Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID	:	2NXG
Title	:	Structural and mechanistic changes along an engineered path from metallo to non-metallo KDO8P synthase.
Authors	:	Kona, F.; Xu, X.; Martin, P.; Kuzmic, P.; Gatti, D.L.
Deposited on	:	2006-11-17
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references ⓘ) 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 1.95 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.
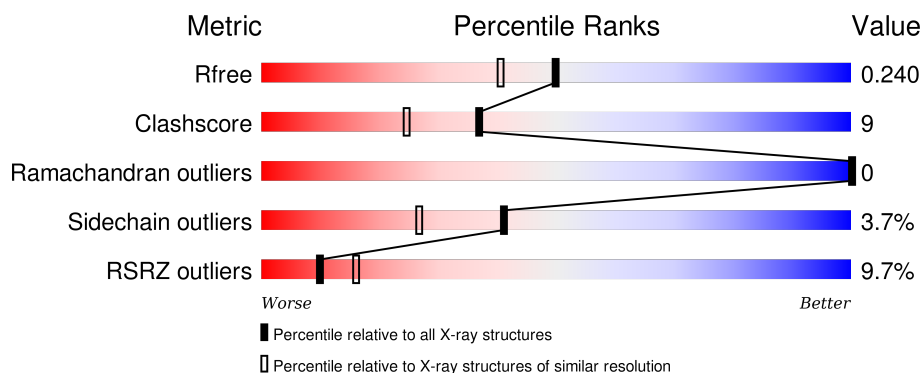
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	263	6% / 80% / 18% / •
1	B	263	13% / 76% / 21% / • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4349 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2065	1332	345	383	5			
1	B	255	Total	C	N	O	S	0	0	0
			2013	1302	336	370	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	ASN	CYS	ENGINEERED	UNP O66496
A	1235	PRO	SER	ENGINEERED	UNP O66496
A	1237	ALA	GLN	ENGINEERED	UNP O66496
B	1011	ASN	CYS	ENGINEERED	UNP O66496
B	1235	PRO	SER	ENGINEERED	UNP O66496
B	1237	ALA	GLN	ENGINEERED	UNP O66496

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).
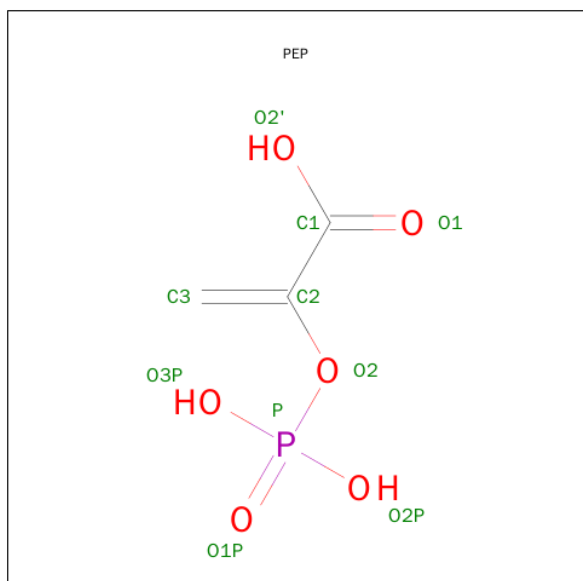
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is ARABINOSE-5-PHOSPHATE (three-letter code: A5P) (formula: $C_5H_{13}O_8P$).
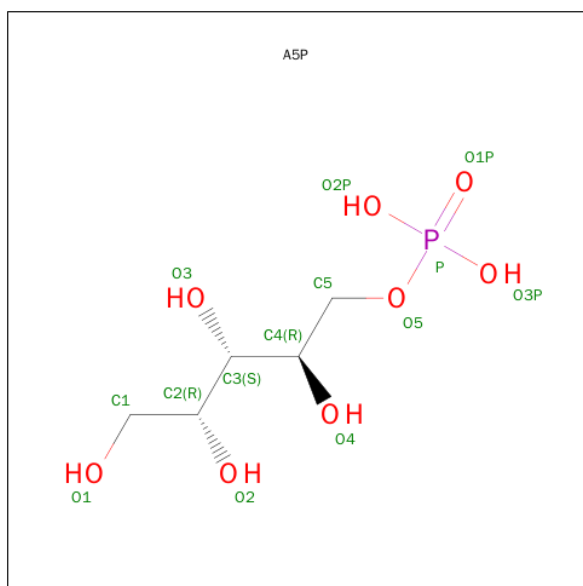
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 4 is (2R,4R,5R,6R,7R)-2,4,5,6,7-PENTAHYDROXY-2,8-BIS(PHOSPHONOOXY)OCTANOIC ACID (three-letter code: 1NT) (formula: $C_8H_{18}O_{15}P_2$).
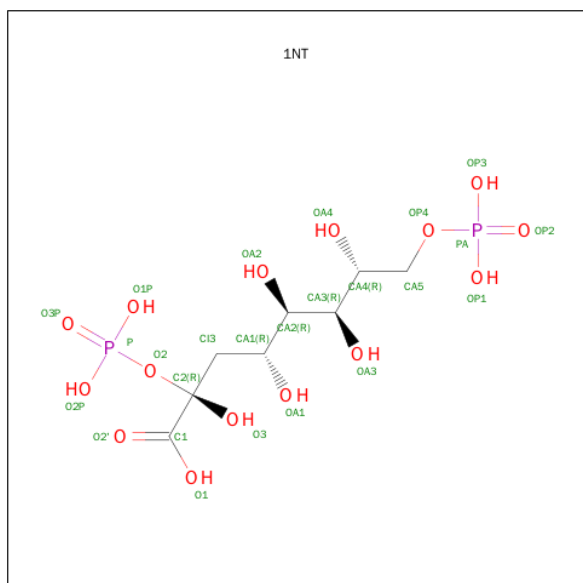
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 25	C 8	O 15	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total 127	O 127	0	0
5	B	95	Total 95	O 95	0	0

