



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:34 AM UTC

PDB ID : 8WWS / pdb_00008wws
Title : Crystal structure of cis-epoxysuccinate hydrolase from *Klebsiella oxytoca* with L(+)-tartaric acid
Authors : Han, Y.; Kong, X.D.; Li, J.; Xu, J.H.
Deposited on : 2023-10-26
Resolution : 1.79 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

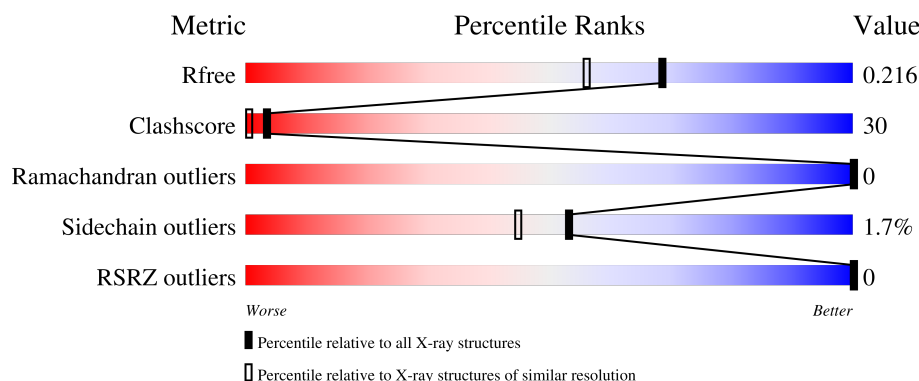
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	278	 50% 33% 16%
1	B	278	 51% 32% 16%
1	C	278	 47% 36% 16%
1	D	278	 45% 38% 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	TLA	A	301	-	X	-	-
2	TLA	D	301	-	X	X	-
4	GOL	B	302	-	X	-	-
5	CO3	C	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8152 atoms, of which 22 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 (S)-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	1	0
			1858	1187	320	346	5			
1	B	234	Total	C	N	O	S	0	0	0
			1849	1182	318	344	5			
1	C	234	Total	C	N	O	S	0	0	0
			1849	1182	318	344	5			
1	D	233	Total	C	N	O	S	9	1	0
			1853	1184	319	345	5			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP W8PFD2
A	275	SER	-	expression tag	UNP W8PFD2
A	276	ASP	-	expression tag	UNP W8PFD2
A	277	PRO	-	expression tag	UNP W8PFD2
A	278	ASN	-	expression tag	UNP W8PFD2
A	279	SER	-	expression tag	UNP W8PFD2
A	280	SER	-	expression tag	UNP W8PFD2
A	281	SER	-	expression tag	UNP W8PFD2
A	282	VAL	-	expression tag	UNP W8PFD2
A	283	ASP	-	expression tag	UNP W8PFD2
A	284	LYS	-	expression tag	UNP W8PFD2
A	285	LEU	-	expression tag	UNP W8PFD2
A	286	ALA	-	expression tag	UNP W8PFD2
A	287	ALA	-	expression tag	UNP W8PFD2
A	288	ALA	-	expression tag	UNP W8PFD2
A	289	LEU	-	expression tag	UNP W8PFD2
A	290	GLU	-	expression tag	UNP W8PFD2
A	291	HIS	-	expression tag	UNP W8PFD2
A	292	HIS	-	expression tag	UNP W8PFD2
A	293	HIS	-	expression tag	UNP W8PFD2
A	294	HIS	-	expression tag	UNP W8PFD2

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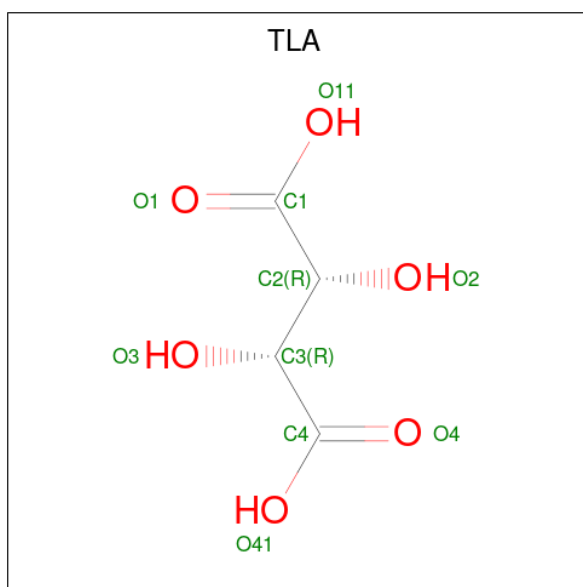
Chain	Residue	Modelled	Actual	Comment	Reference
A	295	HIS	-	expression tag	UNP W8PFD2
A	296	HIS	-	expression tag	UNP W8PFD2
B	19	MET	-	initiating methionine	UNP W8PFD2
B	275	SER	-	expression tag	UNP W8PFD2
B	276	ASP	-	expression tag	UNP W8PFD2
B	277	PRO	-	expression tag	UNP W8PFD2
B	278	ASN	-	expression tag	UNP W8PFD2
B	279	SER	-	expression tag	UNP W8PFD2
B	280	SER	-	expression tag	UNP W8PFD2
B	281	SER	-	expression tag	UNP W8PFD2
B	282	VAL	-	expression tag	UNP W8PFD2
B	283	ASP	-	expression tag	UNP W8PFD2
B	284	LYS	-	expression tag	UNP W8PFD2
B	285	LEU	-	expression tag	UNP W8PFD2
B	286	ALA	-	expression tag	UNP W8PFD2
B	287	ALA	-	expression tag	UNP W8PFD2
B	288	ALA	-	expression tag	UNP W8PFD2
B	289	LEU	-	expression tag	UNP W8PFD2
B	290	GLU	-	expression tag	UNP W8PFD2
B	291	HIS	-	expression tag	UNP W8PFD2
B	292	HIS	-	expression tag	UNP W8PFD2
B	293	HIS	-	expression tag	UNP W8PFD2
B	294	HIS	-	expression tag	UNP W8PFD2
B	295	HIS	-	expression tag	UNP W8PFD2
B	296	HIS	-	expression tag	UNP W8PFD2
C	19	MET	-	initiating methionine	UNP W8PFD2
C	275	SER	-	expression tag	UNP W8PFD2
C	276	ASP	-	expression tag	UNP W8PFD2
C	277	PRO	-	expression tag	UNP W8PFD2
C	278	ASN	-	expression tag	UNP W8PFD2
C	279	SER	-	expression tag	UNP W8PFD2
C	280	SER	-	expression tag	UNP W8PFD2
C	281	SER	-	expression tag	UNP W8PFD2
C	282	VAL	-	expression tag	UNP W8PFD2
C	283	ASP	-	expression tag	UNP W8PFD2
C	284	LYS	-	expression tag	UNP W8PFD2
C	285	LEU	-	expression tag	UNP W8PFD2
C	286	ALA	-	expression tag	UNP W8PFD2
C	287	ALA	-	expression tag	UNP W8PFD2
C	288	ALA	-	expression tag	UNP W8PFD2
C	289	LEU	-	expression tag	UNP W8PFD2
C	290	GLU	-	expression tag	UNP W8PFD2

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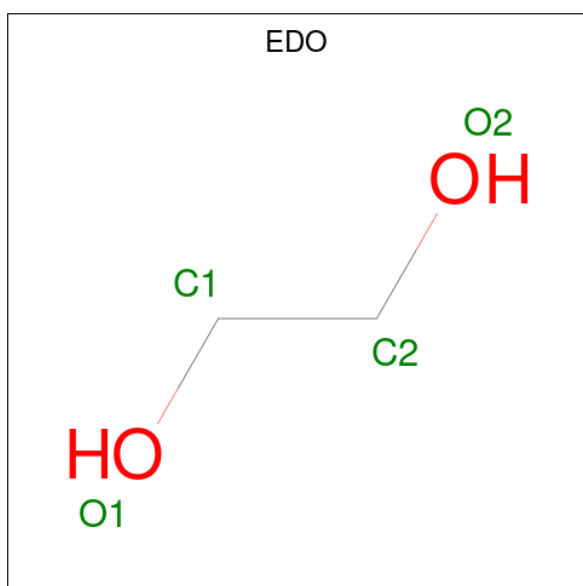
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	HIS	-	expression tag	UNP W8PFD2
C	292	HIS	-	expression tag	UNP W8PFD2
C	293	HIS	-	expression tag	UNP W8PFD2
C	294	HIS	-	expression tag	UNP W8PFD2
C	295	HIS	-	expression tag	UNP W8PFD2
C	296	HIS	-	expression tag	UNP W8PFD2
D	19	MET	-	initiating methionine	UNP W8PFD2
D	275	SER	-	expression tag	UNP W8PFD2
D	276	ASP	-	expression tag	UNP W8PFD2
D	277	PRO	-	expression tag	UNP W8PFD2
D	278	ASN	-	expression tag	UNP W8PFD2
D	279	SER	-	expression tag	UNP W8PFD2
D	280	SER	-	expression tag	UNP W8PFD2
D	281	SER	-	expression tag	UNP W8PFD2
D	282	VAL	-	expression tag	UNP W8PFD2
D	283	ASP	-	expression tag	UNP W8PFD2
D	284	LYS	-	expression tag	UNP W8PFD2
D	285	LEU	-	expression tag	UNP W8PFD2
D	286	ALA	-	expression tag	UNP W8PFD2
D	287	ALA	-	expression tag	UNP W8PFD2
D	288	ALA	-	expression tag	UNP W8PFD2
D	289	LEU	-	expression tag	UNP W8PFD2
D	290	GLU	-	expression tag	UNP W8PFD2
D	291	HIS	-	expression tag	UNP W8PFD2
D	292	HIS	-	expression tag	UNP W8PFD2
D	293	HIS	-	expression tag	UNP W8PFD2
D	294	HIS	-	expression tag	UNP W8PFD2
D	295	HIS	-	expression tag	UNP W8PFD2
D	296	HIS	-	expression tag	UNP W8PFD2

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆) (labeled as "Ligand of Interest" by depositor).



