wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1ND6
Title	:	Crystal Structures of Human Prostatic Acid Phosphatase in Complex with a Phosphate Ion and alpha-Benzylaminobenzylphosphonic Acid Update the Mechanistic Picture and Offer New Insights into Inhibitor Design
Authors	:	Ortlund, E.; LaCount, M.W.; Lebioda, L.
Deposited on	:	2002-12-07
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

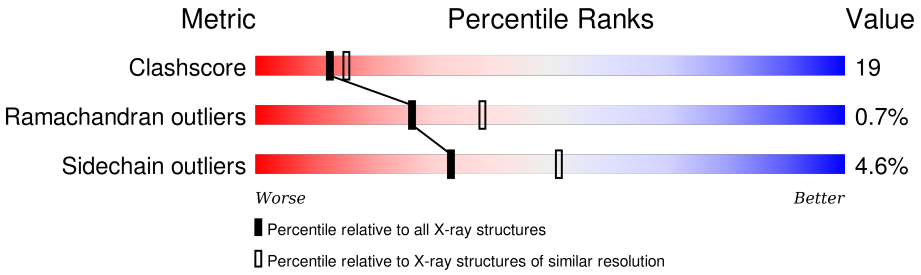
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	354	60% 34%
1	B	354	64% 30%
1	C	354	64% 31%
1	D	354	62% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	5001	X	-	-	-
2	MAN	A	5003	X	-	-	-
3	NAG	A	5005	X	-	-	-
4	NAG	B	5006	X	-	-	-
5	NAG	B	5007	X	-	-	-
5	MAN	B	5010	X	-	-	-
5	MAN	B	5011	X	-	-	-
5	NAG	D	5016	X	-	-	-
6	NAG	C	5012	X	-	-	-
6	NAG	C	5013	X	-	-	-
6	MAN	C	5014	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12048 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 prostatic acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	B	343	Total	C	N	O	S	0	0	0
			2807	1811	462	518	16			
1	C	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	D	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			

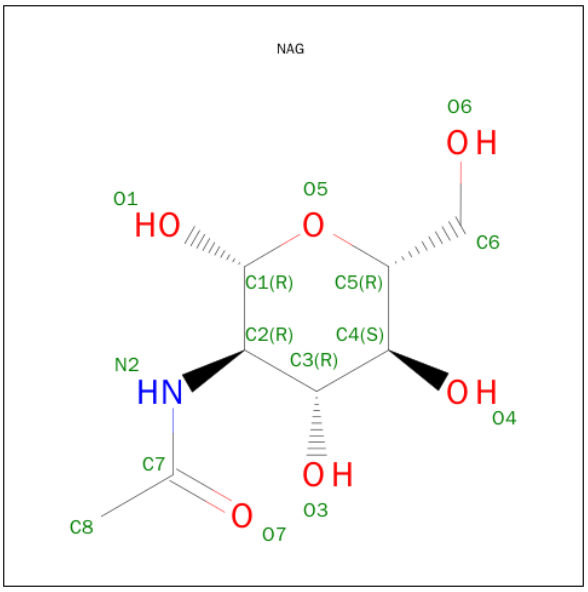
- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			54	28	2	24		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			30	16	2	12		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 15 8 1 6	0	0
4	D	1	Total C N O 15 8 1 6	0	0

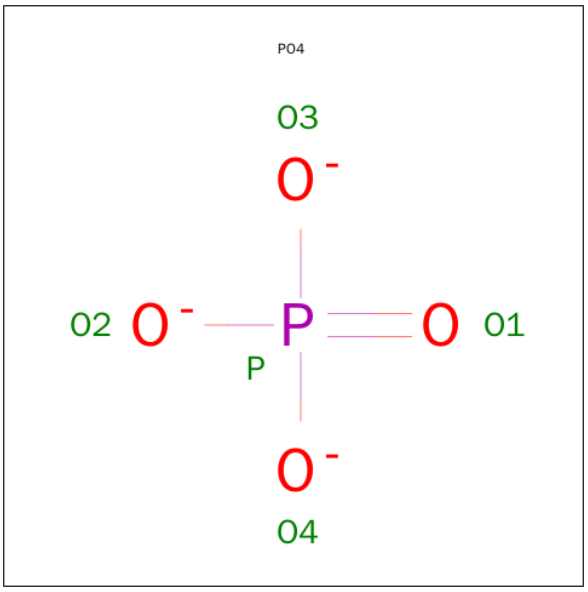
- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total C N O 66 34 2 30	0	0
5	D	5	Total C N O 66 34 2 30	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

