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)
2:B:22:LYS:NZ	3:B:101:HOH:O	2.39	0.52
1:A:81:TRP:CG	1:A:82:PRO:HD3	2.51	0.46

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	124/130 (95%)	123 (99%)	1 (1%)	0	100	100
2	B	10/14 (71%)	9 (90%)	1 (10%)	0	100	100
All	All	134/144 (93%)	132 (98%)	2 (2%)	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	119/122 (98%)	119 (100%)	0	100	100
2	B	8/8 (100%)	8 (100%)	0	100	100
All	All	127/130 (98%)	127 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	62	GLN
1	A	85	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)

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	$\#\|Z\| > 2$
2	ALY	B	20	2	10,11,12	0.77	0	7,12,14	0.38	0
2	ALY	B	23	2	10,11,12	0.89	0	7,12,14	0.93	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	ALY	B	20	2	-	0/9/10/12	-
2	ALY	B	23	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

There are no ligands in this entry.

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, 95^{th} 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	126/130 (96%)	-0.03	4 (3%) 50 53	14, 26, 43, 55	1 (0%)
2	B	10/14 (71%)	0.44	1 (10%) 14 13	18, 22, 29, 55	0
All	All	136/144 (94%)	0.01	5 (3%) 45 48	14, 25, 44, 55	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	26	GLY	7.0
1	A	42	SER	2.4
1	A	61	ASN	2.2
1	A	54	ASN	2.0
1	A	166	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	ALY	B	23	12/13	0.95	0.07	16,24,29,30	0
2	ALY	B	20	12/13	0.98	0.04	13,14,16,17	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2025 – 03:01 PM EST

PDB ID	:	9NN4
Title	:	BET BRD3-BD1 in complex with peptide 7.2
Deposited on	:	2025-03-05
Resolution	:	1.37 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

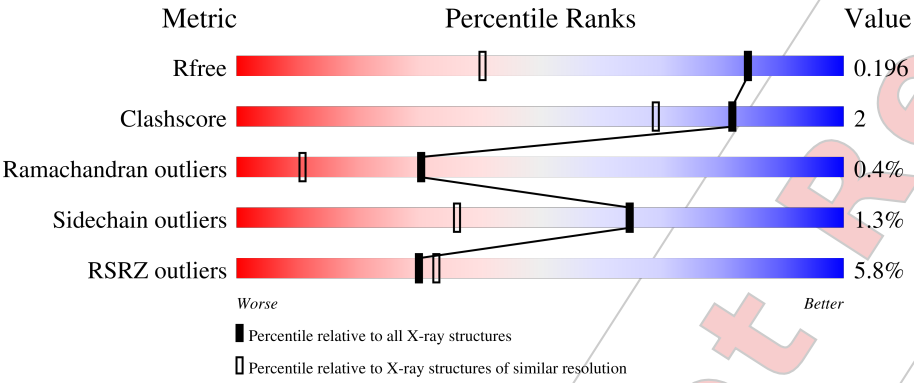
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 1.37 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}	164625	3869 (1.40-1.36)
Clashscore	180529	4183 (1.40-1.36)
Ramachandran outliers	177936	4116 (1.40-1.36)
Sidechain outliers	177891	4115 (1.40-1.36)
RSRZ outliers	164620	3867 (1.40-1.36)

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 <=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	120	2% 90% 6% ·
1	B	120	2% 93% · 5%
2	D	11	45% 73% 27%
2	E	11	45% 64% 27% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4668 atoms, of which 2135 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 Bromodomain-containing protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	115	Total	C	H	N	O	S	30	5	0
			1972	639	982	162	179	10			
1	B	114	Total	C	H	N	O	S	30	4	0
			1948	632	970	160	177	9			

- Molecule 2 is a protein called peptide 7.2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	11	Total	C	H	N	O	S	0	0	1
			185	58	93	19	14	1			
2	E	11	Total	C	H	N	O	S	0	0	1
			182	58	90	19	14	1			

- Molecule 3 is water.

