



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:31 AM GMT

PDB ID : 3EZ0
Title : Crystal structure of protein of unknown function with ferritin-like fold (YP_832262.1) from *Arthrobacter* sp. FB24 at 2.33 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-10-22
Resolution : 2.33 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

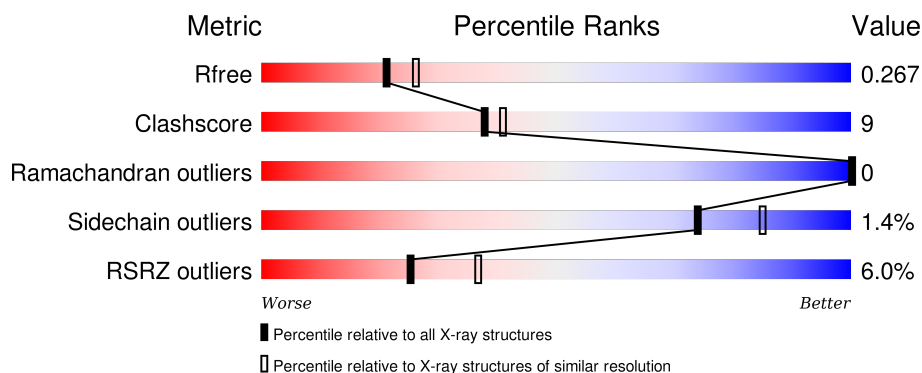
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 $\leq 5\%$. 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	225	<div> <div>4%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
1	B	225	<div> <div>6%</div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>
1	C	225	<div> <div>7%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
1	D	225	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>

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
2	UNL	A	500	-	-	X	-
2	UNL	B	500	-	-	X	-
2	UNL	C	500	-	-	X	-
2	UNL	D	500	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6854 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 uncharacterized protein with ferritin-like fold.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	Se	0	0	0
			1677	1056	304	311	6			
1	B	213	Total	C	N	O	Se	0	0	0
			1665	1054	296	309	6			
1	C	208	Total	C	N	O	Se	0	0	0
			1609	1019	286	298	6			
1	D	210	Total	C	N	O	Se	0	0	0
			1632	1037	290	299	6			

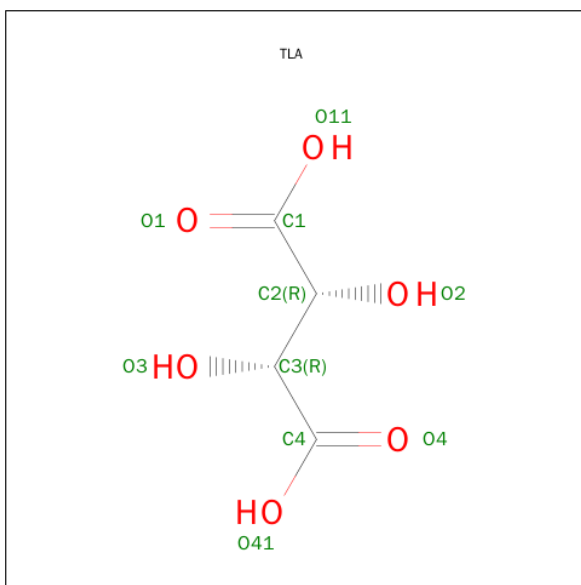
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP A0JYP2
B	0	GLY	-	leader sequence	UNP A0JYP2
C	0	GLY	-	leader sequence	UNP A0JYP2
D	0	GLY	-	leader sequence	UNP A0JYP2

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			22	2	20		
2	A	1	Total	C	O	0	0
			18	2	16		
2	D	1	Total	C	O	0	0
			22	2	20		
2	C	1	Total	C	O	0	0
			22	2	20		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total 51	O 51	0	0
5	B	18	Total 18	O 18	0	0
5	C	50	Total 50	O 50	0	0
5	D	54	Total 54	O 54	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.60Å 96.71Å 71.20Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	29.54 – 2.33 29.54 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-2.33) 99.6 (29.54-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.262 0.214 , 0.267	Depositor DCC
R_{free} test set	1786 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35843 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 37.37 % 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 4.3319e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: TLA, UNL, EDO

