Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:23 PM GMT

PDB ID	:	4LGL
Title	:	Crystal Structure of Glycine Decarboxylase P-protein from Synechocystis sp. PCC 6803, apo form
Authors	:	Hasse, D.; Andersson, E.; Carlsson, G.; Masloboy, A.; Hagemann, M.; Bauwe, H.; Andersson, I.
Deposited on	:	2013-06-28
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
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:

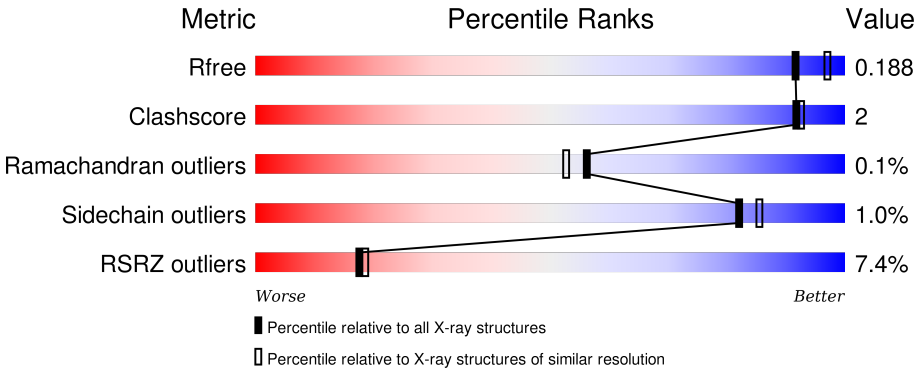
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	983	8% 90% 6% ·
1	B	983	6% 89% 6% 5%

2 Entry composition

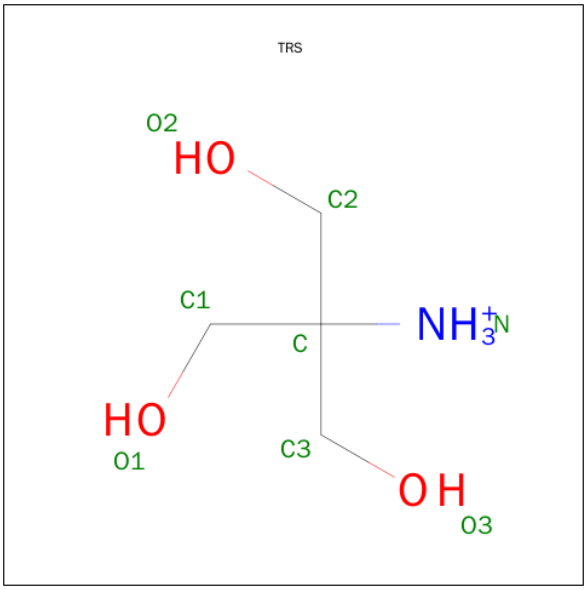
There are 4 unique types of molecules in this entry. The entry contains 15465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycine dehydrogenase [decarboxylating].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	948	Total	C	N	O	S	0	7	0
			7337	4656	1248	1387	46			
1	B	930	Total	C	N	O	S	0	15	0
			7245	4605	1226	1365	49			

- 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	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

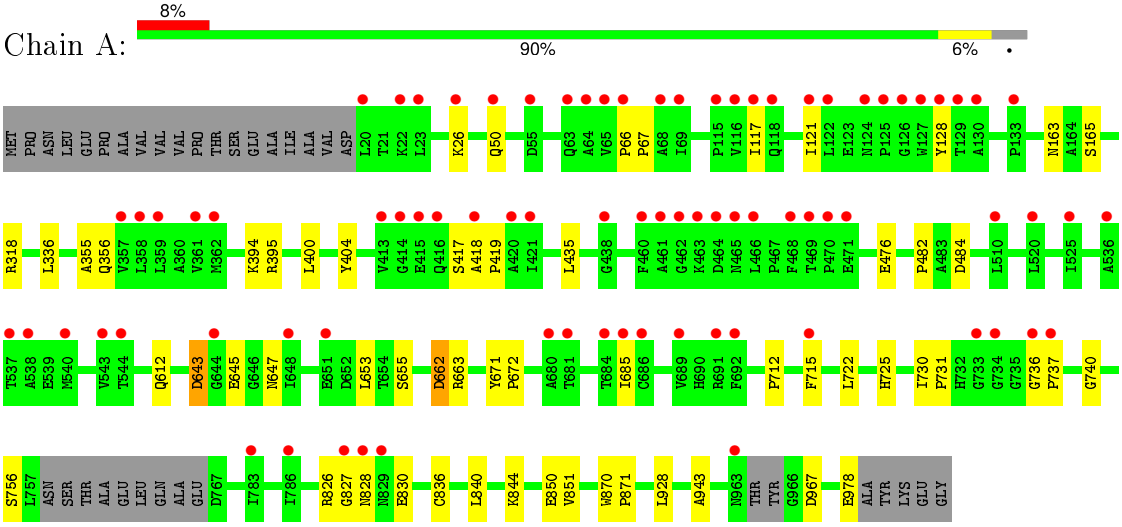
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	405	Total O 405 405	0	0
4	B	460	Total O 460 460	0	0

