wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:58 AM GMT

PDB ID	:	2F1K
Title	:	Crystal structure of Synechocystis arogenate dehydrogenase
Authors	:	Legrand, P.; Dumas, R.; Seux, M.; Rippert, P.; Ravelli, R.; Ferrer, J.-L.; Matringe, M.
Deposited on	:	2005-11-14
Resolution	:	1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

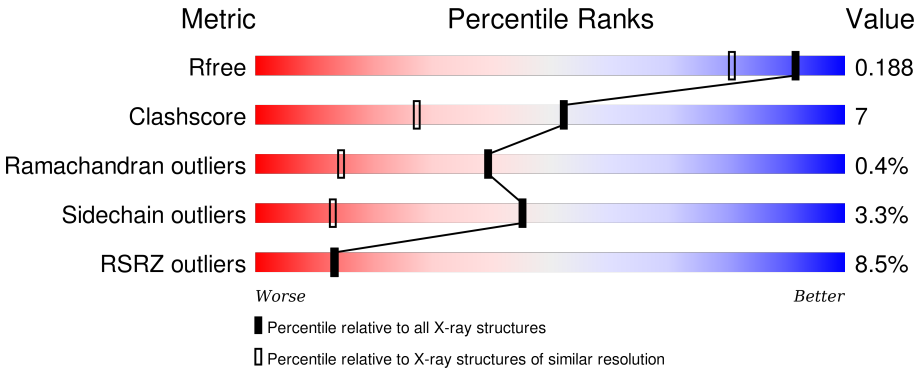
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	279	3% 88% 10%
1	B	279	2% 89% 10%
1	C	279	23% 84% 13%
1	D	279	6% 85% 14%

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	TRS	C	1001	-	-	-	X
2	TRS	D	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9282 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.

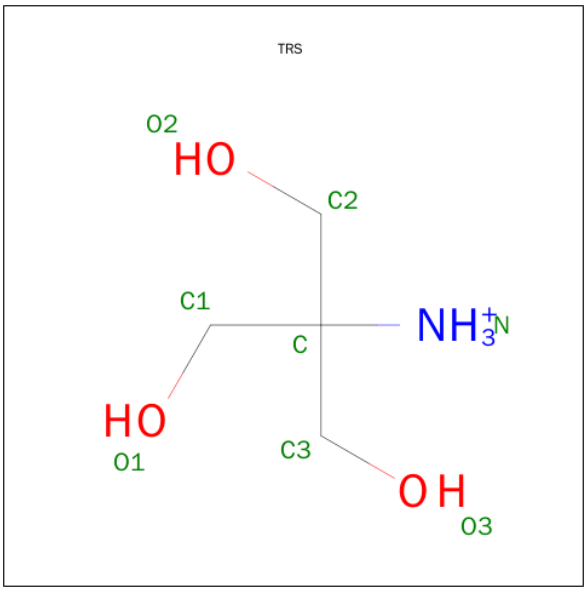
- Molecule 1 is a protein called prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	4	10	0
			2181	1371	381	418	11			
1	B	279	Total	C	N	O	S	0	2	0
			2135	1344	369	410	12			
1	C	278	Total	C	N	O	S	17	4	0
			2133	1341	371	411	10			
1	D	279	Total	C	N	O	S	0	9	0
			2190	1376	381	421	12			

There are 8 discrepancies between the modelled and reference sequences:

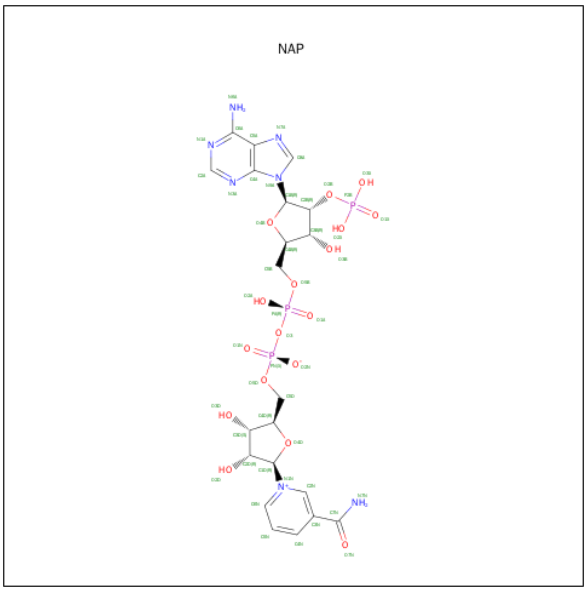
Chain	Residue	Modelled	Actual	Comment	Reference
A	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
A	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
B	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
B	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
C	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
C	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
D	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
D	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			58	22	7	24	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

