



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 02:15 PM EDT

PDB ID : 9MXK / pdb_00009mxk
Title : BRD4-BD1 in complex with cyclic peptide 4.1C
Authors : Patel, K.; Pachl, P.; Mackay, J.P.
Deposited on : 2025-01-20
Resolution : 1.73 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

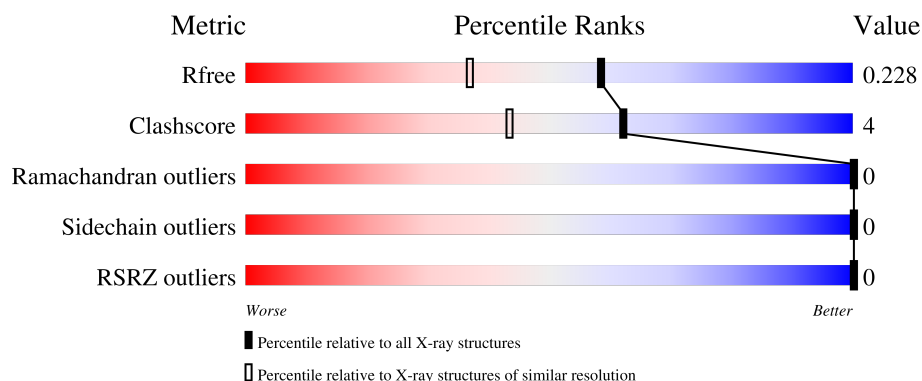
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





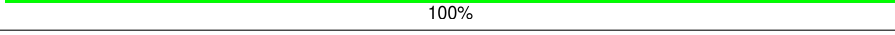
The reported resolution of this entry is 1.73 Å.

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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	133	
1	D	133	
1	I	133	
2	B	18	
2	E	18	

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Mol	Chain	Length	Quality of chain
2	J	18	 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6870 atoms, of which 3366 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	119	Total	C	H	N	O	S	39	0	0
			1895	621	944	149	175	6			
1	D	118	Total	C	H	N	O	S	35	0	0
			1890	619	939	149	177	6			
1	I	119	Total	C	H	N	O	S	42	0	0
			1877	617	930	150	174	6			

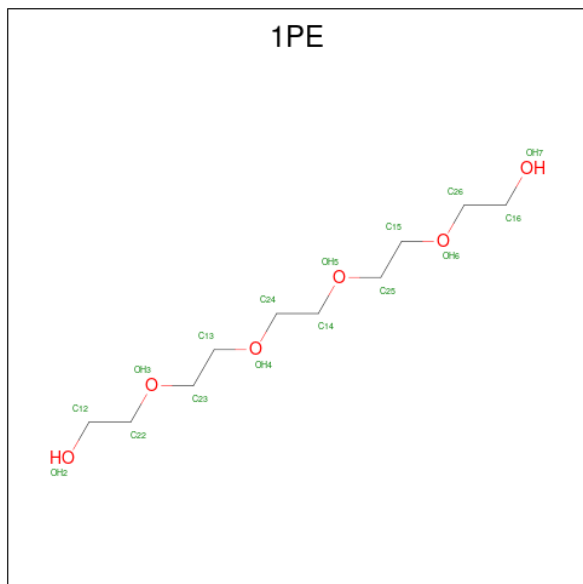
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLN	-	expression tag	UNP O60885
A	37	GLY	-	expression tag	UNP O60885
A	38	PRO	-	expression tag	UNP O60885
A	39	LEU	-	expression tag	UNP O60885
A	40	GLY	-	expression tag	UNP O60885
A	41	SER	-	expression tag	UNP O60885
D	36	GLN	-	expression tag	UNP O60885
D	37	GLY	-	expression tag	UNP O60885
D	38	PRO	-	expression tag	UNP O60885
D	39	LEU	-	expression tag	UNP O60885
D	40	GLY	-	expression tag	UNP O60885
D	41	SER	-	expression tag	UNP O60885
I	36	GLN	-	expression tag	UNP O60885
I	37	GLY	-	expression tag	UNP O60885
I	38	PRO	-	expression tag	UNP O60885
I	39	LEU	-	expression tag	UNP O60885
I	40	GLY	-	expression tag	UNP O60885
I	41	SER	-	expression tag	UNP O60885

- Molecule 2 is a protein called 4.1C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	18	Total 305	C 101	H 155	N 28	O 20	S 1	7	0	1
2	E	18	Total 305	C 101	H 155	N 28	O 20	S 1	7	0	1
2	J	18	Total 305	C 101	H 155	N 28	O 20	S 1	7	0	1

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			38	10	22	6		
3	D	1	Total	C	H	O	2	0
			38	10	22	6		
3	I	1	Total	C	H	O	2	0
			38	10	22	6		
3	I	1	Total	C	H	O	2	0
			38	10	22	6		

- Molecule 4 is water.

