Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:33 PM BST

PDB ID	:	5K3V
Title	:	apo-PDX1.3 (Arabidopsis)
Authors	:	Robinson, G.C.; Kaufmann, M.; Roux, C.; Fitzpatrick, T.B.
Deposited on	:	2016-05-20
Resolution	:	1.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

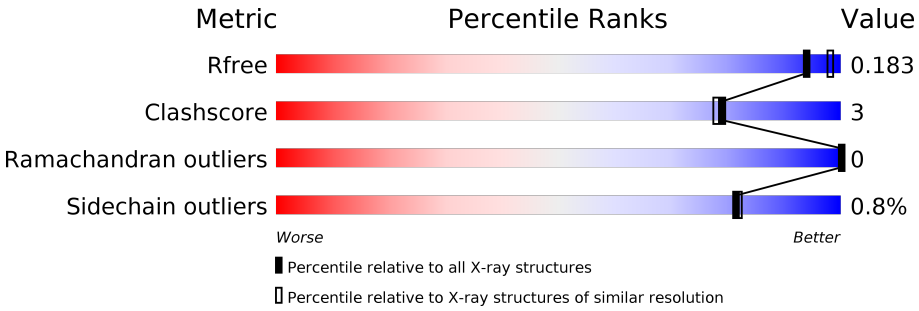
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	315	83% • 12%
1	B	315	82% 5% 13%
1	C	315	83% 5% 12%
1	D	315	84% • • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8956 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 Pyridoxal 5'-phosphate synthase subunit PDX1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	7	0
			2111	1315	389	389	18			
1	B	274	Total	C	N	O	S	0	6	0
			2088	1302	384	384	18			
1	C	277	Total	C	N	O	S	0	5	0
			2115	1318	386	393	18			
1	D	277	Total	C	N	O	S	0	3	0
			2084	1299	382	385	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	expression tag	UNP Q8L940
A	311	HIS	-	expression tag	UNP Q8L940
A	312	HIS	-	expression tag	UNP Q8L940
A	313	HIS	-	expression tag	UNP Q8L940
A	314	HIS	-	expression tag	UNP Q8L940
A	315	HIS	-	expression tag	UNP Q8L940
B	310	HIS	-	expression tag	UNP Q8L940
B	311	HIS	-	expression tag	UNP Q8L940
B	312	HIS	-	expression tag	UNP Q8L940
B	313	HIS	-	expression tag	UNP Q8L940
B	314	HIS	-	expression tag	UNP Q8L940
B	315	HIS	-	expression tag	UNP Q8L940
C	310	HIS	-	expression tag	UNP Q8L940
C	311	HIS	-	expression tag	UNP Q8L940
C	312	HIS	-	expression tag	UNP Q8L940
C	313	HIS	-	expression tag	UNP Q8L940
C	314	HIS	-	expression tag	UNP Q8L940
C	315	HIS	-	expression tag	UNP Q8L940
D	310	HIS	-	expression tag	UNP Q8L940
D	311	HIS	-	expression tag	UNP Q8L940
D	312	HIS	-	expression tag	UNP Q8L940

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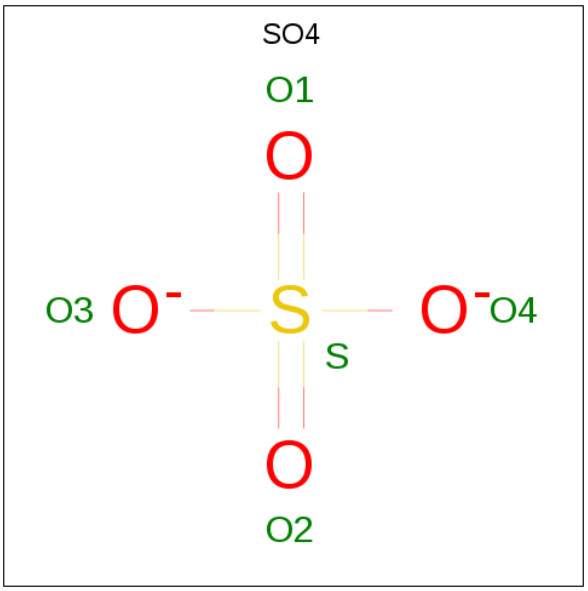
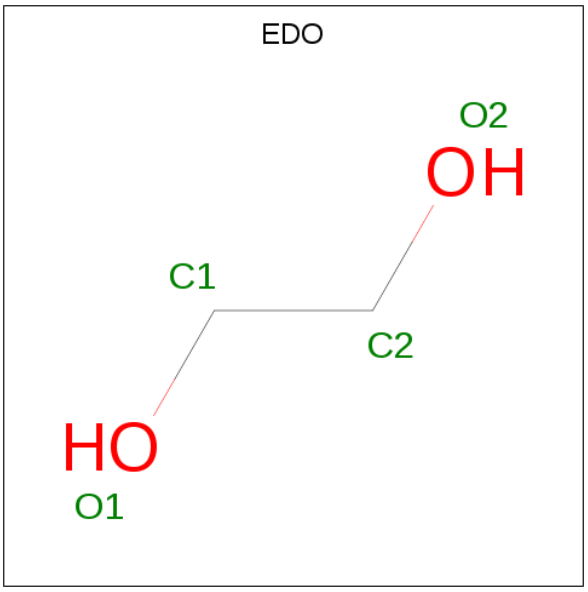
Chain	Residue	Modelled	Actual	Comment	Reference
D	313	HIS	-	expression tag	UNP Q8L940
D	314	HIS	-	expression tag	UNP Q8L940
D	315	HIS	-	expression tag	UNP Q8L940