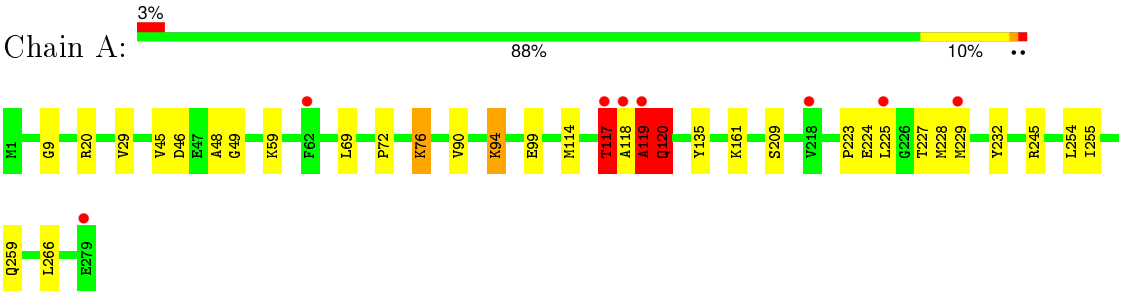
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	129	Total	O	0	0
			129	129		
4	C	43	Total	O	0	0
			43	43		
4	D	125	Total	O	0	1
			126	126		

3 Residue-property plots (i)

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.

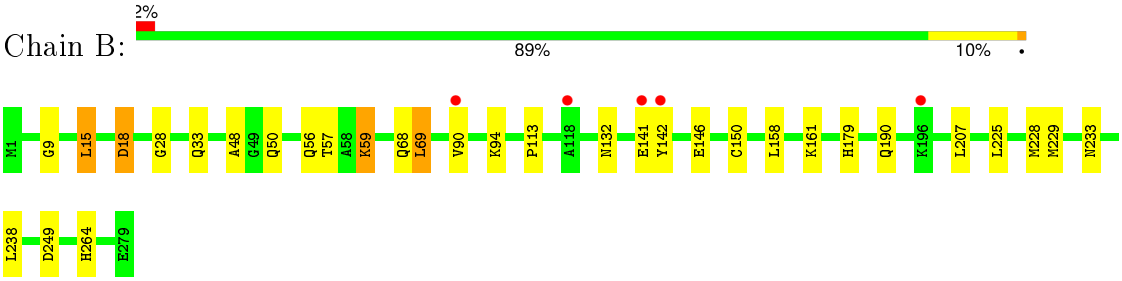
- Molecule 1: prephenate dehydrogenase

Chain A:



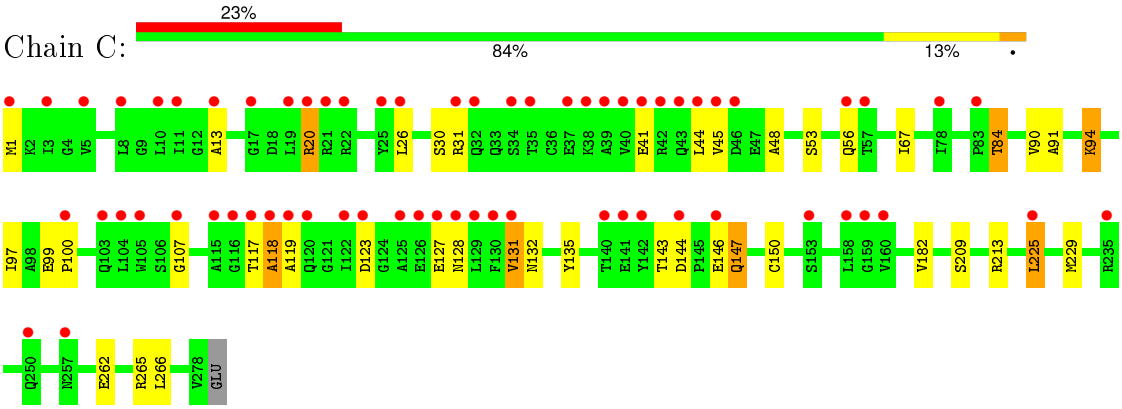
- Molecule 1: prephenate dehydrogenase

Chain B:



