



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 10:51 AM EDT

PDB ID : 2EF9
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 : 2007-02-22
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

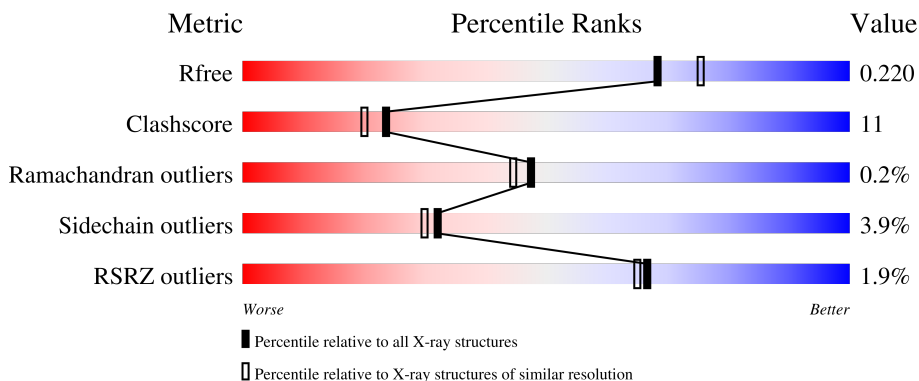
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	267	 3% 75% 21% ..
1	B	267	 3% 73% 22% ..

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
3	A5P	B	2269	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4571 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.

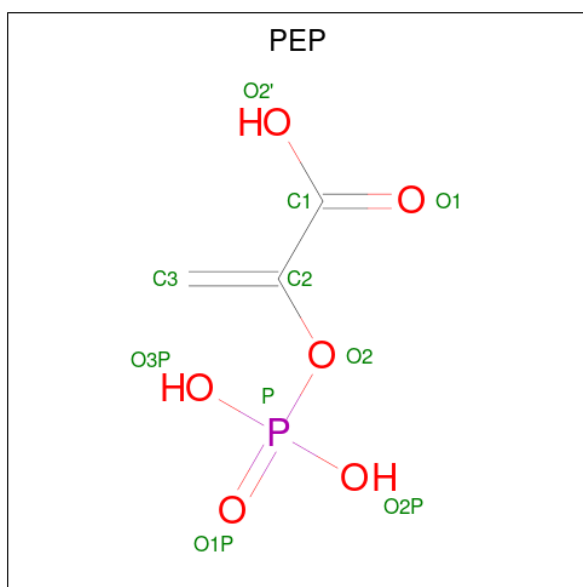
- Molecule 1 is a protein called 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2065	1332	345	382	6	0	0	0
1	B	262	2056	1327	344	379	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

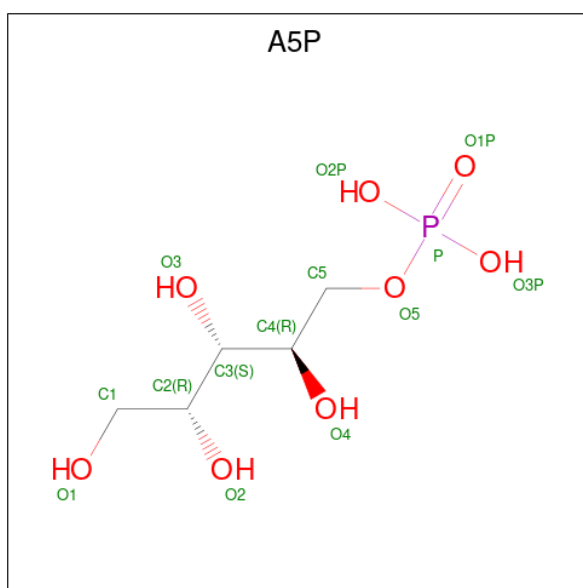
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	PRO	engineered mutation	UNP O66496
A	11	ASN	CYS	engineered mutation	UNP O66496
A	235	PRO	SER	engineered mutation	UNP O66496
A	237	ALA	GLN	engineered mutation	UNP O66496
B	10	MET	PRO	engineered mutation	UNP O66496
B	11	ASN	CYS	engineered mutation	UNP O66496
B	235	PRO	SER	engineered mutation	UNP O66496
B	237	ALA	GLN	engineered mutation	UNP O66496

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C₃H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	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		
3	B	1	Total	C	O	P	0	0
			14	5	8	1		