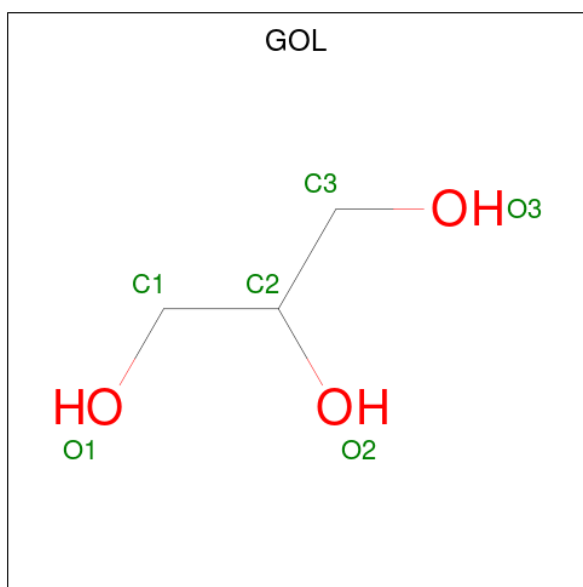
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	4	4	6		
2	D	1	Total	C	H	O	0	0
			14	4	4	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



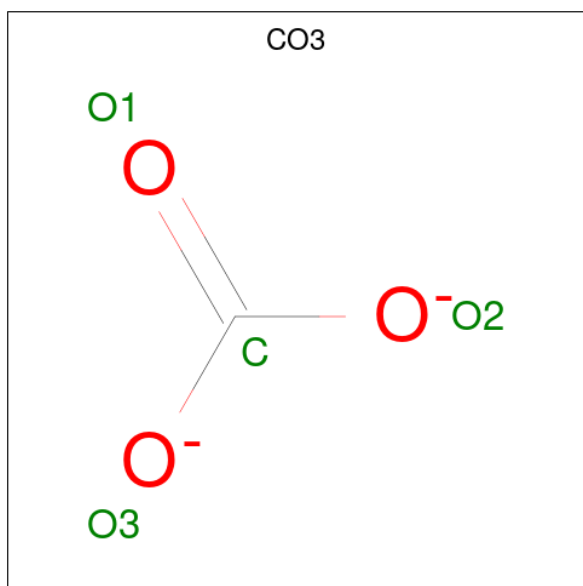
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

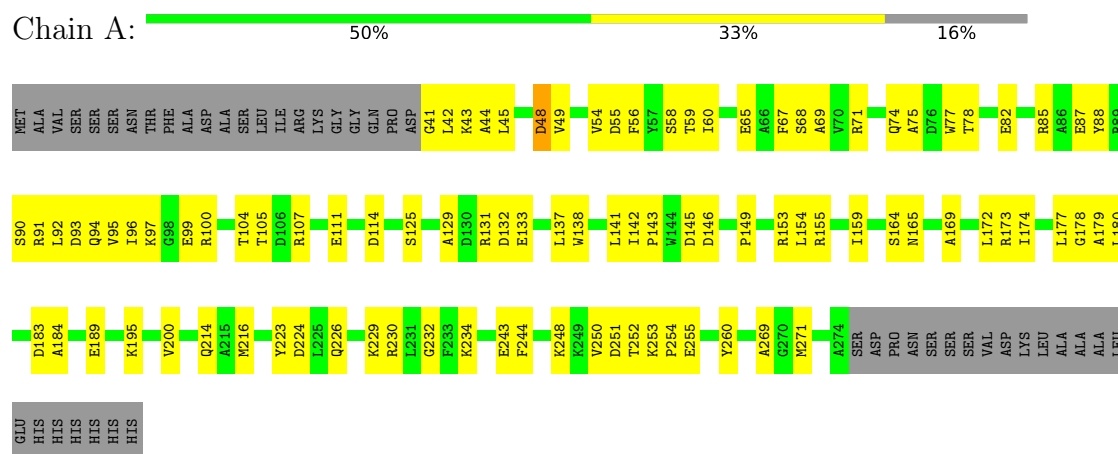
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	211	Total 211	O 211	0	0
6	B	146	Total 146	O 146	0	0
6	C	162	Total 162	O 162	0	0
6	D	164	Total 164	O 164	0	0

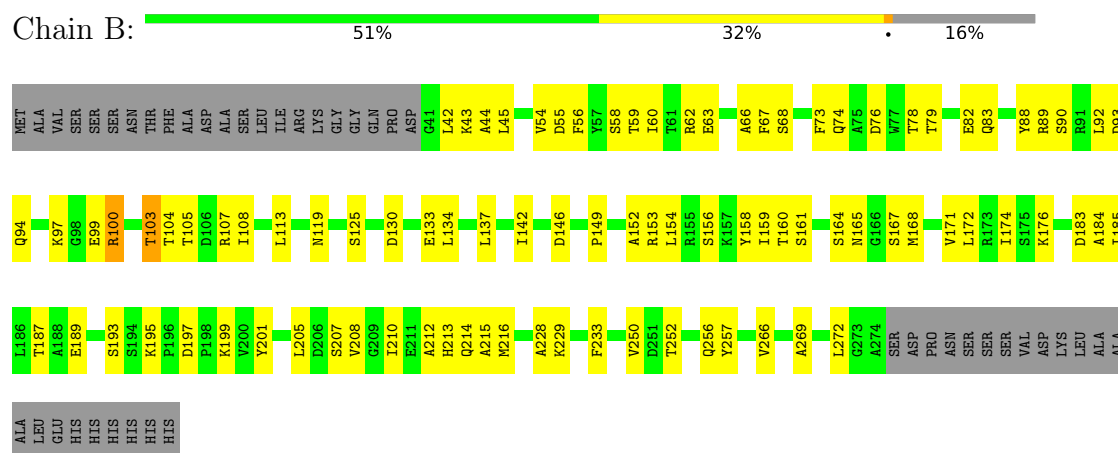
3 Residue-property plots

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.

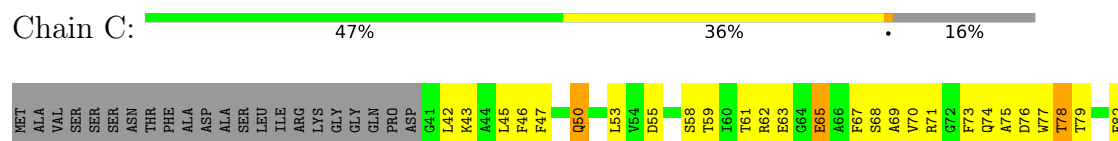
• Molecule 1: (S)-2-haloacid dehalogenase

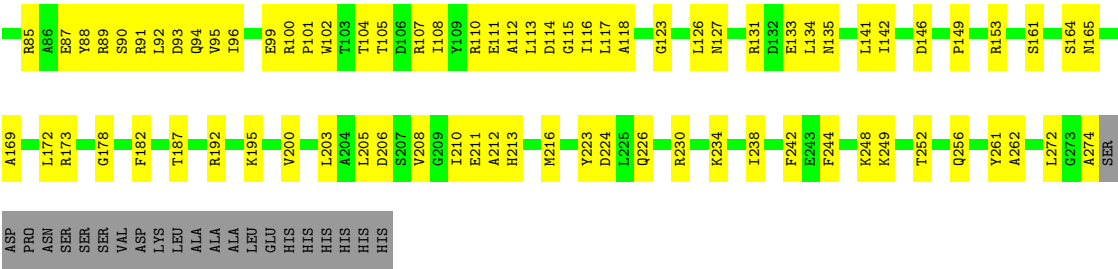


• Molecule 1: (S)-2-haloacid dehalogenase

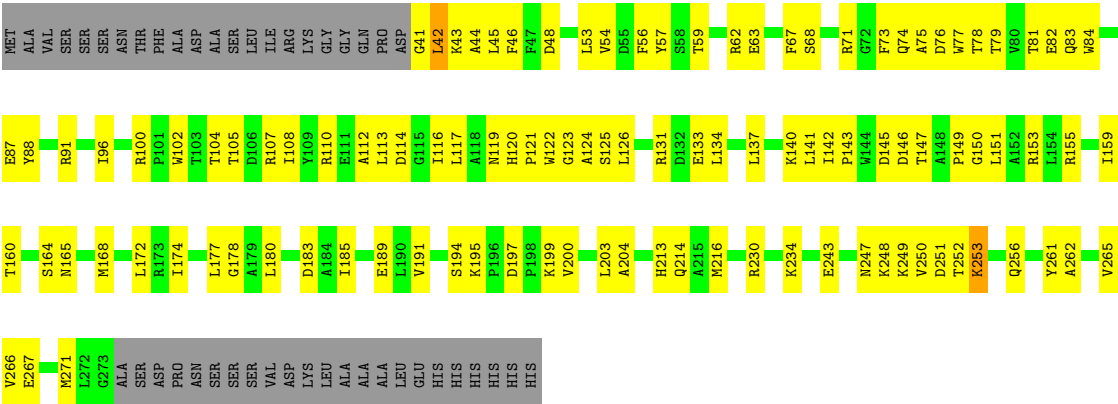


• Molecule 1: (S)-2-haloacid dehalogenase





● Molecule 1: (S)-2-haloacid dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.62Å 114.70Å 86.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.08 – 1.79 44.08 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.08-1.79) 99.0 (44.08-1.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.183 , 0.219 0.185 , 0.216	Depositor DCC
R_{free} test set	5285 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.457 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8152	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 35.73 % 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 5.5780e-04.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, CO3, TLA

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	0.42	0/1902	0.64	2/2580 (0.1%)
1	B	0.42	0/1893	0.57	0/2568
1	C	0.39	0/1893	0.53	0/2568
1	D	0.42	0/1897	0.56	0/2573
All	All	0.41	0/7585	0.58	2/10289 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CA-C-N	-6.06	117.03	122.97
1	A	48	ASP	C-N-CA	-6.06	117.03	122.97

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	1858	0	1836	112	1
1	B	1849	0	1829	96	0
1	C	1849	0	1829	119	0
1	D	1853	0	1831	115	0
2	A	10	4	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10	4	4	5	0
3	B	4	6	6	0	1
4	B	6	8	7	0	0
5	B	4	0	0	0	0
5	C	4	0	0	2	0
6	A	211	0	0	40	2
6	B	146	0	0	29	2
6	C	162	0	0	28	4
6	D	164	0	0	42	4
All	All	8130	22	7346	437	7

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 30.

