



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2019 – 10:06 PM EDT

PDB ID : 6A80
Title : Crystal Structure of putative amino acid binding periplasmic ABC transporter protein from *Candidatus Liberibacter asiaticus* in complex with cystine
Authors : Kumar, P.; Kesari, P.; Ghosh, D.K.; Kumar, P.; Sharma, A.K.
Deposited on : 2018-07-05
Resolution : 1.56 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

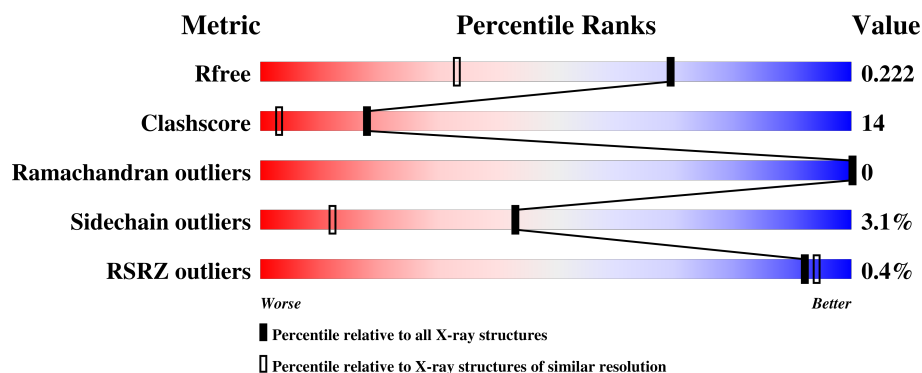
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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}	111664	1224 (1.56-1.56)
Clashscore	122126	1265 (1.56-1.56)
Ramachandran outliers	120053	1240 (1.56-1.56)
Sidechain outliers	120020	1238 (1.56-1.56)
RSRZ outliers	108989	1207 (1.56-1.56)

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	241	 78% 19% . .
1	B	241	 79% 16% . .

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	EDO	A	302	-	-	X	-
2	EDO	B	305	-	-	X	-
4	TRS	A	304	-	-	X	-
6	CYS	A	319[A]	-	-	X	-
6	CYS	A	319[B]	-	-	X	-
6	CYS	A	320[A]	-	-	X	-
6	CYS	B	310[A]	-	-	X	-
6	CYS	B	310[B]	-	-	X	-
6	CYS	B	311[A]	-	-	X	-
6	CYS	B	311[B]	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4478 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

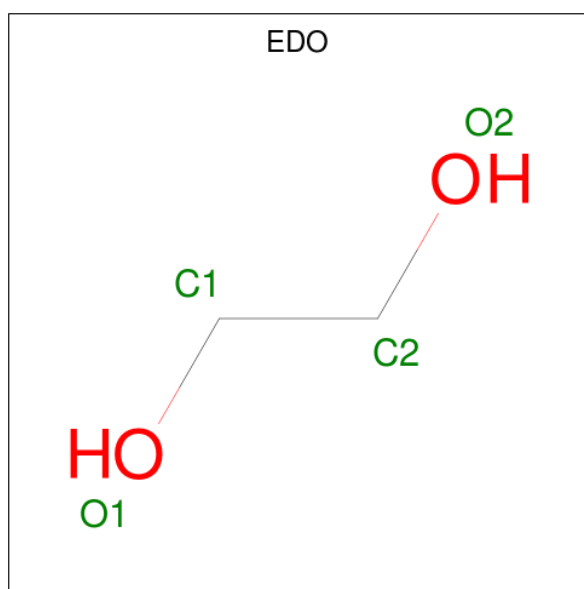
- Molecule 1 is a protein called Putative amino acid-binding periplasmic ABC transporter protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	18	0
			2028	1281	362	377	8			
1	B	234	Total	C	N	O	S	0	12	0
			1974	1248	353	365	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C6XGT2
B	1	MET	-	initiating methionine	UNP C6XGT2

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



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

Continued on next page...

Continued from previous page...