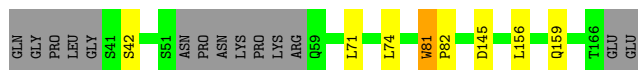
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	7	Total	O	0	0
			7	7		
4	D	39	Total	O	0	0
			39	39		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	8	Total 8	O 8	0	0
4	I	37	Total 37	O 37	0	0
4	J	8	Total 8	O 8	0	0

- Molecule 1: Bromodomain-containing protein 4

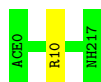


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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|
| GLN | GLY | PRO | LEU | GLY | S41 | S51 | ASN | PRO | ASN | LYS | PRO | LYS | ARG | GLN | T60 | L71 | H77 | A80 | W81 | P82 | A89 | K99 | M107 | K111 | N116 | V147 | E151 | T166 | GLU | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|
| GLM | GLY | PRO | LEU | GLY | S41 | T50 | SER | ASN | PRO | ASN | LYS | PRO | LYS | ARG | Q59 | T60 | L71 | W81 | P82 | D88 | L92 | K112 | T134 | I138 | D144 | K160 | T166 | E167 | GUU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|

- ACEO N11 F15 K16 NH217

- Chain J:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	70.12Å 70.12Å 90.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.75 – 1.73 19.75 – 1.73	Depositor EDS
% Data completeness (in resolution range)	88.2 (19.75-1.73) 90.1 (19.75-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.176 , 0.213 0.190 , 0.228	Depositor DCC
R_{free} test set	2086 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l 0.208 for h,-h-k,-l 0.040 for -k,-h,-l	Xtriage
Reported twinning fraction	0.600 for H, K, L 0.400 for K, H, -L	Depositor
Outliers	0 of 46480 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6197e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NH2, 1PE, ALY, ACE

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	0.83	0/976	1.37	2/1331 (0.2%)
1	D	0.79	1/976 (0.1%)	1.30	2/1332 (0.2%)
1	I	0.75	0/972	1.29	2/1329 (0.2%)
2	B	0.73	0/138	1.08	0/183
2	E	0.68	0/138	0.99	0/183
2	J	0.70	0/138	1.06	0/183
All	All	0.78	1/3338 (0.0%)	1.29	6/4541 (0.1%)

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
2	J	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	HIS	CE1-NE2	-5.05	1.27	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	144	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	145	ASP	CA-CB-CG	6.66	119.25	112.60
1	D	89	ALA	CA-C-N	5.70	127.83	120.88
1	D	89	ALA	C-N-CA	5.70	127.83	120.88
1	A	81	TRP	O-C-N	-5.43	115.61	120.71
1	I	88	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	10	ARG	Sidechain

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	951	944	923	5	0
1	D	951	939	924	10	0
1	I	947	930	905	12	0
2	B	150	155	152	2	0
2	E	150	155	152	0	0
2	J	150	155	152	0	0
3	A	16	22	22	1	0
3	D	16	22	22	0	0
3	I	32	44	44	6	0
4	A	42	0	0	0	0
4	B	7	0	0	0	0
4	D	39	0	0	0	0
4	E	8	0	0	0	0
4	I	37	0	0	0	0
4	J	8	0	0	0	0
All	All	3504	3366	3296	27	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 4.

All (27) 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:I:160:LYS:HZ2	3:I:201:1PE:H222	1.62	0.64
1:D:51:SER:HB3	1:D:116:ASN:HB3	1.79	0.63
1:D:81:TRP:CG	1:D:82:PRO:HD3	2.38	0.58
1:I:112:LYS:HD2	3:I:202:1PE:H252	1.89	0.53
1:I:166:THR:O	1:I:167:GLU:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:LYS:HD3	3:I:202:1PE:H231	1.91	0.51
1:I:112:LYS:HD3	3:I:202:1PE:C23	2.42	0.49
2:B:11:ASN:O	1:D:99:LYS:NZ	2.32	0.48
1:I:81:TRP:CG	1:I:82:PRO:HD3	2.49	0.47
1:D:71:LEU:HD11	1:D:111:LYS:HB2	1.96	0.47
3:I:202:1PE:H132	3:I:202:1PE:H142	1.59	0.47
1:D:80:ALA:HB1	1:D:107:MET:HE1	1.97	0.46
1:A:74:LEU:HD23	1:A:156:LEU:HD22	1.97	0.46
1:D:81:TRP:CD2	1:D:82:PRO:HD3	2.51	0.46
1:A:81:TRP:CG	1:A:82:PRO:HD3	2.51	0.46
1:A:159:GLN:HB3	3:A:201:1PE:H261	1.98	0.45
1:I:59:GLN:C	1:I:60:THR:HG23	2.42	0.45
1:A:71:LEU:C	1:A:71:LEU:HD23	2.42	0.45
1:I:166:THR:O	1:I:167:GLU:O	2.37	0.43
1:I:71:LEU:C	1:I:71:LEU:HD23	2.45	0.42
1:A:42:SER:HA	1:I:92:LEU:HD23	2.01	0.42
1:D:51:SER:HB3	1:D:116:ASN:CB	2.49	0.42
2:B:15:PHE:O	1:D:41:SER:HB2	2.20	0.41
1:I:134:THR:HG22	1:I:138:ILE:HD12	2.02	0.41
1:D:71:LEU:HD23	1:D:71:LEU:C	2.46	0.41
1:I:160:LYS:HZ2	3:I:201:1PE:C22	2.33	0.40
1:D:147:VAL:O	1:D:151:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/133 (86%)	114 (99%)	1 (1%)	0	100	100
1	D	114/133 (86%)	113 (99%)	1 (1%)	0	100	100
1	I	115/133 (86%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	15/18 (83%)	13 (87%)	2 (13%)	0	100	100
2	E	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	J	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
All	All	389/453 (86%)	382 (98%)	7 (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	103/124 (83%)	103 (100%)	0	100	100
1	D	105/124 (85%)	105 (100%)	0	100	100
1	I	101/124 (82%)	101 (100%)	0	100	100
2	B	14/15 (93%)	14 (100%)	0	100	100
2	E	14/15 (93%)	14 (100%)	0	100	100
2	J	14/15 (93%)	14 (100%)	0	100	100
All	All	351/417 (84%)	351 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	93	ASN
1	A	117	ASN
1	A	159	GLN
1	I	62	GLN
1	I	85	GLN
1	I	140	ASN
1	I	159	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	9	2	10,11,12	0.57	0	7,12,14	0.35	0
2	ALY	B	9	2	10,11,12	0.50	0	7,12,14	0.74	0
2	ALY	J	9	2	10,11,12	0.63	0	7,12,14	0.77	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	9	2	-	0/9/10/12	-
2	ALY	B	9	2	-	1/9/10/12	-
2	ALY	J	9	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9	ALY	CG-CD-CE-NZ

