



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:14 PM UTC

PDB ID : 4YTU / pdb_00004ytu
Title : Crystal structure of D-tagatose 3-epimerase C66S from *Pseudomonas cichorii* in complex with L-erythrulose
Authors : Yoshida, H.; Yoshihara, A.; Ishii, T.; Izumori, K.; Kamitori, S.
Deposited on : 2015-03-18
Resolution : 2.20 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
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

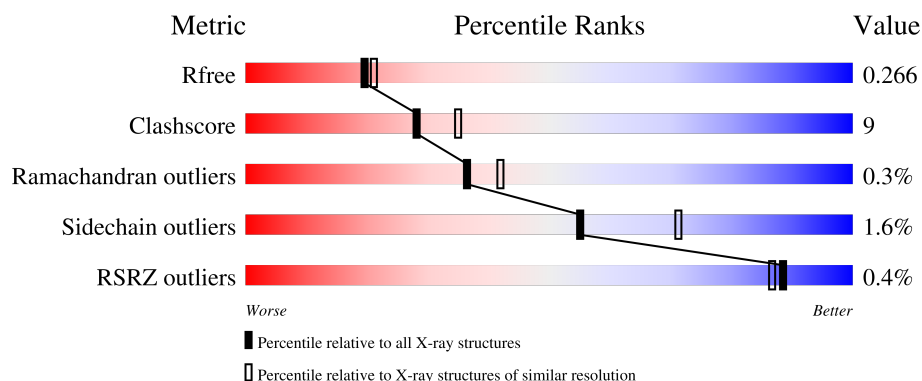
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	300	 79% 18% . .
1	B	300	 74% 21% . .
1	C	300	 83% 16% .
1	D	300	 77% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9985 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 D-tagatose 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2314	1465	399	432	18			
1	B	290	Total	C	N	O	S	0	0	0
			2287	1451	392	426	18			
1	C	297	Total	C	N	O	S	0	0	0
			2344	1483	408	435	18			
1	D	292	Total	C	N	O	S	0	0	0
			2297	1456	394	429	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	SER	CYS	engineered mutation	UNP O50580
A	291	GLY	-	expression tag	UNP O50580
A	292	SER	-	expression tag	UNP O50580
A	293	ARG	-	expression tag	UNP O50580
A	294	SER	-	expression tag	UNP O50580
A	295	HIS	-	expression tag	UNP O50580
A	296	HIS	-	expression tag	UNP O50580
A	297	HIS	-	expression tag	UNP O50580
A	298	HIS	-	expression tag	UNP O50580
A	299	HIS	-	expression tag	UNP O50580
A	300	HIS	-	expression tag	UNP O50580
B	66	SER	CYS	engineered mutation	UNP O50580
B	291	GLY	-	expression tag	UNP O50580
B	292	SER	-	expression tag	UNP O50580
B	293	ARG	-	expression tag	UNP O50580
B	294	SER	-	expression tag	UNP O50580
B	295	HIS	-	expression tag	UNP O50580
B	296	HIS	-	expression tag	UNP O50580
B	297	HIS	-	expression tag	UNP O50580
B	298	HIS	-	expression tag	UNP O50580
B	299	HIS	-	expression tag	UNP O50580