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	0.59	0/1701	0.71	0/2291
1	B	0.62	0/1689	0.70	3/2272 (0.1%)
1	C	0.56	0/1632	0.67	0/2197
1	D	0.64	0/1656	0.74	3/2228 (0.1%)
All	All	0.60	0/6678	0.71	6/8988 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	LEU	CA-CB-CG	5.70	128.40	115.30
1	B	91	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	91	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	91	ARG	CG-CD-NE	5.09	122.48	111.80
1	D	93	ARG	CG-CD-NE	5.07	122.44	111.80
1	B	62	LEU	CA-CB-CG	5.04	126.88	115.30

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	1677	0	1636	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1665	0	1627	17	0
1	C	1609	0	1562	21	0
1	D	1632	0	1595	18	0
2	A	18	0	0	9	0
2	B	22	0	0	13	0
2	C	22	0	0	12	0
2	D	22	0	0	12	0
3	B	10	0	4	1	0
4	B	4	0	6	0	0
5	A	51	0	0	1	0
5	B	18	0	0	0	0
5	C	50	0	0	1	0
5	D	54	0	0	1	0
All	All	6854	0	6430	121	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 (121) 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:B:500:UNL:O20	2:B:500:UNL:O21	1.54	1.26
2:D:500:UNL:O21	2:D:500:UNL:O20	1.53	1.26
2:B:500:UNL:O22	2:B:500:UNL:O21	1.54	1.26
2:A:500:UNL:O16	2:A:500:UNL:O15	1.54	1.26
2:C:500:UNL:O2	2:C:500:UNL:O13	1.52	1.26
2:D:500:UNL:O19	2:D:500:UNL:O20	1.53	1.26
2:D:500:UNL:O15	2:D:500:UNL:O14	1.53	1.26
2:C:500:UNL:O19	2:C:500:UNL:O18	1.54	1.25
2:A:500:UNL:O14	2:A:500:UNL:O13	1.54	1.25
2:C:500:UNL:O21	2:C:500:UNL:O22	1.53	1.25
2:B:500:UNL:O18	2:B:500:UNL:O17	1.54	1.25
2:C:500:UNL:O15	2:C:500:UNL:O16	1.54	1.25
2:D:500:UNL:O15	2:D:500:UNL:O16	1.54	1.25
2:A:500:UNL:O17	2:A:500:UNL:O16	1.53	1.24
2:A:500:UNL:O13	2:A:500:UNL:O2	1.52	1.24
2:D:500:UNL:O22	2:D:500:UNL:O21	1.53	1.24
2:B:500:UNL:O15	2:B:500:UNL:O16	1.54	1.24
2:D:500:UNL:O13	2:D:500:UNL:O14	1.53	1.24
2:C:500:UNL:O19	2:C:500:UNL:O20	1.53	1.24
2:A:500:UNL:O14	2:A:500:UNL:O15	1.54	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:UNL:O2	2:D:500:UNL:O13	1.53	1.24
2:D:500:UNL:O17	2:D:500:UNL:O18	1.53	1.24
2:B:500:UNL:O18	2:B:500:UNL:O19	1.54	1.23
2:B:500:UNL:O11	2:B:500:UNL:O9	1.53	1.23
2:C:500:UNL:O15	2:C:500:UNL:O14	1.53	1.23
2:B:500:UNL:O20	2:B:500:UNL:O19	1.54	1.23
2:B:500:UNL:O14	2:B:500:UNL:O13	1.54	1.23
2:D:500:UNL:O19	2:D:500:UNL:O18	1.53	1.22
2:C:500:UNL:O14	2:C:500:UNL:O13	1.54	1.22
2:B:500:UNL:O16	2:B:500:UNL:O17	1.54	1.22
2:D:500:UNL:O16	2:D:500:UNL:O17	1.53	1.22
2:C:500:UNL:O20	2:C:500:UNL:O21	1.53	1.21
2:A:500:UNL:O17	2:A:500:UNL:O18	1.53	1.21
2:C:500:UNL:O18	2:C:500:UNL:O17	1.53	1.21