All (437) 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:133:GLU:OE1	6:A:401:HOH:O	1.72	1.05
1:B:63:GLU:OE1	6:B:401:HOH:O	1.74	1.03
1:A:75:ALA:O	6:A:403:HOH:O	1.76	1.02
1:C:79:THR:HA	1:C:82:GLU:OE1	1.57	1.02
1:D:59:THR:O	6:D:401:HOH:O	1.79	1.01
1:A:93:ASP:OD1	6:A:402:HOH:O	1.76	1.01
1:B:97:LYS:NZ	6:B:402:HOH:O	1.93	1.01
1:A:183:ASP:OD1	6:A:404:HOH:O	1.79	0.99
1:C:67:PHE:O	6:C:401:HOH:O	1.81	0.99
1:C:42:LEU:HD12	1:C:43:LYS:HG2	1.45	0.98
1:D:87:GLU:OE2	6:D:402:HOH:O	1.82	0.98
1:B:214:GLN:O	6:B:403:HOH:O	1.83	0.96
1:B:93:ASP:OD1	6:B:402:HOH:O	1.81	0.96
1:B:42:LEU:HD11	1:B:214:GLN:HG2	1.47	0.95
1:A:226:GLN:OE1	6:A:406:HOH:O	1.85	0.94
1:A:155:ARG:NH1	6:A:404:HOH:O	2.01	0.94
1:A:184:ALA:HB2	1:B:172:LEU:HD23	1.47	0.94
1:C:63:GLU:OE2	6:C:402:HOH:O	1.85	0.94
1:A:129:ALA:HB2	1:C:249:LYS:HD2	1.49	0.93
1:C:100:ARG:O	6:C:404:HOH:O	1.88	0.92
1:A:178:GLY:HA3	6:A:489:HOH:O	1.69	0.91
1:C:82:GLU:OE2	6:C:403:HOH:O	1.86	0.91
1:B:185:ILE:O	6:B:404:HOH:O	1.87	0.90
1:D:122:TRP:O	1:D:125:SER:OG	1.88	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ASP:OD2	6:D:403:HOH:O	1.88	0.89
1:A:189:GLU:OE2	6:A:407:HOH:O	1.89	0.89
1:A:58:SER:HB2	1:A:142:ILE:HD11	1.55	0.88
1:B:250:VAL:HG12	1:B:252:THR:HG23	1.56	0.88
1:D:71:ARG:O	6:D:404:HOH:O	1.90	0.88
1:A:94:GLN:HA	1:A:97:LYS:HG2	1.54	0.87
1:A:97:LYS:HE3	1:A:99:GLU:HB3	1.53	0.86
1:D:174:ILE:O	6:D:406:HOH:O	1.93	0.86
1:C:78:THR:OG1	6:C:405:HOH:O	1.94	0.86
1:C:50:GLN:OE1	1:C:85:ARG:NH1	2.09	0.85
1:D:42:LEU:HD11	1:D:214:GLN:HG2	1.57	0.85
1:B:152:ALA:O	6:B:406:HOH:O	1.94	0.85
1:A:92:LEU:O	1:A:96:ILE:HG13	1.76	0.84
1:D:145:ASP:OD1	6:D:405:HOH:O	1.93	0.84
1:C:62:ARG:NH2	6:C:412:HOH:O	2.09	0.84
1:D:88:TYR:OH	2:D:301:TLA:O11	1.94	0.84
1:A:189:GLU:OE1	6:A:408:HOH:O	1.95	0.84
1:D:79:THR:O	1:D:83:GLN:HG3	1.77	0.83
1:D:63:GLU:N	6:D:401:HOH:O	1.93	0.83
1:D:63:GLU:OE1	6:D:407:HOH:O	1.96	0.83
1:B:183:ASP:OD1	6:B:407:HOH:O	1.95	0.83
1:D:155:ARG:N	6:D:418:HOH:O	2.12	0.83
1:D:42:LEU:HD13	1:D:43:LYS:HE3	1.59	0.82
1:A:42:LEU:HD12	1:A:43:LYS:HG2	1.61	0.82
1:B:125:SER:HB3	6:B:473:HOH:O	1.78	0.81
1:D:142:ILE:HD11	6:D:487:HOH:O	1.79	0.81
1:D:67:PHE:HB2	6:D:444:HOH:O	1.81	0.81
1:C:63:GLU:OE1	6:C:406:HOH:O	1.99	0.80
1:C:74:GLN:OE1	6:C:407:HOH:O	1.99	0.80
1:B:42:LEU:HD12	1:B:43:LYS:HG2	1.62	0.80
1:A:78:THR:OG1	6:A:405:HOH:O	1.79	0.80
1:D:134:LEU:O	1:D:137:LEU:HG	1.82	0.80
1:B:62:ARG:NH2	6:B:409:HOH:O	2.12	0.79
1:B:78:THR:O	1:B:82:GLU:HG3	1.81	0.79
1:D:62:ARG:NH2	6:D:417:HOH:O	2.12	0.79
1:C:43:LYS:HA	6:C:463:HOH:O	1.81	0.79
1:D:82:GLU:HG3	6:D:454:HOH:O	1.82	0.79
1:C:89:ARG:NH2	6:C:415:HOH:O	2.15	0.78
1:A:195:LYS:HG3	1:A:200:VAL:HG11	1.65	0.78
1:B:59:THR:HA	6:B:454:HOH:O	1.84	0.77
1:D:81:THR:HB	6:D:425:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:MET:N	6:A:415:HOH:O	2.17	0.77
1:B:42:LEU:HD13	1:B:43:LYS:HE2	1.66	0.77
1:C:42:LEU:CD1	1:C:43:LYS:HG2	2.15	0.77
1:B:119:ASN:OD1	6:B:408:HOH:O	2.02	0.77
1:D:121:PRO:O	6:D:412:HOH:O	2.01	0.77
1:B:44:ALA:O	6:B:403:HOH:O	2.03	0.77
1:B:88:TYR:HE2	1:B:105:THR:HG23	1.50	0.77
1:C:62:ARG:NH1	6:C:419:HOH:O	2.18	0.76
1:D:168:MET:HE1	1:D:185:ILE:O	1.85	0.76
1:A:269:ALA:O	6:A:409:HOH:O	2.04	0.76
1:C:90:SER:OG	6:C:408:HOH:O	2.00	0.76
1:D:75:ALA:HB2	1:D:122:TRP:NE1	2.01	0.75
1:B:43:LYS:HG2	1:B:214:GLN:HB3	1.68	0.75
1:C:62:ARG:NH2	1:D:57:TYR:OH	2.20	0.75
1:D:42:LEU:HD13	1:D:43:LYS:CE	2.17	0.74
1:D:243:GLU:OE2	6:D:414:HOH:O	2.05	0.74
1:D:180:LEU:HG	6:D:406:HOH:O	1.86	0.74
1:A:243:GLU:O	6:A:410:HOH:O	2.05	0.74
1:A:59:THR:OG1	1:A:142:ILE:HG12	1.87	0.74
1:A:260:TYR:HD2	1:A:271:MET:HE3	1.50	0.74
1:B:195:LYS:HG2	1:B:201:TYR:OH	1.87	0.74
1:C:117:LEU:CD1	1:C:131:ARG:HG2	2.17	0.74
1:A:93:ASP:O	1:A:97:LYS:N	2.21	0.73
1:C:244:PHE:HB2	1:C:248:LYS:HD3	1.69	0.73
1:A:145:ASP:OD2	6:A:411:HOH:O	2.07	0.73
1:D:122:TRP:CZ3	1:D:126:LEU:HD11	2.23	0.73
1:B:215:ALA:HA	6:B:403:HOH:O	1.87	0.73
1:C:88:TYR:O	1:C:92:LEU:HB2	1.88	0.73
1:A:226:GLN:O	1:A:230:ARG:HG2	1.88	0.73
1:D:164:SER:OG	2:D:301:TLA:O4	2.07	0.73
1:C:61:THR:O	6:C:410:HOH:O	2.06	0.72
1:D:41:GLY:N	1:D:234:LYS:HG3	2.04	0.72
1:C:70:VAL:HB	6:C:401:HOH:O	1.89	0.72
1:A:125:SER:OG	6:A:412:HOH:O	2.08	0.72
1:B:195:LYS:HG2	1:B:201:TYR:CZ	2.24	0.72
1:A:143:PRO:HG3	6:A:489:HOH:O	1.89	0.72
1:B:104:THR:HG23	1:B:107:ARG:H	1.56	0.70
1:C:211:GLU:OE2	6:C:411:HOH:O	2.08	0.70
1:D:178:GLY:HA2	6:D:470:HOH:O	1.91	0.70
1:A:65:GLU:OE1	6:A:413:HOH:O	2.08	0.70
1:A:177:LEU:O	6:A:414:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:VAL:HG12	1:D:252:THR:HG23	1.73	0.70
1:A:141:LEU:HB3	6:A:435:HOH:O	1.91	0.69
1:C:117:LEU:HD12	1:C:131:ARG:HG2	1.73	0.69
1:A:68:SER:OG	1:A:69:ALA:N	2.21	0.69
1:C:91:ARG:HE	1:C:112:ALA:HA	1.56	0.69
1:C:153:ARG:NH2	1:C:274:ALA:O	2.18	0.69
1:D:125:SER:N	6:D:423:HOH:O	2.25	0.69
1:C:68:SER:HB2	1:C:73:PHE:CE1	2.28	0.68
1:D:142:ILE:HD11	6:D:452:HOH:O	1.92	0.68
1:A:260:TYR:HD2	1:A:271:MET:CE	2.05	0.68
1:C:117:LEU:HD12	1:C:131:ARG:HD3	1.75	0.68
1:A:75:ALA:HB3	1:A:77:TRP:CE2	2.29	0.67
1:D:126:LEU:HB2	1:D:131:ARG:HE	1.59	0.67
1:D:137:LEU:O	6:D:416:HOH:O	2.12	0.67
1:B:88:TYR:CE2	1:B:105:THR:HG23	2.29	0.67
1:B:42:LEU:CD1	1:B:43:LYS:HG2	2.23	0.67
1:C:146:ASP:O	1:C:149:PRO:HD2	1.95	0.66
1:D:160:THR:HG21	6:D:418:HOH:O	1.95	0.66
1:B:130:ASP:OD2	6:B:410:HOH:O	2.14	0.66
1:C:178:GLY:O	6:C:414:HOH:O	2.13	0.66
1:A:44:ALA:O	6:A:415:HOH:O	2.13	0.66
1:D:151:LEU:O	6:D:418:HOH:O	2.12	0.66
1:C:89:ARG:NH2	6:C:409:HOH:O	2.05	0.66
1:D:122:TRP:HZ3	1:D:126:LEU:HD11	1.61	0.65
1:D:124:ALA:HB3	6:D:423:HOH:O	1.97	0.65
1:D:197:ASP:OD1	1:D:199:LYS:HB2	1.96	0.65
1:B:168:MET:HG3	6:B:411:HOH:O	1.96	0.65
1:C:212:ALA:N	6:C:413:HOH:O	2.13	0.65
1:C:105:THR:HG21	1:C:165:ASN:O	1.96	0.64
1:C:252:THR:O	1:C:261:TYR:OH	2.12	0.64
1:A:179:ALA:HB2	6:A:541:HOH:O	1.97	0.64
1:B:205:LEU:HD11	1:B:212:ALA:HB2	1.80	0.64
1:D:73:PHE:C	1:D:74:GLN:HG2	2.22	0.64
1:B:168:MET:HG2	1:B:189:GLU:HG2	1.78	0.64
1:C:238:ILE:HD13	1:C:262:ALA:HB3	1.80	0.64
1:C:71:ARG:NH1	6:C:401:HOH:O	2.10	0.64
1:D:42:LEU:HD12	1:D:43:LYS:HG2	1.80	0.64
1:B:189:GLU:OE2	6:B:411:HOH:O	2.15	0.64
1:B:164:SER:OG	6:B:405:HOH:O	1.93	0.63
1:D:42:LEU:O	1:D:43:LYS:HE2	1.98	0.63