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.

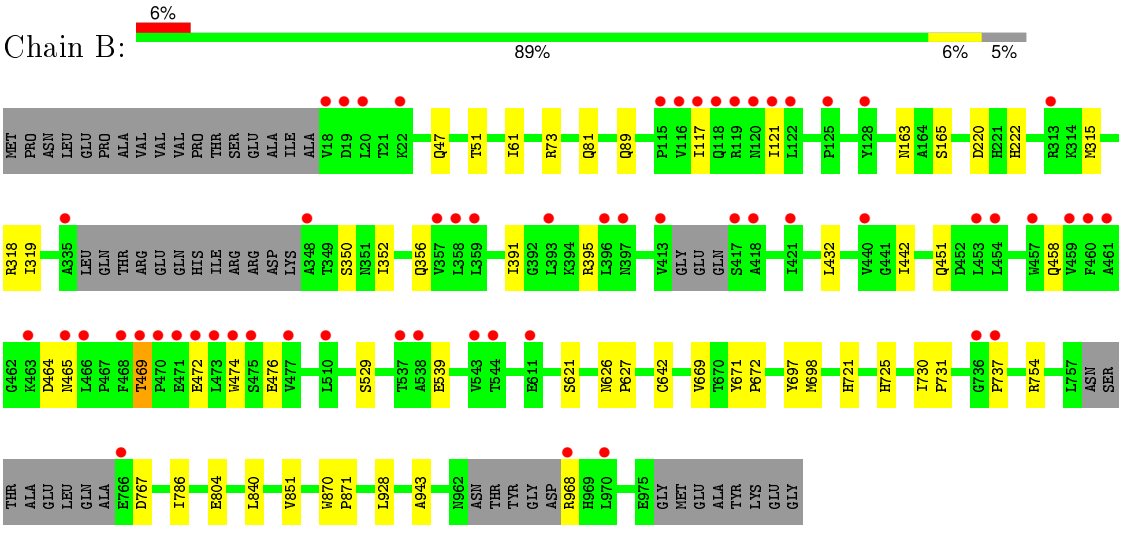
- Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain A:



- Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.30Å 135.81Å 179.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.11 – 2.00 54.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.11-2.00) 99.8 (54.11-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.161 , 0.192 0.154 , 0.188	Depositor DCC
R_{free} test set	7941 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 158214 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15465	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: CME, TRS, CL

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	0.35	0/7485	0.51	0/10172
1	B	0.37	0/7397	0.50	0/10052
All	All	0.36	0/14882	0.50	0/20224

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	7337	0	7213	29	0
1	B	7245	0	7128	32	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	405	0	0	0	0
4	B	460	0	0	2	0
All	All	15465	0	14365	60	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 2.