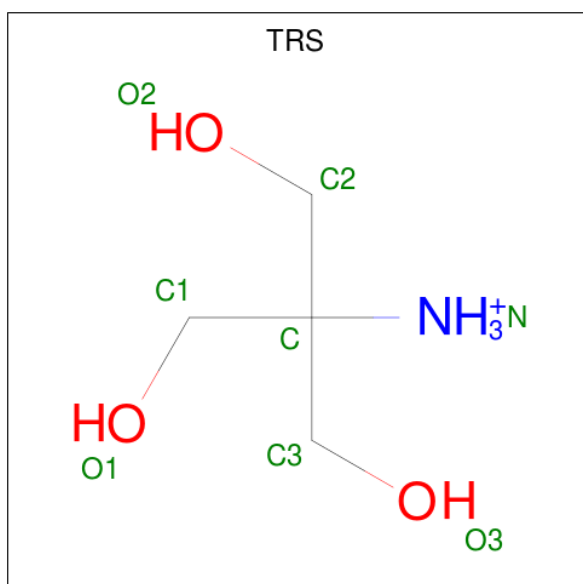
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



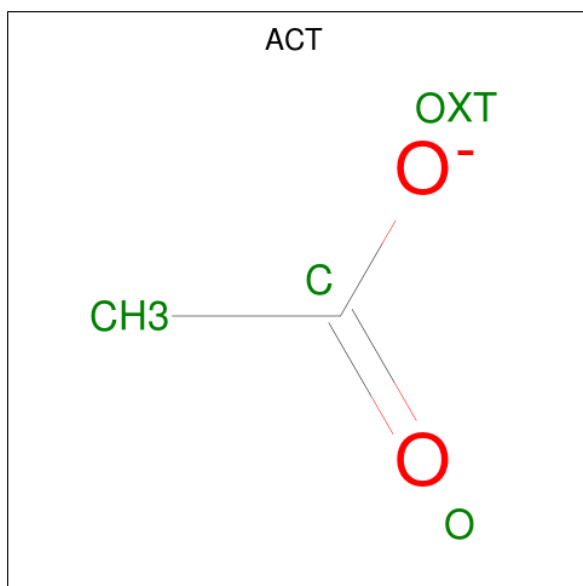
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



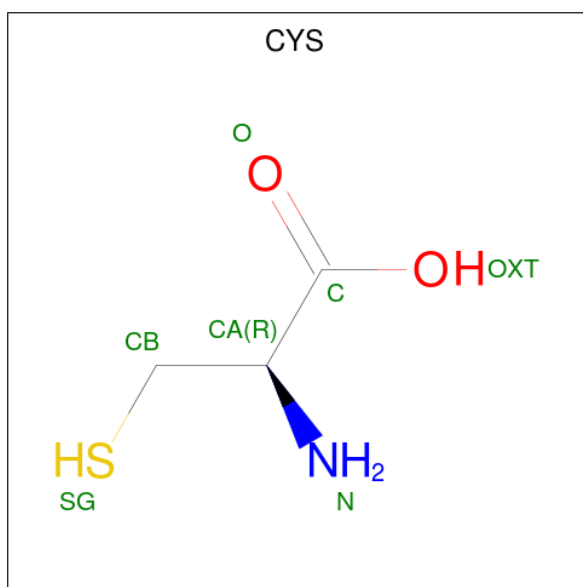
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	1
			14	6	2	4	2		
6	A	1	Total	C	N	O	S	0	1
			14	6	2	4	2		
6	B	1	Total	C	N	O	S	0	1
			14	6	2	4	2		
6	B	1	Total	C	N	O	S	0	1
			14	6	2	4	2		

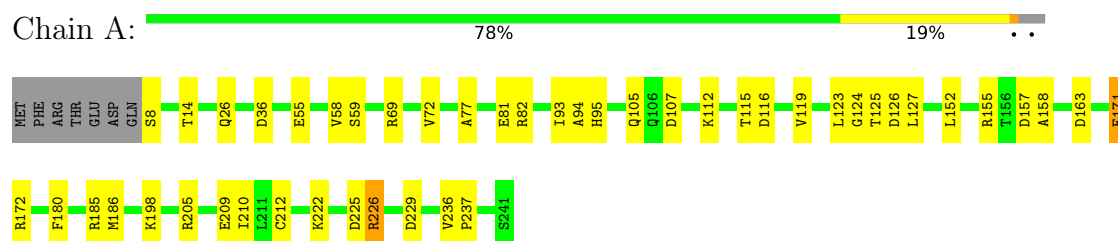
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	148	Total	O	0	0
			148	148		
7	B	144	Total	O	0	0
			144	144		