1:C:88:TYR:CE2	1:C:92:LEU:HD22	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HD3	6:A:457:HOH:O	1.97	0.63
1:B:168:MET:HE1	6:B:404:HOH:O	1.98	0.63
1:A:107:ARG:O	1:A:111:GLU:HG3	1.98	0.63
1:A:138:TRP:HA	1:A:141:LEU:HD21	1.78	0.63
1:C:173:ARG:HH21	5:C:301:CO3:C	2.12	0.63
1:B:153:ARG:NH1	1:B:266:VAL:HG23	2.14	0.62
1:D:78:THR:HA	6:D:425:HOH:O	1.99	0.62
1:C:76:ASP:OD2	1:C:79:THR:OG1	2.17	0.62
1:C:78:THR:O	1:C:82:GLU:HG3	2.00	0.62
1:D:42:LEU:CD1	1:D:43:LYS:HG2	2.30	0.62
1:A:114:ASP:OD1	1:A:131:ARG:NH1	2.31	0.62
1:C:59:THR:OG1	1:C:142:ILE:HG12	1.99	0.62
1:B:76:ASP:OD1	1:B:78:THR:HB	2.00	0.61
1:A:180:LEU:HG	6:A:489:HOH:O	1.99	0.61
1:A:41:GLY:N	1:A:234:LYS:HG3	2.16	0.61
1:C:208:VAL:O	1:C:208:VAL:HG12	2.01	0.60
1:C:213:HIS:O	1:C:234:LYS:HE2	2.00	0.60
1:D:153:ARG:NH1	1:D:266:VAL:HG13	2.16	0.60
1:C:113:LEU:HD21	1:C:134:LEU:HD23	1.83	0.60
1:C:117:LEU:HD12	1:C:131:ARG:CD	2.32	0.60
1:C:74:GLN:HG2	6:C:425:HOH:O	2.00	0.60
1:A:251:ASP:OD1	1:A:253:LYS:NZ	2.33	0.60
1:D:110:ARG:NH1	1:D:114:ASP:OD1	2.33	0.60
1:C:87:GLU:O	1:C:90:SER:N	2.34	0.60
1:D:140:LYS:NZ	6:D:415:HOH:O	2.05	0.60
1:A:45:LEU:HD23	6:A:415:HOH:O	2.01	0.59
1:C:91:ARG:HH21	1:C:115:GLY:HA3	1.67	0.59
1:C:182:PHE:O	6:C:417:HOH:O	2.16	0.59
1:A:78:THR:O	1:A:82:GLU:HG3	2.02	0.59
1:D:41:GLY:CA	1:D:234:LYS:HG3	2.32	0.59
1:D:74:GLN:NE2	6:D:410:HOH:O	1.98	0.59
1:A:54:VAL:HG23	6:A:435:HOH:O	2.02	0.59
1:B:79:THR:O	1:B:83:GLN:HG3	2.03	0.59
1:D:46:PHE:CE1	1:D:204:ALA:HB1	2.36	0.59
1:C:58:SER:HB2	1:C:142:ILE:HD11	1.83	0.59
1:A:94:GLN:HA	1:A:97:LYS:CG	2.30	0.59
1:A:138:TRP:O	1:A:174:ILE:HD11	2.02	0.59
1:A:92:LEU:HG	1:A:96:ILE:HD11	1.85	0.58
1:A:93:ASP:O	1:A:96:ILE:N	2.36	0.58
1:A:104:THR:HG21	6:A:510:HOH:O	2.03	0.58
1:A:250:VAL:HG23	1:A:252:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:THR:HG21	1:D:141:LEU:HD23	1.85	0.58
1:A:244:PHE:HB3	6:A:432:HOH:O	2.02	0.58
1:A:99:GLU:HG2	1:A:100:ARG:NH1	2.18	0.58
1:B:44:ALA:HB3	1:B:210:ILE:CD1	2.34	0.58
1:B:76:ASP:OD2	6:B:412:HOH:O	2.16	0.58
1:B:208:VAL:HG12	1:B:210:ILE:HG23	1.86	0.58
1:D:230:ARG:HG3	6:D:509:HOH:O	2.04	0.58
1:C:79:THR:CA	1:C:82:GLU:OE1	2.43	0.58
1:A:55:ASP:HB3	1:A:142:ILE:HG13	1.85	0.58
1:A:172:LEU:C	1:A:172:LEU:HD23	2.29	0.57
1:D:248:LYS:O	6:D:421:HOH:O	2.17	0.57
1:A:153:ARG:HE	1:A:269:ALA:HB1	1.69	0.57
1:D:96:ILE:O	6:D:420:HOH:O	2.17	0.57
1:B:42:LEU:HD11	1:B:214:GLN:CG	2.28	0.57
1:D:79:THR:HG21	6:D:455:HOH:O	2.03	0.57
1:A:216:MET:HG3	1:A:234:LYS:C	2.30	0.56
1:A:137:LEU:HD21	6:A:425:HOH:O	2.05	0.56
1:A:105:THR:HG21	1:A:165:ASN:O	2.06	0.56
1:D:59:THR:HG21	1:D:141:LEU:HA	1.87	0.56
1:D:262:ALA:HB1	1:D:267:GLU:HB2	1.87	0.56
1:C:87:GLU:HG2	1:C:112:ALA:CA	2.35	0.56
1:D:105:THR:HA	1:D:108:ILE:HD12	1.87	0.56
1:C:173:ARG:HG3	1:C:173:ARG:HH11	1.69	0.56
1:A:260:TYR:HB3	1:A:271:MET:HE1	1.88	0.56
1:B:103:THR:OG1	1:B:108:ILE:HG13	2.05	0.56
1:C:74:GLN:NE2	6:C:429:HOH:O	2.38	0.56
1:D:261:TYR:O	1:D:271:MET:HE1	2.05	0.56
1:D:75:ALA:HB2	1:D:122:TRP:HE1	1.71	0.56
1:A:254:PRO:C	1:A:255:GLU:HG2	2.31	0.56
1:C:146:ASP:C	1:C:149:PRO:HD2	2.31	0.56
1:A:42:LEU:HD11	1:A:214:GLN:HG2	1.87	0.56
1:A:43:LYS:HD2	6:B:474:HOH:O	2.06	0.55
1:A:69:ALA:HB2	6:A:458:HOH:O	2.06	0.55
2:D:301:TLA:O2	6:D:408:HOH:O	1.97	0.55
1:B:88:TYR:HD2	1:B:108:ILE:HG22	1.73	0.54
1:D:41:GLY:HA3	1:D:234:LYS:HG3	1.89	0.54
1:D:117:LEU:HD13	1:D:126:LEU:HD12	1.88	0.54
1:A:169:ALA:O	1:A:173:ARG:HD2	2.07	0.54
1:D:140:LYS:HB2	6:D:416:HOH:O	2.08	0.54
1:C:117:LEU:HD12	1:C:131:ARG:CG	2.36	0.54
1:B:146:ASP:O	1:B:149:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLN:OE1	6:A:419:HOH:O	2.19	0.53
1:B:197:ASP:OD2	1:B:199:LYS:HD2	2.08	0.53
1:A:45:LEU:HD22	1:A:216:MET:HB3	1.89	0.53
1:A:172:LEU:HD23	1:A:172:LEU:O	2.08	0.53
1:D:87:GLU:O	1:D:91:ARG:HG3	2.09	0.53
1:C:216:MET:HE1	1:C:272:LEU:HD11	1.91	0.53
1:A:41:GLY:HA2	6:A:415:HOH:O	2.08	0.53
1:C:87:GLU:HG2	1:C:112:ALA:HA	1.90	0.53
1:C:107:ARG:O	1:C:111:GLU:HG3	2.09	0.53
1:D:41:GLY:N	1:D:213:HIS:O	2.42	0.53
1:D:68:SER:HB3	1:D:77:TRP:HZ2	1.75	0.52
1:A:92:LEU:O	1:A:95:VAL:HB	2.09	0.52
1:B:78:THR:HG22	1:B:82:GLU:OE2	2.10	0.52
1:D:44:ALA:C	1:D:45:LEU:HD23	2.34	0.52
1:C:91:ARG:NE	1:C:112:ALA:HA	2.24	0.52
1:C:172:LEU:HD23	1:C:172:LEU:C	2.35	0.52
1:C:67:PHE:CE1	1:C:133:GLU:HG2	2.44	0.52
1:A:132:ASP:OD1	6:A:418:HOH:O	2.18	0.51
1:D:117:LEU:CD1	1:D:131:ARG:HG2	2.41	0.51
1:C:43:LYS:HD3	6:C:463:HOH:O	2.09	0.51
1:D:102:TRP:HZ2	1:D:189:GLU:HB2	1.75	0.51
1:C:76:ASP:OD1	1:C:78:THR:CG2	2.58	0.51
1:D:146:ASP:C	1:D:149:PRO:HD2	2.36	0.51
1:A:59:THR:HG1	1:A:142:ILE:HG12	1.73	0.51
1:D:178:GLY:HA3	6:D:406:HOH:O	2.09	0.51
1:D:191:VAL:HG13	1:D:203:LEU:HD13	1.91	0.51
1:A:153:ARG:HE	1:A:269:ALA:CB	2.24	0.51
1:C:76:ASP:OD1	1:C:78:THR:HG22	2.09	0.51
1:A:260:TYR:CD2	1:A:271:MET:CE	2.91	0.51
1:B:97:LYS:HD3	1:B:99:GLU:OE2	2.10	0.51
1:D:189:GLU:HB3	6:D:460:HOH:O	2.11	0.51
1:A:48:ASP:OD1	2:A:301:TLA:C1	2.59	0.51
1:A:216:MET:HG3	1:A:234:LYS:HB2	1.93	0.51
1:D:53:LEU:HD22	1:D:147:THR:HG23	1.93	0.51
1:D:133:GLU:HG3	6:D:508:HOH:O	2.11	0.51
1:A:99:GLU:HG2	1:A:100:ARG:HH12	1.74	0.50
1:D:42:LEU:CD1	1:D:214:GLN:HG2	2.36	0.50
1:A:260:TYR:HB3	1:A:271:MET:CE	2.42	0.50
1:D:96:ILE:HD11	1:D:194:SER:HB3	1.94	0.50
1:D:177:LEU:HD13	6:D:534:HOH:O	2.10	0.50
1:B:142:ILE:HG23	6:B:454:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ILE:HD11	1:D:194:SER:O	2.12	0.50
1:A:85:ARG:NH1	1:A:244:PHE:HE1	2.11	0.49
1:C:95:VAL:HG13	1:C:102:TRP:HA	1.94	0.49
1:A:216:MET:HA	1:A:234:LYS:O	2.12	0.49
1:B:54:VAL:HG11	1:B:174:ILE:HG21	1.95	0.49
1:C:87:GLU:HB3	1:C:112:ALA:HB1	1.95	0.49
1:B:56:PHE:O	1:B:60:ILE:HG22	2.11	0.49
1:A:226:GLN:HG2	1:A:230:ARG:HH21	1.78	0.49
1:C:102:TRP:HB3	1:C:192:ARG:NH2	2.27	0.49
1:D:249:LYS:HD3	1:D:249:LYS:C	2.38	0.49
1:A:229:LYS:NZ	6:A:417:HOH:O	2.17	0.48
1:C:223:TYR:CG	1:C:224:ASP:N	2.81	0.48
1:B:74:GLN:NE2	6:B:415:HOH:O	2.25	0.48
1:D:150:GLY:HA3	1:D:265:VAL:HG12	1.95	0.48
1:A:87:GLU:O	1:A:91:ARG:HG3	2.12	0.48
1:B:45:LEU:HB2	1:B:160:THR:HG22	1.95	0.48
1:B:58:SER:HB2	1:B:142:ILE:HD11	1.94	0.48
1:B:88:TYR:CD2	1:B:108:ILE:HG22	2.48	0.48
1:C:91:ARG:NH2	1:C:115:GLY:HA3	2.28	0.48
1:D:249:LYS:N	6:D:431:HOH:O	2.43	0.48
1:C:226:GLN:NE2	6:C:433:HOH:O	2.46	0.48
1:B:44:ALA:N	6:B:403:HOH:O	2.08	0.48
1:C:59:THR:O	1:C:63:GLU:HB2	2.14	0.48