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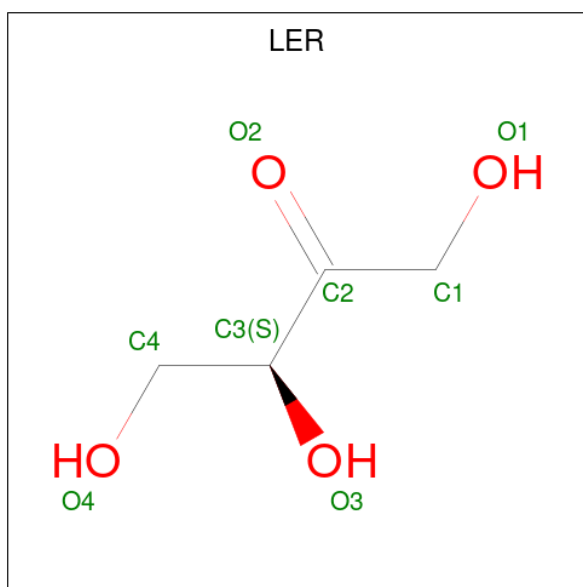
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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	HIS	-	expression tag	UNP O50580
C	66	SER	CYS	engineered mutation	UNP O50580
C	291	GLY	-	expression tag	UNP O50580
C	292	SER	-	expression tag	UNP O50580
C	293	ARG	-	expression tag	UNP O50580
C	294	SER	-	expression tag	UNP O50580
C	295	HIS	-	expression tag	UNP O50580
C	296	HIS	-	expression tag	UNP O50580
C	297	HIS	-	expression tag	UNP O50580
C	298	HIS	-	expression tag	UNP O50580
C	299	HIS	-	expression tag	UNP O50580
C	300	HIS	-	expression tag	UNP O50580
D	66	SER	CYS	engineered mutation	UNP O50580
D	291	GLY	-	expression tag	UNP O50580
D	292	SER	-	expression tag	UNP O50580
D	293	ARG	-	expression tag	UNP O50580
D	294	SER	-	expression tag	UNP O50580
D	295	HIS	-	expression tag	UNP O50580
D	296	HIS	-	expression tag	UNP O50580
D	297	HIS	-	expression tag	UNP O50580
D	298	HIS	-	expression tag	UNP O50580
D	299	HIS	-	expression tag	UNP O50580
D	300	HIS	-	expression tag	UNP O50580

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is L-Erythrulose (CCD ID: LER) (formula: C₄H₈O₄).



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

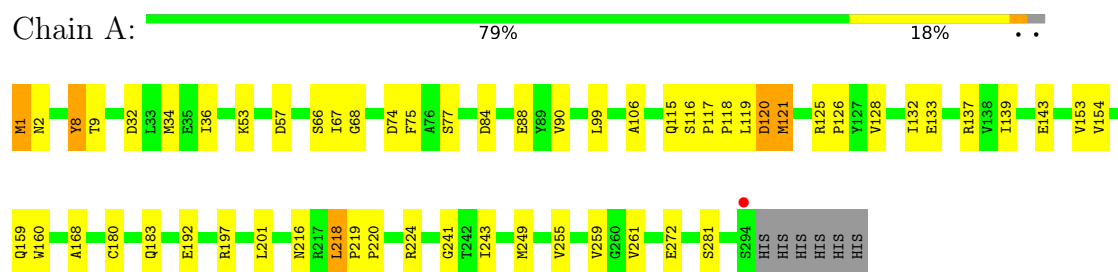
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	184	Total	O	0	0
			184	184		
4	C	181	Total	O	0	0
			181	181		
4	D	133	Total	O	0	0
			133	133		

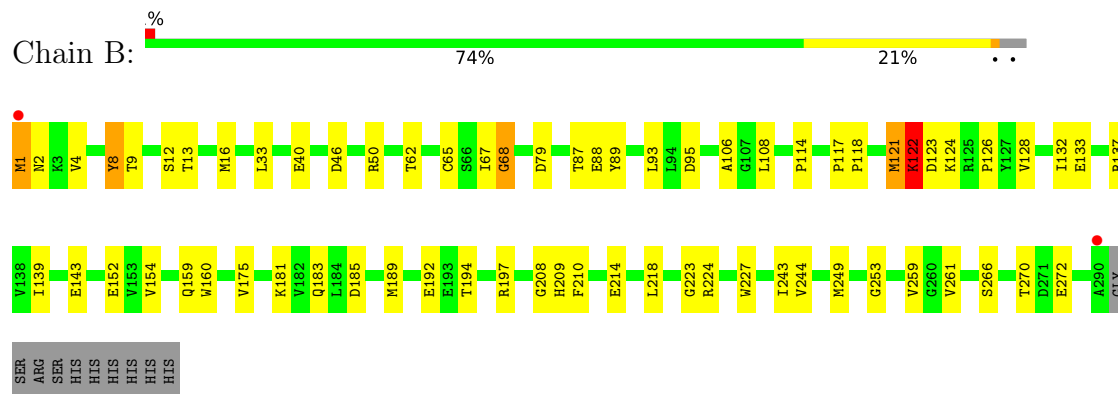
3 Residue-property plots

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.