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](#)

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	$\# Z > 2$
3	1PE	A	201	-	15,15,15	0.37	0	14,14,14	0.47	0
3	1PE	I	202	-	15,15,15	0.47	0	14,14,14	0.38	0
3	1PE	D	201	-	15,15,15	0.56	0	14,14,14	0.47	0
3	1PE	I	201	-	15,15,15	0.39	0	14,14,14	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	201	-	-	6/13/13/13	-
3	1PE	I	202	-	-	8/13/13/13	-
3	1PE	D	201	-	-	5/13/13/13	-
3	1PE	I	201	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	201	1PE	C13-C23-OH3-C22
3	I	202	1PE	C13-C23-OH3-C22

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Mol	Chain	Res	Type	Atoms
3	I	201	1PE	OH5-C14-C24-OH4
3	I	202	1PE	OH4-C13-C23-OH3
3	I	202	1PE	C14-C24-OH4-C13
3	I	201	1PE	OH2-C12-C22-OH3
3	I	202	1PE	OH7-C16-C26-OH6
3	D	201	1PE	OH4-C13-C23-OH3
3	A	201	1PE	OH4-C13-C23-OH3
3	A	201	1PE	C12-C22-OH3-C23
3	D	201	1PE	OH7-C16-C26-OH6
3	I	202	1PE	OH6-C15-C25-OH5
3	I	201	1PE	OH6-C15-C25-OH5
3	I	202	1PE	C24-C14-OH5-C25
3	D	201	1PE	C23-C13-OH4-C24
3	A	201	1PE	OH6-C15-C25-OH5
3	A	201	1PE	C23-C13-OH4-C24
3	A	201	1PE	C13-C23-OH3-C22
3	D	201	1PE	C14-C24-OH4-C13
3	I	202	1PE	C25-C15-OH6-C26
3	I	202	1PE	OH5-C14-C24-OH4
3	I	201	1PE	C24-C14-OH5-C25
3	A	201	1PE	OH2-C12-C22-OH3
3	D	201	1PE	OH2-C12-C22-OH3
3	I	201	1PE	OH4-C13-C23-OH3
3	I	201	1PE	C15-C25-OH5-C14

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	1PE	1	0
3	I	202	1PE	4	0
3	I	201	1PE	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	119/133 (89%)	-0.95	0 100 100	17, 26, 39, 49	0
1	D	118/133 (88%)	-0.87	0 100 100	19, 28, 44, 58	0
1	I	119/133 (89%)	-0.84	0 100 100	20, 29, 42, 68	0
2	B	15/18 (83%)	-0.87	0 100 100	21, 26, 34, 42	0
2	E	15/18 (83%)	-0.66	0 100 100	26, 30, 35, 40	0
2	J	15/18 (83%)	-0.78	0 100 100	24, 29, 38, 40	0
All	All	401/453 (88%)	-0.87	0 100 100	17, 28, 42, 68	0

There are no RSRZ outliers to report.

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
2	ALY	E	9	12/13	0.98	0.04	20,22,24,29	3
2	ALY	B	9	12/13	0.99	0.03	15,17,24,26	3
2	ALY	J	9	12/13	0.99	0.03	19,25,29,29	3

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
3	1PE	I	202	16/16	0.96	0.05	25,31,37,44	2
3	1PE	I	201	16/16	0.98	0.04	23,26,29,30	2
3	1PE	D	201	16/16	0.98	0.04	21,28,32,35	2
3	1PE	A	201	16/16	0.99	0.03	27,31,34,36	2

6.5 Other polymers [i](#)

There are no such residues in this entry.