Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 05:34 PM EDT

PDB ID	:	4PVB
Title	:	Crystal structure of Aminopeptidase N in complex with the phosphonic acid analogue of leucine (D-(S)-LeuP)
Authors	:	Nocek, B.; Vassiliou, S.; Berlicki, L.; Mulligan, R.; Mucha, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2014-03-16
Resolution	:	2.10 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 (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:

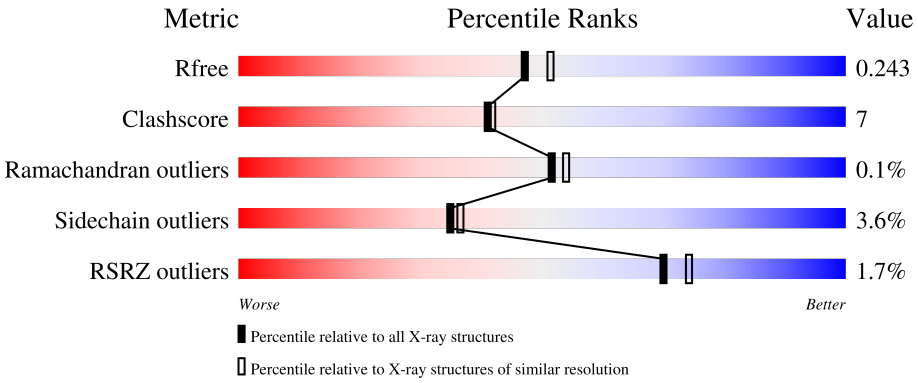
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

2 Entry composition

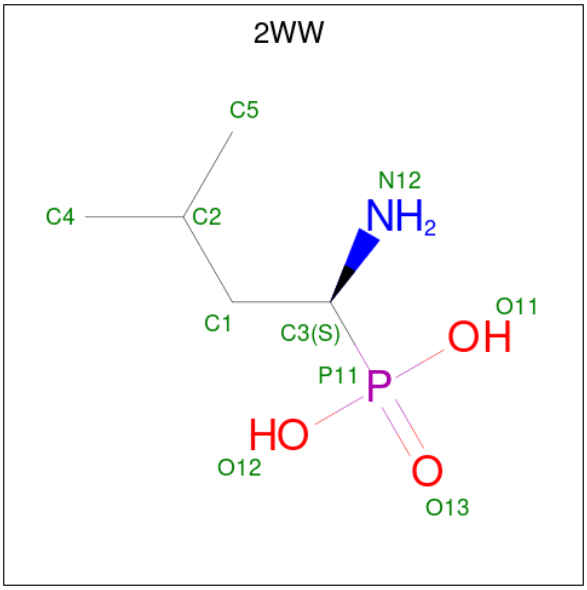
There are 6 unique types of molecules in this entry. The entry contains 7259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminopeptidase N.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	864	6864	4352	1186	1303	5	18	0	1	0

- Molecule 2 is [(1S)-1-amino-3-methylbutyl]phosphonic acid (three-letter code: 2WW) (formula: $C_5H_{14}NO_3P$).

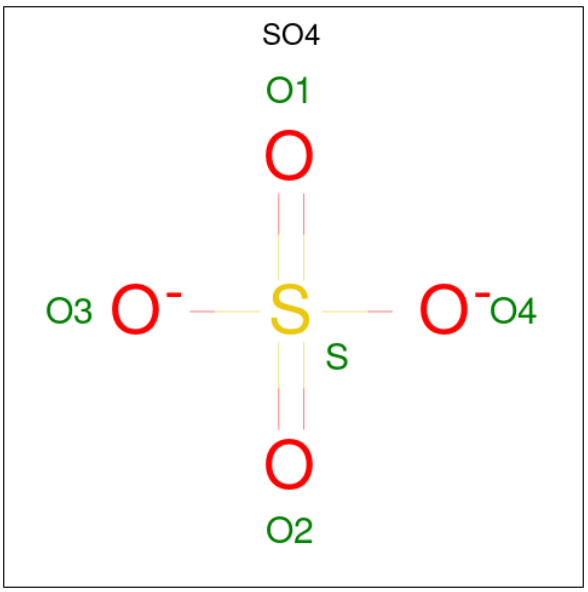


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	10	5	1	3	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

