Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 01:27 AM EDT

PDB ID	:	4G22
Title	:	Structure of a Lys-HCT mutant from Coffea canephora (Crystal form 1)
Authors	:	McCarthy, A.A.; Lallemand, L.A.; McCarthy, J.G.
Deposited on	:	2012-07-11
Resolution	:	1.70 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:

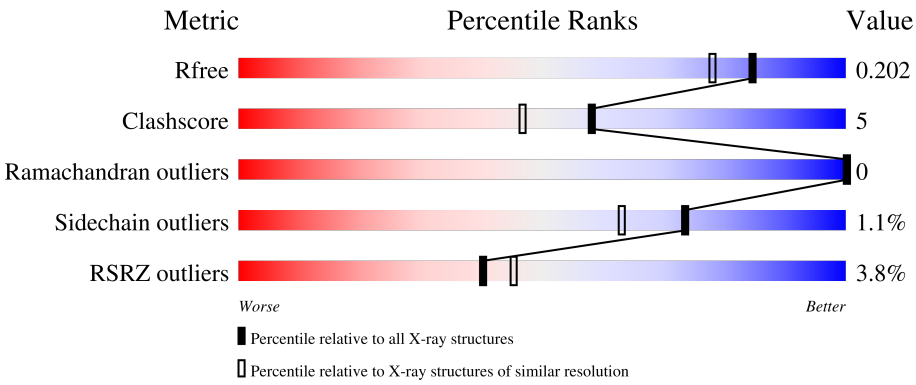
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	439	3% 80% 15% • 5%
1	B	439	4% 81% 14% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7150 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.

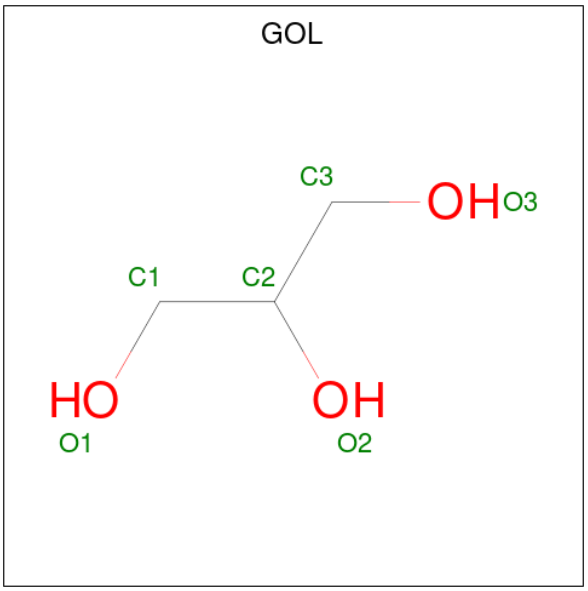
- Molecule 1 is a protein called Hydroxycinnamoyl-CoA shikimate/quinate hydroxycinnamoy ltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3265	2099	546	604	16	0	10	0
1	B	418	3240	2089	541	595	15	0	10	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP A4ZKE4
A	-3	ALA	-	EXPRESSION TAG	UNP A4ZKE4
A	-2	MET	-	EXPRESSION TAG	UNP A4ZKE4
A	-1	GLY	-	EXPRESSION TAG	UNP A4ZKE4
A	0	SER	-	EXPRESSION TAG	UNP A4ZKE4
A	210	ALA	LYS	ENGINEERED MUTATION	UNP A4ZKE4
A	217	ALA	LYS	ENGINEERED MUTATION	UNP A4ZKE4
B	-4	GLY	-	EXPRESSION TAG	UNP A4ZKE4
B	-3	ALA	-	EXPRESSION TAG	UNP A4ZKE4
B	-2	MET	-	EXPRESSION TAG	UNP A4ZKE4
B	-1	GLY	-	EXPRESSION TAG	UNP A4ZKE4
B	0	SER	-	EXPRESSION TAG	UNP A4ZKE4
B	210	ALA	LYS	ENGINEERED MUTATION	UNP A4ZKE4
B	217	ALA	LYS	ENGINEERED MUTATION	UNP A4ZKE4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 4 is water.