2:B:500:UNL:O2	2:B:500:UNL:O13	1.53	1.20
2:C:500:UNL:O17	2:C:500:UNL:O16	1.53	1.19
2:B:500:UNL:O14	2:B:500:UNL:O15	1.54	1.18
2:B:500:UNL:O12	2:B:500:UNL:O9	1.62	1.18
2:D:500:UNL:O9	2:D:500:UNL:O8	1.63	1.17
2:A:500:UNL:O12	2:A:500:UNL:O9	1.62	1.16
2:A:500:UNL:O8	2:A:500:UNL:O9	1.63	1.15
2:C:500:UNL:O9	2:C:500:UNL:O12	1.62	1.15
2:D:500:UNL:O9	2:D:500:UNL:O12	1.63	1.15
2:C:500:UNL:O9	2:C:500:UNL:O8	1.64	1.15
2:B:500:UNL:O8	2:B:500:UNL:O9	1.63	1.14
1:C:52:ILE:HD11	1:C:143:LEU:HD21	1.34	1.04
1:A:174:THR:HG23	1:C:177:GLN:NE2	1.88	0.89
1:B:48:VAL:HG21	1:B:146:ARG:NH2	1.89	0.88
1:D:154:ASP:OD1	1:D:156:ARG:HD3	1.73	0.88
1:D:186:LEU:HD22	1:D:202:VAL:HG22	1.58	0.86
1:C:102:MSE:HE2	1:C:147:LEU:HD22	1.61	0.82
1:A:102:MSE:HE2	1:A:147:LEU:HD22	1.62	0.79
1:A:163:LEU:HD12	1:C:211:GLU:OE2	1.86	0.75
1:D:190:ILE:HD12	1:D:201:LEU:HD22	1.68	0.74
1:A:102:MSE:HE2	1:A:147:LEU:CD2	2.19	0.73
1:D:102:MSE:HE2	1:D:161:LEU:HD13	1.73	0.70
1:B:102:MSE:HE3	1:B:161:LEU:HB3	1.74	0.70
1:B:180:SER:O	1:B:184:ALA:HB2	1.91	0.69
1:C:52:ILE:HD11	1:C:143:LEU:CD2	2.19	0.68
1:D:102:MSE:HE3	1:D:161:LEU:HB3	1.79	0.65
1:B:154:ASP:OD1	1:B:156:ARG:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:CZ	1:B:126:THR:HG23	2.33	0.63
1:B:36:ASP:HB2	1:B:49:LEU:HD13	1.82	0.61
1:B:121:TYR:CD2	1:B:190:ILE:HG22	2.37	0.59
1:A:102:MSE:CE	1:A:147:LEU:HD22	2.32	0.59
1:B:102:MSE:CE	1:B:161:LEU:HD13	2.33	0.59
1:D:19:PHE:CZ	1:D:126:THR:HG23	2.39	0.58
1:A:52:ILE:CD1	1:A:104:ALA:HB1	2.34	0.57
1:D:108:ASP:HB2	5:D:359:HOH:O	2.04	0.57
1:C:63:VAL:CG2	1:C:133:ILE:HD11	2.34	0.56
1:A:163:LEU:HD23	5:A:295:HOH:O	2.05	0.56
1:B:48:VAL:HG21	1:B:146:ARG:HH22	1.67	0.56
1:A:63:VAL:CG2	1:A:133:ILE:HD11	2.36	0.56
1:D:66:ARG:HG2	1:D:129:VAL:HG21	1.89	0.55
1:D:180:SER:O	1:D:184:ALA:HB2	2.07	0.55
1:C:16:ALA:HB2	1:C:72:ILE:CD1	2.40	0.52
1:D:154:ASP:OD2	1:D:157:LEU:HD13	2.09	0.52
1:D:115:TYR:HB3	1:D:130:ILE:CG2	2.40	0.52
1:D:87:TYR:O	1:D:91:ARG:HG2	2.10	0.51
1:D:186:LEU:HD23	1:D:186:LEU:O	2.10	0.51
1:C:205:LEU:C	1:C:205:LEU:HD23	2.30	0.51
1:D:5:PRO:N	1:D:8:THR:HG1	2.09	0.51
1:A:116:ARG:HG3	1:A:134:GLN:NE2	2.26	0.51
1:A:52:ILE:HD13	1:A:104:ALA:HB1	1.93	0.50
1:B:102:MSE:HE2	1:B:161:LEU:HD13	1.93	0.50
1:A:102:MSE:HE3	1:A:161:LEU:HD13	1.95	0.49
1:A:184:ALA:CB	1:A:199:LYS:HZ3	2.26	0.49
1:B:62:LEU:CD2	1:B:129:VAL:HG13	2.43	0.48
1:C:102:MSE:HE1	1:C:220:LEU:HD13	1.95	0.48
1:B:121:TYR:HB3	1:B:189:LEU:O	2.13	0.48
1:A:163:LEU:CD1	1:C:211:GLU:OE2	2.56	0.48
1:A:75:GLU:HA	1:A:78:MSE:HE3	1.96	0.47