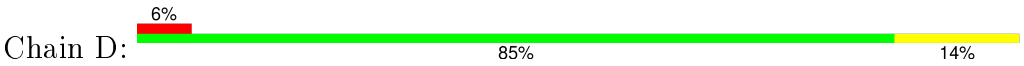
- Molecule 1: prephenate dehydrogenase

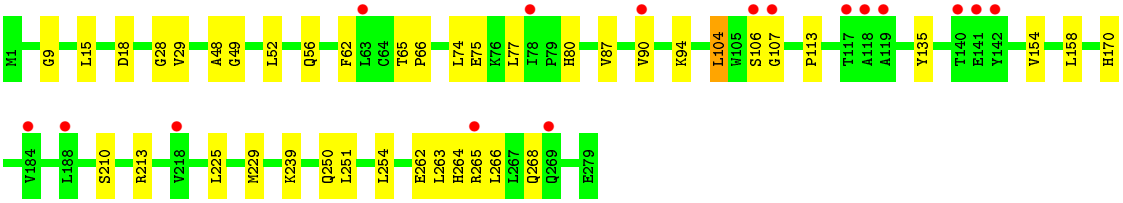
Chain C:



- Molecule 1: prephenate dehydrogenase

Chain D:




M1
G9
L15
D18
G28
V29
A48
G49
L52
Q56
F62
L63
G64
T65
P66
L74
E75
K76
L77
I78
P79
H80
V87
V90
K94
L104
W105
S106
G107
P113
T117
A118
A119
Y135
T140
E141
Y142
V154
L158
H170
V184
L188
S210
R213
V218
L225
M229
K239
Q250
L251
L254
E262
L263
H264
R265
L266
L267
Q268
Q269
E279

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.15Å 70.85Å 104.49Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 29.94 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.55) 99.0 (29.94-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.222 0.189 , 0.188	Depositor DCC
R_{free} test set	6960 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 138618 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9282	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OCS, TRS, NAP, OMT

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	0.61	0/2225	0.75	1/3017 (0.0%)
1	B	0.56	0/2159	0.67	2/2931 (0.1%)
1	C	0.99	8/2161 (0.4%)	1.12	5/2936 (0.2%)
1	D	0.56	0/2218	0.71	0/3008
All	All	0.70	8/8763 (0.1%)	0.83	8/11892 (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	A	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLN	CD-NE2	21.12	1.85	1.32
1	C	1	MET	CA-CB	18.64	1.95	1.53
1	C	147	GLN	CG-CD	13.93	1.83	1.51
1	C	84	THR	CB-OG1	11.10	1.65	1.43
1	C	123	ASP	CG-OD1	9.53	1.47	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	MET	N-CA-CB	-48.15	23.92	110.60
1	A	120	GLN	CB-CG-CD	8.71	134.25	111.60
1	C	1	MET	CB-CA-C	-8.49	93.41	110.40
1	C	147	GLN	CG-CD-NE2	-7.18	99.48	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	GLN	CG-CD-OE1	6.06	133.72	121.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	119	ALA	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	2181	0	2210	31	0
1	B	2135	0	2160	38	0
1	C	2133	0	2154	33	1
1	D	2190	0	2211	30	1
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	A	58	0	10	2	0
3	B	48	0	25	4	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	127	0	0	3	0
4	B	129	0	0	3	0
4	C	43	0	0	0	0
4	D	126	0	0	3	0
All	All	9282	0	8844	119	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 7.