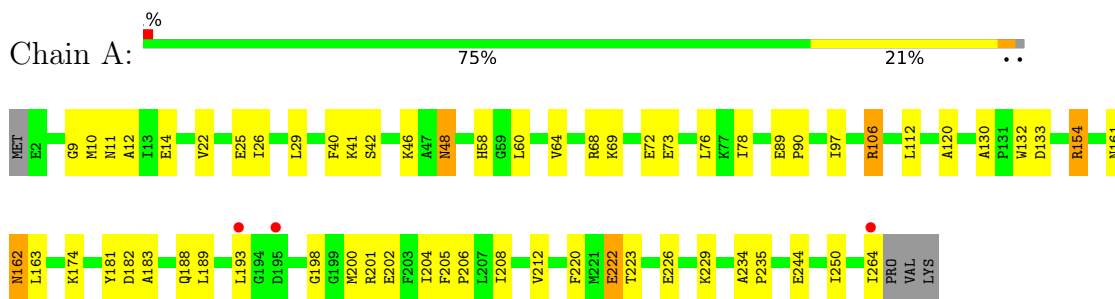
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total 216	O 216	0	0
4	B	186	Total 186	O 186	0	0

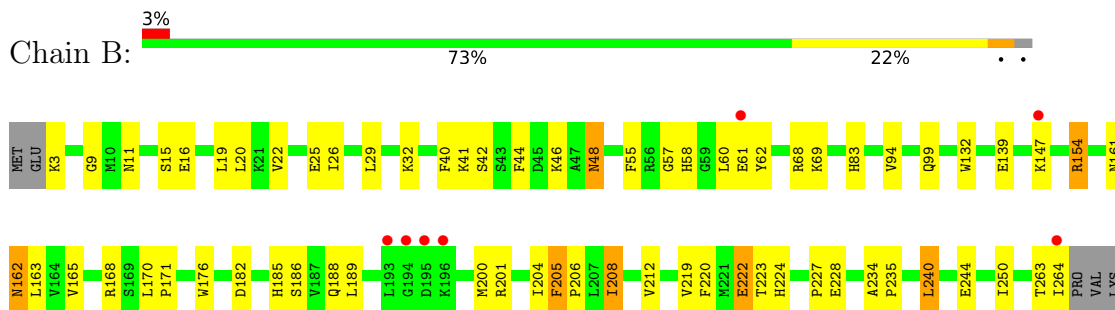
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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	84.57Å 84.57Å 159.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.16 – 2.00 26.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (26.16-2.00) 98.1 (26.16-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.99Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.222 0.183 , 0.220	Depositor DCC
R_{free} test set	4489 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.434	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.33	0/2106	0.57	0/2840
1	B	0.32	0/2097	0.56	0/2828
All	All	0.33	0/4203	0.56	0/5668

There are no bond length outliers.

There are no bond angle outliers.

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	2065	0	2103	45	0
1	B	2056	0	2097	50	0
2	A	10	0	2	1	0
2	B	10	0	2	0	0
3	A	14	0	10	2	0
3	B	14	0	10	0	0
4	A	216	0	0	2	0
4	B	186	0	0	3	0
All	All	4571	0	4224	94	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 11.