1:D:96:ASP:OD2	1:D:160:ARG:NH1	2.48	0.47
1:D:87:TYR:CE2	1:D:91:ARG:HD3	2.49	0.47
1:C:52:ILE:HD13	1:C:143:LEU:HD11	1.95	0.47
1:B:87:TYR:O	1:B:91:ARG:HG2	2.14	0.47
1:B:48:VAL:O	1:B:52:ILE:HD12	2.15	0.46
1:A:184:ALA:HB3	1:A:199:LYS:HZ3	1.81	0.46
1:B:41:PRO:HD3	1:B:97:TRP:CD2	2.49	0.46
1:C:58:ARG:HD3	5:C:360:HOH:O	2.15	0.46
1:C:24:TYR:CE2	1:C:82:GLN:HA	2.51	0.45
1:B:93:ARG:HH11	3:B:225:TLA:H3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLU:O	1:C:79:LEU:HD13	2.16	0.45
1:C:109:THR:HB	1:C:216:ARG:CZ	2.46	0.45
1:A:115:TYR:HB3	1:A:130:ILE:CG2	2.47	0.44
1:A:21:MSE:HE3	2:A:500:UNL:O1	2.18	0.43
1:A:9:ALA:O	1:A:13:ARG:HG3	2.18	0.43
1:A:121:TYR:CD2	1:A:190:ILE:HD13	2.54	0.43
1:A:33:PHE:CD2	1:A:52:ILE:HD12	2.54	0.43
1:D:10:ARG:O	1:D:14:PHE:CD2	2.72	0.43
1:A:184:ALA:CB	1:A:199:LYS:NZ	2.82	0.42
1:D:102:MSE:CE	1:D:161:LEU:HD13	2.45	0.42
1:B:115:TYR:HB3	1:B:130:ILE:CG2	2.48	0.42
1:A:81:PHE:O	1:A:85:VAL:HG23	2.20	0.42
1:C:16:ALA:CB	1:C:72:ILE:HD13	2.50	0.41
1:C:40:SER:HA	1:C:97:TRP:CD1	2.56	0.41
1:C:115:TYR:HB3	1:C:130:ILE:HG23	2.02	0.41
1:A:62:LEU:HD23	1:A:62:LEU:C	2.41	0.41
1:C:63:VAL:HG23	1:C:133:ILE:HD11	2.02	0.40
1:C:40:SER:HA	1:C:97:TRP:CG	2.57	0.40
1:C:104:ALA:O	1:C:108:ASP:HB2	2.21	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	212/225 (94%)	208 (98%)	4 (2%)	0	100	100
1	B	207/225 (92%)	200 (97%)	7 (3%)	0	100	100
1	C	204/225 (91%)	201 (98%)	3 (2%)	0	100	100
1	D	204/225 (91%)	198 (97%)	6 (3%)	0	100	100
All	All	827/900 (92%)	807 (98%)	20 (2%)	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	164/170 (96%)	163 (99%)	1 (1%)	90	96
1	B	164/170 (96%)	162 (99%)	2 (1%)	78	88
1	C	155/170 (91%)	153 (99%)	2 (1%)	76	86
1	D	158/170 (93%)	154 (98%)	4 (2%)	55	68
All	All	641/680 (94%)	632 (99%)	9 (1%)	74	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	B	133	ILE
1	B	178	ARG
1	C	180	SER
1	C	188	SER
1	D	68	GLU
1	D	75	GLU
1	D	133	ILE
1	D	178	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	C	134	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are unknown - leaving 2 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	TLA	B	225	-	3,9,9	0.24	0	6,12,12	1.44	1 (16%)
4	EDO	B	226	-	3,3,3	0.46	0	2,2,2	0.34	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	TLA	B	225	-	-	0/4/12/12	0/0/0/0
4	EDO	B	226	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	225	TLA	C4-C3-C2	-2.10	109.04	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	225	TLA	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 ⓘ