The worst 5 of 119 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:C:147:GLN:CG	1:C:147:GLN:CD	1.83	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:CB	1:C:84:THR:OG1	1.65	1.39
1:C:147:GLN:CD	1:C:147:GLN:NE2	1.85	1.28
1:A:266:LEU:HD11	1:B:190:GLN:NE2	1.78	0.97
1:A:255:ILE:HG22	1:B:238:LEU:CD2	2.11	0.81

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)
1:C:41:GLU:OE2	1:D:265:ARG:NH2[2_656]	2.19	0.01

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	285/279 (102%)	275 (96%)	7 (2%)	3 (1%)	17 2
1	B	277/279 (99%)	273 (99%)	4 (1%)	0	100 100
1	C	278/279 (100%)	271 (98%)	6 (2%)	1 (0%)	39 14
1	D	284/279 (102%)	275 (97%)	9 (3%)	0	100 100
All	All	1124/1116 (101%)	1094 (97%)	26 (2%)	4 (0%)	39 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	A	118	ALA
1	C	118	ALA
1	A	120	GLN

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	237/227 (104%)	227 (96%)	10 (4%)	36 7
1	B	229/227 (101%)	223 (97%)	6 (3%)	54 20
1	C	229/227 (101%)	220 (96%)	9 (4%)	39 9
1	D	235/227 (104%)	228 (97%)	7 (3%)	48 15
All	All	930/908 (102%)	898 (97%)	32 (3%)	45 12

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	TYR
1	C	26	LEU
1	D	154	VAL
1	C	20	ARG
1	C	30	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	205	GLN
1	B	257	ASN
1	C	258	GLN
1	B	179	HIS
1	B	190	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OMT	A	114	1	8,9,10	2.64	2 (25%)	8,12,14	2.43	2 (25%)
1	OCS	A	150	1	7,8,9	0.93	0	7,11,13	1.35	1 (14%)
1	OMT	B	114	1	8,9,10	3.00	1 (12%)	8,12,14	15.91	5 (62%)
1	OCS	B	150	1	7,8,9	0.87	0	7,11,13	1.81	2 (28%)
1	OMT	C	114	1	8,9,10	2.72	1 (12%)	8,12,14	17.65	6 (75%)
1	OCS	C	150	1	7,8,9	6.46	4 (57%)	7,11,13	3.77	2 (28%)
1	OMT	D	114	1	8,9,10	2.90	1 (12%)	8,12,14	17.12	5 (62%)
1	OCS	D	150	1	7,8,9	0.91	0	7,11,13	1.29	1 (14%)

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
1	OMT	A	114	1	-	0/6/8/10	0/0/0/0
1	OCS	A	150	1	-	1/4/7/9	0/0/0/0
1	OMT	B	114	1	-	0/6/8/10	0/0/0/0
1	OCS	B	150	1	-	1/4/7/9	0/0/0/0
1	OMT	C	114	1	-	0/6/8/10	0/0/0/0
1	OCS	C	150	1	-	1/4/7/9	0/0/0/0
1	OMT	D	114	1	-	0/6/8/10	0/0/0/0
1	OCS	D	150	1	-	1/4/7/9	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	OMT	CG-SD	-8.13	1.68	1.78
1	D	114	OMT	CG-SD	-7.82	1.68	1.78
1	C	114	OMT	CG-SD	-7.27	1.69	1.78
1	A	114	OMT	CG-SD	-6.90	1.69	1.78
1	A	114	OMT	CE-SD	-2.07	1.65	1.75

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	114	OMT	OD2-SD-CG	-38.05	83.95	108.28
1	D	114	OMT	OD2-SD-CG	-30.56	88.74	108.28
1	C	114	OMT	OD2-SD-CE	-23.50	82.95	108.92
1	B	114	OMT	OD2-SD-CG	-22.55	93.86	108.28
1	D	114	OMT	OD2-SD-CE	-18.93	88.00	108.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	150	OCS	SG-CB-CA-N
1	D	150	OCS	SG-CB-CA-N
1	B	150	OCS	SG-CB-CA-N
1	A	150	OCS	SG-CB-CA-N