All (60) 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:B:73[B]:ARG:NH2	4:B:1531:HOH:O	2.21	0.73
1:A:612:GLN:O	1:A:663:ARG:NH1	2.22	0.72
1:B:754:ARG:NH2	1:B:767:ASP:OD1	2.23	0.71
1:A:394:LYS:HE2	1:A:400:LEU:HD12	1.73	0.70
1:A:662:ASP:N	1:A:662:ASP:OD1	2.26	0.68
1:A:643:ASP:HB3	1:A:645:GLU:H	1.60	0.66
1:A:395:ARG:NH2	1:A:476:GLU:OE2	2.30	0.64
1:B:356:GLN:OE1	1:B:737[B]:PRO:HB3	1.99	0.62
1:B:870:TRP:CD1	1:B:871:PRO:HA	2.38	0.59
1:B:395:ARG:NH1	4:B:1466:HOH:O	2.35	0.59
1:B:315:MET:SD	1:B:319[B]:ILE:HD11	2.46	0.56
1:A:870:TRP:CD1	1:A:871:PRO:HA	2.42	0.53
1:A:840:LEU:HD22	1:A:851:VAL:HG23	1.90	0.53
1:B:117:ILE:HG23	1:B:121:ILE:HD12	1.91	0.53
1:B:725:HIS:HA	1:B:730:ILE:HB	1.91	0.52
1:B:163:ASN:HA	1:B:319[B]:ILE:HG12	1.92	0.51
1:B:451:GLN:OE1	1:B:451:GLN:N	2.39	0.51
1:A:643:ASP:HB2	1:A:647:ASN:H	1.75	0.50
1:A:356:GLN:OE1	1:A:737[B]:PRO:HB3	2.11	0.50
1:B:697:TYR:OH	1:B:721:HIS:ND1	2.40	0.50
1:A:404:TYR:CG	1:A:482:PRO:HD3	2.47	0.50
1:B:458:GLN:HG2	1:B:464:ASP:HA	1.95	0.49
1:B:928:LEU:CD1	1:B:943:ALA:HB2	2.43	0.48
1:B:626:ASN:HB2	1:B:627:PRO:HD3	1.94	0.48
1:B:621:SER:HG	1:B:642:CME:HH	1.60	0.48
1:B:870:TRP:CG	1:B:871:PRO:HA	2.49	0.46
1:B:469:THR:O	1:B:472:GLU:HB3	2.16	0.46
1:B:840:LEU:HD22	1:B:851:VAL:HG23	1.98	0.46
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.73	0.45
1:A:418:ALA:HB3	1:A:419:PRO:HD3	1.98	0.45
1:A:712:PRO:HA	1:A:715:PHE:CE2	2.52	0.45
1:B:220:ASP:OD1	1:B:222:HIS:ND1	2.48	0.45
1:B:163:ASN:HB2	1:B:318:ARG:O	2.17	0.45
1:A:26:LYS:HD3	1:B:474:TRP:CD1	2.53	0.44
1:A:117:ILE:HG23	1:A:121:ILE:HD12	2.00	0.44
1:A:826:ARG:HD3	1:A:830:GLU:HB3	1.98	0.44
1:A:725:HIS:HA	1:A:730:ILE:HB	1.99	0.44
1:A:163:ASN:HB2	1:A:318:ARG:O	2.18	0.43
1:B:81:GLN:NE2	1:B:89:GLN:OE1	2.39	0.43
1:A:355:ALA:O	1:A:736[A]:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HG13	1:B:804:GLU:HG2	2.01	0.43
1:B:350:SER:OG	1:B:352:ILE:HG22	2.18	0.42
1:A:928:LEU:CD1	1:A:943:ALA:HB2	2.49	0.42
1:A:128:TYR:O	1:A:731:PRO:HB2	2.19	0.42
1:A:827:GLY:HA3	1:A:828:ASN:HB2	2.02	0.42
1:B:671:TYR:HA	1:B:672:PRO:C	2.38	0.42
1:B:539:GLU:HB3	1:B:786:ILE:HG23	2.00	0.42
1:A:844:LYS:HE3	1:A:850:GLU:OE2	2.19	0.42
1:B:391:ILE:HD13	1:B:476:GLU:HB2	2.02	0.42
1:B:469:THR:HG23	1:B:472:GLU:HB2	2.00	0.42
1:A:722:LEU:O	1:A:740:GLY:HA2	2.21	0.41
1:B:47:GLN:O	1:B:51:THR:HG23	2.20	0.41
1:A:336:LEU:O	1:A:978:GLU:HG2	2.20	0.41
1:A:643:ASP:HB2	1:A:647:ASN:N	2.36	0.41
1:A:66:PRO:HA	1:A:67:PRO:HD3	1.93	0.41
1:B:731:PRO:HD2	1:B:786:ILE:HD13	2.02	0.41
1:B:669:VAL:O	1:B:698:MET:HA	2.21	0.41
1:B:432:LEU:HD22	1:B:442:ILE:HG12	2.03	0.41
1:A:671:TYR:HA	1:A:672:PRO:C	2.41	0.41
1:A:826:ARG:HB3	1:A:830:GLU:HA	2.02	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	947/983 (96%)	923 (98%)	23 (2%)	1 (0%)	56	53
1	B	933/983 (95%)	911 (98%)	21 (2%)	1 (0%)	56	53
All	All	1880/1966 (96%)	1834 (98%)	44 (2%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	165	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	773/797 (97%)	762 (99%)	11 (1%)	74 77
1	B	766/797 (96%)	762 (100%)	4 (0%)	92 94
All	All	1539/1594 (96%)	1524 (99%)	15 (1%)	82 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	417	SER
1	A	484	ASP
1	A	643	ASP
1	A	653	LEU
1	A	655	SER
1	A	662	ASP
1	A	685	ILE
1	A	756	SER
1	A	836	CYS
1	A	967	ASP
1	B	465	ASN
1	B	469	THR
1	B	529	SER
1	B	968	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	256	GLN
1	A	416	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	CME	A	642	1	8,9,10	0.92	0	6,9,11	1.67	2 (33%)
1	CME	A	974	1	8,9,10	0.99	0	6,9,11	1.92	2 (33%)
1	CME	B	642	1	8,9,10	0.95	0	6,9,11	1.71	2 (33%)
1	CME	B	974	1	8,9,10	0.89	0	6,9,11	1.63	2 (33%)

