Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2024 – 01:16 pm BST

PDB ID	:	8RUA
Title	:	Crystal structure of Rhizobium etli L-asparaginase ReAV C135A mutant
Authors	:	Pokrywka, K.; Grzechowiak, M.; Sliwiak, J.; Worsztynowicz, P.; Loch, J.I.; Ruszkowski, M.; Gilski, M.; Jaskolski, M.
Deposited on	:	2024-01-30
Resolution	:	1.71 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

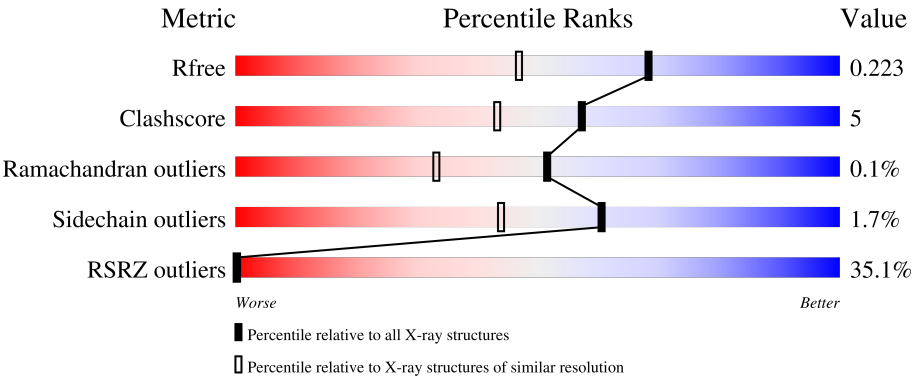
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	373	33% 84% 9% 6%
1	B	373	34% 91% 7%

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	A	401	-	-	-	X
3	PEG	A	407	-	-	X	-
4	GOL	A	403	-	-	-	X
4	GOL	A	410	-	-	-	X
4	GOL	B	402	-	-	-	X
4	GOL	B	404	-	-	-	X
4	GOL	B	406	-	-	-	X
4	GOL	B	410	-	-	-	X
5	EDO	B	405	-	-	-	X
5	EDO	B	411	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5976 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.

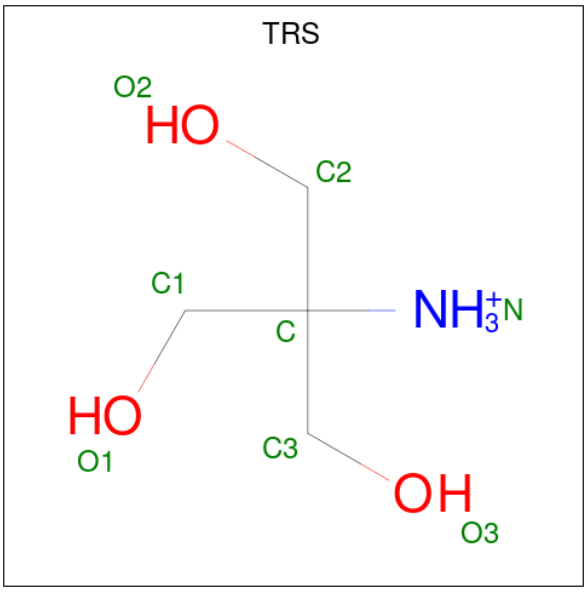
- Molecule 1 is a protein called L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	9	0
			2647	1637	492	499	19			
1	B	367	Total	C	N	O	S	0	11	0
			2773	1718	507	528	20			

There are 14 discrepancies between the modelled and reference sequences:

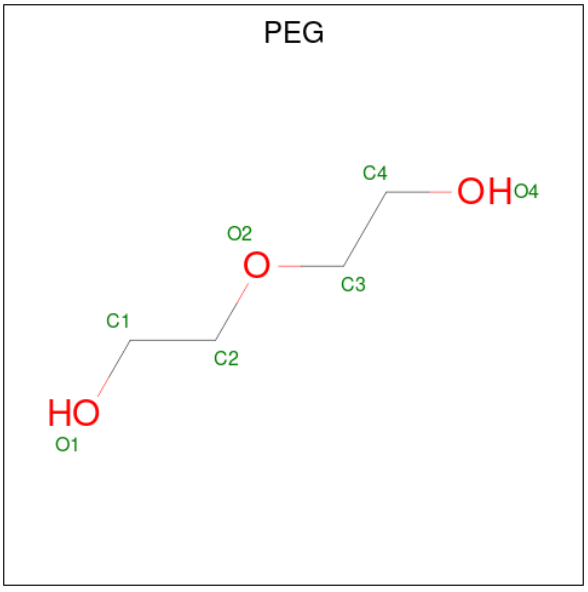
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q2K0Z2
A	-4	ILE	-	expression tag	UNP Q2K0Z2
A	-3	ASP	-	expression tag	UNP Q2K0Z2
A	-2	PRO	-	expression tag	UNP Q2K0Z2
A	-1	PHE	-	expression tag	UNP Q2K0Z2
A	0	THR	-	expression tag	UNP Q2K0Z2
A	135	ALA	CYS	engineered mutation	UNP Q2K0Z2
B	-5	GLY	-	expression tag	UNP Q2K0Z2
B	-4	ILE	-	expression tag	UNP Q2K0Z2
B	-3	ASP	-	expression tag	UNP Q2K0Z2
B	-2	PRO	-	expression tag	UNP Q2K0Z2
B	-1	PHE	-	expression tag	UNP Q2K0Z2
B	0	THR	-	expression tag	UNP Q2K0Z2
B	135	ALA	CYS	engineered mutation	UNP Q2K0Z2

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



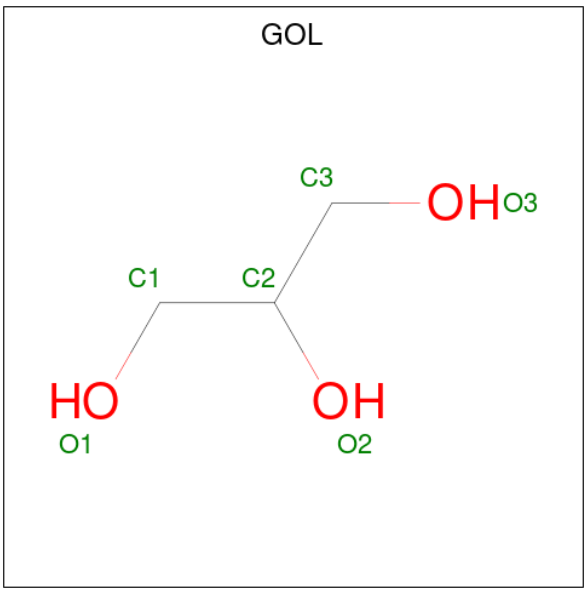
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 8 4 1 3	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



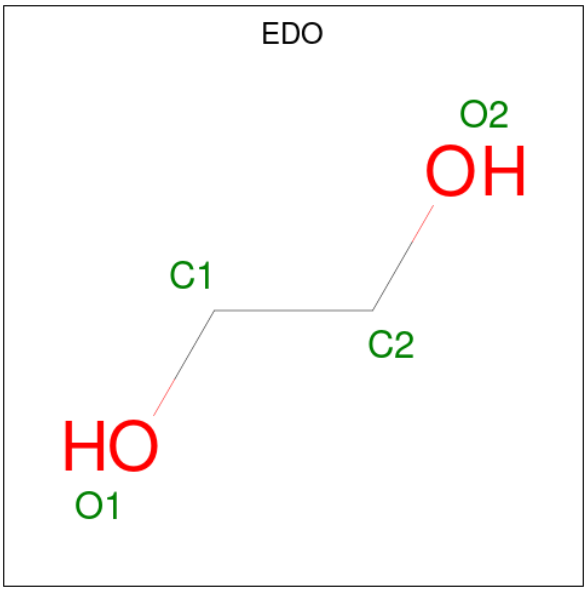
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is water.