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	114	OMT	2	0
1	B	150	OCS	1	0
1	C	150	OCS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	NAP	A	1350[A]	-	42,52,52	1.57	4 (9%)	54,80,80	2.18	4 (7%)
3	NAP	A	1350[B]	-	42,52,52	1.54	3 (7%)	54,80,80	2.11	3 (5%)
3	NAP	B	2350	-	42,52,52	1.59	3 (7%)	54,80,80	2.26	5 (9%)
2	TRS	C	1001	-	7,7,7	0.99	1 (14%)	9,9,9	0.85	0
3	NAP	C	3350	-	42,52,52	1.60	3 (7%)	54,80,80	1.98	4 (7%)
2	TRS	D	1002	-	7,7,7	1.13	1 (14%)	9,9,9	0.81	0
3	NAP	D	4350	-	42,52,52	1.62	3 (7%)	54,80,80	2.19	6 (11%)

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	NAP	A	1350[A]	-	-	0/27/67/67	0/5/5/5
3	NAP	A	1350[B]	-	-	0/27/67/67	0/5/5/5
3	NAP	B	2350	-	-	0/27/67/67	0/5/5/5
2	TRS	C	1001	-	-	0/9/9/9	0/0/0/0
3	NAP	C	3350	-	-	0/27/67/67	0/5/5/5
2	TRS	D	1002	-	-	0/9/9/9	0/0/0/0
3	NAP	D	4350	-	-	0/27/67/67	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1002	TRS	C-N	-2.90	1.46	1.50
2	C	1001	TRS	C-N	-2.51	1.47	1.50
3	A	1350[A]	NAP	PN-O2N	-2.33	1.45	1.54
3	B	2350	NAP	C2A-N1A	2.32	1.38	1.33
3	C	3350	NAP	C2A-N1A	2.68	1.39	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2350	NAP	N3A-C2A-N1A	-14.24	117.99	128.89
3	A	1350[A]	NAP	N3A-C2A-N1A	-13.94	118.22	128.89
3	A	1350[B]	NAP	N3A-C2A-N1A	-13.94	118.22	128.89
3	D	4350	NAP	N3A-C2A-N1A	-12.56	119.28	128.89
3	C	3350	NAP	N3A-C2A-N1A	-12.20	119.55	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1350[A]	NAP	2	0
3	B	2350	NAP	4	0
3	C	3350	NAP	2	0
3	D	4350	NAP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	277/279 (99%)	0.27	8 (2%) 55 59	11, 16, 24, 39	3 (1%)
1	B	277/279 (99%)	0.22	5 (1%) 71 75	11, 16, 24, 33	1 (0%)
1	C	276/279 (98%)	1.32	65 (23%) 1 1	10, 16, 24, 29	4 (1%)
1	D	277/279 (99%)	0.41	16 (5%) 26 27	11, 16, 24, 35	0
All	All	1107/1116 (99%)	0.55	94 (8%) 13 13	10, 16, 24, 39	8 (0%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ALA	23.7
1	C	119	ALA	17.5
1	B	142	TYR	10.8
1	D	118	ALA	9.4
1	A	117	THR	8.4

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

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, 95^{th} 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
1	OMT	D	114	10/11	0.97	0.09	-	14,15,24,24	2
1	OMT	B	114	10/11	0.97	0.13	-	14,16,20,21	2
1	OMT	C	114	10/11	0.76	0.18	-	18,21,29,30	2
1	OMT	A	114	10/11	0.86	0.16	-	20,25,36,37	2
1	OCS	C	150	9/10	0.90	0.19	-	21,22,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	OCS	A	150	9/10	0.95	0.07	-	15,16,24,25	0
1	OCS	B	150	9/10	0.94	0.08	-	19,20,23,26	0
1	OCS	D	150	9/10	0.96	0.07	-	17,17,21,24	0

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, 95^{th} 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	TRS	C	1001	8/8	0.83	0.21	4.66	25,26,26,27	0
2	TRS	D	1002	8/8	0.86	0.19	3.69	25,25,26,26	0
3	NAP	A	1350[B]	48/48	0.90	0.12	0.52	15,19,24,30	10
3	NAP	C	3350	48/48	0.82	0.18	0.03	21,26,35,36	0
3	NAP	D	4350	48/48	0.91	0.10	-0.11	15,22,26,28	0
3	NAP	A	1350[A]	48/48	0.90	0.12	-0.11	14,20,24,30	10
3	NAP	B	2350	48/48	0.92	0.11	-0.14	16,19,27,30	0

6.5 Other polymers (i)

There are no such residues in this entry.