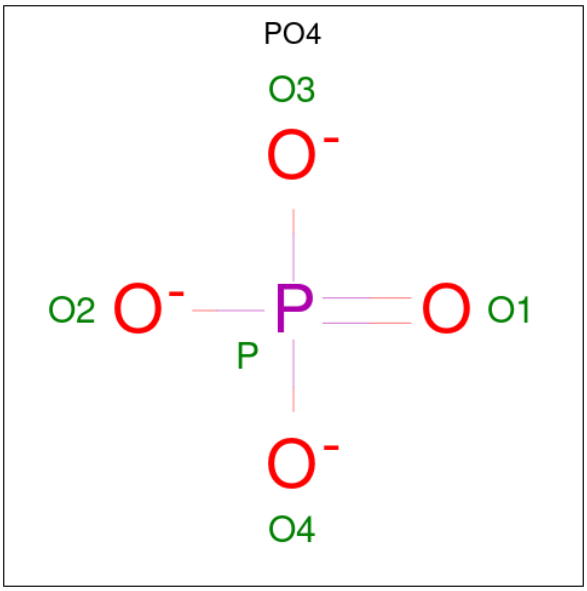
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

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



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	351	Total O 354 354	0	3

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	224.26Å 224.26Å 57.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.00 – 2.10 32.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (32.00-2.10) 85.9 (32.37-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.233 0.191 , 0.243	Depositor DCC
R_{free} test set	2753 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7259	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, 2WW, SO4

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	0.86	1/7001 (0.0%)	0.89	4/9463 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	GLU	CD-OE1	5.18	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	277	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	85	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	85	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	6864	0	6716	97	0
2	A	10	0	13	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	0	0	0
5	A	5	0	0	0	0
6	A	354	0	0	12	0
All	All	7259	0	6729	97	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 7.