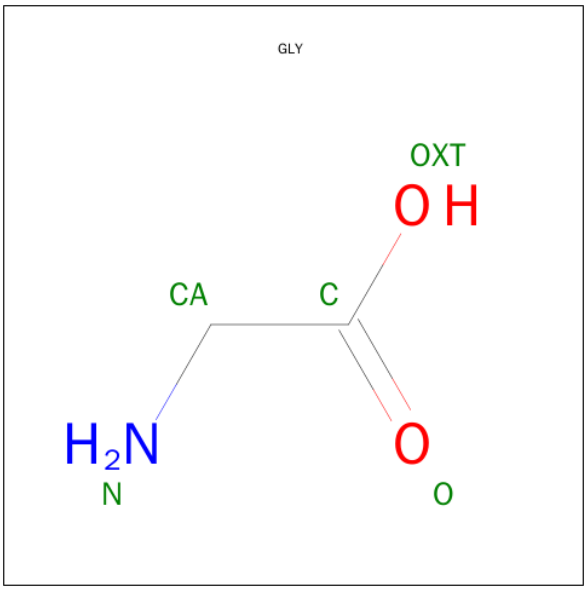
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total C N O 42 22 2 18	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



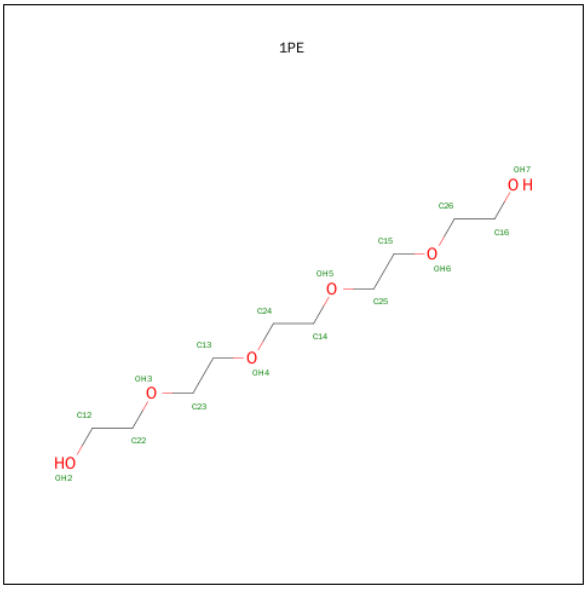
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0

- Molecule 8 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 16 10 6	0	0
9	B	1	Total C O 16 10 6	0	0
9	C	1	Total C O 16 10 6	0	0
9	D	1	Total C O 16 10 6	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	147	Total O 147 147	0	0
10	B	134	Total O 134 134	0	0
10	C	89	Total O 89 89	0	0
10	D	94	Total O 94 94	0	0