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	CME	A	642	1	-	0/5/8/10	0/0/0/0
1	CME	A	974	1	-	0/5/8/10	0/0/0/0
1	CME	B	642	1	-	0/5/8/10	0/0/0/0
1	CME	B	974	1	-	0/5/8/10	0/0/0/0

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	B	642	CME	O-C-CA	-2.38	119.30	125.49
1	B	974	CME	O-C-CA	-2.16	119.86	125.49
1	A	974	CME	O-C-CA	-2.11	119.98	125.49
1	A	642	CME	CZ-CE-SD	2.14	118.39	113.16
1	A	642	CME	CB-SG-SD	2.20	108.25	103.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	642	CME	CZ-CE-SD	2.24	118.64	113.16
1	B	974	CME	CB-SG-SD	2.54	108.90	103.95
1	A	974	CME	CB-SG-SD	3.33	110.44	103.95

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
1	B	642	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - 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	$\#\|Z\| > 2$
2	TRS	A	1001	-	7,7,7	0.96	1 (14%)	9,9,9	0.72	0
2	TRS	B	1001	-	7,7,7	0.84	1 (14%)	9,9,9	0.40	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
2	TRS	A	1001	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	B	1001	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	TRS	C-N	-2.52	1.47	1.50
2	B	1001	TRS	C-N	-2.01	1.47	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	946/983 (96%)	0.23	81 (8%) 13 14	21, 39, 72, 111	2 (0%)
1	B	928/983 (94%)	0.05	57 (6%) 25 26	21, 35, 65, 102	0
All	All	1874/1966 (95%)	0.14	138 (7%) 17 18	21, 37, 69, 111	2 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737[A]	PRO	12.4
1	B	737[A]	PRO	9.7
1	B	18	VAL	6.7
1	A	736[A]	GLY	6.1
1	A	416	GLN	5.9
1	A	414	GLY	5.7
1	B	736[A]	GLY	5.5
1	A	828	ASN	5.5
1	A	827	GLY	5.0
1	B	19	ASP	4.7
1	A	415	GLU	4.5
1	B	474	TRP	4.3
1	A	122	LEU	4.1
1	A	69	ILE	4.1
1	B	460	PHE	4.1
1	A	829	ASN	3.9
1	B	122	LEU	3.9
1	A	686	CYS	3.8
1	A	121	ILE	3.7
1	A	468	PHE	3.7
1	A	685	ILE	3.6
1	B	466	LEU	3.5
1	A	469	THR	3.5
1	A	128	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	473	LEU	3.4
1	A	127	TRP	3.3
1	A	689	VAL	3.3
1	A	648	ILE	3.3
1	B	421	ILE	3.3
1	A	544	THR	3.3
1	A	22	LYS	3.2
1	A	644	GLY	3.2
1	B	116	VAL	3.2
1	B	477	VAL	3.2
1	A	691	ARG	3.1
1	B	358	LEU	3.1
1	A	461	ALA	3.0
1	A	466	LEU	3.0
1	A	358	LEU	3.0
1	B	465	ASN	3.0
1	A	684	THR	3.0
1	A	543	VAL	3.0
1	B	470	PRO	3.0
1	A	537	THR	3.0
