Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 02:28 AM GMT

PDB ID	:	2HAW
Title	:	Crystal structure of family II Inorganic pyrophosphatase in complex with PNP
Authors	:	Fabrichniy, I.P.; Lehtio, L.; Oksanen, E.; Goldman, A.
Deposited on	:	2006-06-13
Resolution	:	1.75 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
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 (1)) were used in the production of this report:

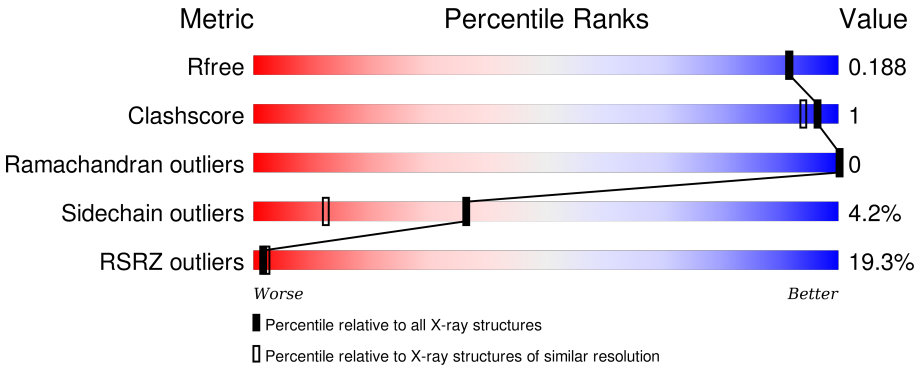
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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.

Mol	Chain	Length	Quality of chain
1	A	309	19%, 94%, 5% ••
1	B	309	19%, 93%, 5% •

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	MG	A	1001	-	-	-	X
3	F	A	3001	-	-	-	X
3	F	B	3002	-	-	-	X
4	SO4	B	4001	-	-	-	X
7	PG4	A	6002	-	-	-	X
7	PG4	B	1002	-	-	-	X
9	GOL	B	5001	-	-	-	X
9	GOL	B	5002	-	-	-	X
9	GOL	B	5003	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5483 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 Manganese-dependent inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	8	0
			2431	1533	403	488	7			
1	B	308	Total	C	N	O	S	0	16	0
			2507	1575	413	511	8			

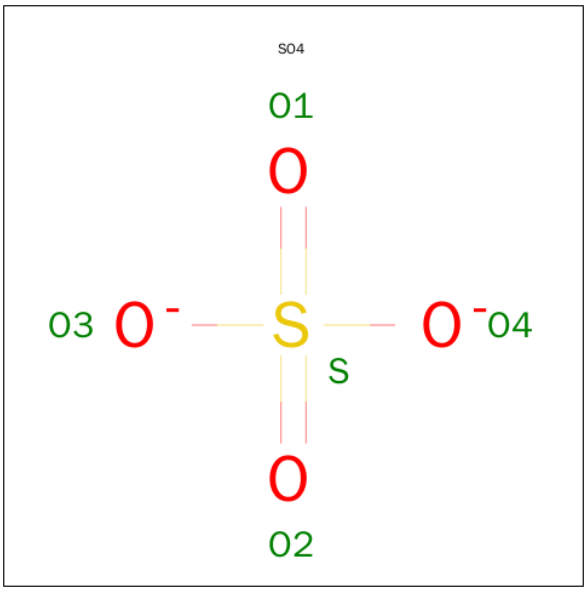
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Mg	0	0
			4	4		
2	A	4	Total	Mg	0	0
			4	4		

- Molecule 3 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	F	0	0
			1	1		
3	A	1	Total	F	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

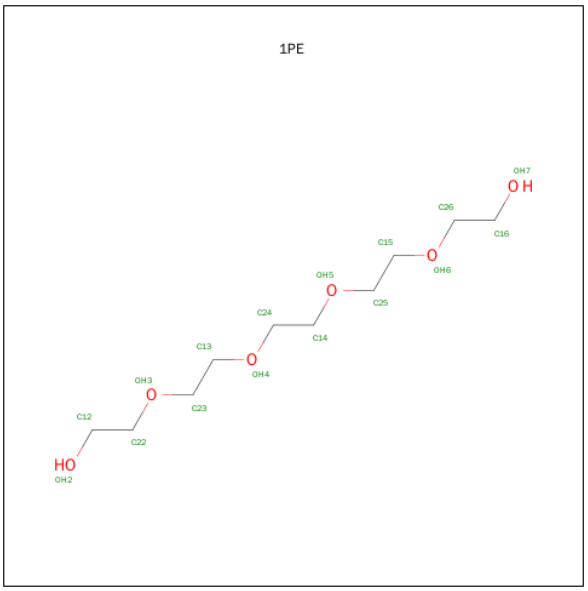


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	1
4	B	1	Total O S 5 4 1	0	1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