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	D	3	Total Cl 3 3	0	0

- Molecule 5 is water.

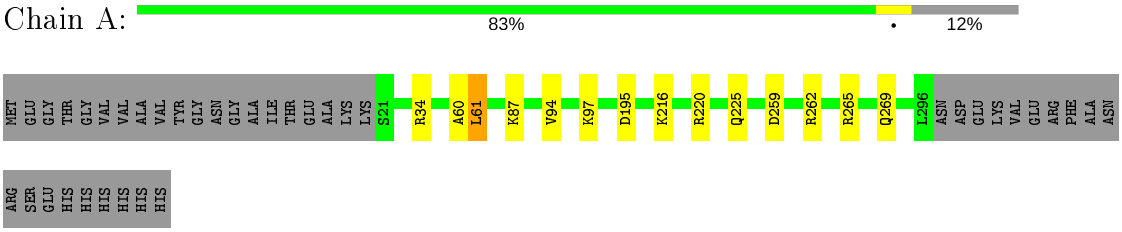
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	143	Total O 143 143	0	0
5	B	125	Total O 125 125	0	0
5	C	125	Total O 125 125	0	0
5	D	108	Total O 108 108	0	0

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. 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. 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.

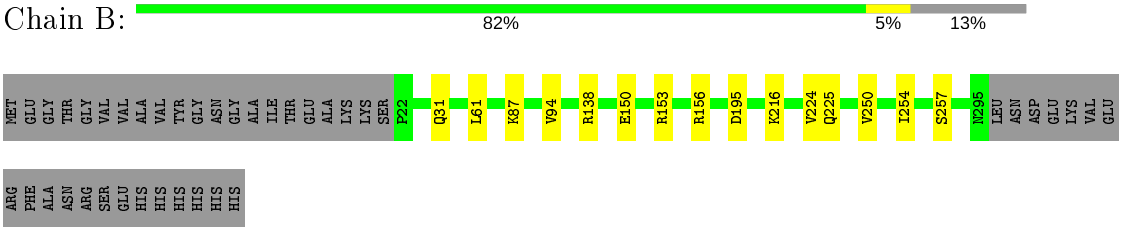
- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain A:



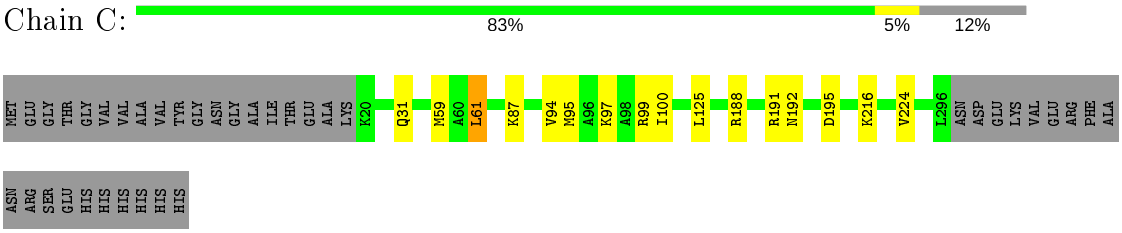
- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain B:



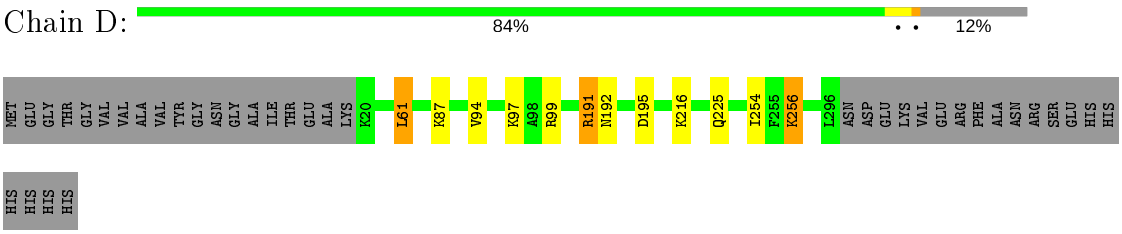
- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain C:



- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	178.22Å 178.22Å 116.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.95 – 1.90 46.47 – 1.46	Depositor EDS
% Data completeness (in resolution range)	98.8 (92.95-1.90) 98.7 (46.47-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.203 0.186 , 0.183	Depositor DCC
R_{free} test set	11527 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, 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	0.75	0/2147	0.92	2/2895 (0.1%)
1	B	0.73	0/2121	0.90	1/2860 (0.0%)
1	C	0.76	0/2145	0.92	3/2893 (0.1%)
1	D	0.74	0/2114	0.88	2/2852 (0.1%)
All	All	0.75	0/8527	0.90	8/11500 (0.1%)

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
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	188	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	192	ASN	CB-CA-C	-5.67	99.07	110.40
1	C	99	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	34	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	220	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	99	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	192	ASN	CB-CA-C	-5.11	100.19	110.40
1	B	138	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	254	ILE	Peptide
1	D	254	ILE	Peptide

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	2111	0	2135	14	0
1	B	2088	0	2112	8	0
1	C	2115	0	2130	11	0
1	D	2084	0	2101	14	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
4	A	2	0	0	0	0
4	D	3	0	0	0	0
5	A	143	0	0	1	1
5	B	125	0	0	2	1
5	C	125	0	0	0	0
5	D	108	0	0	1	0
All	All	8956	0	8496	47	1

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 3.