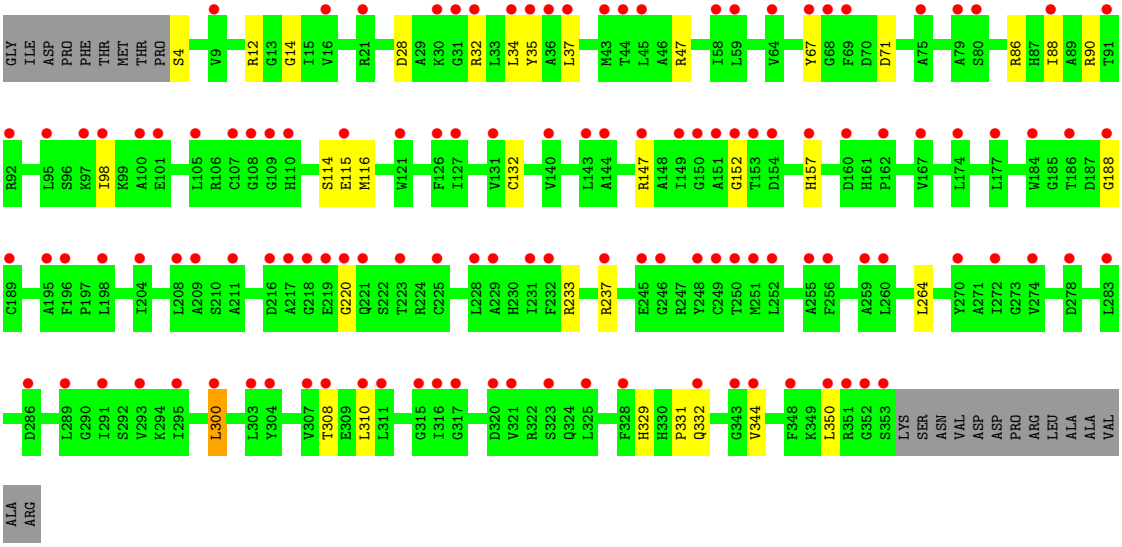
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	214	Total O 214 214	0	0
7	B	226	Total O 226 226	0	0

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 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.

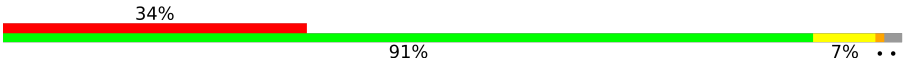
• Molecule 1: L-asparaginase II protein

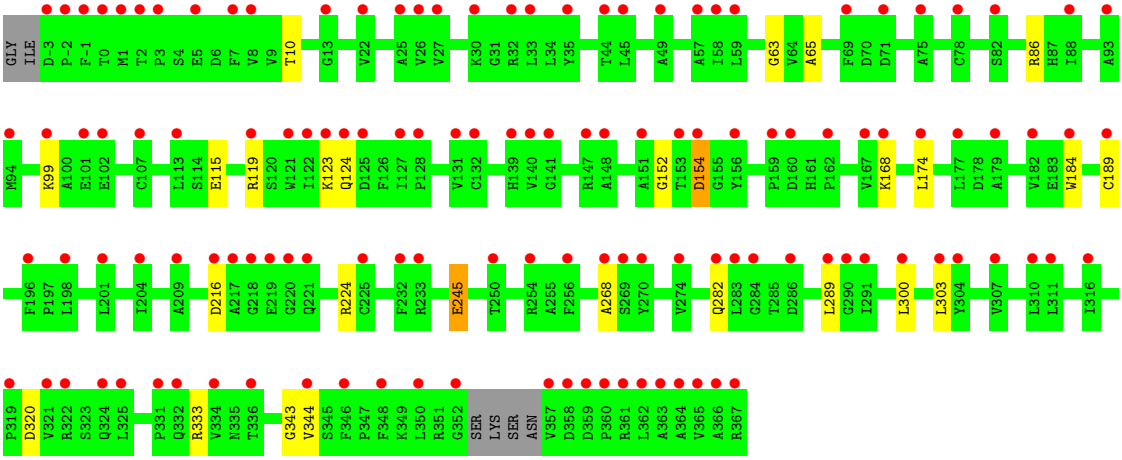
Chain A:



• Molecule 1: L-asparaginase II protein

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	78.06Å 91.18Å 106.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.84 – 1.71 62.87 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.84-1.71) 99.8 (62.87-1.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.224 0.200 , 0.223	Depositor DCC
R_{free} test set	1027 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5976	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 21.62 % 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 6.7518e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, PEG, CL, EDO, TRS

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	0.49	0/2718	0.69	0/3668
1	B	0.52	0/2853	0.68	0/3853
All	All	0.50	0/5571	0.68	0/7521

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	2647	0	2649	29	0
1	B	2773	0	2775	24	0
2	A	8	0	12	5	0
3	A	14	0	20	5	0
3	B	7	0	10	0	0
4	A	30	0	40	4	0
4	B	24	0	32	6	0
5	A	12	0	18	2	0
5	B	20	0	30	8	0
6	B	1	0	0	0	0
7	A	214	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	226	0	0	1	0
All	All	5976	0	5586	54	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 5.