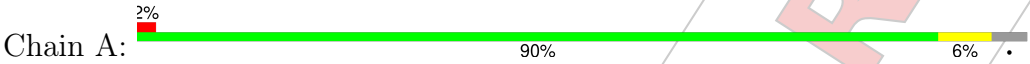
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	185	Total	O	0	0
			185	185		
3	D	6	Total	O	0	0
			6	6		
3	E	9	Total	O	0	0
			9	9		

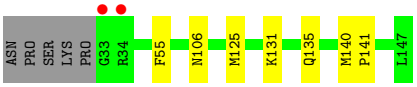
3 Residue-property plots (i)

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: Bromodomain-containing protein 3

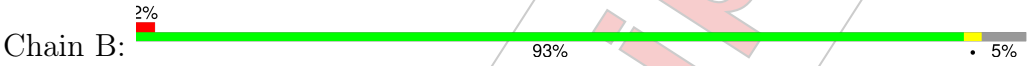
Chain A:

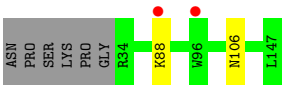




• Molecule 1: Bromodomain-containing protein 3

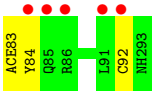
Chain B:





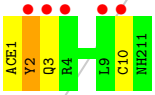
• Molecule 2: peptide 7.2

Chain D:



• Molecule 2: peptide 7.2

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.83Å 30.07Å 77.85Å 90.00° 108.53° 90.00°	Depositor
Resolution (Å)	42.63 – 1.37 42.63 – 1.37	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.63-1.37) 99.3 (42.63-1.37)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.156 , 0.195 0.157 , 0.196	Depositor DCC
R_{free} test set	62321 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 51.5	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	0.97	EDS
Total number of atoms	4668	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALY, ACE, NH2

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	0.47	0/1036	0.64	0/1402
1	B	0.44	0/1024	0.63	0/1386
2	D	0.34	0/64	0.85	0/81
2	E	0.53	0/64	1.02	0/81
All	All	0.45	0/2188	0.66	0/2950

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	990	982	960	5	0
1	B	978	970	948	0	0
2	D	92	93	96	2	0
2	E	92	90	96	3	0
3	A	181	0	0	0	2
3	B	185	0	0	0	1
3	D	6	0	0	0	0
3	E	9	0	0	1	0
All	All	2533	2135	2100	10	3

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 (10) 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)
2:D:83:ACE:H1	2:D:84:TYR:CD1	2.27	0.69
2:E:1:ACE:H3	2:E:10:CYS:N	2.16	0.60
2:E:3:GLN:O	3:E:101:HOH:O	2.17	0.59
2:E:1:ACE:O	2:E:2:TYR:HB2	2.09	0.53
1:A:131:LYS:O	1:A:135:GLN:HG3	2.15	0.47
1:A:140[A]:MET:CG	1:A:141:PRO:HD2	2.47	0.45
1:A:55:PHE:CG	1:A:125:MET:HG2	2.51	0.45
1:A:140[A]:MET:HG3	1:A:141:PRO:HD2	2.00	0.44
2:D:83:ACE:H3	2:D:92:CYS:HA	1.74	0.43

All (3) 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)
3:B:327:HOH:O	3:B:362:HOH:O[2_655]	1.96	0.24
3:A:316:HOH:O	3:A:334:HOH:O[1_545]	2.12	0.08
3:A:331:HOH:O	3:A:356:HOH:O[2_545]	2.19	0.01

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	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
1	B	116/120 (97%)	115 (99%)	1 (1%)	0	100	100
2	D	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
2	E	7/11 (64%)	4 (57%)	2 (29%)	1 (14%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	248/262 (95%)	242 (98%)	5 (2%)	1 (0%)	30 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	2	TYR

