W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 11:29 PM EDT

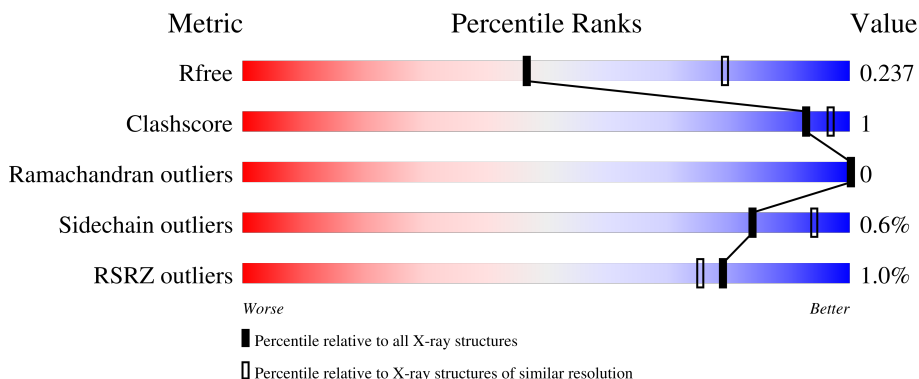|		
PDB ID	:	3P1T
Title	:	Crystal structure of a putative aminotransferase (BPSL1724) from Burkholderia pseudomallei K96243 at 2.60 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2010-09-30
Resolution	:	2.60 Å(reported)

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 2.60 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.

| | Percentile relative to all X-ray structures |
| | Percentile relative to X-ray structures of similar resolution |

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 <=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	337	92%
1	B	337	91% · 5%
1	C	337	93% · 5%
1	D	337	90% · 6%

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	TLA	A	343	-	X	-	-
3	TLA	B	342	-	X	-	-
3	TLA	C	344	-	X	-	-
3	TLA	C	345	-	X	-	-
3	TLA	D	341	-	X	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10750 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 Putative histidinol-phosphate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	Se	0	3	0
			2512	1573	459	471	5	4			
1	B	319	Total	C	N	O	S	Se	0	4	0
			2515	1572	464	470	5	4			
1	C	321	Total	C	N	O	S	Se	0	4	0
			2530	1582	472	467	5	4			
1	D	317	Total	C	N	O	S	Se	0	2	0
			2492	1557	464	462	5	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q63U92
B	0	GLY	-	expression tag	UNP Q63U92
C	0	GLY	-	expression tag	UNP Q63U92
D	0	GLY	-	expression tag	UNP Q63U92

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

SO4

O1

O

O3 O⁻ —— S —— O⁻ O4

S

O

O2

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

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).

TLA

O11
OH

O1 O == C1

C2(R) ·······OH O2

O3 HO|||||· C3(R)

C4 == O O4

HO

O41
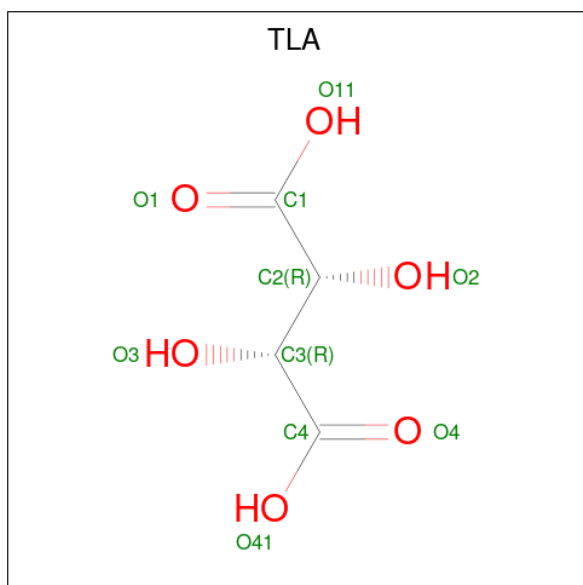
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 9	C 4	O 5	0	0
3	B	1	Total 10	C 4	O 6	0	0
3	C	1	Total 10	C 4	O 6	0	0
3	C	1	Total 10	C 4	O 6	0	0
3	D	1	Total 10	C 4	O 6	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
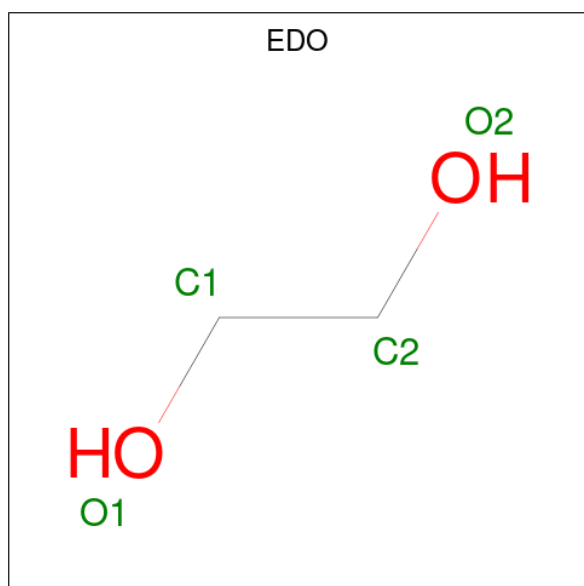
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 8	C 4	O 4	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 8	C 4	O 4	0	1
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 8	C 4	O 4	0	1