3 Residue-property plots ⓘ

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: 2-dehydro-3-deoxyphosphooctonate aldolase
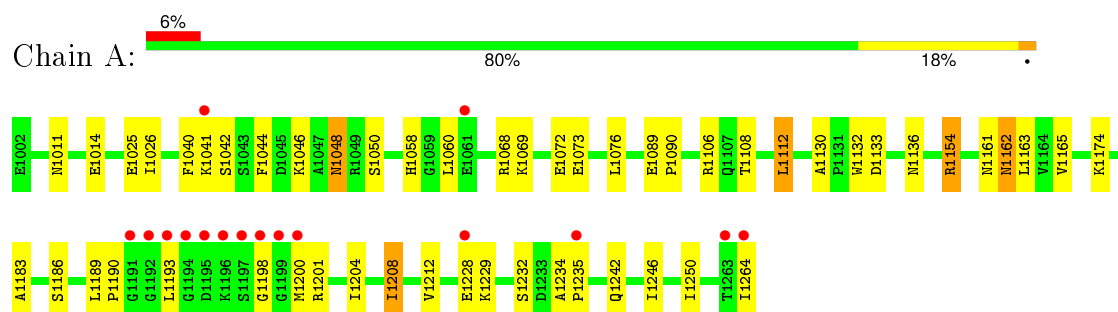
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase
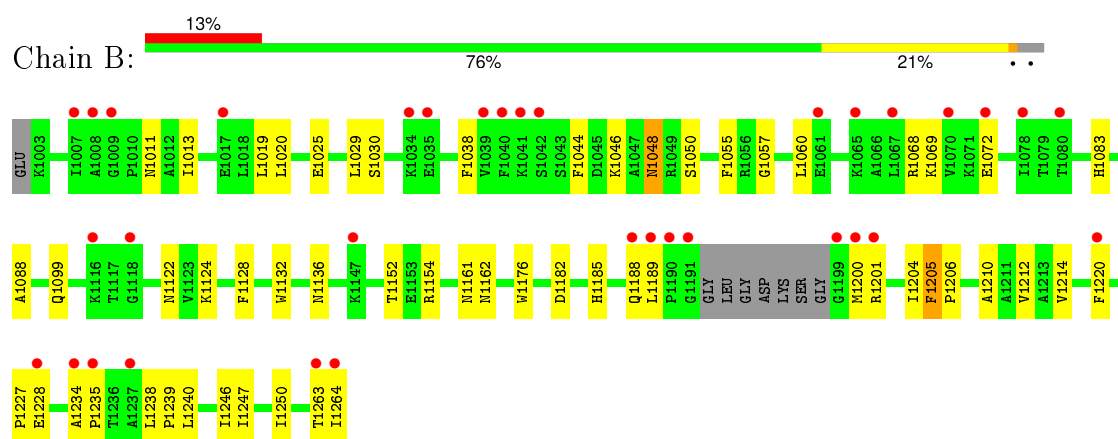
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.16Å 84.16Å 160.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.13 – 1.95 25.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.9 (25.13-1.95) 80.8 (25.13-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.243 0.207 , 0.240	Depositor DCC
R_{free} test set	4244 reflections (10.12%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 45187 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4349	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1NT, A5P, PEP