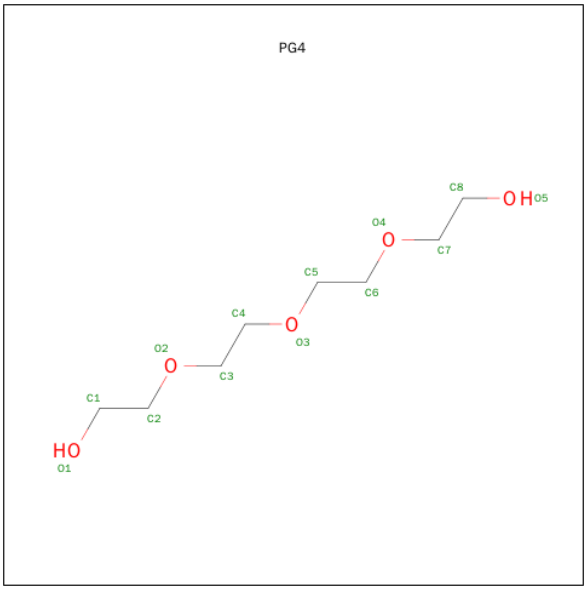
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



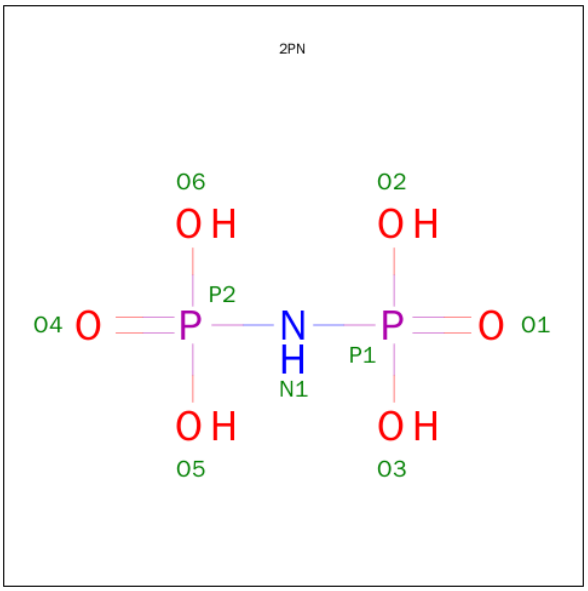
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 16 10 6	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



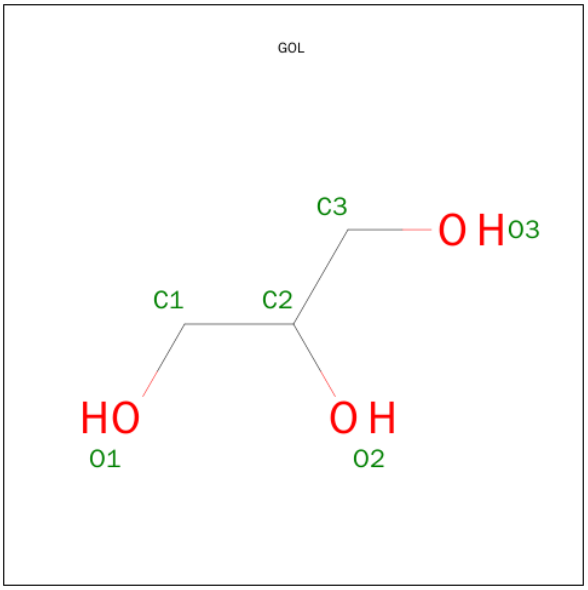
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

- Molecule 8 is IMIDODIPHOSPHORIC ACID (three-letter code: 2PN) (formula: $H_5NO_6P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total N O P 9 1 6 2	0	1
8	B	1	Total N O P 9 1 6 2	0	1