1:C:87:GLU:HG2	1:C:112:ALA:HB1	1.94	0.48
1:C:47:PHE:HB3	1:C:53:LEU:HD11	1.95	0.48
1:C:67:PHE:HE1	1:C:133:GLU:HG2	1.78	0.48
1:D:142:ILE:HD12	1:D:143:PRO:O	2.14	0.48
1:C:104:THR:HG1	1:C:107:ARG:HG3	1.79	0.48
1:D:46:PHE:CZ	1:D:204:ALA:HB1	2.49	0.47
1:A:216:MET:CB	6:A:415:HOH:O	2.62	0.47
1:D:104:THR:HG23	1:D:107:ARG:H	1.78	0.47
1:B:42:LEU:HD13	1:B:43:LYS:CE	2.42	0.47
1:C:42:LEU:HD12	1:C:42:LEU:C	2.39	0.47
1:C:116:ILE:C	1:C:118:ALA:H	2.23	0.47
1:B:55:ASP:HB3	1:B:142:ILE:HG13	1.96	0.47
1:C:244:PHE:HB2	1:C:248:LYS:CD	2.41	0.47
1:D:48:ASP:OD1	2:D:301:TLA:C4	2.63	0.47
1:D:56:PHE:HA	1:D:141:LEU:HD22	1.97	0.47
1:D:75:ALA:CB	1:D:122:TRP:NE1	2.75	0.47
1:B:205:LEU:HB3	1:B:210:ILE:O	2.15	0.47
1:A:195:LYS:HG3	1:A:200:VAL:CG1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ALA:HB3	1:C:77:TRP:NE1	2.30	0.46
1:D:123:GLY:O	1:D:131:ARG:NH2	2.37	0.46
1:B:164:SER:OG	1:B:165:ASN:N	2.48	0.46
1:C:208:VAL:O	1:C:208:VAL:CG1	2.64	0.46
1:D:112:ALA:O	1:D:116:ILE:HG12	2.15	0.46
1:D:63:GLU:HG2	6:D:401:HOH:O	2.15	0.46
1:A:59:THR:HG21	1:A:141:LEU:HA	1.98	0.46
1:A:56:PHE:N	6:A:435:HOH:O	2.49	0.46
1:D:172:LEU:C	1:D:172:LEU:HD23	2.40	0.46
1:B:113:LEU:HD11	1:B:134:LEU:HD23	1.98	0.46
1:B:133:GLU:OE2	6:B:413:HOH:O	2.21	0.46
1:A:94:GLN:HB3	1:A:100:ARG:HB2	1.98	0.45
1:A:223:TYR:CG	1:A:224:ASP:N	2.84	0.45
1:C:164:SER:O	1:C:187:THR:HB	2.16	0.45
1:C:173:ARG:NH2	5:C:301:CO3:O1	2.45	0.45
1:C:169:ALA:O	1:C:173:ARG:HG3	2.17	0.45
1:C:208:VAL:HG12	1:C:210:ILE:HG23	1.96	0.45
1:C:89:ARG:O	1:C:93:ASP:OD1	2.34	0.45
1:A:85:ARG:O	1:A:88:TYR:HB3	2.16	0.45
1:B:94:GLN:OE1	1:B:100:ARG:NH2	2.43	0.45
1:C:110:ARG:HB2	1:C:135:ASN:ND2	2.32	0.45
1:D:119:ASN:O	1:D:120:HIS:HD2	1.98	0.45
1:A:55:ASP:OD2	1:A:58:SER:OG	2.21	0.45
1:B:137:LEU:HD21	6:B:485:HOH:O	2.16	0.45
1:A:49:VAL:HG23	1:A:164:SER:HB2	1.99	0.45
1:A:68:SER:HG	1:A:69:ALA:N	2.12	0.45
1:C:46:PHE:HA	1:C:161:SER:O	2.16	0.45
1:C:87:GLU:HG2	1:C:112:ALA:CB	2.47	0.45
1:C:205:LEU:HD13	6:C:413:HOH:O	2.16	0.45
1:D:87:GLU:HG2	1:D:91:ARG:HE	1.82	0.45
1:C:114:ASP:OD1	1:C:131:ARG:CD	2.65	0.44
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.82	0.44
1:B:67:PHE:HA	6:B:444:HOH:O	2.17	0.44
1:C:101:PRO:HA	6:C:404:HOH:O	2.17	0.44
1:D:177:LEU:HD12	1:D:177:LEU:O	2.18	0.44
1:A:180:LEU:CG	6:A:489:HOH:O	2.63	0.44
1:C:195:LYS:HE3	1:C:195:LYS:HB2	1.81	0.44
1:C:104:THR:O	1:C:108:ILE:HG13	2.17	0.44
1:C:226:GLN:O	1:C:230:ARG:HG2	2.18	0.44
1:A:250:VAL:CG2	1:A:252:THR:HG23	2.46	0.44
1:C:87:GLU:CG	1:C:112:ALA:HB1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LYS:HD3	1:D:253:LYS:HA	1.53	0.44
1:A:146:ASP:C	1:A:149:PRO:HD2	2.42	0.44
1:D:153:ARG:HH12	1:D:266:VAL:HG13	1.83	0.44
1:C:248:LYS:HE3	1:C:249:LYS:O	2.17	0.44
1:C:100:ARG:NH2	6:C:416:HOH:O	2.16	0.43
1:B:142:ILE:CG2	6:B:454:HOH:O	2.66	0.43
1:B:156:SER:HA	6:B:430:HOH:O	2.18	0.43
1:B:167:SER:O	1:B:171:VAL:HG23	2.18	0.43
1:B:216:MET:HE1	1:B:272:LEU:HD11	2.01	0.43
1:C:200:VAL:O	1:C:203:LEU:HB3	2.18	0.43
1:B:193:SER:OG	1:B:197:ASP:OD2	2.28	0.43
1:D:84:TRP:CZ2	1:D:113:LEU:HB2	2.52	0.43
1:D:247:ASN:HB3	6:D:442:HOH:O	2.17	0.43
1:B:44:ALA:HB3	1:B:210:ILE:HD13	2.00	0.43
1:B:45:LEU:HD13	1:B:158:TYR:HB2	1.99	0.43
1:D:75:ALA:CB	1:D:122:TRP:HE1	2.32	0.43
1:C:71:ARG:HD3	1:C:73:PHE:HE2	1.84	0.43
1:D:76:ASP:HB3	1:D:79:THR:HB	2.00	0.43
1:D:113:LEU:HD21	1:D:134:LEU:HD23	2.01	0.43
1:D:165:ASN:N	2:D:301:TLA:O41	2.45	0.43
1:A:45:LEU:CD2	1:A:216:MET:HE2	2.48	0.43
1:B:94:GLN:HB3	1:B:100:ARG:HB2	2.01	0.43
1:C:45:LEU:HD22	1:C:216:MET:HE2	2.01	0.43
1:C:59:THR:HG21	1:C:141:LEU:HA	2.01	0.43
1:B:42:LEU:HD12	1:B:214:GLN:HB3	2.01	0.43
1:B:66:ALA:HB1	6:B:436:HOH:O	2.19	0.43
1:B:44:ALA:HA	1:B:159:ILE:O	2.19	0.43
1:D:54:VAL:HG11	1:D:174:ILE:HG21	2.00	0.43
1:C:75:ALA:HB3	1:C:77:TRP:CE2	2.53	0.43
1:B:105:THR:HA	1:B:108:ILE:HB	2.01	0.42
1:B:256:GLN:HG2	1:B:257:TYR:N	2.33	0.42
1:C:94:GLN:HB3	1:C:99:GLU:HB2	2.01	0.42
1:A:232:GLY:HA2	6:A:492:HOH:O	2.18	0.42
1:B:142:ILE:HG13	1:B:142:ILE:O	2.17	0.42
1:B:228:ALA:O	1:B:233:PHE:HB2	2.19	0.42
1:B:250:VAL:CG1	1:B:252:THR:HG23	2.37	0.42
1:C:205:LEU:HD21	1:C:212:ALA:HA	2.01	0.42
1:B:104:THR:CG2	1:B:107:ARG:HB2	2.50	0.42
1:B:161:SER:OG	1:B:184:ALA:O	2.33	0.42
1:A:146:ASP:O	1:A:149:PRO:HD2	2.20	0.42
1:B:45:LEU:HD13	1:B:158:TYR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LYS:N	6:D:409:HOH:O	1.98	0.42
1:B:213:HIS:CD2	1:B:214:GLN:HG3	2.55	0.42
1:A:74:GLN:OE1	6:A:420:HOH:O	2.21	0.42
1:C:123:GLY:O	1:C:126:LEU:N	2.49	0.42
1:D:195:LYS:HG3	1:D:200:VAL:HG11	2.02	0.42
1:B:93:ASP:OD1	1:B:97:LYS:NZ	2.46	0.42
1:C:104:THR:OG1	1:C:107:ARG:HG3	2.20	0.42
1:A:44:ALA:HA	1:A:159:ILE:O	2.19	0.41
1:C:206:ASP:HB3	6:C:492:HOH:O	2.19	0.41
1:D:82:GLU:HG2	6:D:499:HOH:O	2.20	0.41
1:A:45:LEU:CD2	6:A:415:HOH:O	2.66	0.41
1:A:67:PHE:O	1:A:71:ARG:HG3	2.21	0.41
1:C:87:GLU:OE1	1:C:116:ILE:HG23	2.20	0.41
1:C:127:ASN:OD1	1:C:127:ASN:C	2.62	0.41
1:B:88:TYR:CZ	1:B:92:LEU:HD22	2.55	0.41
1:A:45:LEU:HD12	1:A:154:LEU:HD13	2.01	0.41
1:D:45:LEU:HD22	1:D:216:MET:HB3	2.02	0.41
1:A:55:ASP:C	6:A:435:HOH:O	2.64	0.41
1:B:168:MET:HB3	1:B:168:MET:HE3	1.59	0.41
1:A:271:MET:HE2	1:A:271:MET:HB2	1.94	0.41
1:B:229:LYS:NZ	1:B:233:PHE:O	2.38	0.41
1:C:55:ASP:OD2	1:C:58:SER:OG	2.34	0.41
1:C:244:PHE:CB	1:C:248:LYS:HD3	2.45	0.41
1:C:256:GLN:H	1:C:256:GLN:HG2	1.57	0.41
1:B:94:GLN:OE1	1:B:100:ARG:NE	2.46	0.41
1:C:42:LEU:HD12	1:C:43:LYS:N	2.36	0.41
1:C:173:ARG:HH11	1:C:173:ARG:CG	2.34	0.41
1:A:183:ASP:OD2	1:B:176:LYS:HD2	2.21	0.41
1:B:99:GLU:H	1:B:99:GLU:HG2	1.57	0.41
1:D:137:LEU:N	1:D:137:LEU:HD23	2.35	0.41
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.86	0.41
1:B:68:SER:HB2	1:B:73:PHE:O	2.21	0.41
1:C:82:GLU:HG3	1:C:82:GLU:H	1.74	0.41
1:A:169:ALA:N	1:B:207:SER:O	2.54	0.40
1:D:159:ILE:HA	1:D:183:ASP:OD2	2.22	0.40
1:D:256:GLN:H	1:D:256:GLN:HG2	1.71	0.40
1:B:171:VAL:HG21	1:B:187:THR:CG2	2.51	0.40
1:C:65:GLU:O	1:C:69:ALA:HB2	2.22	0.40
1:C:92:LEU:O	1:C:96:ILE:HD12	2.21	0.40
1:D:122:TRP:CE3	1:D:126:LEU:HD11	2.55	0.40
1:B:44:ALA:CB	1:B:210:ILE:HD13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HD21	1:B:269:ALA:HA	2.03	0.40
1:A:56:PHE:O	1:A:60:ILE:HG12	2.21	0.40
1:A:183:ASP:O	1:B:172:LEU:CD2	2.69	0.40