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	0.39	1/2107 (0.0%)	0.58	0/2842
1	B	0.34	0/2054	0.57	0/2771
All	All	0.37	1/4161 (0.0%)	0.58	0/5613

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1072	GLU	CD-OE2	7.28	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

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	2065	0	2101	38	0
1	B	2013	0	2052	39	0
2	A	10	0	2	3	0
3	A	14	0	10	2	0
4	B	25	0	13	2	0
5	A	127	0	0	2	0
5	B	95	0	0	2	0
All	All	4349	0	4178	78	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 9.

All (78) 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:A:1268:PEP:C3	3:A:1269:A5P:H12	2.09	0.82
1:A:1132:TRP:HE1	1:B:1161:ASN:HD21	1.28	0.82
1:A:1161:ASN:HD21	1:B:1132:TRP:HE1	1.26	0.81
1:B:1025:GLU:HG2	1:B:1240:LEU:HD22	1.68	0.76
1:A:1189:LEU:HD21	1:A:1200:MET:CE	2.23	0.68
1:B:1238:LEU:HD21	1:B:1246:ILE:HD12	1.75	0.67
1:B:1185:HIS:O	1:B:1188:GLN:HG2	1.94	0.67
1:B:1011:ASN:HD21	1:B:1046:LYS:HE2	1.60	0.66
1:A:1234:ALA:HB3	1:A:1235:PRO:HD3	1.78	0.65
1:A:1228:GLU:OE2	1:A:1229:LYS:HG3	1.96	0.65
1:B:1182:ASP:HA	1:B:1220:PHE:HB3	1.79	0.64
1:B:1044:PHE:CZ	1:B:1060:LEU:HD13	2.33	0.63
1:A:1048:ASN:HD22	1:A:1048:ASN:H	1.47	0.63
1:A:1183:ALA:HB2	1:A:1208:ILE:HG13	1.81	0.61
1:B:1044:PHE:CE1	1:B:1060:LEU:HD13	2.35	0.61
4:B:2269:1NT:HI31	4:B:2269:1NT:O2P	1.99	0.61
1:B:1201:ARG:HG3	1:B:1204:ILE:HD12	1.81	0.61
1:A:1011:ASN:HD21	1:A:1046:LYS:HE2	1.67	0.60
1:A:1189:LEU:HD21	1:A:1200:MET:HE3	1.84	0.58
1:B:1205:PHE:HB3	1:B:1206:PRO:HD3	1.86	0.57
1:A:1068:ARG:HB2	1:A:1068:ARG:NH1	2.21	0.54
5:A:3036:HOH:O	1:B:1083:HIS:HD2	1.90	0.54
1:A:1044:PHE:CZ	1:A:1060:LEU:HD23	2.43	0.54
1:A:1068:ARG:HB2	1:A:1068:ARG:HH11	1.72	0.53
1:B:1246:ILE:O	1:B:1250:ILE:HG23	2.08	0.53
1:A:1011:ASN:HD21	1:A:1046:LYS:CE	2.20	0.53
1:A:1212:VAL:HG11	1:A:1250:ILE:HB	1.91	0.53
1:B:1227:PRO:HG2	1:B:1239:PRO:HG3	1.92	0.52
1:B:1048:ASN:H	1:B:1048:ASN:HD22	1.57	0.51
1:B:1011:ASN:HD21	1:B:1046:LYS:CE	2.24	0.51
1:A:1026:ILE:HD12	1:A:1040:PHE:HD1	1.76	0.50
1:A:1154:ARG:HD3	1:A:1154:ARG:O	2.11	0.50
1:A:1026:ILE:HD12	1:A:1040:PHE:CD1	2.47	0.49
1:A:1041:LYS:C	1:A:1041:LYS:HD3	2.33	0.49
1:B:1234:ALA:N	1:B:1235:PRO:HD2	2.28	0.49
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.07	0.49
1:A:1193:LEU:HD13	1:A:1198:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1268:PEP:H32	3:A:1269:A5P:H12	1.94	0.48