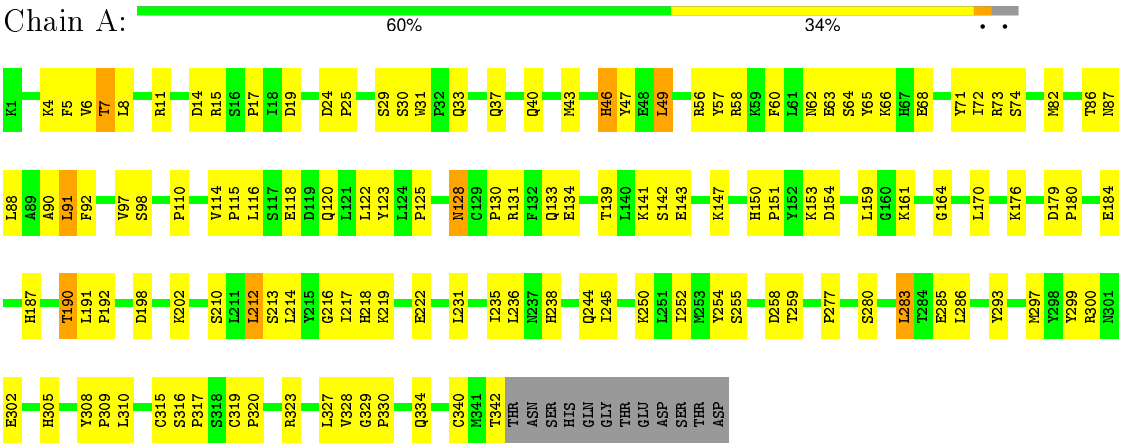
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

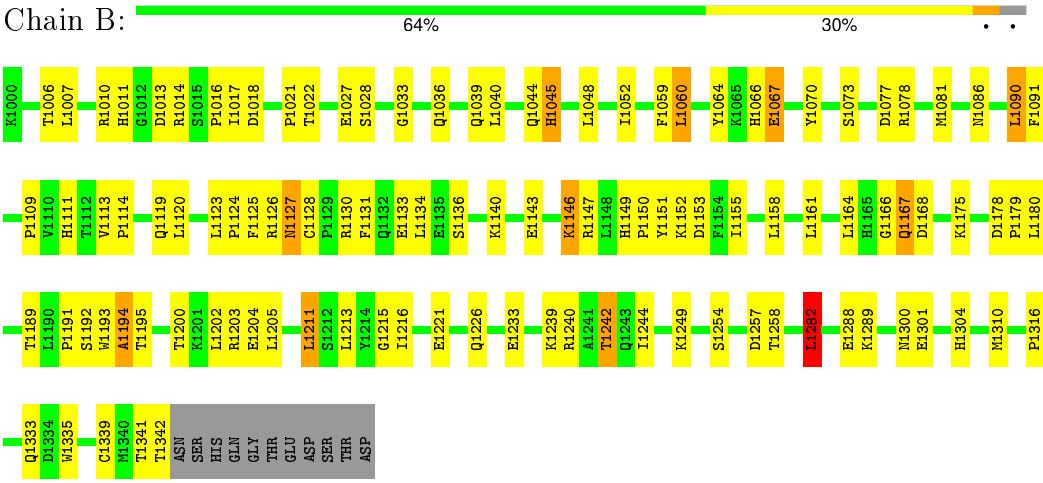
- Molecule 1: prostatic acid phosphatase

Chain A:



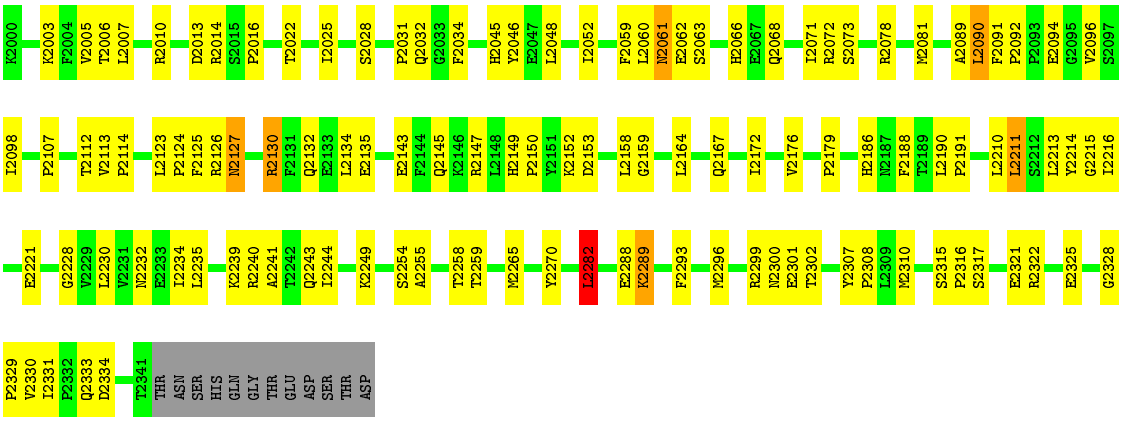
- Molecule 1: prostatic acid phosphatase