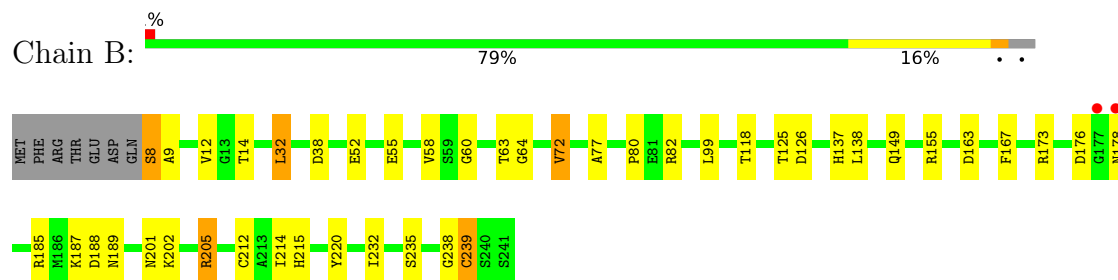
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative amino acid-binding periplasmic ABC transporter protein



- Molecule 1: Putative amino acid-binding periplasmic ABC transporter protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.16Å 86.78Å 122.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.76 – 1.56 70.76 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.76-1.56) 99.8 (70.76-1.56)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.185 , 0.221 0.186 , 0.222	Depositor DCC
R_{free} test set	3614 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4478	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, TRS, EDO, ACT

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	0.97	1/2066 (0.0%)	1.09	12/2785 (0.4%)
1	B	0.97	3/2012 (0.1%)	1.08	6/2713 (0.2%)
All	All	0.97	4/4078 (0.1%)	1.08	18/5498 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	LEU	C-O	5.81	1.34	1.23
1	A	171	GLU	CD-OE2	5.43	1.31	1.25
1	B	239[A]	CYS	N-CA	5.42	1.57	1.46
1	B	239[B]	CYS	N-CA	5.42	1.57	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ASP	CB-CG-OD1	9.73	127.05	118.30
1	A	157	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	163	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	157	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	225	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	226	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	226	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	239[A]	CYS	N-CA-CB	5.97	121.34	110.60
1	B	239[B]	CYS	N-CA-CB	5.97	121.34	110.60
1	A	36	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	229	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	155[A]	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	155[B]	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	38	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	32	LEU	CB-CG-CD2	-5.28	102.02	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	MET	CG-SD-CE	-5.23	91.83	100.20
1	A	72	VAL	CA-CB-CG1	5.20	118.69	110.90
1	A	69	ARG	NE-CZ-NH1	-5.06	117.77	120.30

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	2028	0	2013	60	0
1	B	1974	0	1964	44	0
2	A	44	0	66	13	0
2	B	28	0	42	12	0
3	A	18	0	24	2	0
3	B	6	0	8	1	0
4	A	8	0	12	6	0
5	A	20	0	15	0	0
5	B	4	0	3	0	0
6	A	28	0	14	25	0
6	B	28	0	14	22	0
7	A	148	0	0	10	0
7	B	144	0	0	4	0
All	All	4478	0	4175	122	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 14.