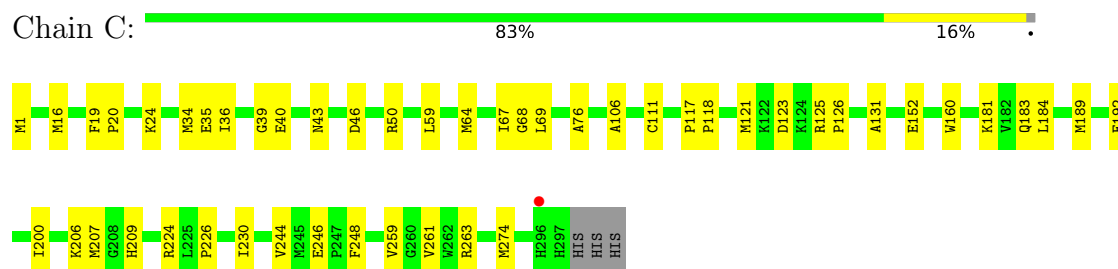
• Molecule 1: D-tagatose 3-epimerase



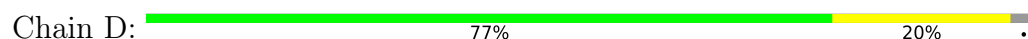
• Molecule 1: D-tagatose 3-epimerase

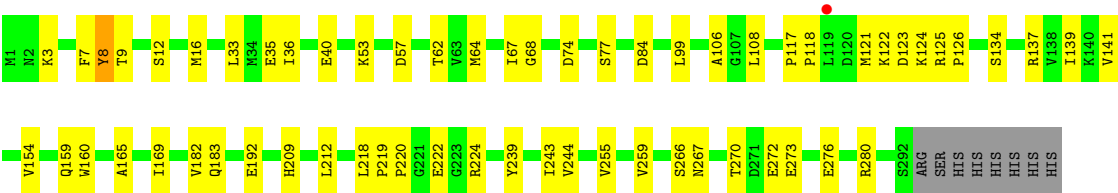


• Molecule 1: D-tagatose 3-epimerase



• Molecule 1: D-tagatose 3-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.72Å 124.80Å 94.72Å 90.00° 99.09° 90.00°	Depositor
Resolution (Å)	20.86 – 2.20 20.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.86-2.20) 96.3 (20.86-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.223 , 0.266 0.223 , 0.266	Depositor DCC
R_{free} test set	5993 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9985	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 3.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, LER

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	0.46	0/2365	0.91	3/3190 (0.1%)
1	B	0.49	0/2338	0.96	10/3155 (0.3%)
1	C	0.46	0/2398	0.91	4/3235 (0.1%)
1	D	0.44	0/2348	0.93	7/3168 (0.2%)
All	All	0.46	0/9449	0.93	24/12748 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	N-CA-C	-8.19	102.45	110.72
1	A	8	TYR	N-CA-C	7.28	121.61	112.87
1	B	8	TYR	N-CA-C	6.83	121.22	112.34
1	C	224	ARG	N-CA-C	6.76	121.69	113.17
1	A	224	ARG	N-CA-C	6.41	120.81	112.92
1	D	224	ARG	N-CA-C	6.36	121.04	113.16
1	C	244	VAL	N-CA-C	6.26	116.88	108.11
1	D	8	TYR	N-CA-C	6.14	119.87	112.38
1	C	192	GLU	N-CA-C	6.13	120.78	113.12
1	B	244	VAL	N-CA-C	6.06	116.59	108.11
1	B	224	ARG	N-CA-C	5.90	119.45	112.72
1	D	244	VAL	N-CA-C	5.80	116.47	108.12
1	B	227	TRP	N-CA-C	5.71	117.51	111.28
1	B	192	GLU	N-CA-C	5.66	120.31	113.41
1	B	68	GLY	N-CA-C	-5.59	99.93	113.18
1	B	95	ASP	N-CA-C	-5.54	105.33	111.36
1	D	192	GLU	N-CA-C	5.36	119.95	113.41
1	D	12	SER	N-CA-C	5.35	118.54	109.76
1	D	139	ILE	N-CA-C	5.33	116.70	110.62
1	B	270	THR	N-CA-C	-5.33	103.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLU	N-CA-C	5.18	119.69	112.90
1	C	274	MET	N-CA-C	-5.11	105.71	111.28
1	B	65	CYS	N-CA-C	5.07	117.38	109.52
1	D	141	VAL	N-CA-C	-5.04	105.58	110.42