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(Å ²)	Q<0.9
1	A	210/225 (93%)	0.32	10 (4%) 34 47	28, 45, 66, 78	0
1	B	207/225 (92%)	0.33	14 (6%) 20 30	32, 43, 62, 76	0
1	C	202/225 (89%)	0.40	16 (7%) 15 23	33, 45, 68, 77	0
1	D	204/225 (90%)	0.20	9 (4%) 38 50	31, 44, 64, 74	0
All	All	823/900 (91%)	0.31	49 (5%) 25 37	28, 45, 66, 78	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	6.8
1	D	6	ALA	4.3
1	B	153	ASP	4.3
1	D	7	ASP	4.1
1	C	12	ASN	3.8
1	A	124	ALA	3.7
1	D	163	LEU	3.6
1	B	4	SER	3.6
1	C	179	VAL	3.4
1	B	157	LEU	3.4
1	B	6	ALA	3.4
1	B	201	LEU	3.4
1	C	11	TYR	3.3
1	C	152	ALA	3.3
1	C	184	ALA	3.3
1	B	5	PRO	3.3
1	D	197	ALA	3.3
1	D	190	ILE	3.1
1	A	8	THR	3.1
1	A	6	ALA	3.1
1	D	198	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	8	THR	3.0
1	A	4	SER	3.0
1	B	142	VAL	3.0
1	C	196	ALA	3.0
1	A	137	ASP	2.8
1	C	133	ILE	2.7
1	B	8	THR	2.7
1	C	180	SER	2.7
1	C	183	HIS	2.7
1	B	158	ALA	2.6
1	B	194	ASP	2.5
1	C	156	ARG	2.5
1	C	181	TYR	2.5
1	D	10	ARG	2.4
1	A	9	ALA	2.4
1	C	14	PHE	2.4
1	B	223	THR	2.4
1	A	7	ASP	2.3
1	B	145	GLU	2.3
1	A	12	ASN	2.3
1	A	120	ARG	2.2
1	C	190	ILE	2.2
1	B	139	THR	2.2
1	C	122	VAL	2.2
1	C	155	PRO	2.2
1	D	9	ALA	2.1
1	B	222	LEU	2.1
1	C	198	ALA	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(Å ²)	Q<0.9
2	UNL	C	500	22/-	0.84	0.23	1.72	46,80,87,88	0
2	UNL	D	500	22/-	0.85	0.21	1.63	41,74,79,83	0
2	UNL	B	500	22/-	0.85	0.18	1.25	44,80,89,91	0
2	UNL	A	500	18/-	0.83	0.22	1.20	46,78,83,83	0
4	EDO	B	226	4/4	0.97	0.13	-0.53	28,31,34,34	0
3	TLA	B	225	10/10	0.96	0.12	-0.89	28,34,36,38	0

6.5 Other polymers

There are no such residues in this entry.