All (122) 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)
6:B:310[B]:CYS:N	6:B:311[B]:CYS:CB	1.76	1.46
6:B:310[B]:CYS:N	6:B:311[B]:CYS:HB3	1.23	1.41
6:B:310[A]:CYS:HB3	6:B:311[A]:CYS:HA	1.17	1.13
1:A:26:GLN:H	4:A:304:TRS:H21	1.16	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126[B]:ASP:H	6:A:319[B]:CYS:HB3	0.95	1.07
6:B:310[B]:CYS:N	6:B:311[B]:CYS:CA	2.19	1.06
1:A:126[B]:ASP:N	6:A:319[B]:CYS:HB3	1.71	1.02
1:A:123[B]:LEU:O	2:A:302:EDO:H12	1.62	0.99
1:A:126[B]:ASP:H	6:A:319[B]:CYS:CB	1.77	0.98
1:B:149:GLN:HG2	7:B:458:HOH:O	1.64	0.97
1:B:63[A]:THR:HG22	2:B:305:EDO:H11	1.46	0.96
6:B:310[B]:CYS:N	6:B:311[B]:CYS:HA	1.80	0.93
1:A:212[B]:CYS:SG	1:B:80:PRO:HD3	2.11	0.91
1:A:123[A]:LEU:O	2:A:302:EDO:H12	1.68	0.90
2:A:302:EDO:O1	7:A:401:HOH:O	1.87	0.90
1:B:12:VAL:HG22	1:B:72[B]:VAL:CG2	2.02	0.90
1:B:205[A]:ARG:HH11	1:B:205[A]:ARG:HB3	1.38	0.88
1:B:32:LEU:H	2:B:306:EDO:H22	1.38	0.87
6:B:310[A]:CYS:O	6:B:310[A]:CYS:SG	2.33	0.86
6:B:310[A]:CYS:CB	6:B:311[A]:CYS:HA	2.02	0.83
1:B:64:GLY:N	2:B:305:EDO:H21	1.93	0.83
1:B:63[A]:THR:CG2	2:B:305:EDO:H11	2.08	0.82
1:B:205[A]:ARG:NH1	1:B:205[A]:ARG:HB3	1.94	0.82
6:A:319[A]:CYS:OXT	6:A:319[A]:CYS:SG	2.38	0.82
6:B:310[B]:CYS:N	6:B:311[B]:CYS:HB2	1.90	0.80
2:A:321:EDO:H12	7:A:521:HOH:O	1.81	0.79
1:B:215[B]:HIS:CD2	1:B:239[B]:CYS:H	2.00	0.79
1:A:82:ARG:HH22	6:A:319[B]:CYS:HA	1.47	0.78
1:A:26:GLN:N	4:A:304:TRS:H21	1.98	0.77
1:A:155[B]:ARG:HH11	2:A:318:EDO:C2	1.99	0.76
1:B:64:GLY:CA	2:B:305:EDO:H21	2.15	0.76
1:A:155[B]:ARG:HH11	2:A:318:EDO:H22	1.52	0.75
6:A:319[A]:CYS:HA	7:A:507:HOH:O	1.87	0.74
2:B:303:EDO:O2	6:B:310[A]:CYS:HB2	1.88	0.74
1:B:205[A]:ARG:HH11	1:B:205[A]:ARG:CB	2.01	0.73
1:B:63[A]:THR:HB	2:B:305:EDO:H22	1.71	0.72
2:A:314:EDO:O1	6:A:319[A]:CYS:HB2	1.90	0.71
6:B:310[A]:CYS:HB3	6:B:311[A]:CYS:CA	2.10	0.71
1:A:126[B]:ASP:CB	6:A:319[B]:CYS:HB3	2.21	0.70
1:A:155[B]:ARG:HG3	7:A:406:HOH:O	1.93	0.68
1:A:222[A]:LYS:HE2	7:A:496:HOH:O	1.93	0.68