All (97) 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:453:ASN:HD21	1:A:520:THR:HG23	1.38	0.88
1:A:655:ASN:OD1	1:A:679:ARG:CD	2.28	0.82
1:A:508:THR:H	1:A:512:GLN:HE22	1.28	0.82
1:A:655:ASN:OD1	1:A:679:ARG:HD2	1.82	0.80
1:A:453:ASN:ND2	1:A:520:THR:HG23	1.98	0.77
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.50	0.76
1:A:438:GLN:HE22	1:A:473:GLN:H	1.34	0.74
1:A:322:ARG:HG2	1:A:322:ARG:NH1	2.03	0.73
1:A:31:GLN:H	1:A:31:GLN:NE2	1.89	0.70
1:A:255:ASN:O	1:A:781:ARG:NH2	2.24	0.69
1:A:31:GLN:H	1:A:31:GLN:HE21	1.40	0.69
1:A:553:ASP:O	1:A:559:ARG:HD2	1.94	0.67
1:A:459:VAL:CG1	1:A:507:LEU:HD22	2.26	0.65
1:A:450:LEU:HD12	1:A:454:ILE:O	1.97	0.64
1:A:62:ILE:HD11	1:A:78:ILE:HD13	1.78	0.64
1:A:174:ASP:OD2	1:A:178:LYS:NZ	2.31	0.62
1:A:386:MSE:HE1	1:A:435:TRP:CD2	2.35	0.61
1:A:459:VAL:HG12	1:A:507:LEU:HD22	1.80	0.61
1:A:483:LEU:HD23	1:A:525:PRO:HA	1.82	0.60
1:A:508:THR:H	1:A:512:GLN:NE2	1.98	0.60
1:A:386:MSE:HE1	1:A:435:TRP:CE2	2.36	0.60
1:A:203:ARG:NH2	6:A:1411:HOH:O	2.20	0.60
1:A:256:MSE:HG3	2:A:1001:2WW:H6	1.85	0.58
1:A:588:GLU:HG3	6:A:1101:HOH:O	2.02	0.58
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.17	0.57
1:A:347:HIS:HB2	1:A:374:MSE:HE2	1.87	0.57
1:A:588:GLU:CG	6:A:1101:HOH:O	2.53	0.57
1:A:374:MSE:CE	1:A:378:GLU:HG3	2.37	0.55
1:A:31:GLN:HE21	1:A:31:GLN:N	2.04	0.55
1:A:781:ARG:NE	6:A:1403:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:SER:O	1:A:771:LYS:HE3	2.10	0.51
1:A:115:GLN:OE1	2:A:1001:2WW:H3	2.11	0.51
1:A:427:ILE:HG12	1:A:428:ASN:N	2.24	0.50
1:A:100:LYS:NZ	6:A:1377:HOH:O	2.43	0.50
1:A:115:GLN:NE2	6:A:1129:HOH:O	2.43	0.50
1:A:205:VAL:HG11	1:A:230:MSE:HE1	1.94	0.50
1:A:661:GLN:HG3	1:A:675:TRP:CH2	2.47	0.50
1:A:16:TYR:CD1	1:A:42:PRO:HA	2.46	0.49
1:A:605:ASN:HD22	1:A:606:ALA:N	2.11	0.49
1:A:481:VAL:HG12	1:A:527:LEU:HD23	1.95	0.49
1:A:115:GLN:NE2	1:A:115:GLN:HA	2.28	0.49
1:A:697:VAL:HG22	1:A:704:MSE:HE1	1.95	0.49
1:A:148:TYR:O	1:A:168:HIS:HE1	1.96	0.49
1:A:831[A]:ASN:ND2	6:A:1393:HOH:O	2.46	0.48
1:A:605:ASN:HD22	1:A:606:ALA:H	1.60	0.48
1:A:655:ASN:OD1	1:A:679:ARG:HD3	2.09	0.48
1:A:375:THR:O	1:A:379:LYS:HB3	2.14	0.47
1:A:459:VAL:HG11	1:A:507:LEU:HD22	1.95	0.47
1:A:661:GLN:HB3	1:A:675:TRP:CE2	2.49	0.47
1:A:45:VAL:CG1	1:A:83:SER:OG	2.63	0.47
1:A:309:TRP:HB3	1:A:368:MSE:SE	2.65	0.47
1:A:483:LEU:HD23	1:A:525:PRO:CA	2.45	0.47
1:A:62:ILE:HG12	1:A:67:ALA:HB2	1.97	0.46
1:A:797:GLU:O	1:A:836:HIS:HE1	1.97	0.46
1:A:119:GLU:O	1:A:122:ARG:HG2	2.15	0.46
1:A:206:LYS:HD3	6:A:1380:HOH:O	2.16	0.46
1:A:182:LEU:O	1:A:261:ASN:HB3	2.16	0.46
1:A:509:GLU:HG3	1:A:512:GLN:HG3	1.98	0.46
1:A:553:ASP:OD1	1:A:554:SER:N	2.49	0.46
1:A:860:GLU:O	1:A:864:LYS:HG2	2.16	0.46
1:A:509:GLU:HG2	1:A:512:GLN:NE2	2.31	0.45
1:A:630:LEU:HD13	1:A:837:ARG:HH21	1.82	0.45
1:A:53:GLY:HA3	1:A:126:PHE:CD2	2.52	0.45
1:A:338:ILE:HD11	1:A:557:PHE:HA	1.97	0.45
1:A:648:LEU:HB3	1:A:649:PRO:HD3	1.99	0.45
1:A:52:ASP:O	1:A:126:PHE:HA	2.18	0.44
1:A:250:ALA:HB2	1:A:272:VAL:HG11	2.00	0.44
1:A:509:GLU:CG	1:A:512:GLN:HE21	2.30	0.44
1:A:664:GLN:HA	1:A:666:TYR:CZ	2.53	0.44
1:A:842:LYS:NZ	6:A:1393:HOH:O	2.51	0.44
1:A:374:MSE:HE1	1:A:378:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:O	1:A:114:THR:HA	2.18	0.43
1:A:230:MSE:HG2	1:A:295:TYR:CZ	2.53	0.43
1:A:60:VAL:CG1	1:A:69:TYR:CE2	3.02	0.42
1:A:755:ARG:HG3	6:A:1341:HOH:O	2.18	0.42
1:A:459:VAL:HG12	1:A:507:LEU:CD2	2.48	0.42
1:A:588:GLU:HG2	6:A:1101:HOH:O	2.19	0.42
1:A:366:GLU:HB2	1:A:860:GLU:CD	2.40	0.42
1:A:198:THR:OG1	1:A:204:ASN:ND2	2.53	0.42
1:A:531:PHE:CZ	1:A:534:PRO:HA	2.54	0.41
1:A:598:ILE:HG23	1:A:654:LEU:HD22	2.02	0.41
1:A:767:LEU:HD21	1:A:784:ILE:HD11	2.02	0.41
1:A:9:LYS:NZ	6:A:1257:HOH:O	2.53	0.41
1:A:265:ASN:N	1:A:265:ASN:HD22	2.18	0.41
1:A:509:GLU:CG	1:A:512:GLN:NE2	2.83	0.41
1:A:62:ILE:HD11	1:A:78:ILE:CD1	2.45	0.41
1:A:178:LYS:HB2	1:A:179:PRO:HD2	2.01	0.41
1:A:444:LEU:HD22	1:A:535:VAL:HG21	2.01	0.41
1:A:509:GLU:H	1:A:512:GLN:HE21	1.69	0.41
1:A:653:GLU:O	1:A:657:GLN:HG3	2.21	0.41
1:A:349:PHE:HB2	1:A:350:PRO:HD3	2.03	0.41
1:A:539:TYR:CD2	1:A:540:PRO:HD2	2.56	0.41
1:A:314:LEU:HD21	1:A:412:VAL:HG23	2.02	0.41
1:A:100:LYS:HB2	1:A:815:PHE:HB2	2.03	0.41
1:A:726:ARG:C	1:A:726:ARG:HD3	2.41	0.41
1:A:38:LEU:O	1:A:87:THR:HA	2.22	0.40
1:A:586:LYS:O	1:A:587:HIS:C	2.59	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	863/867 (100%)	838 (97%)	24 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	830	CYS