Chain B:



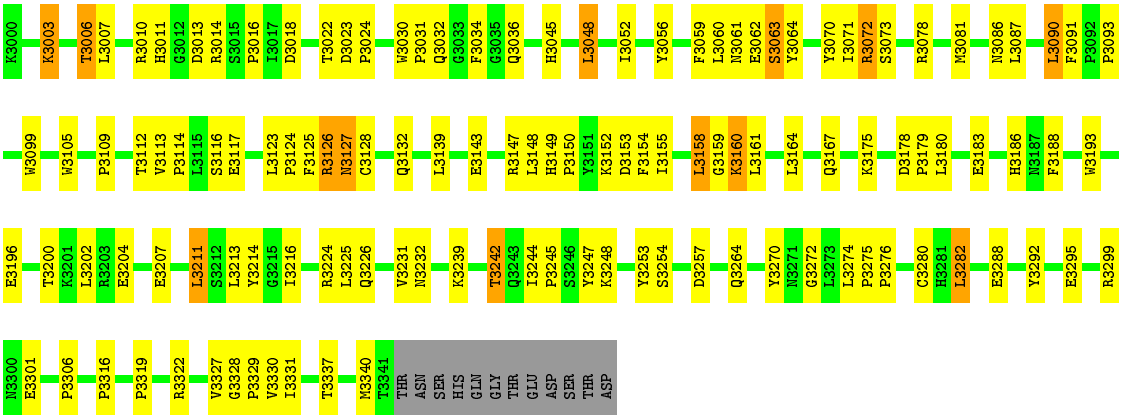
- Molecule 1: prostatic acid phosphatase

Chain C:



- Molecule 1: prostatic acid phosphatase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.89Å 203.32Å 70.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.27 – 2.40	Depositor
% Data completeness (in resolution range)	90.6 (35.27-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12048	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 1PE, NAG, MAN

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	0.35	0/2882	0.59	0/3914
1	B	0.34	0/2889	0.60	1/3924 (0.0%)
1	C	0.34	0/2882	0.59	1/3914 (0.0%)
1	D	0.34	0/2882	0.59	0/3914
All	All	0.34	0/11535	0.59	2/15666 (0.0%)

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	A	2	0
3	A	1	0
5	B	3	0
5	D	1	0
6	C	3	0
All	All	10	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2282	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	1282	LEU	CA-CB-CG	5.68	128.36	115.30

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5001	NAG	C1

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Mol	Chain	Res	Type	Atom
2	A	5003	MAN	C1
3	A	5005	NAG	C1
5	B	5007	NAG	C1
5	B	5010	MAN	C1

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	2800	0	2749	110	0
1	B	2807	0	2753	122	0
1	C	2800	0	2747	115	0
1	D	2800	0	2746	118	0
2	A	54	0	47	4	0
3	A	30	0	27	1	0
4	B	15	0	14	1	0
4	D	15	0	14	0	0
5	B	66	0	57	2	0
5	D	66	0	59	1	0
6	C	42	0	37	4	0
7	A	5	0	0	1	0
7	B	5	0	0	1	0
7	C	5	0	0	1	0
7	D	5	0	0	1	0
8	B	5	0	2	3	0
9	A	16	0	22	1	0
9	B	16	0	22	3	0
9	C	16	0	22	2	0
9	D	16	0	22	2	0
10	A	147	0	0	7	0
10	B	134	0	0	9	0
10	C	89	0	0	3	0
10	D	94	0	0	4	0
All	All	12048	0	11340	445	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 19.