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	2314	0	2271	42	0
1	B	2287	0	2245	46	0
1	C	2344	0	2292	37	0
1	D	2297	0	2253	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	1	0
3	D	16	0	0	0	0
4	A	185	0	0	2	0
4	B	184	0	0	4	0
4	C	181	0	0	2	0
4	D	133	0	0	6	0
All	All	9985	0	9061	163	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 9.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:HD3	1:B:122:LYS:H	1.04	1.15
1:B:117:PRO:HB2	1:B:121:MET:HG3	1.55	0.89
1:B:122:LYS:HD3	1:B:122:LYS:N	1.88	0.88
1:C:125:ARG:HB3	1:C:126:PRO:HD3	1.62	0.81
1:A:84:ASP:O	1:A:88:GLU:HG2	1.82	0.80
1:A:118:PRO:HD2	1:A:121:MET:HB2	1.66	0.77
1:D:183:GLN:HG3	1:D:209:HIS:HB3	1.70	0.73
1:D:276:GLU:HG3	1:D:280:ARG:HH22	1.53	0.73
1:B:118:PRO:O	1:B:121:MET:HB2	1.89	0.72
1:C:67:ILE:HG13	1:C:68:GLY:N	2.05	0.71
1:B:106:ALA:HB1	1:B:183:GLN:OE1	1.90	0.71
1:C:67:ILE:HG13	1:C:68:GLY:H	1.55	0.70
1:C:183:GLN:HG3	1:C:209:HIS:HB3	1.73	0.69
1:D:16:MET:HE2	1:D:40:GLU:HB3	1.72	0.69
1:B:1:MET:HG2	1:B:2:ASN:N	2.08	0.69
1:C:184:LEU:HD12	1:C:207:MET:HE1	1.76	0.67
1:A:2:ASN:ND2	1:A:243:ILE:HD11	2.10	0.67
1:A:216:ASN:OD1	1:A:218:LEU:HD23	1.96	0.65
1:A:106:ALA:HB1	1:A:183:GLN:OE1	1.98	0.64
1:D:84:ASP:HA	4:D:502:HOH:O	1.97	0.64
1:D:122:LYS:HA	4:D:598:HOH:O	1.98	0.63
1:A:197:ARG:O	1:A:201:LEU:HD23	1.98	0.63
1:C:39:GLY:HA3	3:C:403:LER:O3	1.99	0.63
1:D:276:GLU:HG3	1:D:280:ARG:NH2	2.14	0.61
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.66	0.61
1:C:259:VAL:HG23	1:C:261:VAL:HG23	1.82	0.60
1:B:152:GLU:HA	1:B:183:GLN:HB3	1.84	0.60
1:C:125:ARG:HB2	1:C:125:ARG:CZ	2.32	0.60
1:B:122:LYS:H	1:B:122:LYS:CD	1.87	0.59
1:B:122:LYS:HG2	1:B:123:ASP:H	1.68	0.59
1:C:152:GLU:HA	1:C:183:GLN:HB3	1.84	0.59
1:D:125:ARG:HB3	1:D:126:PRO:HD3	1.84	0.59
1:C:117:PRO:HG3	1:C:160:TRP:CD2	2.38	0.58
1:D:99:LEU:C	1:D:99:LEU:HD23	2.29	0.58
1:D:165:ALA:O	1:D:169:ILE:HG13	2.04	0.58
1:A:216:ASN:HD21	1:B:194:THR:CG2	2.16	0.58
1:C:19:PHE:HB2	1:C:20:PRO:HD3	1.85	0.58
1:D:8:TYR:CE1	1:D:9:THR:HG23	2.40	0.57
1:B:16:MET:HE2	1:B:40:GLU:HB3	1.86	0.56
1:D:106:ALA:HB1	1:D:183:GLN:OE1	2.06	0.56
1:B:33:LEU:HD12	1:B:62:THR:O	2.06	0.56
1:D:118:PRO:O	1:D:121:MET:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG2	1:B:2:ASN:H	1.72	0.55