All (54) 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:115:GLU:H	2:A:401:TRS:H21	1.36	0.90
1:B:154:ASP:H	5:B:403:EDO:H21	1.48	0.79
1:B:189:CYS:H	4:B:404:GOL:H31	1.54	0.72
1:A:264:LEU:HD11	1:A:300:LEU:HD11	1.71	0.71
1:B:10:THR:HG22	1:B:344:VAL:HG22	1.73	0.70
1:A:86:ARG:HB2	4:A:408:GOL:H31	1.82	0.62
1:A:71:ASP:HB2	3:A:402:PEG:H42	1.81	0.61
1:B:86:ARG:NH2	1:B:245[A]:GLU:OE1	2.34	0.59
1:A:114:SER:OG	2:A:401:TRS:H12	2.04	0.58
1:A:90:ARG:HH21	4:A:408:GOL:H2	1.68	0.57
1:A:157:HIS:H	1:A:157:HIS:HD1	1.52	0.57
1:B:333:ARG:HD2	4:B:406:GOL:H31	1.85	0.57
1:A:147[B]:ARG:HH21	1:A:152:GLY:HA2	1.70	0.55
1:A:12:ARG:HH22	5:A:411:EDO:H12	1.74	0.53
1:B:224:ARG:HH11	5:B:407:EDO:H11	1.73	0.52
1:A:28:ASP:HB3	1:A:34:LEU:HD11	1.92	0.52
1:A:233[A]:ARG:HG2	1:A:237:ARG:HD3	1.92	0.51
1:A:14:GLY:HA2	4:A:403:GOL:H12	1.95	0.49
3:A:407:PEG:C1	4:B:406:GOL:H2	2.43	0.49
1:B:282:GLN:HG3	7:B:643:HOH:O	2.14	0.48
1:A:88:ILE:HD12	1:A:132:CYS:HA	1.95	0.48
1:B:189:CYS:N	4:B:404:GOL:H31	2.27	0.47
1:A:67:TYR:CG	1:A:98:ILE:HG22	2.50	0.47
1:A:331:PRO:HD2	1:A:344:VAL:HG11	1.95	0.47
1:B:268:ALA:HA	1:B:303:LEU:HD22	1.97	0.46
1:B:168[B]:LYS:HD3	1:B:184:TRP:CE2	2.50	0.46
1:A:35:TYR:HB3	1:A:350:LEU:HD22	1.98	0.45
1:A:32:ARG:HH21	5:A:405:EDO:H22	1.82	0.45
1:A:67:TYR:CD1	1:A:98:ILE:HG22	2.51	0.45
1:B:63:GLY:H	5:B:409:EDO:H21	1.82	0.45
1:A:90:ARG:HH21	4:A:408:GOL:C2	2.30	0.44
1:A:47:ARG:HH21	3:A:407:PEG:C4	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:THR:HG21	1:A:329:HIS:HB2	2.00	0.44
1:B:174:LEU:HD23	5:B:407:EDO:H22	2.00	0.44
1:B:168[A]:LYS:HG2	1:B:184:TRP:CZ2	2.53	0.43
1:A:37:LEU:HD11	1:A:310[B]:LEU:HD21	1.99	0.43
1:B:99[B]:LYS:HB3	1:B:99[B]:LYS:HE2	1.51	0.43
1:A:115:GLU:N	2:A:401:TRS:H21	2.19	0.43
1:A:116:MET:H	2:A:401:TRS:H31	1.83	0.43
1:A:188:GLY:H	3:A:407:PEG:H41	1.84	0.43
1:A:116:MET:HB2	2:A:401:TRS:H32	2.01	0.43
1:B:154:ASP:N	5:B:403:EDO:H21	2.27	0.42
1:A:310[B]:LEU:HD23	1:A:310[B]:LEU:HA	1.83	0.42
1:B:343:GLY:N	4:B:402:GOL:H2	2.35	0.42
1:B:115:GLU:O	1:B:119:ARG:HG3	2.20	0.42
1:A:47:ARG:HH21	3:A:407:PEG:H42	1.85	0.41
1:B:63:GLY:H	5:B:409:EDO:C2	2.33	0.41
1:B:300[A]:LEU:HD23	1:B:300[A]:LEU:HA	1.88	0.41
1:B:123:LYS:HB2	1:B:123:LYS:HE2	1.87	0.41
1:B:65:ALA:H	5:B:409:EDO:C1	2.34	0.41
1:B:115:GLU:HG2	1:B:119:ARG:HH11	1.85	0.41
1:A:71:ASP:OD2	1:A:237:ARG:NH1	2.53	0.41
1:B:333:ARG:HD3	4:B:406:GOL:H12	2.03	0.41
1:B:152:GLY:HA3	5:B:403:EDO:H22	2.03	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	357/373 (96%)	346 (97%)	10 (3%)	1 (0%)	41 24
1	B	374/373 (100%)	366 (98%)	8 (2%)	0	100 100
All	All	731/746 (98%)	712 (97%)	18 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	GLY