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	112/112 (100%)	111 (99%)	1 (1%)	75 52
1	B	111/112 (99%)	109 (98%)	2 (2%)	54 23
2	D	7/7 (100%)	7 (100%)	0	100 100
2	E	7/7 (100%)	7 (100%)	0	100 100
All	All	237/238 (100%)	234 (99%)	3 (1%)	65 36

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

Mol	Chain	Res	Type
1	A	106	ASN
1	B	88	LYS
1	B	106	ASN

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	135	GLN
1	B	92	ASN
1	B	135	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\|>2$
2	ALY	E	8	2	10,11,12	0.82	0	7,12,14	0.52	0
2	ALY	D	90	2	10,11,12	0.91	0	7,12,14	0.27	0
2	ALY	D	87	2	10,11,12	1.01	0	7,12,14	0.77	0
2	ALY	E	5	2	10,11,12	0.74	0	7,12,14	0.52	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	ALY	E	8	2	-	0/9/10/12	-
2	ALY	D	90	2	-	0/9/10/12	-
2	ALY	D	87	2	-	4/9/10/12	-
2	ALY	E	5	2	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	ALY	CE-CD-CG-CB
2	D	87	ALY	OH-CH-NZ-CE
2	D	87	ALY	CH3-CH-NZ-CE

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Mol	Chain	Res	Type	Atoms
2	D	87	ALY	C-CA-CB-CG
2	D	87	ALY	CE-CD-CG-CB

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)

There are no ligands in this entry.

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, 95^{th} 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	115/120 (95%)	-0.11	2 (1%)	69	74	8, 16, 31, 64	5 (4%)
1	B	114/120 (95%)	-0.19	2 (1%)	67	72	8, 15, 29, 39	4 (3%)
2	D	7/11 (63%)	2.82	5 (71%)	0	0	20, 29, 81, 85	0
2	E	7/11 (63%)	3.43	5 (71%)	0	0	21, 30, 75, 84	0
All	All	243/262 (92%)	0.04	14 (5%)	30	33	8, 16, 36, 85	9 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	TYR	8.5
2	D	84	TYR	7.8
1	A	33	GLY	6.5
2	E	10	CYS	5.9
2	D	85	GLN	3.5
2	E	3	GLN	3.5
2	D	92	CYS	3.3
2	E	4	ARG	3.1
2	D	86	ARG	2.8
2	D	91	LEU	2.7
1	B	96	TRP	2.6
1	A	34	ARG	2.6
2	E	9	LEU	2.4
1	B	88	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	ALY	D	87	12/13	0.89	0.14	22,35,43,43	0
2	ALY	E	5	12/13	0.90	0.13	21,37,43,45	0
2	ALY	E	8	12/13	0.97	0.06	14,16,19,19	0
2	ALY	D	90	12/13	0.98	0.05	13,17,18,19	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2025 – 07:59 AM EDT

PDB ID	:	9NNT
Title	:	BET BRD4-BD1 in complex with peptide 6.1
Deposited on	:	2025-03-06
Resolution	:	1.59 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

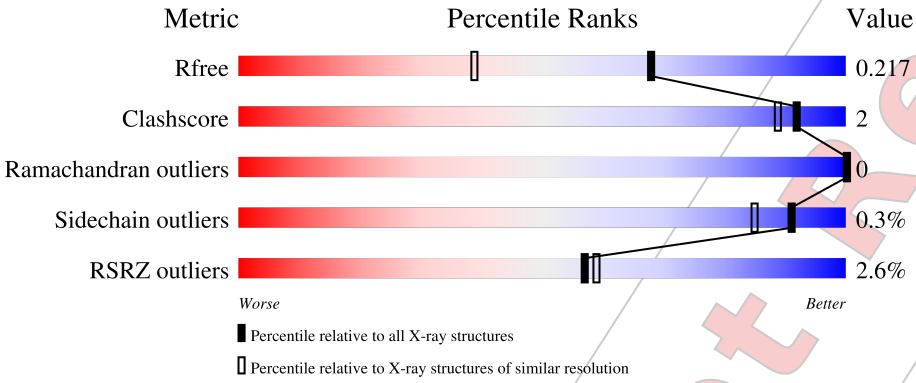
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 1.59 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 <=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	129	95%
1	B	129	3% 97%
1	C	129	5% 93% 5%
2	D	10	80% 10% 10%