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total 112	O 112	0	0
5	B	159	Total 159	O 159	0	0
5	C	151	Total 151	O 151	0	0
5	D	146	Total 146	O 146	0	0

3 Residue-property plots ⓘ

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.
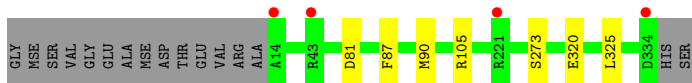
• Molecule 1: Putative histidinol-phosphate aminotransferase
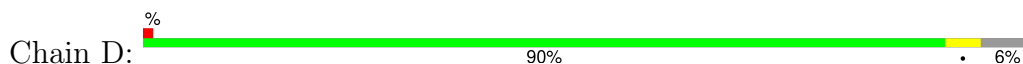

Chain A:

• Molecule 1: Putative histidinol-phosphate aminotransferase

Chain B:

• Molecule 1: Putative histidinol-phosphate aminotransferase

Chain C:

• Molecule 1: Putative histidinol-phosphate aminotransferase

Chain D:
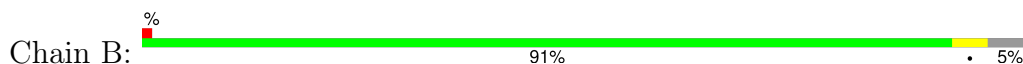
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	167.55Å 167.55Å 290.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 2.60 29.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.65-2.60) 97.8 (29.65-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.200 , 0.234 0.203 , 0.237	Depositor DCC
R_{free} test set	3131 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10750	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1359e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: EDO, SO4, TLA

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	0.48	0/2561	0.61	0/3454
1	B	0.51	0/2567	0.63	0/3460
1	C	0.49	0/2582	0.61	0/3478
1	D	0.52	0/2538	0.61	0/3420
All	All	0.50	0/10248	0.62	0/13812

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	2512	0	2464	8	0
1	B	2515	0	2476	9	0
1	C	2530	0	2504	3	0
1	D	2492	0	2461	8	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	D	5	0	0	0	0
3	A	9	0	5	0	0
3	B	10	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	20	0	10	1	0
3	D	10	0	5	1	0
4	A	12	0	18	3	0
4	B	20	0	30	3	0
4	C	20	0	30	0	0
4	D	12	0	18	2	0
5	A	112	0	0	2	0
5	B	159	0	0	1	0
5	C	151	0	0	1	0
5	D	146	0	0	1	0
All	All	10750	0	10026	28	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.

The worst 5 of 28 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:69:ASN:HD21	4:A:349:EDO:H12	1.46	0.81
1:B:43:ARG:NE	5:B:804:HOH:O	2.33	0.62
1:B:257:ARG:HH21	3:B:342:TLA:H3	1.65	0.62
1:D:274:SER:O	3:D:341:TLA:H3	2.05	0.56
1:B:171:THR:HG21	4:B:353:EDO:H12	1.89	0.54