1:A:59:SER:N	2:A:302:EDO:H21	2.09	0.67
1:B:12:VAL:HG22	1:B:72[B]:VAL:HG21	1.76	0.67
1:B:58:VAL:HG13	6:B:311[B]:CYS:N	2.10	0.67
1:A:59:SER:H	2:A:302:EDO:H21	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63[B]:THR:OG1	2:B:305:EDO:H22	1.98	0.62
1:A:26:GLN:HA	4:A:304:TRS:H11	1.81	0.62
1:A:26:GLN:CA	4:A:304:TRS:H11	2.30	0.61
1:A:152:LEU:HG	1:A:180:PHE:CZ	2.36	0.61
1:B:63[A]:THR:HG22	2:B:305:EDO:C1	2.27	0.60
1:A:82:ARG:NH2	6:A:320[A]:CYS:HB2	2.16	0.60
1:B:82:ARG:NH2	6:B:311[A]:CYS:HB3	2.16	0.59
1:A:172:ARG:HD3	2:A:322:EDO:H21	1.85	0.58
1:A:155[B]:ARG:NH2	7:A:406:HOH:O	2.37	0.58
1:A:26:GLN:H	4:A:304:TRS:C2	2.03	0.58
1:B:118[A]:THR:HG21	7:B:518:HOH:O	2.03	0.57
1:A:171:GLU:HG3	7:A:464:HOH:O	2.03	0.57
1:A:115:THR:O	1:A:116[B]:ASP:HB2	2.05	0.56
1:B:126:ASP:H	6:B:310[B]:CYS:HB2	1.70	0.56
6:A:319[A]:CYS:O	7:A:402:HOH:O	2.19	0.54
1:B:189:ASN:HB3	7:B:513:HOH:O	2.07	0.54
1:A:212[B]:CYS:SG	1:B:80:PRO:CD	2.91	0.54
1:A:126[B]:ASP:HB3	6:A:319[B]:CYS:CB	2.38	0.53
1:B:167:PHE:CE2	1:B:232:ILE:CG2	2.91	0.53
1:A:105:GLN:NE2	1:A:107:ASP:OD1	2.33	0.53
1:A:236:VAL:HB	1:A:237:PRO:HD2	1.90	0.53
1:B:9:ALA:HB1	1:B:52:GLU:HG3	1.90	0.53
1:A:82:ARG:NH2	6:A:320[A]:CYS:SG	2.73	0.52
1:B:201:ASN:O	1:B:205[A]:ARG:HG3	2.10	0.52
2:B:303:EDO:H21	6:B:311[B]:CYS:HA	1.92	0.52
1:A:77:ALA:H	6:A:319[A]:CYS:N	2.08	0.51
1:B:77:ALA:H	6:B:310[A]:CYS:N	2.08	0.51
1:A:126[B]:ASP:CA	6:A:319[B]:CYS:HB3	2.40	0.51
1:B:235:SER:OG	3:B:308:GOL:H32	2.11	0.51
2:A:314:EDO:O1	6:A:319[A]:CYS:CB	2.59	0.50
1:A:126[B]:ASP:HB3	6:A:319[B]:CYS:HB3	1.93	0.50
1:A:123[B]:LEU:C	1:A:123[B]:LEU:HD23	2.32	0.50
2:B:303:EDO:H21	6:B:310[A]:CYS:HB3	1.93	0.50
1:A:222[A]:LYS:HE3	1:A:226:ARG:NH2	2.27	0.50
1:A:126[B]:ASP:N	6:A:319[B]:CYS:CB	2.53	0.49
1:A:152:LEU:HG	1:A:180:PHE:HZ	1.77	0.49
1:A:26:GLN:N	4:A:304:TRS:H11	2.28	0.49
1:A:155[B]:ARG:NH2	1:A:155[B]:ARG:HG3	2.28	0.48
1:A:209:GLU:OE1	7:A:403:HOH:O	2.20	0.48
1:A:198:LYS:HD3	1:B:205[A]:ARG:NH2	2.28	0.48