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	272/282 (96%)	269 (99%)	3 (1%)	73	62
1	B	288/282 (102%)	280 (97%)	8 (3%)	43	23
All	All	560/564 (99%)	549 (98%)	11 (2%)	60	37

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	300	LEU
1	A	332	GLN
1	B	124	GLN
1	B	154	ASP
1	B	216	ASP
1	B	245[A]	GLU
1	B	245[B]	GLU
1	B	289	LEU
1	B	320[A]	ASP
1	B	320[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	GOL	A	403	-	5,5,5	0.83	0	5,5,5	1.01	0
4	GOL	B	406	-	5,5,5	0.72	0	5,5,5	0.84	0
4	GOL	A	410	-	5,5,5	0.98	0	5,5,5	0.86	0
4	GOL	B	402	-	5,5,5	0.97	0	5,5,5	0.99	0
5	EDO	B	411	-	3,3,3	0.55	0	2,2,2	0.13	0
4	GOL	A	408	-	5,5,5	0.87	0	5,5,5	0.78	0
5	EDO	B	405	-	3,3,3	0.53	0	2,2,2	0.38	0
2	TRS	A	401	-	7,7,7	0.36	0	9,9,9	0.65	0
3	PEG	B	401	-	6,6,6	0.13	0	5,5,5	0.15	0
5	EDO	A	406	-	3,3,3	0.52	0	2,2,2	0.25	0
5	EDO	A	411	-	3,3,3	0.53	0	2,2,2	0.05	0
4	GOL	A	404	-	5,5,5	0.72	0	5,5,5	1.03	0
5	EDO	B	407	-	3,3,3	0.50	0	2,2,2	0.63	0
4	GOL	B	410	-	5,5,5	1.09	0	5,5,5	0.94	0
3	PEG	A	402	-	6,6,6	0.20	0	5,5,5	0.12	0
5	EDO	B	403	-	3,3,3	0.52	0	2,2,2	0.12	0
5	EDO	B	409	-	3,3,3	0.59	0	2,2,2	0.18	0
4	GOL	B	404	-	5,5,5	0.66	0	5,5,5	1.02	0
4	GOL	A	409	-	5,5,5	0.77	0	5,5,5	1.00	0
3	PEG	A	407	-	6,6,6	0.14	0	5,5,5	0.21	0
5	EDO	A	405	-	3,3,3	0.48	0	2,2,2	0.31	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
4	GOL	A	403	-	-	4/4/4/4	-
4	GOL	B	406	-	-	3/4/4/4	-
4	GOL	A	410	-	-	3/4/4/4	-
4	GOL	B	402	-	-	1/4/4/4	-
5	EDO	B	411	-	-	1/1/1/1	-
4	GOL	A	408	-	-	2/4/4/4	-
5	EDO	B	405	-	-	1/1/1/1	-
2	TRS	A	401	-	-	5/9/9/9	-
3	PEG	B	401	-	-	3/4/4/4	-
5	EDO	A	406	-	-	1/1/1/1	-
5	EDO	A	411	-	-	0/1/1/1	-
4	GOL	A	404	-	-	2/4/4/4	-
5	EDO	B	407	-	-	1/1/1/1	-
4	GOL	B	410	-	-	0/4/4/4	-
3	PEG	A	402	-	-	1/4/4/4	-
5	EDO	B	403	-	-	0/1/1/1	-
5	EDO	B	409	-	-	1/1/1/1	-
4	GOL	B	404	-	-	4/4/4/4	-
4	GOL	A	409	-	-	4/4/4/4	-
3	PEG	A	407	-	-	3/4/4/4	-
5	EDO	A	405	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TRS	N-C-C2-O2
2	A	401	TRS	C1-C-C3-O3
4	A	403	GOL	O1-C1-C2-C3
4	A	404	GOL	C1-C2-C3-O3
4	A	409	GOL	O1-C1-C2-C3
4	A	409	GOL	C1-C2-C3-O3
4	A	410	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	404	GOL	C1-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	A	409	GOL	O2-C2-C3-O3
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O2-C2-C3-O3
3	A	402	PEG	O2-C3-C4-O4
4	A	403	GOL	C1-C2-C3-O3
4	A	408	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-C3
4	A	409	GOL	O1-C1-C2-O2
4	A	410	GOL	O1-C1-C2-O2
5	B	405	EDO	O1-C1-C2-O2
5	B	411	EDO	O1-C1-C2-O2
2	A	401	TRS	C1-C-C2-O2
2	A	401	TRS	C2-C-C3-O3
3	B	401	PEG	O2-C3-C4-O4
4	A	403	GOL	O2-C2-C3-O3
4	A	408	GOL	O2-C2-C3-O3
4	B	406	GOL	C1-C2-C3-O3
4	A	410	GOL	O2-C2-C3-O3
4	B	406	GOL	O1-C1-C2-O2
3	B	401	PEG	C4-C3-O2-C2
3	A	407	PEG	C4-C3-O2-C2
3	B	401	PEG	C1-C2-O2-C3
3	A	407	PEG	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
5	B	407	EDO	O1-C1-C2-O2
3	A	407	PEG	C1-C2-O2-C3
5	B	409	EDO	O1-C1-C2-O2
4	B	406	GOL	O1-C1-C2-C3
4	A	404	GOL	O2-C2-C3-O3
4	B	402	GOL	O2-C2-C3-O3
2	A	401	TRS	N-C-C3-O3