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	323/337 (96%)	312 (97%)	11 (3%)	0	100	100
1	B	321/337 (95%)	312 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	323/337 (96%)	313 (97%)	10 (3%)	0	100	100
1	D	317/337 (94%)	309 (98%)	8 (2%)	0	100	100
All	All	1284/1348 (95%)	1246 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	252/259 (97%)	251 (100%)	1 (0%)	89	96
1	B	255/259 (98%)	254 (100%)	1 (0%)	89	96
1	C	255/259 (98%)	253 (99%)	2 (1%)	79	91
1	D	253/259 (98%)	251 (99%)	2 (1%)	79	91
All	All	1015/1036 (98%)	1009 (99%)	6 (1%)	84	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	325	LEU
1	D	32	ARG
1	D	325	LEU
1	B	325	LEU
1	A	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	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 ⓘ

There are no oligosaccharides in this entry.

5.6　Ligand geometry ⓘ

25 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	$\#|Z| > 2$
3	TLA	A	343	-	6,8,9	6.76	5 (83%)	7,10,12	4.77	6 (85%)
4	EDO	B	353	-	3,3,3	0.59	0	2,2,2	0.18	0
4	EDO	C	357[B]	-	3,3,3	0.55	0	2,2,2	0.24	0
4	EDO	C	352	-	3,3,3	0.47	0	2,2,2	0.44	0
4	EDO	C	355	-	3,3,3	0.51	0	2,2,2	0.18	0
3	TLA	C	345	-	9,9,9	7.88	7 (77%)	12,12,12	3.69	7 (58%)
4	EDO	C	348	-	3,3,3	0.57	0	2,2,2	0.24	0
4	EDO	D	358[B]	-	3,3,3	0.43	0	2,2,2	0.41	0
3	TLA	D	341	-	9,9,9	7.46	7 (77%)	12,12,12	3.74	8 (66%)
4	EDO	B	356[B]	-	3,3,3	0.45	0	2,2,2	0.26	0
4	EDO	A	350	-	3,3,3	0.54	0	2,2,2	0.12	0
2	SO4	B	339	-	4,4,4	0.35	0	6,6,6	0.16	0
2	SO4	D	337	-	4,4,4	0.44	0	6,6,6	0.28	0
3	TLA	C	344	-	9,9,9	7.08	7 (77%)	12,12,12	4.49	8 (66%)
2	SO4	A	338	-	4,4,4	0.42	0	6,6,6	0.18	0
4	EDO	B	347	-	3,3,3	0.74	0	2,2,2	0.23	0
2	SO4	B	340	-	4,4,4	0.38	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	D	358[A]	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	B	351	-	3,3,3	0.47	0	2,2,2	0.41	0
4	EDO	C	357[A]	-	3,3,3	0.51	0	2,2,2	0.25	0
4	EDO	A	349	-	3,3,3	0.51	0	2,2,2	0.15	0
4	EDO	B	356[A]	-	3,3,3	0.50	0	2,2,2	0.08	0
4	EDO	A	346	-	3,3,3	0.64	0	2,2,2	0.32	0
4	EDO	D	354	-	3,3,3	0.55	0	2,2,2	0.05	0
3	TLA	B	342	-	9,9,9	6.43	7 (77%)	12,12,12	3.55	6 (50%)

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	TLA	A	343	-	-	3/9/10/12	-
4	EDO	B	353	-	-	0/1/1/1	-
4	EDO	C	357[B]	-	-	0/1/1/1	-
4	EDO	C	352	-	-	1/1/1/1	-
4	EDO	C	355	-	-	0/1/1/1	-
3	TLA	C	345	-	-	7/12/12/12	-
4	EDO	C	348	-	-	0/1/1/1	-
4	EDO	D	358[B]	-	-	0/1/1/1	-
3	TLA	D	341	-	-	4/12/12/12	-
4	EDO	B	356[B]	-	-	0/1/1/1	-
4	EDO	A	350	-	-	0/1/1/1	-
3	TLA	C	344	-	-	11/12/12/12	-
4	EDO	B	347	-	-	0/1/1/1	-
4	EDO	D	358[A]	-	-	0/1/1/1	-
4	EDO	B	351	-	-	0/1/1/1	-
4	EDO	C	357[A]	-	-	0/1/1/1	-
4	EDO	A	349	-	-	0/1/1/1	-
4	EDO	B	356[A]	-	-	0/1/1/1	-
4	EDO	A	346	-	-	0/1/1/1	-
4	EDO	D	354	-	-	1/1/1/1	-
3	TLA	B	342	-	-	7/12/12/12	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	345	TLA	C3-C4	14.12	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	341	TLA	C3-C4	12.26	1.70	1.52
3	C	345	TLA	C2-C1	10.55	1.67	1.52
3	C	344	TLA	O3-C3	10.53	1.62	1.42
3	C	345	TLA	O2-C2	9.89	1.61	1.42