All (94) 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:132:TRP:HE1	1:B:161:ASN:HD21	1.25	0.83
1:A:154:ARG:HH22	1:A:188:GLN:NE2	1.76	0.83
1:B:208:ILE:HD12	1:B:250:ILE:HG21	1.62	0.81
1:A:161:ASN:HD21	1:B:132:TRP:HE1	1.29	0.80
1:A:202:GLU:HG3	4:A:3379:HOH:O	1.81	0.80
1:A:154:ARG:HH22	1:A:188:GLN:HE22	1.29	0.80
1:A:174:LYS:HG3	1:A:264:ILE:HD13	1.72	0.70
1:A:48:ASN:HD22	1:A:48:ASN:H	1.41	0.68
1:B:20:LEU:HD21	1:B:69:LYS:HG3	1.75	0.67
1:A:205:PHE:O	1:A:208:ILE:HG22	1.95	0.67
1:A:154:ARG:HH12	1:A:188:GLN:HE21	1.42	0.66
1:B:25:GLU:HG2	1:B:240:LEU:HD22	1.78	0.64
1:B:189:LEU:HD21	1:B:200:MET:HE2	1.81	0.63
1:B:228:GLU:CD	1:B:228:GLU:H	2.02	0.62
1:A:205:PHE:HB3	1:A:206:PRO:HD3	1.82	0.61
1:B:185:HIS:O	1:B:188:GLN:HG2	2.01	0.61
1:B:48:ASN:HD22	1:B:48:ASN:H	1.49	0.61
1:B:208:ILE:HD11	1:B:219:VAL:HG21	1.82	0.60
1:B:182:ASP:HA	1:B:220:PHE:HB3	1.82	0.60
1:A:9:GLY:O	1:A:223:THR:HG22	2.03	0.58
1:A:226:GLU:OE1	1:A:229:LYS:HE2	2.03	0.58
1:A:10:MET:HE2	1:A:22:VAL:HG21	1.86	0.57
1:B:263:THR:HG22	1:B:264:ILE:HG22	1.85	0.57
1:B:44:PHE:CE1	1:B:60:LEU:HD23	2.39	0.57
1:B:201:ARG:HG3	1:B:204:ILE:HD12	1.86	0.57
1:A:201:ARG:HG3	1:A:204:ILE:HD12	1.86	0.56
1:A:182:ASP:HA	1:A:220:PHE:HB3	1.87	0.56
1:A:212:VAL:HG11	1:A:250:ILE:HB	1.87	0.55
1:B:205:PHE:O	1:B:208:ILE:HG22	2.06	0.55
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.88	0.55
1:A:12:ALA:HB2	1:A:46:LYS:HD3	1.91	0.53
1:B:44:PHE:CZ	1:B:60:LEU:HD23	2.44	0.53
1:A:48:ASN:HD22	1:A:48:ASN:N	2.03	0.53
1:B:205:PHE:HB3	1:B:206:PRO:HD3	1.91	0.52
1:A:41:LYS:HD3	1:A:42:SER:N	2.24	0.52
1:A:189:LEU:HD21	1:A:200:MET:HE2	1.91	0.52
1:A:189:LEU:HD21	1:A:200:MET:CE	2.41	0.51
1:A:40:PHE:HB3	1:A:78:ILE:HD13	1.92	0.50
1:A:69:LYS:HE3	1:A:73:GLU:OE1	2.12	0.50
1:A:26:ILE:HD12	1:A:40:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:O	1:B:223:THR:HG22	2.12	0.49
4:A:3193:HOH:O	1:B:83:HIS:HD2	1.96	0.49
1:B:26:ILE:HD12	1:B:40:PHE:CD1	2.47	0.49
1:B:55:PHE:CZ	1:B:57:GLY:HA2	2.48	0.49
1:A:60:LEU:O	1:A:64:VAL:HG23	2.13	0.48
1:A:68:ARG:O	1:A:72:GLU:HG3	2.15	0.47
1:A:193:LEU:HD13	1:A:198:GLY:CA	2.44	0.47
1:B:11:ASN:HD21	1:B:46:LYS:HE2	1.80	0.46
1:B:41:LYS:HD3	1:B:42:SER:N	2.30	0.46
1:A:41:LYS:HD3	1:A:41:LYS:C	2.36	0.46
1:B:224:HIS:O	1:B:227:PRO:HD3	2.15	0.46
1:A:11:ASN:N	1:A:222:GLU:HG2	2.31	0.46
1:A:10:MET:O	1:A:42:SER:HA	2.16	0.45
1:B:234:ALA:HB3	1:B:235:PRO:HD3	1.99	0.45
1:B:48:ASN:HD22	1:B:48:ASN:N	2.10	0.45
1:B:41:LYS:HD3	1:B:41:LYS:C	2.38	0.45
1:B:168:ARG:O	1:B:171:PRO:HD2	2.17	0.45
1:A:234:ALA:N	1:A:235:PRO:CD	2.80	0.44
1:B:58:HIS:HB2	1:B:62:TYR:CD2	2.52	0.44
1:B:11:ASN:N	1:B:222:GLU:HG2	2.32	0.44
2:A:1268:PEP:O2P	3:A:1269:A5P:H11	2.18	0.44
1:B:22:VAL:HA	1:B:240:LEU:HD11	1.99	0.44
1:B:162:ASN:HD22	1:B:163:LEU:H	1.66	0.43
1:B:32:LYS:HE2	1:B:244:GLU:OE2	2.18	0.43
1:A:97:ILE:HG12	1:A:120:ALA:HB3	2.00	0.43
1:B:61:GLU:HB2	4:B:3134:HOH:O	2.18	0.43
1:A:29:LEU:HD21	1:A:244:GLU:HB2	2.01	0.43
1:B:234:ALA:N	1:B:235:PRO:CD	2.82	0.43
1:A:26:ILE:HD12	1:A:40:PHE:HD1	1.84	0.42
1:A:162:ASN:HD22	1:A:163:LEU:H	1.67	0.42
1:A:181:TYR:CE2	1:A:183:ALA:HA	2.54	0.42
1:B:60:LEU:C	1:B:60:LEU:HD13	2.39	0.42
1:A:10:MET:HE2	1:A:10:MET:HB2	1.85	0.42
1:B:170:LEU:CB	1:B:171:PRO:HD3	2.49	0.42
1:B:212:VAL:HG11	1:B:250:ILE:HB	2.02	0.42
1:A:193:LEU:HD13	1:A:198:GLY:HA3	2.01	0.42
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.20	0.41
1:B:139:GLU:HG3	4:B:3318:HOH:O	2.21	0.41
1:B:154:ARG:HD3	1:B:154:ARG:O	2.19	0.41
1:B:189:LEU:HD21	1:B:200:MET:CE	2.48	0.41
3:A:1269:A5P:HC4	3:A:1269:A5P:H12	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:O	1:B:20:LEU:HG	2.21	0.41
1:A:89:GLU:HB3	1:A:90:PRO:CD	2.51	0.41
1:B:165:VAL:CG2	1:B:186:SER:HB3	2.50	0.41
1:B:3:LYS:HE3	4:B:3283:HOH:O	2.21	0.41
1:A:14:GLU:O	1:A:58:HIS:HE1	2.03	0.41
1:A:48:ASN:N	1:A:48:ASN:ND2	2.69	0.41
1:B:99:GLN:HE22	1:B:220:PHE:HE2	1.67	0.41
1:A:106:ARG:NH1	1:B:48:ASN:O	2.54	0.40
1:A:130:ALA:HB3	1:A:133:ASP:OD2	2.21	0.40
1:B:68:ARG:HG3	1:B:94:VAL:CG2	2.52	0.40
1:A:234:ALA:HB3	1:A:235:PRO:HD3	2.03	0.40
1:B:19:LEU:HD22	1:B:40:PHE:CZ	2.56	0.40
1:B:162:ASN:ND2	1:B:163:LEU:H	2.19	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	261/267 (98%)	255 (98%)	6 (2%)	0	100	100
1	B	260/267 (97%)	251 (96%)	8 (3%)	1 (0%)	34	30
All	All	521/534 (98%)	506 (97%)	14 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	SER