The worst 5 of 445 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:1304:HIS:HB3	8:B:9000:GLY:OXT	1.47	1.12
1:B:1146:LYS:HE3	1:B:1146:LYS:HA	1.38	1.03
1:C:2310:MET:HE2	1:C:2315:SER:HA	1.45	0.98
1:B:1127:ASN:HD22	1:B:1127:ASN:H	1.02	0.97
1:C:2127:ASN:H	1:C:2127:ASN:HD22	1.07	0.97

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	340/354 (96%)	319 (94%)	19 (6%)	2 (1%)	30	43
1	B	341/354 (96%)	311 (91%)	28 (8%)	2 (1%)	30	43
1	C	340/354 (96%)	310 (91%)	28 (8%)	2 (1%)	30	43
1	D	340/354 (96%)	318 (94%)	19 (6%)	3 (1%)	21	30
All	All	1361/1416 (96%)	1258 (92%)	94 (7%)	9 (1%)	26	38

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	B	1064	TYR
1	C	2289	LYS
1	D	3064	TYR
1	A	65	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	314/325 (97%)	295 (94%)	19 (6%)	23	36
1	B	315/325 (97%)	304 (96%)	11 (4%)	43	64
1	C	314/325 (97%)	300 (96%)	14 (4%)	34	52
1	D	314/325 (97%)	300 (96%)	14 (4%)	34	52
All	All	1257/1300 (97%)	1199 (95%)	58 (5%)	33	51

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1167	GLN
1	C	2060	LEU
1	D	3160	LYS
1	B	1211	LEU
1	B	1282	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1303	GLN
1	C	2061	ASN
1	D	3186	HIS
1	B	1333	GLN
1	C	2066	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

19 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	5000	1,2	15,15,15	0.47	0	17,21,21	0.77	0
2	NAG	A	5001	2	15,15,15	0.51	0	17,21,21	0.61	0
2	MAN	A	5002	2	12,12,12	0.48	0	17,17,17	0.47	0
2	MAN	A	5003	2	12,12,12	0.37	0	17,17,17	0.69	0
3	NAG	A	5004	1,3	15,15,15	0.41	0	17,21,21	0.74	1 (5%)
3	NAG	A	5005	3	15,15,15	0.41	0	17,21,21	0.58	0
5	NAG	B	5007	1,5	15,15,15	0.47	0	17,21,21	0.65	0
5	NAG	B	5008	5	15,15,15	0.56	0	17,21,21	0.65	0
5	MAN	B	5009	5	12,12,12	0.52	0	17,17,17	0.59	0
5	MAN	B	5010	5	12,12,12	0.37	0	17,17,17	0.43	0
5	MAN	B	5011	5	12,12,12	0.36	0	17,17,17	0.46	0
6	NAG	C	5012	1,6	15,15,15	0.52	0	17,21,21	1.25	2 (11%)
6	NAG	C	5013	6	15,15,15	0.81	0	17,21,21	1.05	1 (5%)
6	MAN	C	5014	6	12,12,12	0.50	0	17,17,17	0.43	0
5	NAG	D	5016	1,5	15,15,15	0.44	0	17,21,21	0.62	0
5	NAG	D	5017	5	15,15,15	0.44	0	17,21,21	0.67	0
5	MAN	D	5018	5	12,12,12	0.44	0	17,17,17	0.49	0
5	MAN	D	5019	5	12,12,12	0.47	0	17,17,17	0.41	0
5	MAN	D	5020	5	12,12,12	0.29	0	17,17,17	0.67	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	NAG	A	5000	1,2	-	0/6/26/26	0/1/1/1
2	NAG	A	5001	2	1/1/6/7	0/6/26/26	0/1/1/1
2	MAN	A	5002	2	-	0/2/22/22	0/1/1/1
2	MAN	A	5003	2	1/1/5/5	0/2/22/22	0/1/1/1
3	NAG	A	5004	1,3	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	5005	3	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	B	5007	1,5	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	B	5008	5	-	0/6/26/26	0/1/1/1
5	MAN	B	5009	5	-	0/2/22/22	0/1/1/1
5	MAN	B	5010	5	1/1/5/5	0/2/22/22	0/1/1/1
5	MAN	B	5011	5	1/1/5/5	0/2/22/22	0/1/1/1
6	NAG	C	5012	1,6	1/1/6/7	0/6/26/26	0/1/1/1
6	NAG	C	5013	6	1/1/6/7	0/6/26/26	0/1/1/1
6	MAN	C	5014	6	1/1/5/5	0/2/22/22	0/1/1/1
5	NAG	D	5016	1,5	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	D	5017	5	-	0/6/26/26	0/1/1/1
5	MAN	D	5018	5	-	0/2/22/22	0/1/1/1
5	MAN	D	5019	5	-	0/2/22/22	0/1/1/1
5	MAN	D	5020	5	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5004	NAG	O1-C1-O5	-2.18	104.28	110.25
6	C	5012	NAG	O4-C4-C3	-2.05	105.71	110.34
6	C	5013	NAG	C3-C4-C5	2.56	114.66	110.20
6	C	5012	NAG	C4-C3-C2	3.46	115.22	110.43