1:A:1069:LYS:HE3	1:A:1073:GLU:OE1	2.13	0.47
2:A:1268:PEP:H32	2:A:1268:PEP:O1P	2.13	0.46
1:B:1247:ILE:O	1:B:1250:ILE:HG12	2.15	0.46
1:B:1099:GLN:HE22	1:B:1220:PHE:HE2	1.62	0.46
1:A:1189:LEU:HD21	1:A:1200:MET:HE2	1.97	0.46
1:A:1011:ASN:ND2	1:A:1232:SER:OG	2.48	0.46
1:B:1200:MET:HA	5:B:3072:HOH:O	2.15	0.45
1:B:1055:PHE:CZ	1:B:1057:GLY:HA2	2.51	0.45
1:A:1136:ASN:HB3	1:B:1050:SER:O	2.17	0.45
1:B:1068:ARG:O	1:B:1072:GLU:HG3	2.17	0.45
1:A:1041:LYS:HD3	1:A:1042:SER:N	2.31	0.45
1:B:1263:THR:HG22	1:B:1264:ILE:HG22	1.97	0.45
1:B:1124:LYS:HD3	1:B:1152:THR:HB	1.98	0.45
1:A:1201:ARG:HG3	1:A:1204:ILE:HD12	2.00	0.44
1:B:1189:LEU:HD21	1:B:1200:MET:CE	2.48	0.44
1:B:1210:ALA:O	1:B:1214:VAL:HG23	2.17	0.44
1:A:1242:GLN:O	1:A:1246:ILE:HG12	2.18	0.43
1:A:1108:THR:HG22	1:A:1112:LEU:HD22	2.00	0.43
1:A:1025:GLU:OE1	1:A:1025:GLU:HA	2.17	0.43
1:B:1048:ASN:N	1:B:1048:ASN:HD22	2.15	0.43
1:B:1020:LEU:HD21	1:B:1069:LYS:HG3	2.00	0.43
1:B:1263:THR:O	1:B:1264:ILE:OXT	2.37	0.43
1:B:1013:ILE:HG23	1:B:1019:LEU:HD11	2.01	0.43
1:A:1174:LYS:HD2	1:A:1174:LYS:HA	1.80	0.43
1:A:1089:GLU:HB3	1:A:1090:PRO:CD	2.50	0.42
1:A:1014:GLU:O	1:A:1058:HIS:HE1	2.02	0.42
1:A:1130:ALA:HB3	1:A:1133:ASP:OD2	2.20	0.42
1:B:1068:ARG:HB2	1:B:1068:ARG:NH1	2.34	0.42
5:A:3006:HOH:O	1:B:1128:PHE:HB3	2.20	0.42
1:A:1165:VAL:CG2	1:A:1186:SER:HB3	2.50	0.42
1:A:1050:SER:O	1:B:1136:ASN:HB3	2.20	0.41
1:A:1044:PHE:CE1	1:A:1060:LEU:HD23	2.56	0.41
1:A:1161:ASN:OD1	1:A:1190:PRO:O	2.37	0.41
4:B:2269:1NT:CI3	4:B:2269:1NT:O2P	2.67	0.41
1:B:1212:VAL:HG11	1:B:1250:ILE:HB	2.02	0.41
1:B:1264:ILE:OXT	1:B:1264:ILE:HG23	2.20	0.41
1:B:1030:SER:HA	1:B:1038:PHE:CE1	2.56	0.41
1:B:1189:LEU:HD21	1:B:1200:MET:HE2	2.03	0.40
1:B:1088:ALA:HB3	5:B:3131:HOH:O	2.20	0.40
1:A:1162:ASN:HD22	1:A:1163:LEU:H	1.70	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	261/263 (99%)	257 (98%)	4 (2%)	0	100	100
1	B	251/263 (95%)	240 (96%)	11 (4%)	0	100	100
All	All	512/526 (97%)	497 (97%)	15 (3%)	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	219/219 (100%)	211 (96%)	8 (4%)	41	27
1	B	214/219 (98%)	206 (96%)	8 (4%)	41	27
All	All	433/438 (99%)	417 (96%)	16 (4%)	41	27

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	ASN
1	A	1076	LEU
1	A	1106	ARG
1	A	1112	LEU
1	A	1154	ARG