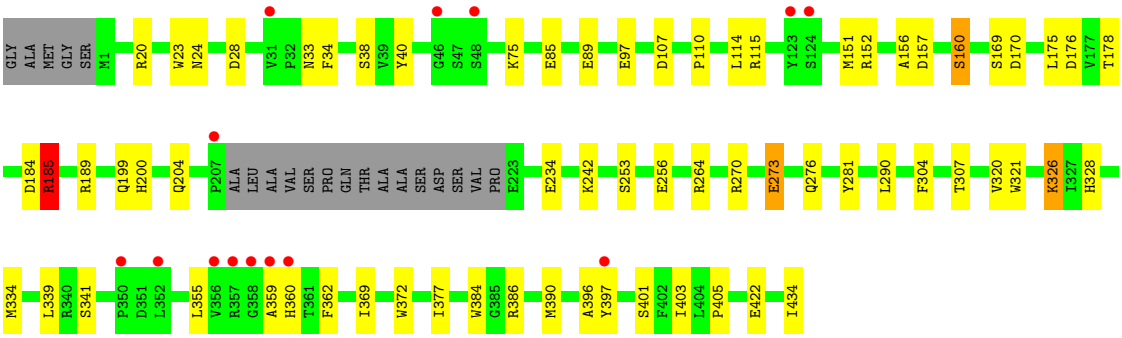
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	322	322	322	0	0
			Total	O		
4	B	303	303	303	0	0

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.

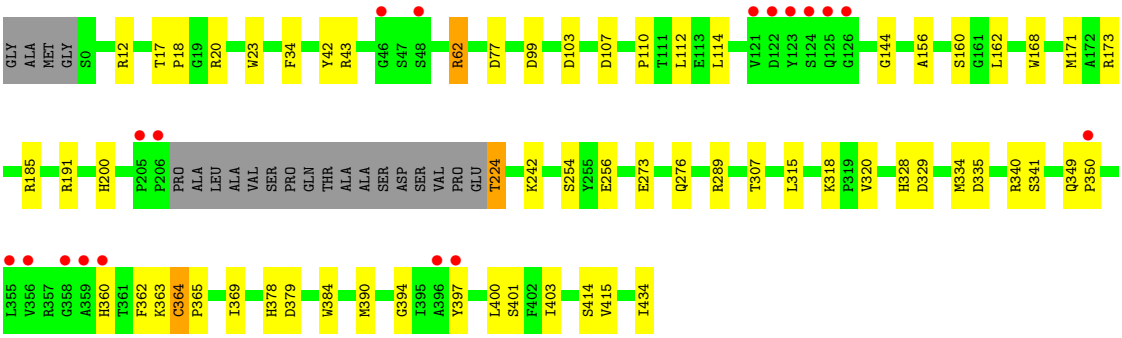
• Molecule 1: Hydroxycinnamoyl-CoA shikimate/quinate hydroxycinnamoyltransferase

Chain A:



• Molecule 1: Hydroxycinnamoyl-CoA shikimate/quinate hydroxycinnamoyltransferase

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	63.55Å 116.48Å 118.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 1.70 40.54 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.94-1.70) 99.8 (40.54-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.168 , 0.203 0.167 , 0.202	Depositor DCC
R_{free} test set	952 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7150	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, CSO