1:A:118:PRO:HD2	1:A:121:MET:CB	2.35	0.55
1:B:4:VAL:HA	1:B:243:ILE:HG23	1.89	0.55
1:D:276:GLU:CG	1:D:280:ARG:HH22	2.20	0.55
1:B:259:VAL:HG23	1:B:261:VAL:HG23	1.89	0.55
1:B:1:MET:CG	1:B:2:ASN:N	2.70	0.54
1:A:67:ILE:HG13	1:A:68:GLY:N	2.23	0.54
1:B:183:GLN:HG3	1:B:209:HIS:HB3	1.87	0.54
1:B:128:VAL:O	1:B:132:ILE:HG13	2.07	0.54
1:B:123:ASP:O	1:B:126:PRO:HD2	2.08	0.54
1:C:16:MET:HE2	1:C:40:GLU:HB3	1.90	0.54
1:C:246:GLU:HG2	1:C:248:PHE:CE2	2.43	0.54
1:B:67:ILE:HG13	1:B:68:GLY:N	2.23	0.54
1:B:1:MET:CG	1:B:2:ASN:H	2.21	0.53
1:D:272:GLU:HG2	4:D:594:HOH:O	2.08	0.53
1:D:123:ASP:O	1:D:126:PRO:HD2	2.09	0.53
1:D:67:ILE:HG13	1:D:68:GLY:N	2.24	0.53
1:C:106:ALA:HB1	1:C:183:GLN:OE1	2.09	0.52
1:C:1:MET:N	1:C:1:MET:HE2	2.24	0.52
1:D:124:LYS:HB2	1:D:160:TRP:HZ3	1.74	0.52
1:C:117:PRO:HB3	1:C:121:MET:HE2	1.90	0.52
1:C:263:ARG:HD3	4:D:513:HOH:O	2.09	0.51
1:D:266:SER:O	1:D:267:ASN:HB2	2.10	0.51
1:A:99:LEU:O	1:A:99:LEU:HD23	2.10	0.51
1:A:115:GLN:HG2	1:A:116:SER:N	2.24	0.51
1:C:76:ALA:HB2	1:C:131:ALA:HB2	1.91	0.51
4:A:617:HOH:O	1:B:194:THR:HG22	2.09	0.51
1:B:133:GLU:O	1:B:137:ARG:HG3	2.11	0.51
1:B:12:SER:HB2	4:B:600:HOH:O	2.10	0.51
1:B:1:MET:HG2	1:B:2:ASN:CG	2.36	0.50
1:C:35:GLU:HG3	1:C:64:MET:HG3	1.93	0.50
1:C:125:ARG:HH21	1:C:125:ARG:HG2	1.76	0.50
1:C:20:PRO:O	1:C:24:LYS:HG3	2.11	0.50
1:B:117:PRO:CB	1:B:121:MET:HG3	2.36	0.50
1:A:117:PRO:HG3	1:A:160:TRP:CD2	2.47	0.49
1:D:212:LEU:HD11	1:D:243:ILE:HD11	1.95	0.49
1:A:216:ASN:HD21	1:B:194:THR:HG23	1.77	0.49
1:A:74:ASP:HB3	1:A:77:SER:HB2	1.95	0.49
1:D:117:PRO:HG3	1:D:160:TRP:CD2	2.48	0.49
1:B:50:ARG:HG2	1:B:50:ARG:NH1	2.25	0.48
1:A:180:CYS:HB3	4:A:593:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:CE2	1:B:93:LEU:HD11	2.48	0.48
1:B:243:ILE:HG23	1:B:243:ILE:O	2.14	0.48
1:D:7:PHE:HB3	4:D:606:HOH:O	2.13	0.47
1:A:8:TYR:CE1	1:A:9:THR:HG23	2.50	0.47
1:A:34:MET:HE3	1:A:36:ILE:CG2	2.44	0.47
1:A:120:ASP:O	1:A:121:MET:C	2.57	0.47
1:C:69:LEU:HB2	1:C:111:CYS:O	2.15	0.47
1:A:139:ILE:O	1:A:143:GLU:HG3	2.15	0.47
1:A:133:GLU:O	1:A:137:ARG:HG3	2.15	0.47
1:A:119:LEU:HD12	1:A:119:LEU:N	2.30	0.47
1:C:189:MET:HE1	1:C:200:ILE:HG13	1.98	0.46
1:A:255:VAL:O	1:A:259:VAL:HG22	2.16	0.46
1:C:117:PRO:HG3	1:C:160:TRP:CG	2.50	0.46
1:B:181:LYS:HB2	1:B:208:GLY:HA3	1.96	0.46