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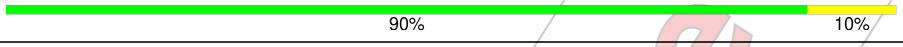
Mol	Chain	Length	Quality of chain
2	E	10	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7093 atoms, of which 3294 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	126	Total	C	H	N	O	S	10	0	0
			2099	681	1048	173	191	6			
1	B	128	Total	C	H	N	O	S	10	0	0
			2118	686	1057	175	194	6			
1	C	126	Total	C	H	N	O	S	10	0	0
			2099	681	1048	173	191	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP O60885
A	41	SER	-	expression tag	UNP O60885
B	40	GLY	-	expression tag	UNP O60885
B	41	SER	-	expression tag	UNP O60885
C	40	GLY	-	expression tag	UNP O60885
C	41	SER	-	expression tag	UNP O60885

- Molecule 2 is a protein called peptide 6.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	10	Total	C	H	N	O	S	0	0	1
			143	50	63	15	14	1			
2	E	10	Total	C	H	N	O	S	0	0	1
			158	50	78	15	14	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	153	Total	O	0	0
			153	153		

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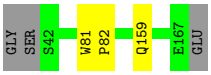
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	124	Total O 124 124	0	0
3	D	7	Total O 7 7	0	0
3	E	10	Total O 10 10	0	0

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.

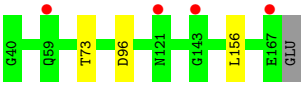
• Molecule 1: Bromodomain-containing protein 4

Chain A:



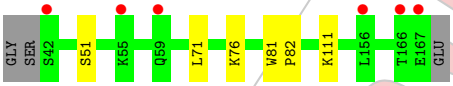
• Molecule 1: Bromodomain-containing protein 4

Chain B:



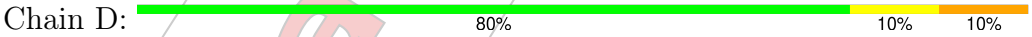
• Molecule 1: Bromodomain-containing protein 4

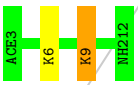
Chain C:



• Molecule 2: peptide 6.1

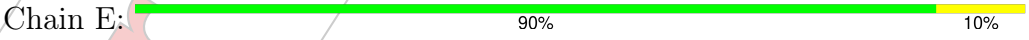
Chain D:





• Molecule 2: peptide 6.1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.56Å 41.63Å 86.63Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	48.33 – 1.59 48.33 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.33-1.59) 98.3 (48.33-1.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.172 , 0.217 0.172 , 0.217	Depositor DCC
R_{free} test set	52279 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7093	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ALY, NH2

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	0.57	0/1081	0.71	0/1472
1	B	0.51	0/1091	0.64	0/1485
1	C	0.54	0/1081	0.68	0/1472
2	D	0.65	0/51	0.96	0/65
2	E	0.58	0/51	0.95	0/65
All	All	0.54	0/3355	0.69	0/4559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1051	1048	1048	2	0
1	B	1061	1057	1056	2	0
1	C	1051	1048	1048	4	0
2	D	80	63	81	1	0
2	E	80	78	81	2	0
3	A	182	0	0	1	0
3	B	153	0	0	0	1
3	C	124	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	0	1	0
3	E	10	0	0	0	0
All	All	3799	3294	3314	10	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 2.