There are no ring outliers.

13 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	GOL	1	0
4	B	406	GOL	3	0
4	B	402	GOL	1	0
4	A	408	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TRS	5	0
5	A	411	EDO	1	0
5	B	407	EDO	2	0
3	A	402	PEG	1	0
5	B	403	EDO	3	0
5	B	409	EDO	3	0
4	B	404	GOL	2	0
3	A	407	PEG	4	0
5	A	405	EDO	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, 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	350/373 (93%)	1.86	124 (35%)	0	0	18, 29, 43, 67	0
1	B	367/373 (98%)	1.89	128 (34%)	0	0	18, 28, 44, 60	0
All	All	717/746 (96%)	1.87	252 (35%)	0	0	18, 28, 44, 67	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	PHE	13.3
1	A	220	GLY	12.1
1	B	-2	PRO	9.5
1	B	127	ILE	9.0
1	B	325	LEU	8.3
1	B	366	ALA	6.9
1	B	151	ALA	6.9
1	A	151	ALA	6.3
1	A	221	GLN	6.2
1	A	69	PHE	6.0
1	A	216	ASP	5.9
1	A	217	ALA	5.6
1	B	362	LEU	5.6
1	A	64	VAL	5.6
1	B	218	GLY	5.4
1	A	289	LEU	5.3
1	A	101	GLU	5.3
1	B	358	ASP	5.3
1	A	126	PHE	5.2
1	A	143	LEU	5.1
1	B	0	THR	5.1
1	B	357	VAL	4.9
1	A	144	ALA	4.8
1	A	286	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	4.5
1	B	365	VAL	4.5
1	B	147	ARG	4.5
1	A	154	ASP	4.5
1	A	332	GLN	4.5
1	B	107	CYS	4.5
1	A	67	TYR	4.5
1	A	310[A]	LEU	4.4
1	B	168[A]	LYS	4.3
1	B	324	GLN	4.3
1	B	334	VAL	4.3
1	A	218	GLY	4.3
1	B	217	ALA	4.3
1	B	3	PRO	4.3
1	A	351	ARG	4.2
1	A	323	SER	4.2
1	A	348	PHE	4.2
1	B	352	GLY	4.2
1	B	153	THR	4.1
1	A	131	VAL	4.1
1	A	35	TYR	4.1
1	B	1	MET	4.1
1	A	32	ARG	4.1
1	B	321	VAL	4.0
1	A	304	TYR	4.0
1	A	100	ALA	4.0
1	B	359	ASP	3.9
1	B	101	GLU	3.9
1	B	32	ARG	3.9
1	B	350	LEU	3.9
1	B	160	ASP	3.9
1	A	108	GLY	3.8
1	B	274	VAL	3.8
1	B	303	LEU	3.7
1	B	30	LYS	3.6
1	B	331	PRO	3.6
1	A	252	LEU	3.6
1	B	282	GLN	3.6
1	B	361	ARG	3.6
1	B	121	TRP	3.6
1	B	364	ALA	3.5
1	A	31	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	125	ASP	3.5
1	A	353	SER	3.5
1	A	34	LEU	3.5
1	B	300[A]	LEU	3.4
1	A	237	ARG	3.4
1	A	174	LEU	3.3
1	B	233	ARG	3.3
1	A	325	LEU	3.3
1	B	35	TYR	3.3
1	B	189	CYS	3.3
1	A	109	GLY	3.3
1	A	245	GLU	3.3