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

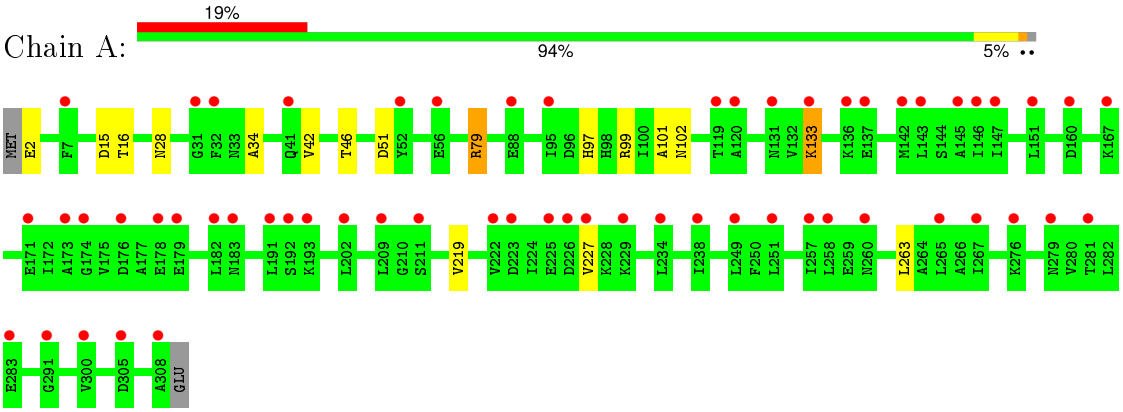
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	166	Total	O	0	0
			166	166		
10	B	270	Total	O	0	0
			270	270		

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.

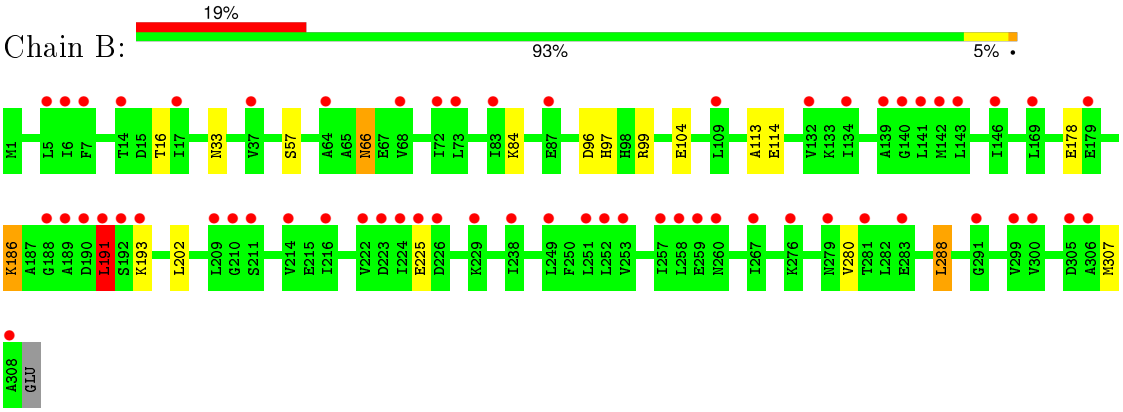
- Molecule 1: Manganese-dependent inorganic pyrophosphatase

Chain A:



- Molecule 1: Manganese-dependent inorganic pyrophosphatase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.01Å 115.87Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 1.75 19.80 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-1.75) 100.0 (19.80-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.186 0.170 , 0.188	Depositor DCC
R_{free} test set	5228 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 104551 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, F, CL, 1PE, PG4, SO4, 2PN

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	0.60	1/2456 (0.0%)	0.68	1/3324 (0.0%)
1	B	0.80	1/2532 (0.0%)	0.78	2/3426 (0.1%)
All	All	0.71	2/4988 (0.0%)	0.73	3/6750 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ASP	CG-OD1	6.18	1.39	1.25
1	B	114	GLU	CB-CG	5.09	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	191	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	288	LEU	CB-CG-CD2	5.04	119.56	111.00