All (10) 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)
3:C:267:HOH:O	2:E:9:ALY:HH32	1.84	0.78
1:C:76:LYS:HA	1:C:76:LYS:HE3	1.83	0.59
1:A:81:TRP:CG	1:A:82:PRO:HD3	2.49	0.47
2:D:9:ALY:HH32	3:D:104:HOH:O	2.14	0.47
1:B:73:THR:HG22	1:B:156:LEU:HD21	1.96	0.46
1:B:96:ASP:OD1	1:B:96:ASP:N	2.41	0.44
1:C:82:PRO:HB3	2:E:9:ALY:HH33	2.00	0.44
1:C:81:TRP:CG	1:C:82:PRO:HD3	2.54	0.43
1:A:159:GLN:NE2	3:A:206:HOH:O	2.53	0.42
1:C:71:LEU:HD11	1:C:111:LYS:HD3	2.02	0.42

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)
3:B:219:HOH:O	3:C:297:HOH:O[2_354]	2.19	0.01

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	124/129 (96%)	123 (99%)	1 (1%)	0	100	100
1	B	126/129 (98%)	126 (100%)	0	0	100	100
1	C	124/129 (96%)	123 (99%)	1 (1%)	0	100	100
2	D	6/10 (60%)	6 (100%)	0	0	100	100
2	E	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
All	All	386/407 (95%)	383 (99%)	3 (1%)	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	119/121 (98%)	119 (100%)	0	100	100
1	B	120/121 (99%)	120 (100%)	0	100	100
1	C	119/121 (98%)	118 (99%)	1 (1%)	79	66
2	D	6/6 (100%)	6 (100%)	0	100	100
2	E	6/6 (100%)	6 (100%)	0	100	100
All	All	370/375 (99%)	369 (100%)	1 (0%)	91	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	SER

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	123	GLN
1	A	159	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
2	ALY	E	6	2	10,11,12	0.70	0	7,12,14	0.58	0
2	ALY	D	9	2	10,11,12	1.06	0	7,12,14	1.24	1 (14%)
2	ALY	D	6	2	10,11,12	0.94	1 (10%)	7,12,14	1.06	0
2	ALY	E	9	2	10,11,12	1.30	0	7,12,14	1.07	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	ALY	E	6	2	-	2/9/10/12	-
2	ALY	D	9	2	-	3/9/10/12	-
2	ALY	D	6	2	-	1/9/10/12	-
2	ALY	E	9	2	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	ALY	CH-NZ	2.12	1.39	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	9	ALY	CE-NZ-CH	2.69	126.53	122.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	6	ALY	O-C-CA-CB
2	E	6	ALY	O-C-CA-CB
2	D	9	ALY	OH-CH-NZ-CE
2	D	9	ALY	CH3-CH-NZ-CE
2	E	9	ALY	OH-CH-NZ-CE
2	E	9	ALY	CH3-CH-NZ-CE
2	E	9	ALY	CA-CB-CG-CD
2	D	9	ALY	CA-CB-CG-CD
2	E	6	ALY	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9	ALY	1	0
2	E	9	ALY	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	126/129 (97%)	-0.35	0 100 100	13, 19, 34, 41	1 (0%)
1	B	128/129 (99%)	0.09	4 (3%) 51 52	14, 26, 47, 73	1 (0%)
1	C	126/129 (97%)	0.16	6 (4%) 36 36	10, 25, 42, 80	1 (0%)
2	D	6/10 (60%)	0.79	0 100 100	20, 25, 31, 41	0
2	E	6/10 (60%)	0.66	0 100 100	18, 24, 33, 36	0
All	All	392/407 (96%)	-0.01	10 (2%) 57 59	10, 23, 42, 80	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLY	3.6
1	C	42	SER	3.0
1	B	59	GLN	2.8
1	C	167	GLU	2.8
1	C	156	LEU	2.6
1	C	166	THR	2.3
1	B	121	ASN	2.1
1	C	55	LYS	2.1
1	B	167	GLU	2.1
1	C	59	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	ALY	D	9	12/13	0.93	0.08	17,26,34,36	0
2	ALY	E	9	12/13	0.94	0.08	14,21,28,31	0
2	ALY	D	6	12/13	0.96	0.06	12,18,24,29	0
2	ALY	E	6	12/13	0.97	0.05	13,18,23,24	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.