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Mol	Chain	Res	Type
1	A	1162	ASN
1	A	1208	ILE
1	A	1264	ILE
1	B	1029	LEU
1	B	1048	ASN
1	B	1122	ASN
1	B	1154	ARG
1	B	1162	ASN
1	B	1176	TRP
1	B	1205	PHE
1	B	1228	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	ASN
1	A	1048	ASN
1	A	1058	HIS
1	A	1099	GLN
1	A	1161	ASN
1	A	1162	ASN
1	A	1175	GLN
1	B	1011	ASN
1	B	1048	ASN
1	B	1053	HIS
1	B	1083	HIS
1	B	1122	ASN
1	B	1161	ASN
1	B	1162	ASN

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)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#|Z| > 2$
2	PEP	A	1268	-	5,9,9	1.97	1 (20%)	8,13,13	1.76	2 (25%)
3	A5P	A	1269	-	13,13,13	1.69	2 (15%)	14,18,18	1.53	2 (14%)
4	1NT	B	2269	-	19,24,24	1.39	2 (10%)	19,37,37	0.88	1 (5%)

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	PEP	A	1268	-	-	0/5/9/9	0/0/0/0
3	A5P	A	1269	-	-	0/16/16/16	0/0/0/0
4	1NT	B	2269	-	-	0/25/35/35	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1269	A5P	O1-C1	-4.38	1.23	1.42
3	A	1269	A5P	P-O1P	3.09	1.61	1.51
4	B	2269	1NT	P-O3P	3.10	1.61	1.51
4	B	2269	1NT	O3-C2	3.29	1.43	1.40
2	A	1268	PEP	C3-C2	3.31	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1268	PEP	P-O2-C2	-4.06	113.93	122.96
2	A	1268	PEP	O2-C2-C3	-2.18	120.33	124.73
3	A	1269	A5P	O3P-P-O5	2.15	112.75	106.56
4	B	2269	1NT	OP4-PA-OP2	2.24	112.85	107.14
3	A	1269	A5P	O1-C1-C2	4.74	121.41	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1268	PEP	3	0
3	A	1269	A5P	2	0
4	B	2269	1NT	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(Å²)	Q<0.9
1	A	263/263 (100%)	0.39	16 (6%)	25	34	30, 42, 65, 85	0
1	B	255/263 (96%)	0.58	34 (13%)	4	7	31, 47, 68, 74	0
All	All	518/526 (98%)	0.48	50 (9%)	10	16	30, 44, 67, 85	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1264	ILE	8.4
1	B	1264	ILE	8.1
1	A	1193	LEU	7.5
1	A	1198	GLY	6.9
1	A	1195	ASP	5.9
1	A	1197	SER	5.6
1	A	1263	THR	5.5
1	B	1199	GLY	5.2
1	A	1196	LYS	5.0
1	B	1235	PRO	4.6
1	B	1147	LYS	4.5
1	A	1194	GLY	4.4
1	B	1200	MET	4.1
1	A	1199	GLY	4.0
1	A	1192	GLY	3.9
1	B	1008	ALA	3.9
1	A	1235	PRO	3.7
1	B	1191	GLY	3.7
1	B	1189	LEU	3.6
1	A	1200	MET	3.3
1	B	1237	ALA	3.1
1	B	1035	GLU	3.0
1	B	1228	GLU	3.0
1	B	1040	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1007	ILE	2.8
1	B	1041	LYS	2.8
1	A	1228	GLU	2.8
1	B	1072	GLU	2.8
1	B	1116	LYS	2.7
1	B	1263	THR	2.7
1	B	1078	ILE	2.7
1	B	1188	GLN	2.7
1	B	1061	GLU	2.6
1	B	1067	LEU	2.6
1	B	1190	PRO	2.5
1	B	1070	VAL	2.4
1	B	1234	ALA	2.3
1	B	1042	SER	2.3
1	B	1220	PHE	2.3
1	A	1041	LYS	2.3
1	B	1201	ARG	2.3
1	B	1065	LYS	2.2
1	B	1039	VAL	2.2
1	A	1061	GLU	2.2
1	A	1191	GLY	2.1
1	B	1118	GLY	2.1
1	B	1034	LYS	2.1
1	B	1017	GLU	2.1
1	B	1080	THR	2.1
1	B	1009	GLY	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, 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	LLDF	B-factors(Å²)	Q<0.9
2	PEP	A	1268	10/10	0.94	0.16	0.29	44,51,55,56	0
4	1NT	B	2269	25/25	0.92	0.14	-0.17	50,58,61,61	0
3	A5P	A	1269	14/14	0.89	0.15	-0.22	62,66,69,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.