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	1.32	9/3368 (0.3%)	1.21	14/4579 (0.3%)
1	B	1.30	8/3339 (0.2%)	1.18	16/4535 (0.4%)
All	All	1.31	17/6707 (0.3%)	1.20	30/9114 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	SER	CB-OG	6.73	1.51	1.42
1	A	23	TRP	CD2-CE2	6.44	1.49	1.41
1	B	23	TRP	CD2-CE2	6.30	1.49	1.41
1	A	234	GLU	CD-OE1	6.22	1.32	1.25
1	B	144	GLY	N-CA	6.20	1.55	1.46
1	B	168	TRP	CE3-CZ3	6.05	1.48	1.38
1	A	321	TRP	CD2-CE2	5.84	1.48	1.41
1	B	414	SER	CB-OG	5.67	1.49	1.42
1	A	89	GLU	CD-OE1	-5.60	1.19	1.25
1	B	384	TRP	CZ2-CH2	5.57	1.48	1.37
1	A	169	SER	CB-OG	5.49	1.49	1.42
1	B	42	TYR	CE1-CZ	5.44	1.45	1.38
1	B	384	TRP	CD2-CE2	5.44	1.47	1.41
1	A	160	SER	CA-CB	5.43	1.61	1.52
1	A	372	TRP	CD2-CE2	5.32	1.47	1.41
1	B	254	SER	CA-CB	5.27	1.60	1.52
1	A	384	TRP	CG-CD1	5.25	1.44	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	B	335	ASP	CB-CG-OD1	8.06	125.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	191	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	340	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	28	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	107	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	107	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	20	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	318	LYS	CD-CE-NZ	-6.29	97.23	111.70
1	A	270	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	386	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	77	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	171	MET	CA-CB-CG	-5.68	103.64	113.30
1	A	157	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	173	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	315	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	A	189	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	184	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	379	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	334	MET	CA-CB-CG	5.36	122.41	113.30
1	B	162	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	12	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	326	LYS	CD-CE-NZ	5.25	123.78	111.70
1	B	99	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	62	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	20	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	151	MET	CG-SD-CE	5.02	108.23	100.20
1	A	290	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	A	40	TYR	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3185	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3240	0	3164	27	0
2	A	12	0	16	2	0
2	B	6	0	7	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	322	0	0	6	0
4	B	303	0	0	9	1
All	All	7150	0	6372	62	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 5.