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	219/223 (98%)	212 (97%)	7 (3%)	39	38
1	B	218/223 (98%)	208 (95%)	10 (5%)	27	23
All	All	437/446 (98%)	420 (96%)	17 (4%)	32	30

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	LEU
1	A	106	ARG
1	A	112	LEU
1	A	154	ARG
1	A	162	ASN
1	A	222	GLU
1	B	29	LEU
1	B	48	ASN
1	B	147	LYS
1	B	154	ARG
1	B	162	ASN
1	B	176	TRP
1	B	205	PHE
1	B	208	ILE
1	B	222	GLU
1	B	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	58	HIS
1	A	99	GLN
1	A	136	ASN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	175	GLN
1	A	188	GLN
1	B	11	ASN
1	B	48	ASN
1	B	53	HIS
1	B	58	HIS
1	B	83	HIS
1	B	107	GLN
1	B	122	ASN
1	B	161	ASN
1	B	162	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 monosaccharides 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	$\# Z > 2$
2	PEP	B	2268	-	9,9,9	1.12	0	11,13,13	1.40	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A5P	A	1269	-	13,13,13	2.44	3 (23%)	18,18,18	2.40	7 (38%)
3	A5P	B	2269	-	13,13,13	2.55	2 (15%)	18,18,18	2.58	6 (33%)
2	PEP	A	1268	-	9,9,9	1.16	1 (11%)	11,13,13	1.19	1 (9%)