1:A:125:THR:HB	6:A:319[B]:CYS:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PHE:CE2	1:B:232:ILE:HG22	2.49	0.47
1:B:118[A]:THR:HG22	1:B:137:HIS:HB3	1.97	0.47
1:B:58:VAL:HG13	6:B:311[A]:CYS:N	2.30	0.47
1:B:82:ARG:HH22	6:B:311[A]:CYS:CB	2.27	0.47
1:A:126[B]:ASP:HB3	6:A:319[B]:CYS:SG	2.55	0.46
1:A:59:SER:H	2:A:302:EDO:C2	2.26	0.46
1:B:82:ARG:NH2	6:B:311[A]:CYS:CB	2.79	0.46
1:A:58:VAL:HB	2:A:302:EDO:H21	1.98	0.46
6:A:319[A]:CYS:N	6:A:320[A]:CYS:HB3	2.30	0.46
1:A:124:GLY:O	6:A:320[B]:CYS:SG	2.73	0.46
1:B:163:ASP:HB2	1:B:167:PHE:CE2	2.50	0.46
1:A:93:ILE:HG13	1:A:94:ALA:N	2.31	0.45
1:B:60:GLY:O	2:B:305:EDO:C2	2.65	0.45
1:A:125:THR:HB	6:A:319[B]:CYS:SG	2.57	0.45
3:A:303:GOL:H32	7:A:453:HOH:O	2.15	0.45
1:B:14:THR:O	1:B:55:GLU:HA	2.15	0.45
1:A:185:ARG:HH22	3:A:315:GOL:H2	1.82	0.45
1:A:155[B]:ARG:HH21	1:A:155[B]:ARG:HG3	1.82	0.44
1:B:126:ASP:H	6:B:310[B]:CYS:CB	2.30	0.44
1:A:205[B]:ARG:CZ	1:A:205[B]:ARG:HB3	2.48	0.44
1:B:214:ILE:HG22	1:B:220:TYR:HB2	2.00	0.44
1:B:125:THR:HB	6:B:310[B]:CYS:SG	2.58	0.44
1:A:205[B]:ARG:CZ	1:A:205[B]:ARG:CB	2.92	0.44
1:B:8:SER:N	7:B:408:HOH:O	2.51	0.43
1:A:125:THR:HB	6:A:319[B]:CYS:CB	2.48	0.43
1:A:82:ARG:NH2	6:A:320[A]:CYS:CB	2.81	0.43
1:A:81[B]:GLU:CD	1:A:81[B]:GLU:H	2.21	0.43
1:B:178:ASN:ND2	1:B:178:ASN:H	2.15	0.42
1:A:14:THR:O	1:A:55:GLU:HA	2.19	0.42
1:A:82:ARG:HH22	6:A:320[A]:CYS:CB	2.33	0.42
1:B:173:ARG:O	1:B:176:ASP:HB2	2.19	0.42
1:B:215[B]:HIS:NE2	1:B:238:GLY:HA3	2.35	0.41
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.89	0.40
1:B:126:ASP:HB2	6:B:310[B]:CYS:HB3	2.03	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.92	0.40
1:A:119[B]:VAL:HG12	1:A:158:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/241 (104%)	241 (96%)	9 (4%)	0	100	100
1	B	244/241 (101%)	237 (97%)	7 (3%)	0	100	100
All	All	494/482 (102%)	478 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/216 (105%)	224 (99%)	3 (1%)	71	46
1	B	221/216 (102%)	209 (95%)	12 (5%)	24	3
All	All	448/432 (104%)	433 (97%)	15 (3%)	43	11