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	5011	MAN	C1
5	D	5016	NAG	C1
3	A	5005	NAG	C1
5	B	5010	MAN	C1
6	C	5013	NAG	C1

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5000	NAG	3	0
2	A	5001	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5002	MAN	1	0
2	A	5003	MAN	1	0
3	A	5004	NAG	1	0
5	B	5008	NAG	2	0
5	B	5009	MAN	2	0
6	C	5012	NAG	3	0
6	C	5013	NAG	1	0
6	C	5014	MAN	1	0
5	D	5016	NAG	1	0

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	$\#\|Z\| > 2$
9	1PE	A	6000	-	15,15,15	0.80	0	14,14,14	1.48	4 (28%)
7	PO4	A	8000	-	4,4,4	1.09	0	6,6,6	0.27	0
4	NAG	B	5006	1	15,15,15	0.38	0	17,21,21	0.72	0
9	1PE	B	7000	-	15,15,15	0.76	0	14,14,14	1.48	4 (28%)
7	PO4	B	8001	-	4,4,4	1.12	0	6,6,6	0.27	0
8	GLY	B	9000	-	1,4,4	0.55	0	0,4,4	0.00	-
9	1PE	C	7001	-	15,15,15	0.80	0	14,14,14	1.46	4 (28%)
7	PO4	C	8002	-	4,4,4	1.08	0	6,6,6	0.27	0
4	NAG	D	5015	1	15,15,15	0.44	0	17,21,21	0.75	1 (5%)
9	1PE	D	7002	-	15,15,15	0.81	0	14,14,14	1.46	4 (28%)
7	PO4	D	8003	-	4,4,4	1.01	0	6,6,6	0.27	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
9	1PE	A	6000	-	-	0/13/13/13	0/0/0/0
7	PO4	A	8000	-	-	0/0/0/0	0/0/0/0
4	NAG	B	5006	1	1/1/6/7	0/6/26/26	0/1/1/1
9	1PE	B	7000	-	-	0/13/13/13	0/0/0/0
7	PO4	B	8001	-	-	0/0/0/0	0/0/0/0
8	GLY	B	9000	-	-	0/0/2/2	0/0/0/0
9	1PE	C	7001	-	-	0/13/13/13	0/0/0/0
7	PO4	C	8002	-	-	0/0/0/0	0/0/0/0
4	NAG	D	5015	1	-	0/6/26/26	0/1/1/1
9	1PE	D	7002	-	-	0/13/13/13	0/0/0/0
7	PO4	D	8003	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5015	NAG	O1-C1-O5	-2.10	104.52	110.25
9	C	7001	1PE	OH3-C22-C12	2.04	119.81	110.43
9	D	7002	1PE	OH3-C22-C12	2.08	119.99	110.43
9	A	6000	1PE	OH3-C22-C12	2.10	120.08	110.43
9	B	7000	1PE	OH3-C22-C12	2.11	120.14	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	5006	NAG	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	6000	1PE	1	0
7	A	8000	PO4	1	0
4	B	5006	NAG	1	0
9	B	7000	1PE	3	0
7	B	8001	PO4	1	0
8	B	9000	GLY	3	0
9	C	7001	1PE	2	0
7	C	8002	PO4	1	0
9	D	7002	1PE	2	0
7	D	8003	PO4	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.