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	B	2268	-	-	4/9/9/9	-
3	A5P	A	1269	-	-	7/16/16/16	-
3	A5P	B	2269	-	-	13/16/16/16	-
2	PEP	A	1268	-	-	0/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2269	A5P	O1-C1	-6.19	1.16	1.42
3	A	1269	A5P	O1-C1	-5.39	1.19	1.42
3	B	2269	A5P	P-O5	-5.38	1.42	1.60
3	A	1269	A5P	P-O5	-4.68	1.45	1.60
3	A	1269	A5P	C5-C4	-3.95	1.46	1.51
2	A	1268	PEP	P-O2	2.06	1.62	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1269	A5P	O1-C1-C2	5.49	123.03	111.07
3	B	2269	A5P	O1-C1-C2	5.07	122.12	111.07
3	B	2269	A5P	C1-C2-C3	-5.02	101.52	112.41
3	B	2269	A5P	P-O5-C5	5.02	132.12	118.30
3	A	1269	A5P	O2-C2-C1	3.86	118.20	109.14
3	A	1269	A5P	O4-C4-C3	3.82	118.38	109.10
2	B	2268	PEP	O2'-C1-C2	3.52	119.92	113.91
3	B	2269	A5P	O4-C4-C3	3.25	117.00	109.10
3	B	2269	A5P	O5-C5-C4	-3.19	100.86	109.36
3	A	1269	A5P	P-O5-C5	3.05	126.70	118.30
2	A	1268	PEP	O2'-C1-C2	2.99	119.00	113.91
3	B	2269	A5P	O3P-P-O5	2.98	114.67	106.73
3	A	1269	A5P	O5-C5-C4	-2.69	102.19	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1269	A5P	C1-C2-C3	-2.61	106.76	112.41
3	A	1269	A5P	O2-C2-C3	2.26	114.61	109.10
2	B	2268	PEP	O1-C1-C2	-2.26	118.38	121.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2268	PEP	O1-C1-C2-C3
2	B	2268	PEP	O2'-C1-C2-C3
3	A	1269	A5P	O1-C1-C2-O2
3	A	1269	A5P	O1-C1-C2-C3
3	A	1269	A5P	C5-O5-P-O1P
3	A	1269	A5P	C5-O5-P-O2P
3	A	1269	A5P	C5-O5-P-O3P
3	B	2269	A5P	O1-C1-C2-O2
3	B	2269	A5P	O1-C1-C2-C3
3	B	2269	A5P	C1-C2-C3-O3
3	B	2269	A5P	C1-C2-C3-C4
3	B	2269	A5P	O2-C2-C3-O3
3	B	2269	A5P	O2-C2-C3-C4
3	B	2269	A5P	C2-C3-C4-O4
3	B	2269	A5P	C2-C3-C4-C5
3	B	2269	A5P	O3-C3-C4-O4
3	B	2269	A5P	C5-O5-P-O2P
3	B	2269	A5P	O3-C3-C4-C5
3	A	1269	A5P	C2-C3-C4-O4
3	B	2269	A5P	C5-O5-P-O1P
2	B	2268	PEP	O1-C1-C2-O2
3	A	1269	A5P	C3-C4-C5-O5
2	B	2268	PEP	O2'-C1-C2-O2
3	B	2269	A5P	C5-O5-P-O3P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1269	A5P	2	0
2	A	1268	PEP	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 [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	263/267 (98%)	-0.44	3 (1%) 80 79	12, 22, 38, 60	0
1	B	262/267 (98%)	-0.25	7 (2%) 54 53	13, 25, 44, 58	0
All	All	525/534 (98%)	-0.35	10 (1%) 66 65	12, 23, 42, 60	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ILE	5.2
1	B	193	LEU	3.9
1	B	196	LYS	3.6
1	A	195	ASP	3.4
1	B	264	ILE	2.9
1	A	193	LEU	2.9
1	B	194	GLY	2.6
1	B	61	GLU	2.6
1	B	195	ASP	2.4
1	B	147	LYS	2.4

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 monosaccharides 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(\AA^2)	Q<0.9
3	A5P	B	2269	14/14	0.92	0.16	35,45,51,52	0
3	A5P	A	1269	14/14	0.94	0.14	27,40,46,48	0
2	PEP	A	1268	10/10	0.98	0.09	21,24,26,27	0
2	PEP	B	2268	10/10	0.98	0.08	20,22,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.