All (7) 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)
6:C:467:HOH:O	6:D:524:HOH:O[4_555]	1.80	0.40
6:C:539:HOH:O	6:D:539:HOH:O[4_555]	1.80	0.40
6:A:608:HOH:O	6:C:552:HOH:O[3_455]	1.96	0.24
6:B:462:HOH:O	6:D:437:HOH:O[4_555]	2.02	0.18
1:A:74:GLN:NE2	3:B:301:EDO:O1[4_454]	2.13	0.07
6:A:521:HOH:O	6:B:412:HOH:O[4_454]	2.18	0.02
6:C:539:HOH:O	6:D:517:HOH:O[4_555]	2.18	0.02

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	233/278 (84%)	226 (97%)	7 (3%)	0	100	100
1	B	232/278 (84%)	222 (96%)	10 (4%)	0	100	100
1	C	232/278 (84%)	218 (94%)	14 (6%)	0	100	100
1	D	232/278 (84%)	226 (97%)	6 (3%)	0	100	100
All	All	929/1112 (84%)	892 (96%)	37 (4%)	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	194/229 (85%)	192 (99%)	2 (1%)	68	64
1	B	193/229 (84%)	189 (98%)	4 (2%)	47	36
1	C	193/229 (84%)	189 (98%)	4 (2%)	47	36
1	D	194/229 (85%)	191 (98%)	3 (2%)	57	49
All	All	774/916 (84%)	761 (98%)	13 (2%)	53	45