4.3.2 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	730/715 (102%)	704 (96%)	26 (4%)	35 36

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

Mol	Chain	Res	Type
1	A	31	GLN
1	A	41	GLU
1	A	83	SER
1	A	84	GLU
1	A	164	SER
1	A	177	SER
1	A	219	VAL
1	A	261	ASN
1	A	270	LYS
1	A	289	SER
1	A	322	ARG
1	A	323	ASP
1	A	352	ASP
1	A	462	THR
1	A	496	GLN
1	A	499	ARG
1	A	509	GLU
1	A	517	GLU
1	A	520	THR
1	A	596	LYS

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Mol	Chain	Res	Type
1	A	605	ASN
1	A	679	ARG
1	A	755	ARG
1	A	822	ARG
1	A	856	LYS
1	A	857	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	115	GLN
1	A	168	HIS
1	A	204	ASN
1	A	261	ASN
1	A	265	ASN
1	A	346	GLN
1	A	347	HIS
1	A	438	GLN
1	A	453	ASN
1	A	512	GLN
1	A	605	ASN
1	A	732	GLN
1	A	818	GLN
1	A	836	HIS

4.3.3 RNA

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
4	SO4	A	1005	-	4,4,4	0.31	0	6,6,6	0.51	0
4	SO4	A	1007	-	4,4,4	0.57	0	6,6,6	0.43	0
5	PO4	A	1008	-	4,4,4	0.70	0	6,6,6	1.12	0
4	SO4	A	1004	-	4,4,4	0.37	0	6,6,6	0.73	0
4	SO4	A	1003	-	4,4,4	0.22	0	6,6,6	0.75	0
2	2WW	A	1001	3	8,9,9	4.15	3 (37%)	8,13,13	2.69	3 (37%)
4	SO4	A	1006	-	4,4,4	0.47	0	6,6,6	0.38	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	2WW	A	1001	3	-	6/9/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	2WW	P11-C3	9.87	1.93	1.84
2	A	1001	2WW	P11-O11	-4.96	1.47	1.54
2	A	1001	2WW	P11-O12	-3.37	1.49	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	2WW	C1-C3-N12	5.07	122.15	110.17
2	A	1001	2WW	O12-P11-O11	3.85	118.00	107.64
2	A	1001	2WW	O12-P11-O13	3.22	121.54	113.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	2WW	C1-C3-P11-O11
2	A	1001	2WW	C1-C3-P11-O12
2	A	1001	2WW	C1-C3-P11-O13
2	A	1001	2WW	C2-C1-C3-N12
2	A	1001	2WW	C3-C1-C2-C5
2	A	1001	2WW	C3-C1-C2-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	2WW	2	0

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	846/867 (97%)	-0.24	14 (1%) 70 74	18, 30, 56, 78	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	GLY	3.7
1	A	852	GLU	3.4
1	A	451	LYS	3.3
1	A	182	LEU	3.3
1	A	500	ALA	2.8
1	A	452	ASN	2.5
1	A	582	VAL	2.5
1	A	181	TYR	2.4
1	A	583	GLU	2.4
1	A	453	ASN	2.2
1	A	584	LEU	2.1
1	A	586	LYS	2.1
1	A	578	LEU	2.0
1	A	449	ARG	2.0

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

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

5.3 Carbohydrates

There are no monosaccharides in this entry.

5.4 Ligands

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
3	ZN	A	1002	1/1	0.93	0.05	34,34,34,34	1
4	SO4	A	1007	5/5	0.93	0.23	59,60,65,68	0
4	SO4	A	1006	5/5	0.94	0.21	61,65,73,74	0
4	SO4	A	1005	5/5	0.94	0.26	59,61,67,70	0
2	2WW	A	1001	10/10	0.96	0.14	27,30,34,39	0
4	SO4	A	1004	5/5	0.97	0.08	53,53,60,71	0
5	PO4	A	1008	5/5	0.97	0.06	40,47,55,58	0
4	SO4	A	1003	5/5	0.99	0.08	32,36,39,47	0

5.5 Other polymers

There are no such residues in this entry.