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	2431	0	2472	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2507	0	2530	7	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
6	B	16	0	22	1	0
7	A	13	0	18	1	0
7	B	13	0	18	0	0
8	A	9	0	1	0	0
8	B	9	0	1	0	0
9	B	18	0	24	1	0
10	A	166	0	0	0	0
10	B	270	0	0	0	0
All	All	5483	0	5086	14	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 (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:HD21	1:A:34:ALA:H	1.30	0.79
1:A:101:ALA:HA	1:B:104[B]:GLU:HG2	1.69	0.73
1:B:66:ASN:H	1:B:66:ASN:HD22	1.39	0.71
1:B:66:ASN:H	1:B:66:ASN:ND2	2.03	0.54
1:A:79:ARG:NH2	1:A:102[B]:ASN:OD1	2.42	0.53
6:B:1001:1PE:H251	6:B:1001:1PE:H122	1.94	0.49
1:B:191:LEU:C	1:B:193:LYS:H	2.18	0.47
1:B:96:ASP:O	1:B:113:ALA:HA	2.16	0.45
1:A:15:ASP:HB3	3:A:3001:F:F	2.06	0.45
1:A:133:LYS:CD	1:A:133:LYS:H	2.28	0.45
7:A:6002:PG4:H62	7:A:6002:PG4:H42	1.52	0.44
1:B:186:LYS:HE2	1:B:186:LYS:HB3	1.73	0.43
1:B:57[B]:SER:HB3	9:B:5003:GOL:H2	2.01	0.42
1:A:42:VAL:HG13	1:A:46:THR:HB	2.01	0.42

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	313/309 (101%)	305 (97%)	8 (3%)	0	100	100
1	B	322/309 (104%)	314 (98%)	8 (2%)	0	100	100
All	All	635/618 (103%)	619 (98%)	16 (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	268/262 (102%)	259 (97%)	9 (3%)	44	18
1	B	277/262 (106%)	260 (94%)	17 (6%)	23	5
All	All	545/524 (104%)	519 (95%)	26 (5%)	36	9

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	16	THR
1	A	97	HIS
1	A	99	ARG
1	A	133	LYS
1	A	219[A]	VAL
1	A	219[B]	VAL
1	A	227	VAL