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	248	LYS
1	B	89	ARG
1	B	90	SER
1	B	100	ARG
1	B	103	THR
1	C	50	GLN
1	C	65	GLU
1	C	78	THR
1	C	242	PHE
1	D	42	LEU
1	D	100	ARG
1	D	253	LYS

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	94	GLN
1	A	226	GLN
1	B	119	ASN
1	B	263	ASN
1	C	83	GLN
1	C	120	HIS

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Mol	Chain	Res	Type
1	C	226	GLN
1	D	119	ASN
1	D	214	GLN
1	D	256	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	301	-	3,3,3	0.32	0	2,2,2	0.60	0
5	CO3	B	303	-	3,3,3	0.81	0	2,3,3	0.58	0
5	CO3	C	301	-	3,3,3	0.60	0	2,3,3	0.69	0
4	GOL	B	302	-	5,5,5	1.28	1 (20%)	5,5,5	1.62	1 (20%)
2	TLA	A	301	-	9,9,9	1.36	1 (11%)	12,12,12	2.14	5 (41%)
2	TLA	D	301	-	9,9,9	1.41	1 (11%)	12,12,12	1.79	4 (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
4	GOL	B	302	-	-	4/4/4/4	-
3	EDO	B	301	-	-	1/1/1/1	-
2	TLA	D	301	-	-	10/12/12/12	-
2	TLA	A	301	-	-	10/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	TLA	O11-C1	-2.39	1.23	1.30
4	B	302	GOL	O2-C2	-2.31	1.36	1.43
2	D	301	TLA	O41-C4	-2.23	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	TLA	C3-C2-C1	3.58	117.77	109.82
2	D	301	TLA	O2-C2-C3	3.41	117.11	110.17
4	B	302	GOL	C3-C2-C1	-3.19	100.11	111.80
2	A	301	TLA	C2-C3-C4	-3.18	102.77	109.82
2	D	301	TLA	C3-C2-C1	-2.94	103.30	109.82
2	A	301	TLA	O1-C1-C2	-2.73	114.34	121.62
2	A	301	TLA	O4-C4-C3	-2.70	114.42	121.62
2	D	301	TLA	C2-C3-C4	2.29	114.90	109.82
2	A	301	TLA	O11-C1-O1	2.27	129.22	124.08
2	D	301	TLA	O4-C4-C3	-2.15	115.89	121.62

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TLA	C1-C2-C3-O3
2	A	301	TLA	C1-C2-C3-C4
2	A	301	TLA	O2-C2-C3-O3
2	A	301	TLA	O2-C2-C3-C4
2	A	301	TLA	O3-C3-C4-O4
2	D	301	TLA	O1-C1-C2-O2
2	D	301	TLA	O11-C1-C2-O2
2	D	301	TLA	C1-C2-C3-O3
2	D	301	TLA	C1-C2-C3-C4

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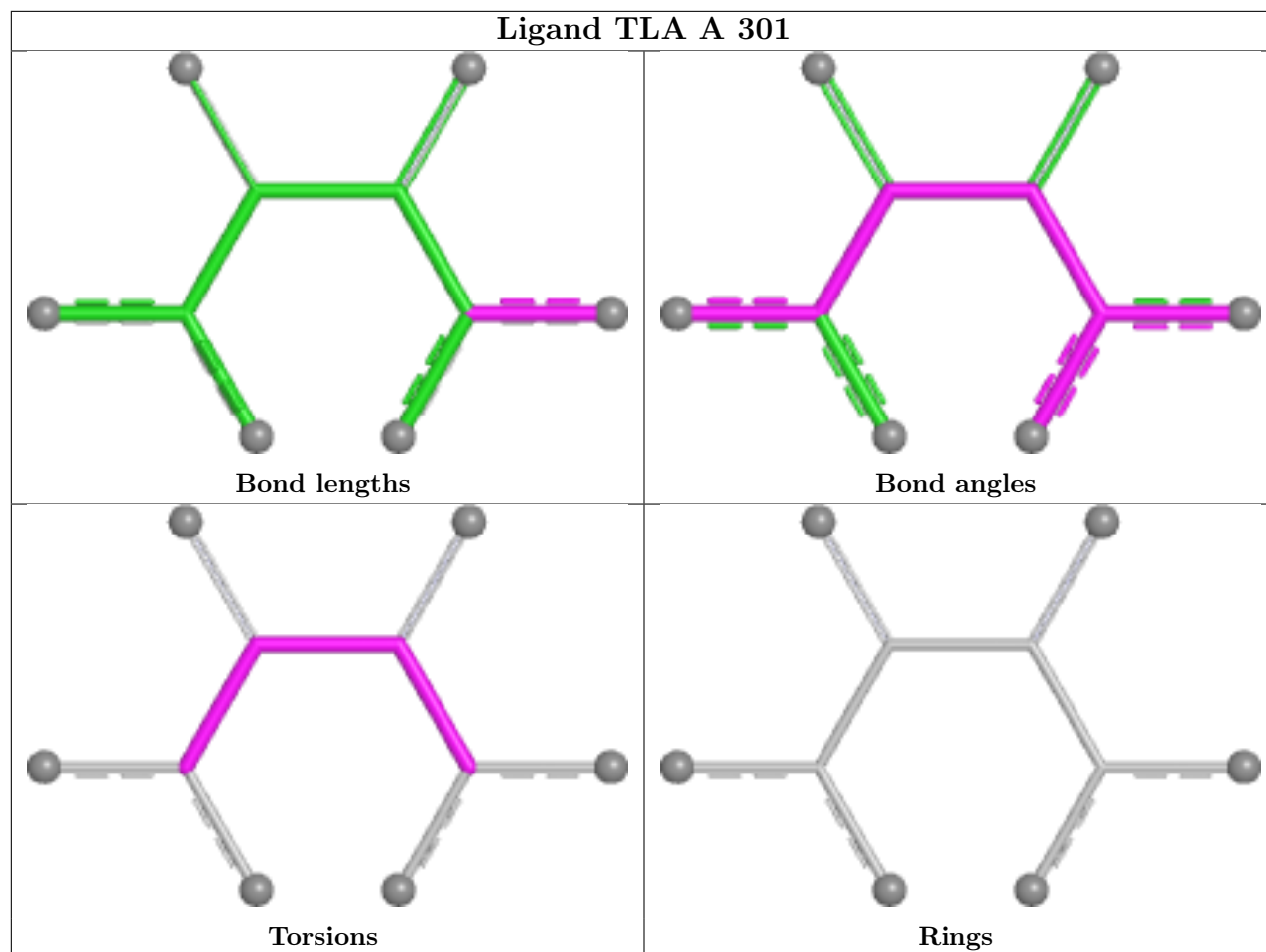
Mol	Chain	Res	Type	Atoms
2	D	301	TLA	O2-C2-C3-O3
2	D	301	TLA	O2-C2-C3-C4
4	B	302	GOL	C1-C2-C3-O3
2	A	301	TLA	O1-C1-C2-O2
2	A	301	TLA	O11-C1-C2-O2
2	A	301	TLA	O3-C3-C4-O41
2	D	301	TLA	O3-C3-C4-O4
2	D	301	TLA	O3-C3-C4-O41
4	B	302	GOL	O2-C2-C3-O3
2	A	301	TLA	O1-C1-C2-C3
2	A	301	TLA	O11-C1-C2-C3
2	D	301	TLA	C2-C3-C4-O41
2	D	301	TLA	C2-C3-C4-O4
3	B	301	EDO	O1-C1-C2-O2
4	B	302	GOL	O1-C1-C2-C3
4	B	302	GOL	O1-C1-C2-O2