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

Mol	Chain	Res	Type
1	A	8	SER
1	A	95	HIS
1	A	112	LYS
1	B	8	SER
1	B	72[A]	VAL
1	B	72[B]	VAL
1	B	99	LEU
1	B	185	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	187	LYS
1	B	188	ASP
1	B	202	LYS
1	B	205[A]	ARG
1	B	205[B]	ARG
1	B	212[A]	CYS
1	B	212[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	178	ASN
1	A	201	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

37 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
2	EDO	A	301	-	3,3,3	0.79	0	2,2,2	0.32	0
2	EDO	A	302	-	3,3,3	0.27	0	2,2,2	0.25	0
3	GOL	A	303	-	5,5,5	0.27	0	5,5,5	0.62	0
4	TRS	A	304	-	7,7,7	0.49	0	9,9,9	1.79	2 (22%)
5	ACT	A	305	-	1,3,3	0.85	0	0,3,3	0.00	-
5	ACT	A	306	-	1,3,3	1.76	0	0,3,3	0.00	-
5	ACT	A	307	-	1,3,3	1.88	0	0,3,3	0.00	-
5	ACT	A	308	-	1,3,3	1.54	0	0,3,3	0.00	-
5	ACT	A	309	-	1,3,3	0.75	0	0,3,3	0.00	-
2	EDO	A	310	-	3,3,3	0.38	0	2,2,2	0.66	0
2	EDO	A	311	-	3,3,3	0.31	0	2,2,2	0.23	0
2	EDO	A	312	-	3,3,3	0.25	0	2,2,2	1.44	0
2	EDO	A	313	-	3,3,3	0.50	0	2,2,2	1.07	0
2	EDO	A	314	-	3,3,3	0.64	0	2,2,2	0.40	0
3	GOL	A	315	-	5,5,5	0.28	0	5,5,5	0.52	0
3	GOL	A	316	-	5,5,5	0.40	0	5,5,5	0.26	0
2	EDO	A	317	-	3,3,3	0.40	0	2,2,2	0.55	0
2	EDO	A	318	-	3,3,3	0.49	0	2,2,2	0.36	0
2	EDO	A	321	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	A	322	-	3,3,3	0.59	0	2,2,2	0.56	0
2	EDO	B	301	-	3,3,3	0.68	0	2,2,2	0.30	0
5	ACT	B	302	-	1,3,3	1.82	0	0,3,3	0.00	-
2	EDO	B	303	-	3,3,3	0.50	0	2,2,2	0.86	0
2	EDO	B	304	-	3,3,3	0.35	0	2,2,2	0.42	0
2	EDO	B	305	-	3,3,3	0.55	0	2,2,2	0.11	0
2	EDO	B	306	-	3,3,3	0.52	0	2,2,2	0.35	0
2	EDO	B	307	-	3,3,3	0.68	0	2,2,2	0.26	0
3	GOL	B	308	-	5,5,5	0.27	0	5,5,5	0.65	0
2	EDO	B	309	-	3,3,3	0.37	0	2,2,2	0.81	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	EDO	A	301	-	-	1/1/1/1	-
2	EDO	A	302	-	-	1/1/1/1	-
3	GOL	A	303	-	-	4/4/4/4	-
4	TRS	A	304	-	-	7/9/9/9	-
2	EDO	A	310	-	-	0/1/1/1	-
2	EDO	A	311	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	312	-	-	1/1/1/1	-
2	EDO	A	313	-	-	0/1/1/1	-
2	EDO	A	314	-	-	1/1/1/1	-
3	GOL	A	315	-	-	2/4/4/4	-
3	GOL	A	316	-	-	2/4/4/4	-
2	EDO	A	317	-	-	1/1/1/1	-
2	EDO	A	318	-	-	1/1/1/1	-
2	EDO	A	321	-	-	1/1/1/1	-
2	EDO	A	322	-	-	0/1/1/1	-
2	EDO	B	301	-	-	1/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	B	304	-	-	0/1/1/1	-
2	EDO	B	305	-	-	1/1/1/1	-
2	EDO	B	306	-	-	1/1/1/1	-
2	EDO	B	307	-	-	1/1/1/1	-
3	GOL	B	308	-	-	4/4/4/4	-
2	EDO	B	309	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	TRS	C2-C-N	3.02	114.15	107.73
4	A	304	TRS	O1-C1-C	-2.93	102.00	110.47