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Mol	Chain	Res	Type
1	A	263	LEU
1	B	16	THR
1	B	33	ASN
1	B	66	ASN
1	B	84	LYS
1	B	97	HIS
1	B	99	ARG
1	B	178[A]	GLU
1	B	178[B]	GLU
1	B	186	LYS
1	B	191	LEU
1	B	202[A]	LEU
1	B	202[B]	LEU
1	B	225[A]	GLU
1	B	225[B]	GLU
1	B	280	VAL
1	B	288	LEU
1	B	307	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	183	ASN
1	A	269	ASN
1	B	33	ASN
1	B	66	ASN
1	B	90	GLN
1	B	284	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
8	2PN	A	2001[A]	2	8,8,8	5.81	6 (75%)	8,13,13	2.95	2 (25%)
4	SO4	A	4002	-	4,4,4	0.26	0	6,6,6	0.43	0
4	SO4	A	4003[B]	2	4,4,4	0.20	0	6,6,6	0.17	0
7	PG4	A	6002	-	12,12,12	0.48	0	11,11,11	0.36	0
6	1PE	B	1001	-	15,15,15	0.55	0	14,14,14	1.06	1 (7%)
7	PG4	B	1002	-	12,12,12	0.63	0	11,11,11	0.47	0
8	2PN	B	2002[A]	2	8,8,8	5.42	5 (62%)	8,13,13	2.19	2 (25%)
4	SO4	B	4001	-	4,4,4	0.29	0	6,6,6	0.97	1 (16%)
4	SO4	B	4004[B]	2	4,4,4	0.33	0	6,6,6	0.10	0
9	GOL	B	5001	-	5,5,5	0.62	0	5,5,5	1.22	1 (20%)
9	GOL	B	5002	-	5,5,5	0.38	0	5,5,5	0.66	0
9	GOL	B	5003	-	5,5,5	0.47	0	5,5,5	0.74	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
8	2PN	A	2001[A]	2	-	0/2/6/6	0/0/0/0
4	SO4	A	4002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	4003[B]	2	-	0/0/0/0	0/0/0/0
7	PG4	A	6002	-	-	0/10/10/10	0/0/0/0
6	1PE	B	1001	-	-	0/13/13/13	0/0/0/0
7	PG4	B	1002	-	-	0/10/10/10	0/0/0/0
8	2PN	B	2002[A]	2	-	1/2/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	4001	-	-	0/0/0/0	0/0/0/0
4	SO4	B	4004[B]	2	-	0/0/0/0	0/0/0/0
9	GOL	B	5001	-	-	0/4/4/4	0/0/0/0
9	GOL	B	5002	-	-	0/4/4/4	0/0/0/0
9	GOL	B	5003	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2001[A]	2PN	P2-N1	-5.86	1.47	1.63
8	A	2001[A]	2PN	P2-O5	-4.49	1.44	1.56
8	B	2002[A]	2PN	P2-O6	-4.37	1.44	1.56
8	A	2001[A]	2PN	P1-O2	2.23	1.62	1.56
8	B	2002[A]	2PN	P1-O2	2.33	1.63	1.56
8	B	2002[A]	2PN	P2-N1	4.33	1.74	1.63
8	A	2001[A]	2PN	P1-O1	5.41	1.52	1.46
8	B	2002[A]	2PN	P2-O4	5.63	1.52	1.46
8	A	2001[A]	2PN	P1-N1	7.64	1.83	1.63
8	A	2001[A]	2PN	P2-O4	11.05	1.58	1.46
8	B	2002[A]	2PN	P1-O1	12.43	1.60	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2001[A]	2PN	O4-P2-N1	-6.68	101.65	111.90
8	B	2002[A]	2PN	O4-P2-N1	-4.94	104.32	111.90
8	A	2001[A]	2PN	O2-P1-O1	-4.70	100.99	113.49
8	B	2002[A]	2PN	O3-P1-O1	-2.33	107.29	113.49
9	B	5001	GOL	O1-C1-C2	-2.01	100.44	110.18
4	B	4001	SO4	O4-S-O3	2.19	117.89	108.98
6	B	1001	1PE	OH4-C24-C14	2.21	120.21	110.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	2002[A]	2PN	O1-P1-N1-P2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6002	PG4	1	0
6	B	1001	1PE	1	0
9	B	5003	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	307/309 (99%)	0.97	59 (19%) 2 2	30, 41, 57, 70	0
1	B	308/309 (99%)	1.00	60 (19%) 1 2	33, 40, 64, 80	0
All	All	615/618 (99%)	0.98	119 (19%) 2 2	30, 40, 60, 80	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	7.0
1	B	192	SER	6.8
1	A	308	ALA	5.1
1	B	308	ALA	4.9
1	A	258	LEU	4.8
1	A	143	LEU	4.6
1	A	193	LYS	4.4
1	B	191	LEU	4.4
1	A	147	ILE	4.4
1	A	211	SER	4.3
1	A	171	GLU	4.2
1	B	226[A]	ASP	4.2
1	B	279[A]	ASN	4.2