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	344	TLA	O4-C4-C3	-8.65	98.59	121.62
3	D	341	TLA	O4-C4-C3	-8.10	100.04	121.62
3	B	342	TLA	O3-C3-C2	8.05	126.55	110.17
3	C	345	TLA	O2-C2-C3	7.59	125.62	110.17
3	A	343	TLA	O2-C2-C1	7.25	126.97	110.48

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	343	TLA	C1-C2-C3-O3
3	A	343	TLA	C1-C2-C3-C4
3	A	343	TLA	O2-C2-C3-C4
3	C	344	TLA	C2-C3-C4-O4
3	C	344	TLA	C2-C3-C4-O41

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	353	EDO	2	0
3	C	345	TLA	1	0
3	D	341	TLA	1	0
4	B	351	EDO	1	0
4	A	349	EDO	2	0
4	A	346	EDO	1	0
4	D	354	EDO	2	0
3	B	342	TLA	2	0

5.7   Other polymers ⓘ

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, 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	318/337 (94%)	-0.12	4 (1%)	74	70	29, 46, 72, 114	3 (0%)
1	B	315/337 (93%)	-0.34	3 (0%)	79	75	24, 39, 55, 94	4 (1%)
1	C	317/337 (94%)	-0.34	4 (1%)	74	70	24, 39, 62, 104	4 (1%)
1	D	313/337 (92%)	-0.41	2 (0%)	85	83	22, 37, 58, 75	2 (0%)
All	All	1263/1348 (93%)	-0.30	13 (1%)	79	75	22, 40, 63, 114	13 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	HIS	6.7
1	A	14	ALA	3.7
1	D	333	SER	3.4
1	A	334	ASP	3.0
1	C	221[A]	ARG	3.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 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, 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(Å^2)	Q<0.9
4	EDO	C	357[A]	4/4	0.56	0.29	34,36,36,40	4
4	EDO	C	357[B]	4/4	0.56	0.29	31,31,33,34	4
4	EDO	D	358[A]	4/4	0.58	0.29	47,48,49,50	4
4	EDO	D	358[B]	4/4	0.58	0.29	52,53,55,59	4
4	EDO	B	356[A]	4/4	0.69	0.18	46,46,48,51	4
4	EDO	B	356[B]	4/4	0.69	0.18	73,75,76,78	4
4	EDO	D	354	4/4	0.70	0.36	72,72,73,79	0
4	EDO	A	350	4/4	0.72	0.21	58,60,60,64	0
4	EDO	A	346	4/4	0.73	0.19	44,48,48,51	0
4	EDO	A	349	4/4	0.73	0.20	64,66,67,69	0
4	EDO	B	351	4/4	0.76	0.17	59,60,63,64	0
3	TLA	C	345	10/10	0.77	0.21	57,69,72,73	0
4	EDO	B	347	4/4	0.79	0.17	41,42,43,47	0
2	SO4	A	338	5/5	0.79	0.25	100,105,105,107	0
4	EDO	C	352	4/4	0.79	0.19	59,61,62,64	0
4	EDO	B	353	4/4	0.79	0.35	71,71,75,77	0
3	TLA	C	344	10/10	0.80	0.16	57,65,73,73	0
3	TLA	D	341	10/10	0.80	0.23	75,81,92,93	0
4	EDO	C	355	4/4	0.81	0.25	74,75,75,80	0
3	TLA	B	342	10/10	0.83	0.20	77,81,87,89	0
2	SO4	B	339	5/5	0.84	0.15	93,97,99,99	0
2	SO4	B	340	5/5	0.86	0.23	47,51,53,53	5
2	SO4	D	337	5/5	0.87	0.14	91,96,97,97	0
3	TLA	A	343	9/10	0.88	0.17	68,73,77,80	0
4	EDO	C	348	4/4	0.89	0.16	44,45,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.