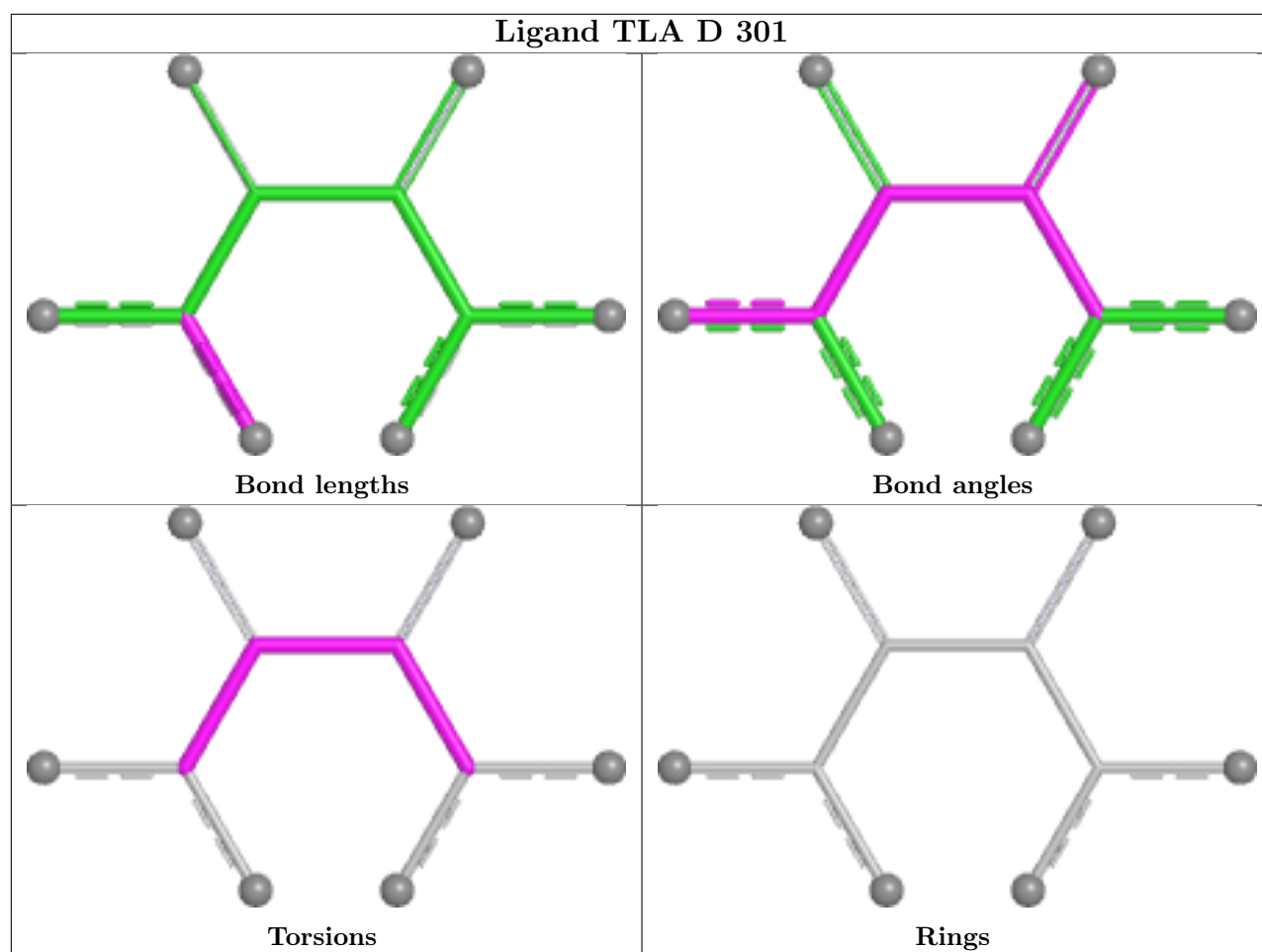
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	EDO	0	1
5	C	301	CO3	2	0
2	A	301	TLA	1	0
2	D	301	TLA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	234/278 (84%)	-1.37	0 100 100	10, 21, 42, 52	1 (0%)
1	B	234/278 (84%)	-1.40	0 100 100	12, 22, 35, 56	0
1	C	234/278 (84%)	-1.34	0 100 100	14, 23, 53, 66	0
1	D	233/278 (83%)	-1.43	0 100 100	8, 20, 35, 50	1 (0%)
All	All	935/1112 (84%)	-1.38	0 100 100	8, 22, 40, 66	2 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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	TLA	A	301	10/10	0.99	0.03	27,37,44,45	0
2	TLA	D	301	10/10	0.99	0.03	21,28,33,34	0
3	EDO	B	301	4/4	0.99	0.03	22,27,29,32	0
4	GOL	B	302	6/6	0.99	0.03	31,36,40,43	0

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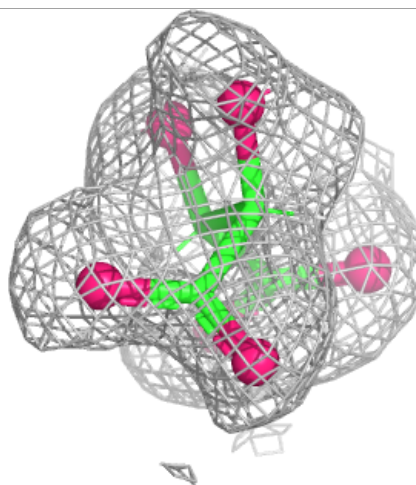
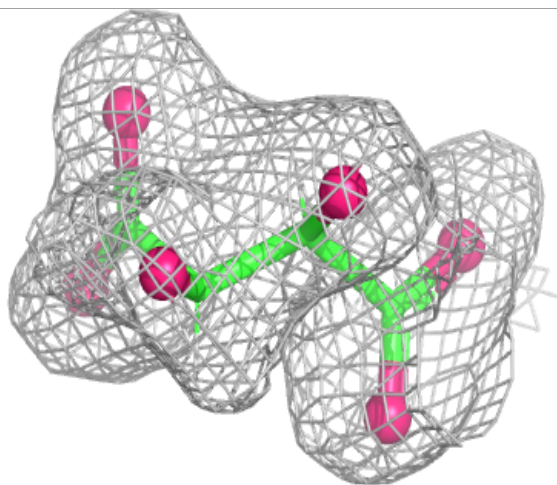
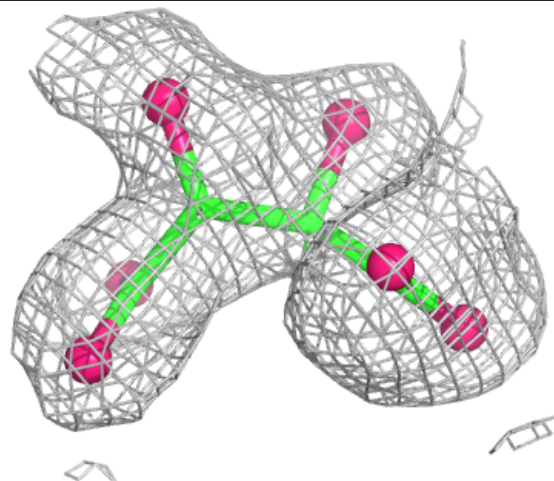
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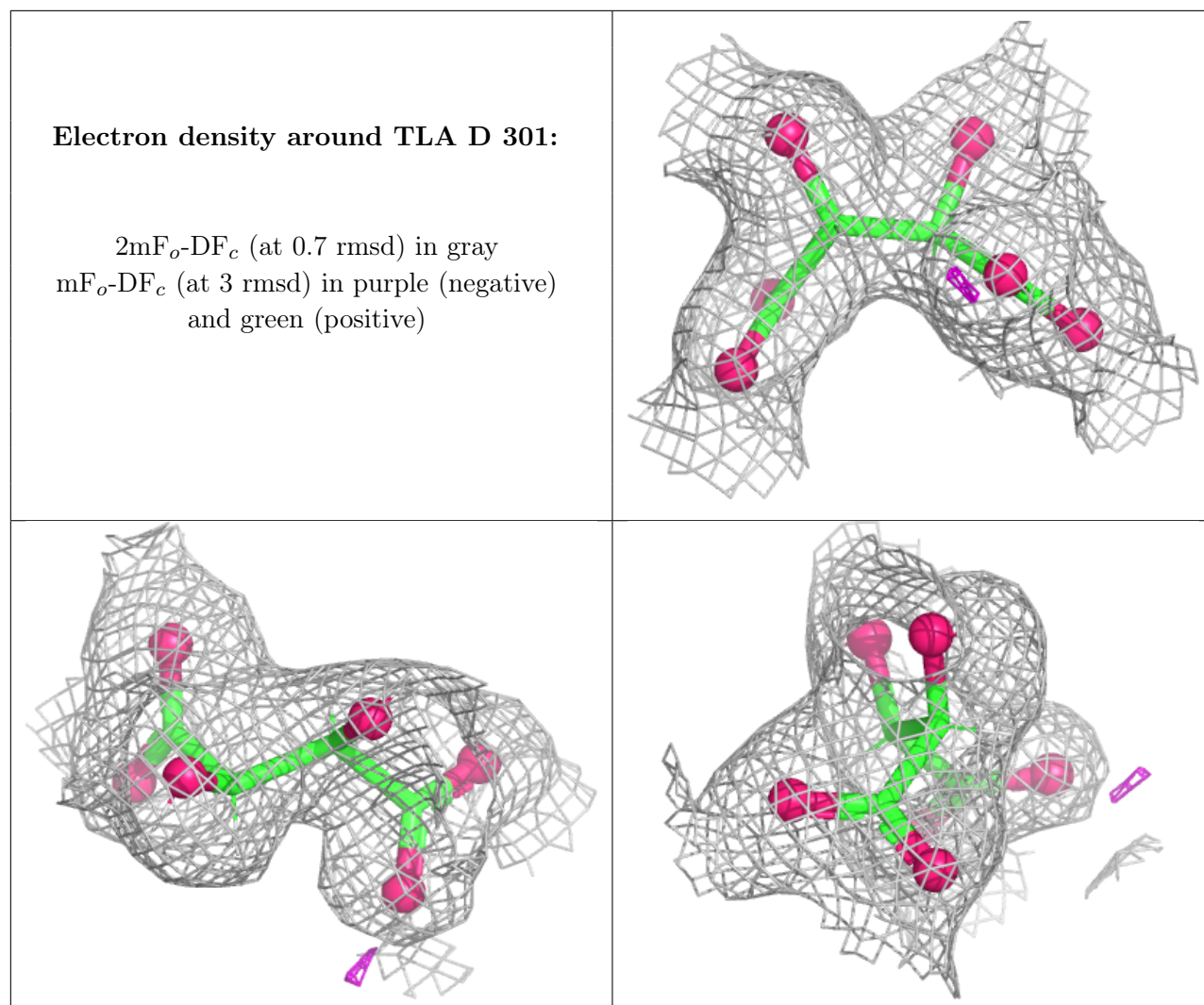
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CO3	B	303	4/4	0.99	0.03	29,31,32,34	0
5	CO3	C	301	4/4	1.00	0.02	26,27,29,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TLA A 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.