1	A	145	ALA	4.2
1	A	305	ASP	4.1
1	B	291	GLY	3.9
1	A	279	ASN	3.8
1	B	210	GLY	3.8
1	A	225	GLU	3.7
1	A	222	VAL	3.6
1	A	257	ILE	3.6
1	B	223	ASP	3.6
1	A	283	GLU	3.6
1	A	176	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	222	VAL	3.6
1	B	257	ILE	3.6
1	B	211	SER	3.5
1	A	251	LEU	3.5
1	A	209	LEU	3.5
1	B	260	ASN	3.5
1	B	252	LEU	3.5
1	A	32	PHE	3.5
1	B	306	ALA	3.4
1	A	31	GLY	3.4
1	A	192	SER	3.4
1	B	188	GLY	3.4
1	A	179	GLU	3.3
1	A	191	LEU	3.3
1	A	41	GLN	3.3
1	A	146	ILE	3.3
1	B	146	ILE	3.2
1	B	132	VAL	3.1
1	A	182	LEU	3.1
1	B	141	LEU	3.1
1	B	251	LEU	3.1
1	A	174	GLY	3.0
1	B	283	GLU	3.0
1	A	281	THR	3.0
1	B	143	LEU	3.0
1	A	229	LYS	3.0
1	B	193	LYS	3.0
1	A	173	ALA	3.0
1	B	224	ILE	3.0
1	B	5	LEU	2.9
1	B	169	LEU	2.9
1	B	225[A]	GLU	2.8
1	B	7	PHE	2.8
1	A	234	LEU	2.8
1	B	73	LEU	2.8
1	A	142	MET	2.8
1	B	68	VAL	2.8
1	A	167	LYS	2.8
1	A	120	ALA	2.7
1	B	281	THR	2.7
1	B	139	ALA	2.7
1	B	216	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	178	GLU	2.7
1	B	253	VAL	2.7
1	A	52	TYR	2.7
1	B	37	VAL	2.6
1	B	209	LEU	2.6
1	A	136	LYS	2.5
1	A	223	ASP	2.5
1	A	226	ASP	2.5
1	A	238	ILE	2.5
1	A	56	GLU	2.5
1	A	249	LEU	2.5
1	A	7	PHE	2.5
1	B	259	GLU	2.5
1	B	190	ASP	2.4
1	B	6	ILE	2.4
1	B	72	ILE	2.4
1	A	227	VAL	2.4
1	A	183	ASN	2.4
1	A	95	ILE	2.4
1	A	267	ILE	2.4
1	B	134	ILE	2.4
1	A	133	LYS	2.4
1	B	229	LYS	2.4
1	A	137	GLU	2.3
1	B	179	GLU	2.3
1	A	151	LEU	2.3
1	A	88[A]	GLU	2.3
1	A	131	ASN	2.3
1	A	160	ASP	2.3
1	A	300	VAL	2.3
1	A	276	LYS	2.2
1	B	276	LYS	2.2
1	B	305	ASP	2.2
1	B	300	VAL	2.2
1	A	291	GLY	2.2
1	A	265	LEU	2.2
1	B	64	ALA	2.2
1	B	140	GLY	2.2
1	A	202[A]	LEU	2.2
1	A	119	THR	2.1
1	B	238	ILE	2.1
1	B	17	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	142	MET	2.1
1	B	249	LEU	2.1
1	B	267	ILE	2.1
1	B	109	LEU	2.1
1	B	214	VAL	2.0
1	B	299	VAL	2.0
1	B	83	ILE	2.0
1	B	87[A]	GLU	2.0
1	B	189	ALA	2.0
1	A	260	ASN	2.0
1	B	14	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	F	A	3001	1/1	0.98	0.33	23.72	35,35,35,35	0
3	F	B	3002	1/1	0.99	0.20	6.78	27,27,27,27	0
4	SO4	B	4001	5/5	0.97	0.29	5.67	51,55,60,63	0
9	GOL	B	5001	6/6	0.84	0.35	5.39	42,54,60,66	0
7	PG4	B	1002	13/13	0.76	0.21	3.19	48,56,81,82	0
2	MG	A	1001	1/1	0.93	0.15	2.88	32,32,32,32	0
9	GOL	B	5002	6/6	0.83	0.26	2.79	72,77,77,79	0
9	GOL	B	5003	6/6	0.84	0.24	2.64	53,62,68,69	0
7	PG4	A	6002	13/13	0.77	0.22	2.52	64,72,82,82	0
6	1PE	B	1001	16/16	0.87	0.16	1.29	44,54,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	2PN	A	2001[A]	9/9	0.98	0.12	0.50	29,32,34,34	9
2	MG	A	1002	1/1	0.95	0.10	-0.62	33,33,33,33	0
4	SO4	A	4003[B]	5/5	0.99	0.10	-0.64	28,29,30,30	5
2	MG	B	1005	1/1	0.99	0.10	-1.16	27,27,27,27	0
8	2PN	B	2002[A]	9/9	0.99	0.09	-1.19	23,28,29,31	9
2	MG	B	1006	1/1	0.98	0.07	-2.04	27,27,27,27	0
4	SO4	B	4004[B]	5/5	0.99	0.08	-2.16	31,31,32,32	5
2	MG	A	1003	1/1	0.98	0.15	-	35,35,35,35	1
4	SO4	A	4002	5/5	0.85	0.35	-	84,85,87,88	0
2	MG	B	1008	1/1	0.96	0.26	-	33,33,33,33	1
5	CL	A	6001	1/1	0.77	0.11	-	86,86,86,86	0
2	MG	A	1004	1/1	0.92	0.48	-	42,42,42,42	1
2	MG	B	1007	1/1	0.99	0.16	-	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.