All (62) 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:175:LEU:HD23	1:A:176:ASP:O	1.55	1.05
1:B:224:THR:N	4:B:721:HOH:O	1.97	0.96
1:A:33:ASN:HB3	1:A:362:PHE:HZ	1.44	0.81
1:B:242:LYS:NZ	4:B:732:HOH:O	2.18	0.76
1:A:33:ASN:HB2	1:A:34:PHE:CE1	2.24	0.72
1:A:175:LEU:CD2	1:A:176:ASP:O	2.33	0.72
1:B:156:ALA:HB1	1:B:160:SER:HB2	1.71	0.72
1:A:38[B]:SER:OG	2:A:501:GOL:H31	1.91	0.71
1:A:152:ARG:NH1	4:A:612:HOH:O	2.24	0.69
1:A:175:LEU:HD21	1:A:178:THR:CG2	2.24	0.67
1:B:200:HIS:HE1	1:B:341:SER:OG	1.79	0.66
1:A:326:LYS:NZ	4:A:765:HOH:O	2.28	0.65
1:B:34:PHE:HD1	1:B:400:LEU:HD11	1.61	0.64
1:A:200:HIS:HE1	1:A:341:SER:OG	1.79	0.64
1:B:378:HIS:HE1	4:B:605:HOH:O	1.81	0.64
1:B:62:ARG:NH1	4:B:827:HOH:O	1.98	0.60
1:B:34:PHE:CD1	1:B:400:LEU:HD11	2.37	0.59
1:A:175:LEU:HD21	1:A:178:THR:HG23	1.85	0.58
1:A:256:GLU:OE2	1:A:328:HIS:HD2	1.87	0.58
1:A:33:ASN:HB2	1:A:34:PHE:CD1	2.39	0.58
1:A:38[B]:SER:OG	2:A:501:GOL:C3	2.52	0.58
1:B:369[A]:ILE:HG12	1:B:401[A]:SER:OG	2.04	0.57
1:A:110:PRO:HA	1:A:114:LEU:HD12	1.86	0.57
1:A:422:GLU:HG3	4:A:878:HOH:O	2.03	0.57
1:A:369[A]:ILE:HG12	1:A:401[A]:SER:OG	2.06	0.56
1:A:170:ASP:HB3	1:A:175:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD21	1:A:178:THR:HG22	1.90	0.54
1:B:273:GLU:H	1:B:276:GLN:HE21	1.56	0.52
1:A:397:TYR:HB3	4:A:795:HOH:O	2.10	0.52
1:B:256:GLU:OE2	1:B:328:HIS:HD2	1.93	0.51
1:B:62:ARG:HD3	4:B:827:HOH:O	2.10	0.51
1:A:264:ARG:HD3	1:A:320[A]:VAL:HG12	1.92	0.51
1:B:329:ASP:OD2	4:B:902:HOH:O	2.19	0.50
1:A:359:ALA:O	1:A:360:HIS:C	2.50	0.49
1:B:362:PHE:HD2	1:B:397:TYR:HE1	1.59	0.49
1:A:24:ASN:OD1	1:A:185:ARG:NH1	2.39	0.49
1:B:434:ILE:O	4:B:826:HOH:O	2.20	0.48
1:A:199:GLN:HE21	1:A:204:GLN:HE22	1.64	0.46
1:A:156:ALA:HB1	1:A:160:SER:HB2	1.98	0.45
1:B:43:ARG:NH2	1:B:103:ASP:OD1	2.45	0.45
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.74	0.45
1:A:75:LYS:HE2	1:A:85:GLU:HB2	1.99	0.44
1:B:360:HIS:O	1:B:363:LYS:HG2	2.17	0.44
1:A:97:GLU:CG	4:A:839:HOH:O	2.65	0.44
1:A:33:ASN:HB3	1:A:362:PHE:CZ	2.36	0.44
1:A:304:PHE:CG	1:A:339:LEU:HD22	2.53	0.44
1:A:369[B]:ILE:HD11	1:A:403:ILE:HD11	2.00	0.44
1:A:115:ARG:HH22	1:A:396:ALA:HB2	1.81	0.43
1:B:320[A]:VAL:HG22	4:B:895:HOH:O	2.18	0.43
1:B:307:THR:HB	4:B:901:HOH:O	2.19	0.43
1:B:364:CSO:HA	1:B:365:PRO:HA	1.84	0.43
1:A:320[B]:VAL:HG23	4:A:634:HOH:O	2.19	0.42
1:A:242:LYS:HE3	1:A:434:ILE:OXT	2.20	0.42
1:B:349:GLN:HA	1:B:350:PRO:HD3	1.94	0.42
1:A:377:ILE:HD11	1:A:405:PRO:HD2	2.03	0.41
1:B:110:PRO:HA	1:B:114:LEU:HD12	2.01	0.41
1:B:289:ARG:HD3	1:B:334:MET:O	2.20	0.41
1:A:273:GLU:H	1:A:276:GLN:HE21	1.69	0.41
1:B:110:PRO:O	1:B:394:GLY:HA2	2.21	0.41
1:A:281:TYR:CD1	1:A:307[B]:THR:HG22	2.56	0.40
1:B:17:THR:HB	1:B:18:PRO:HD2	2.03	0.40
1:B:403[B]:ILE:HD12	1:B:415:VAL:HG22	2.02	0.40

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)
4:B:601:HOH:O	4:B:903:HOH:O[4_455]	2.15	0.05

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	424/439 (97%)	411 (97%)	13 (3%)	0	100	100
1	B	422/439 (96%)	409 (97%)	13 (3%)	0	100	100
All	All	846/878 (96%)	820 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	343/362 (95%)	339 (99%)	4 (1%)	71	59
1	B	335/362 (92%)	332 (99%)	3 (1%)	78	70
All	All	678/724 (94%)	671 (99%)	7 (1%)	73	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	273	GLU
1	A	355	LEU