All (47) 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:265[B]:ARG:CZ	1:A:269[B]:GLN:HE21	1.71	1.01
1:A:265[B]:ARG:CZ	1:A:269[B]:GLN:NE2	2.39	0.84
1:C:59:MET:HE2	1:C:95:MET:HE2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:CE	1:C:95:MET:HE2	2.09	0.81
1:D:191[B]:ARG:HD3	1:D:191[B]:ARG:C	2.01	0.81
1:D:191[A]:ARG:HH11	1:D:191[A]:ARG:HG2	1.48	0.78
1:A:265[B]:ARG:NH2	1:A:269[B]:GLN:NE2	2.32	0.76
1:A:60:ALA:O	1:A:61[B]:LEU:HD12	1.86	0.76
1:C:191[B]:ARG:HG2	1:C:191[B]:ARG:HH11	1.57	0.69
1:D:191[B]:ARG:O	1:D:191[B]:ARG:HD3	1.93	0.68
1:D:191[B]:ARG:CD	1:D:191[B]:ARG:C	2.63	0.65
1:A:259:ASP:OD2	1:A:262:ARG:HD2	2.00	0.61
1:A:61[B]:LEU:HD21	1:A:97:LYS:HD2	1.84	0.59
1:C:195:ASP:OD1	1:C:216:LYS:HE2	2.02	0.59
1:B:195:ASP:OD1	1:B:216:LYS:HE2	2.02	0.58
1:D:195:ASP:OD1	1:D:216:LYS:HE2	2.02	0.58
1:C:59:MET:CE	1:C:95:MET:CE	2.81	0.58
1:A:195:ASP:OD1	1:A:216:LYS:HE2	2.04	0.57
1:B:257:SER:HB2	5:B:559:HOH:O	2.05	0.56
1:B:150[B]:GLU:HG2	1:B:153:ARG:NH2	2.23	0.54
1:A:265[B]:ARG:NH2	1:A:269[B]:GLN:HE22	2.01	0.54
1:A:265[B]:ARG:NE	1:A:269[B]:GLN:HE21	2.04	0.52
1:D:191[A]:ARG:NH1	1:D:191[A]:ARG:HG2	2.17	0.52
1:C:59:MET:HE1	1:C:95:MET:CE	2.41	0.51
1:A:61[B]:LEU:HG	5:A:520:HOH:O	2.11	0.50
1:C:87:LYS:HA	1:C:94:VAL:HG21	1.94	0.49
1:D:225:GLN:OE1	5:D:501:HOH:O	2.19	0.49
1:D:191[A]:ARG:CG	1:D:191[A]:ARG:NH1	2.76	0.48
1:C:100:ILE:HB	1:C:125[B]:LEU:HD23	1.95	0.48
1:D:87:LYS:HA	1:D:94:VAL:HG21	1.95	0.48
1:A:87:LYS:HA	1:A:94:VAL:HG21	1.96	0.47
1:C:191[B]:ARG:HG2	1:C:191[B]:ARG:NH1	2.24	0.47
1:D:256:LYS:H	1:D:256:LYS:HD3	1.80	0.47
1:A:61[B]:LEU:HD11	1:A:97:LYS:HG3	1.97	0.46
1:B:31:GLN:HA	1:B:224:VAL:HG21	1.98	0.46
1:B:87:LYS:HA	1:B:94:VAL:HG21	1.98	0.45
1:A:225:GLN:CG	1:A:225:GLN:O	2.67	0.43
1:B:225:GLN:OE1	5:B:501:HOH:O	2.21	0.43
1:D:191[B]:ARG:HG3	1:D:191[B]:ARG:HH11	1.84	0.42
1:D:61:LEU:HD13	1:D:97:LYS:HE2	2.00	0.42
1:B:225:GLN:CG	1:B:225:GLN:O	2.67	0.42
1:C:61:LEU:HD13	1:C:97:LYS:HE2	2.01	0.41
1:C:31:GLN:HA	1:C:224:VAL:HG21	2.02	0.41
1:D:225:GLN:O	1:D:225:GLN:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:HA	1:B:156:ARG:HD2	1.93	0.41
1:A:60:ALA:C	1:A:61[B]:LEU:HD12	2.41	0.41
1:D:191[B]:ARG:HG3	1:D:191[B]:ARG:NH1	2.36	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:575:HOH:O	5:B:529:HOH:O[5_455]	1.07	1.13

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	281/315 (89%)	276 (98%)	5 (2%)	0	100	100
1	B	278/315 (88%)	271 (98%)	7 (2%)	0	100	100
1	C	281/315 (89%)	275 (98%)	6 (2%)	0	100	100
1	D	278/315 (88%)	271 (98%)	7 (2%)	0	100	100
All	All	1118/1260 (89%)	1093 (98%)	25 (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	216/245 (88%)	214 (99%)	2 (1%)	78 79
1	B	213/245 (87%)	210 (99%)	3 (1%)	67 65
1	C	216/245 (88%)	215 (100%)	1 (0%)	88 89
1	D	212/245 (86%)	208 (98%)	4 (2%)	57 53
All	All	857/980 (87%)	847 (99%)	10 (1%)	81 70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	LEU
1	A	61[B]	LEU
1	B	61	LEU
1	B	250[A]	VAL
1	B	250[B]	VAL
1	C	61	LEU
1	D	61	LEU
1	D	191[A]	ARG
1	D	191[B]	ARG
1	D	256	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	B	71	GLN
1	C	71	GLN
1	D	225	GLN

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)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	EDO	A	403	-	3,3,3	0.52	0	2,2,2	0.25	0
2	SO4	C	402	-	4,4,4	0.50	0	6,6,6	0.61	0
2	SO4	A	401	-	4,4,4	0.21	0	6,6,6	0.68	0
2	SO4	C	401	-	4,4,4	0.17	0	6,6,6	0.66	0
2	SO4	A	402	-	4,4,4	0.51	0	6,6,6	0.61	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.72	0
2	SO4	B	402	-	4,4,4	0.67	0	6,6,6	0.54	0
3	EDO	B	403	-	3,3,3	0.34	0	2,2,2	0.46	0
2	SO4	B	401	-	4,4,4	0.32	0	6,6,6	1.06	1 (16%)
2	SO4	D	402	-	4,4,4	0.53	0	6,6,6	0.80	0
3	EDO	C	403	-	3,3,3	0.37	0	2,2,2	0.24	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
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	C	403	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	SO4	O4-S-O3	-2.14	99.94	109.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	EDO	O1-C1-C2-O2
3	A	403	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.