1	B	148	ALA	3.3
1	B	209	ALA	3.3
1	A	232	PHE	3.3
1	B	82	SER	3.3
1	B	182	VAL	3.3
1	B	2	THR	3.2
1	B	69	PHE	3.2
1	B	367	ARG	3.2
1	B	179	ALA	3.2
1	B	316	ILE	3.2
1	B	75	ALA	3.2
1	B	332	GLN	3.2
1	A	307	VAL	3.1
1	A	350	LEU	3.1
1	A	140	VAL	3.1
1	B	219	GLU	3.1
1	B	26	VAL	3.1
1	A	189	CYS	3.0
1	B	310	LEU	3.0
1	B	201	LEU	3.0
1	A	147[A]	ARG	3.0
1	B	286	ASP	3.0
1	A	9	VAL	3.0
1	A	95	LEU	3.0
1	A	303	LEU	3.0
1	A	311	LEU	3.0
1	B	71	ASP	3.0
1	B	45	LEU	3.0
1	B	363	ALA	2.9
1	A	204	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	316	ILE	2.9
1	B	93	ALA	2.9
1	B	44	THR	2.9
1	B	198	LEU	2.9
1	B	102	GLU	2.9
1	A	107	CYS	2.8
1	A	315	GLY	2.8
1	B	270	TYR	2.8
1	A	246	GLY	2.8
1	A	110	HIS	2.8
1	B	204	ILE	2.8
1	A	321	VAL	2.8
1	B	346	PHE	2.8
1	A	121	TRP	2.8
1	B	232	PHE	2.8
1	A	320	ASP	2.8
1	A	278	ASP	2.7
1	B	131	VAL	2.7
1	B	289	LEU	2.7
1	B	196	PHE	2.7
1	B	256	PHE	2.7
1	A	43	MET	2.7
1	B	216	ASP	2.7
1	A	150	GLY	2.7
1	A	75	ALA	2.7
1	B	344	VAL	2.7
1	A	160	ASP	2.7
1	B	99[A]	LYS	2.7
1	A	37	LEU	2.7
1	B	139	HIS	2.7
1	B	124	GLN	2.7
1	B	88	ILE	2.7
1	B	290	GLY	2.7
1	A	45	LEU	2.7
1	A	274	VAL	2.7
1	A	196	PHE	2.7
1	A	231	ILE	2.6
1	A	248	TYR	2.6
1	A	250	THR	2.6
1	A	272	ILE	2.6
1	A	291	ILE	2.6
1	B	269[A]	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	311	LEU	2.6
1	B	250	THR	2.6
1	A	105	LEU	2.6
1	A	79	ALA	2.6
1	B	94	MET	2.6
1	A	68	GLY	2.6
1	A	152	GLY	2.6
1	A	328	PHE	2.6
1	A	92	ARG	2.6
1	A	127	ILE	2.6
1	B	140	VAL	2.6
1	A	283	LEU	2.6
1	B	162	PRO	2.6
1	B	304	TYR	2.5
1	A	30	LYS	2.5
1	A	256	PHE	2.5
1	B	156	TYR	2.5
1	B	78	CYS	2.5
1	B	132	CYS	2.5
1	A	211	ALA	2.5
1	B	348	PHE	2.5
1	B	119	ARG	2.5
1	B	27	VAL	2.5
1	B	291	ILE	2.5
1	B	59	LEU	2.5
1	A	352	GLY	2.5
1	A	91	THR	2.4
1	B	128	PRO	2.4
1	B	154	ASP	2.4
1	B	159	PRO	2.4
1	A	255	ALA	2.4
1	A	259	ALA	2.4
1	B	122	ILE	2.4
1	A	308	THR	2.4
1	A	317	GLY	2.4
1	B	220	GLY	2.4
1	B	225	CYS	2.4
1	A	300	LEU	2.4
1	B	336	THR	2.4
1	A	209	ALA	2.4
1	A	44	THR	2.4
1	B	307	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	322	ARG	2.3
1	A	295	ILE	2.3