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Mol	Chain	Res	Type
1	A	390	MET
1	B	185	ARG
1	B	224	THR
1	B	390	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	199	GLN
1	A	200	HIS
1	A	276	GLN
1	A	328	HIS
1	B	199	GLN
1	B	200	HIS
1	B	276	GLN
1	B	328	HIS
1	B	378	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	CSO	B	364	1	3,6,7	1.18	0	1,6,8	3.20	1 (100%)
1	CSO	B	142	1	3,6,7	0.93	0	1,6,8	0.88	0
1	CSO	A	364	1	3,6,7	0.77	0	1,6,8	0.20	0
1	CSO	A	142	1	3,6,7	1.10	0	1,6,8	1.76	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
1	CSO	B	364	1	-	0/1/5/7	-
1	CSO	B	142	1	-	0/1/5/7	-
1	CSO	A	364	1	-	0/1/5/7	-
1	CSO	A	142	1	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	364	CSO	CB-CA-C	3.20	119.50	110.80

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	364	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	GOL	B	501	-	5,5,5	0.81	0	5,5,5	1.40	1 (20%)
2	GOL	A	502	-	5,5,5	1.36	1 (20%)	5,5,5	1.23	1 (20%)
2	GOL	A	501	-	5,5,5	0.79	0	5,5,5	1.19	1 (20%)

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	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	GOL	O2-C2	2.76	1.51	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	GOL	O2-C2-C3	-2.37	99.38	109.18
2	A	501	GOL	O2-C2-C3	-2.36	99.42	109.18
2	A	502	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	B	501	GOL	C1-C2-C3-O3
2	A	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	2	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 (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	417/439 (94%)	-0.20	14 (3%)	45	50	14, 23, 48, 90	0
1	B	416/439 (94%)	-0.19	18 (4%)	35	39	13, 24, 54, 101	0
All	All	833/878 (94%)	-0.19	32 (3%)	40	45	13, 24, 53, 101	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	VAL	5.7
1	B	124	SER	5.6
1	A	360	HIS	5.5
1	A	358	GLY	4.8
1	B	356	VAL	4.2
1	B	123	TYR	4.1
1	A	124	SER	4.1
1	B	121	VAL	4.0
1	B	125	GLN	3.7
1	A	357	ARG	3.5
1	A	350	PRO	3.4
1	B	397	TYR	3.4
1	A	359	ALA	3.3
1	B	396	ALA	3.2
1	A	48	SER	3.2
1	B	358	GLY	3.1
1	A	46	GLY	3.0
1	B	48	SER	3.0
1	A	123	TYR	2.9
1	A	397	TYR	2.9
1	B	360	HIS	2.8
1	B	126	GLY	2.7
1	A	31	VAL	2.6
1	A	207	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	122	ASP	2.5
1	B	46	GLY	2.5
1	B	355	LEU	2.3
1	B	350	PRO	2.3
1	B	359	ALA	2.1
1	B	206	PRO	2.1
1	A	352	LEU	2.1
1	B	205	PRO	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. 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
1	CSO	B	142	7/8	0.94	0.06	30,35,42,46	0
1	CSO	A	142	7/8	0.97	0.07	25,26,36,42	0
1	CSO	B	364	7/8	0.97	0.05	24,25,29,33	0
1	CSO	A	364	7/8	0.98	0.06	23,24,27,30	0

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, 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	GOL	A	502	6/6	0.80	0.12	25,34,34,40	0
2	GOL	A	501	6/6	0.90	0.13	25,37,44,52	0
2	GOL	B	501	6/6	0.93	0.12	27,41,45,47	0
3	CL	B	502	1/1	0.98	0.04	28,28,28,28	0
3	CL	A	503	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.