1	A	125	PRO	2.9
1	A	20	LEU	2.9
1	B	393	LEU	2.9
1	A	462	GLY	2.9
1	B	413	VAL	2.9
1	A	680	ALA	2.9
1	A	681	THR	2.9
1	A	715	PHE	2.9
1	A	418	ALA	2.9
1	B	468	PHE	2.8
1	A	117	ILE	2.8
1	B	461	ALA	2.8
1	A	68	ALA	2.8
1	B	970	LEU	2.8
1	B	440	VAL	2.8
1	B	766	GLU	2.7
1	A	420	ALA	2.7
1	A	116	VAL	2.7
1	B	475	SER	2.7
1	B	453	LEU	2.7
1	B	457	TRP	2.6
1	A	963	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	421	ILE	2.6
1	A	465	ASN	2.6
1	B	121	ILE	2.6
1	B	357	VAL	2.6
1	A	438	GLY	2.6
1	B	454	LEU	2.6
1	A	361	VAL	2.6
1	A	413	VAL	2.6
1	B	119	ARG	2.6
1	B	20	LEU	2.6
1	A	464	ASP	2.6
1	A	66	PRO	2.5
1	B	510	LEU	2.5
1	A	359	LEU	2.5
1	B	313	ARG	2.5
1	B	128	TYR	2.5
1	A	786	ILE	2.5
1	A	463	LYS	2.5
1	A	651	GLU	2.5
1	B	471	GLU	2.5
1	B	417	SER	2.5
1	A	520	LEU	2.5
1	B	359	LEU	2.5
1	B	469	THR	2.5
1	B	115	PRO	2.4
1	B	463	LYS	2.4
1	A	540	MET	2.4
1	A	55	ASP	2.4
1	B	117	ILE	2.4
1	B	459	VAL	2.4
1	B	472	GLU	2.4
1	B	537	THR	2.4
1	A	470	PRO	2.3
1	A	50	GLN	2.3
1	A	23	LEU	2.3
1	B	348	ALA	2.3
1	A	733	GLY	2.3
1	A	510	LEU	2.3
1	A	118	GLN	2.3
1	A	64	ALA	2.3
1	A	692	PHE	2.3
1	A	536	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	397	ASN	2.3
1	A	63	GLN	2.3
1	A	26	LYS	2.3
1	A	65	VAL	2.2
1	A	538	ALA	2.2
1	B	118	GLN	2.2
1	B	120	ASN	2.2
1	B	125	PRO	2.2
1	B	544	THR	2.2
1	A	357	VAL	2.2
1	B	611	GLU	2.1
1	A	115	PRO	2.1
1	A	471	GLU	2.1
1	A	783	ILE	2.1
1	A	460	PHE	2.1
1	A	130	ALA	2.1
1	B	335	ALA	2.1
1	B	538	ALA	2.1
1	A	362	MET	2.1
1	A	126	GLY	2.1
1	A	734	GLY	2.1
1	A	133	PRO	2.1
1	B	968	ARG	2.1
1	B	396	LEU	2.1
1	A	124	ASN	2.1
1	B	543	VAL	2.1
1	A	129	THR	2.0
1	B	418	ALA	2.0
1	B	22	LYS	2.0
1	A	525	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	A	642	10/11	0.92	0.13	-	50,62,67,71	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	B	642	10/11	0.95	0.12	-	39,54,60,65	0
1	CME	A	974	10/11	0.96	0.11	-	45,48,69,73	0
1	CME	B	974	10/11	0.90	0.15	-	43,53,70,71	2

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	A	1001	8/8	0.92	0.13	1.20	48,54,57,60	0
2	TRS	B	1001	8/8	0.94	0.11	-0.49	31,39,43,49	0
3	CL	A	1002	1/1	0.98	0.07	-0.64	48,48,48,48	0
3	CL	B	1002	1/1	0.97	0.08	-0.77	33,33,33,33	1

6.5 Other polymers (i)

There are no such residues in this entry.