1	A	223	THR	2.3
1	A	80	SER	2.3
1	B	167	VAL	2.3
1	B	141	GLY	2.3
1	A	188	GLY	2.3
1	B	58	ILE	2.3
1	B	284	GLY	2.3
1	A	186	THR	2.3
1	B	8	VAL	2.3
1	A	249	CYS	2.3
1	A	177	LEU	2.2
1	B	57	ALA	2.2
1	B	268	ALA	2.2
1	B	7	PHE	2.2
1	A	229	ALA	2.2
1	B	174	LEU	2.2
1	B	177	LEU	2.2
1	B	254[A]	ARG	2.2
1	A	115	GLU	2.2
1	A	270	TYR	2.2
1	A	157	HIS	2.2
1	B	13	GLY	2.2
1	B	33	LEU	2.2
1	B	-3	ASP	2.2
1	A	98	ILE	2.2
1	A	293	VAL	2.2
1	B	22	VAL	2.2
1	A	208	LEU	2.2
1	A	195	ALA	2.2
1	B	221	GLN	2.1
1	A	251	MET	2.1
1	B	123	LYS	2.1
1	A	149	ILE	2.1
1	A	97	LYS	2.1
1	B	319	PRO	2.1
1	A	343	GLY	2.1
1	A	219	GLU	2.1
1	A	16	VAL	2.1
1	A	198	LEU	2.1
1	A	167	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLU	2.1
1	B	25	ALA	2.1
1	B	113	LEU	2.1
1	B	283	LEU	2.1
1	A	36	ALA	2.1
1	A	228	LEU	2.1
1	A	162	PRO	2.0
1	B	49	ALA	2.0
1	A	21[A]	ARG	2.0
1	B	184	TRP	2.0
1	A	58	ILE	2.0
1	A	88	ILE	2.0
1	A	153	THR	2.0
1	A	225	CYS	2.0
1	A	344	VAL	2.0
1	A	59	LEU	2.0
1	A	184	TRP	2.0
1	B	360	PRO	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	GOL	B	410	6/6	0.11	0.42	38,45,52,58	0
2	TRS	A	401	8/8	0.34	0.59	38,41,48,50	0
4	GOL	A	403	6/6	0.38	0.50	38,42,44,45	0
5	EDO	B	405	4/4	0.39	0.42	39,41,44,46	0
4	GOL	B	402	6/6	0.40	0.65	33,37,39,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	407	4/4	0.43	0.22	31,33,33,42	0
5	EDO	B	409	4/4	0.43	0.32	35,36,39,49	0
5	EDO	A	405	4/4	0.44	0.30	41,44,46,48	0
4	GOL	A	409	6/6	0.45	0.36	44,45,46,48	0
4	GOL	A	408	6/6	0.52	0.28	31,38,46,48	0
5	EDO	B	411	4/4	0.52	0.52	39,44,45,50	0
4	GOL	B	404	6/6	0.53	0.56	37,39,44,44	0
3	PEG	A	407	7/7	0.54	0.27	37,39,43,48	0
4	GOL	B	406	6/6	0.54	0.54	38,42,44,46	0
3	PEG	B	401	7/7	0.55	0.23	40,46,47,49	0
4	GOL	A	404	6/6	0.58	0.22	39,43,47,48	0
5	EDO	A	406	4/4	0.58	0.24	41,41,42,42	0
5	EDO	B	403	4/4	0.62	0.24	37,41,50,53	0
5	EDO	A	411	4/4	0.67	0.26	32,35,37,39	0
3	PEG	A	402	7/7	0.71	0.22	32,43,50,50	0
4	GOL	A	410	6/6	0.72	0.46	40,47,49,51	0
6	CL	B	408	1/1	0.93	0.14	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.