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	308	GOL	O1-C1-C2-O2
3	B	308	GOL	O1-C1-C2-C3
3	A	303	GOL	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-C3
3	A	316	GOL	C1-C2-C3-O3
4	A	304	TRS	C2-C-C1-O1
4	A	304	TRS	C3-C-C1-O1
4	A	304	TRS	C1-C-C2-O2
4	A	304	TRS	C3-C-C2-O2
3	A	315	GOL	C1-C2-C3-O3
4	A	304	TRS	N-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	304	TRS	N-C-C3-O3
3	B	308	GOL	C1-C2-C3-O3
3	A	303	GOL	C1-C2-C3-O3
3	A	316	GOL	O2-C2-C3-O3
3	A	315	GOL	O2-C2-C3-O3
2	B	306	EDO	O1-C1-C2-O2
2	A	317	EDO	O1-C1-C2-O2
4	A	304	TRS	C2-C-C3-O3
2	A	312	EDO	O1-C1-C2-O2
3	A	303	GOL	O2-C2-C3-O3
2	A	302	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
3	B	308	GOL	O2-C2-C3-O3
2	A	318	EDO	O1-C1-C2-O2
2	A	314	EDO	O1-C1-C2-O2
2	A	321	EDO	O1-C1-C2-O2
2	B	305	EDO	O1-C1-C2-O2
2	B	307	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	EDO	7	0
3	A	303	GOL	1	0
4	A	304	TRS	6	0
2	A	314	EDO	2	0
3	A	315	GOL	1	0
2	A	318	EDO	2	0
2	A	321	EDO	1	0
2	A	322	EDO	1	0
2	B	303	EDO	3	0
2	B	305	EDO	8	0
2	B	306	EDO	1	0
3	B	308	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	234/241 (97%)	-0.27	0 100 100	19, 26, 43, 53	0
1	B	234/241 (97%)	-0.16	2 (0%) 84 87	21, 30, 49, 58	0
All	All	468/482 (97%)	-0.22	2 (0%) 92 94	19, 28, 47, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	ASN	2.7
1	B	177	GLY	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	301	4/4	0.41	0.22	53,53,54,61	0
3	GOL	A	316	6/6	0.69	0.16	53,63,67,75	0
3	GOL	A	315	6/6	0.71	0.12	61,65,67,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	318	4/4	0.71	0.12	55,59,60,68	0
2	EDO	B	301	4/4	0.73	0.14	43,48,51,56	0
3	GOL	A	303	6/6	0.77	0.20	50,65,67,67	0
2	EDO	B	307	4/4	0.80	0.19	43,51,55,59	0
2	EDO	B	306	4/4	0.82	0.11	45,50,54,64	0
6	CYS	A	320[A]	7/7	0.83	0.30	32,44,47,52	7
6	CYS	A	320[B]	7/7	0.83	0.30	97,106,123,133	7
5	ACT	A	305	4/4	0.85	0.12	39,40,49,51	0
6	CYS	B	310[B]	7/7	0.85	0.13	25,29,34,35	7
4	TRS	A	304	8/8	0.85	0.14	34,43,51,52	0
6	CYS	B	310[A]	7/7	0.85	0.13	21,27,30,42	7
2	EDO	B	303	4/4	0.86	0.15	40,40,41,44	0
2	EDO	A	317	4/4	0.86	0.12	61,64,65,68	0
6	CYS	A	319[B]	7/7	0.87	0.15	29,31,38,39	7
6	CYS	A	319[A]	7/7	0.87	0.15	21,28,33,34	7
5	ACT	A	307	4/4	0.88	0.16	59,62,64,68	0
6	CYS	B	311[B]	7/7	0.88	0.22	46,49,55,56	7
5	ACT	A	306	4/4	0.88	0.09	40,48,49,51	0
6	CYS	B	311[A]	7/7	0.88	0.22	36,43,49,51	7
2	EDO	A	302	4/4	0.89	0.36	37,41,42,46	0
2	EDO	A	321	4/4	0.89	0.10	55,55,58,62	0
3	GOL	B	308	6/6	0.89	0.24	44,71,79,88	0
2	EDO	A	313	4/4	0.90	0.21	34,38,51,52	0
5	ACT	A	309	4/4	0.90	0.18	59,62,64,69	0
5	ACT	A	308	4/4	0.90	0.11	42,53,57,67	0
2	EDO	A	322	4/4	0.90	0.21	35,46,54,60	0
2	EDO	B	309	4/4	0.90	0.27	47,58,63,69	0
2	EDO	A	314	4/4	0.91	0.09	36,36,37,39	0
2	EDO	B	304	4/4	0.93	0.11	36,44,47,54	0
2	EDO	A	312	4/4	0.95	0.16	34,38,41,47	0
5	ACT	B	302	4/4	0.95	0.07	61,62,67,68	0
2	EDO	A	310	4/4	0.96	0.07	40,46,49,54	0
2	EDO	B	305	4/4	0.96	0.20	29,34,36,40	0
2	EDO	A	311	4/4	0.97	0.08	32,32,33,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.