1:D:33:LEU:HD12	1:D:62:THR:O	2.16	0.46
1:A:1:MET:HE3	1:A:1:MET:HA	1.97	0.45
1:A:2:ASN:HB3	1:A:241:GLY:O	2.17	0.45
1:B:13:THR:HB	1:B:253:GLY:HA3	1.98	0.45
1:B:185:ASP:O	1:B:189:MET:HG3	2.17	0.45
1:D:243:ILE:HG23	1:D:243:ILE:O	2.16	0.45
1:A:119:LEU:H	1:A:119:LEU:CD1	2.30	0.45
1:C:1:MET:HE2	1:C:1:MET:H1	1.80	0.45
1:A:53:LYS:HE3	1:A:57:ASP:OD2	2.17	0.45
1:A:99:LEU:HD23	1:A:99:LEU:C	2.42	0.45
1:D:239:TYR:HB3	4:D:575:HOH:O	2.16	0.45
1:B:117:PRO:HB3	1:B:160:TRP:CE3	2.52	0.45
1:D:134:SER:O	1:D:137:ARG:HB2	2.17	0.45
1:A:220:PRO:HD2	1:A:281:SER:OG	2.17	0.45
1:B:214:GLU:CD	1:B:223:GLY:HA3	2.42	0.45
1:A:125:ARG:N	1:A:126:PRO:CD	2.79	0.44
1:A:154:VAL:CG2	1:A:159:GLN:HB2	2.48	0.44
1:A:119:LEU:HD12	1:A:119:LEU:H	1.82	0.44
1:B:210:PHE:HD2	1:B:243:ILE:CD1	2.31	0.44
1:A:216:ASN:CG	1:A:218:LEU:HD23	2.43	0.44
1:B:139:ILE:O	1:B:143:GLU:HG3	2.18	0.44
1:D:53:LYS:HE3	1:D:57:ASP:OD2	2.17	0.44
1:D:99:LEU:HD23	1:D:99:LEU:O	2.18	0.44
1:D:154:VAL:CG2	1:D:159:GLN:HB2	2.48	0.44
1:D:118:PRO:HD2	1:D:121:MET:HG3	2.00	0.43
1:D:121:MET:HE1	1:D:124:LYS:HB3	1.99	0.43
1:B:121:MET:HE1	1:B:124:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:O	1:A:132:ILE:HG13	2.19	0.43
1:C:46:ASP:O	1:C:50:ARG:HG3	2.18	0.43
1:A:153:VAL:HG22	1:A:168:ALA:HB2	2.00	0.43
1:D:3:LYS:HE3	1:D:62:THR:HG21	2.00	0.43
1:B:87:THR:HG21	4:B:502:HOH:O	2.19	0.43
1:C:24:LYS:HA	1:C:59:LEU:HD11	2.01	0.43
1:D:64:MET:HE1	1:D:209:HIS:CE1	2.54	0.42
1:B:8:TYR:CE1	1:B:9:THR:HG23	2.53	0.42
1:B:197:ARG:HD3	4:B:625:HOH:O	2.19	0.42
1:A:259:VAL:HG23	1:A:261:VAL:HG23	2.00	0.42
1:C:123:ASP:O	1:C:126:PRO:HD2	2.19	0.42
1:D:182:VAL:HG12	1:D:183:GLN:N	2.34	0.42
1:D:219:PRO:HA	1:D:220:PRO:HD3	1.91	0.42
1:A:218:LEU:HD13	1:A:249:MET:HG2	2.01	0.42
1:A:2:ASN:HD22	1:A:243:ILE:CD1	2.33	0.42
1:C:125:ARG:HD2	4:C:588:HOH:O	2.19	0.42
1:D:36:ILE:O	1:D:36:ILE:HG13	2.18	0.42
1:A:121:MET:HE2	1:A:160:TRP:CZ3	2.55	0.42
1:D:117:PRO:HG3	1:D:160:TRP:CE3	2.54	0.42
1:A:219:PRO:HA	1:A:220:PRO:HD3	1.91	0.42
1:C:24:LYS:HA	1:C:59:LEU:CD1	2.50	0.42
1:B:1:MET:HE2	4:B:673:HOH:O	2.19	0.42
1:C:34:MET:HE3	1:C:36:ILE:CG2	2.50	0.41
1:B:249:MET:HE2	1:B:266:SER:HA	2.01	0.41
1:C:118:PRO:HD2	1:C:121:MET:HG3	2.02	0.41
1:C:125:ARG:HH21	1:C:125:ARG:CG	2.33	0.41
1:C:226:PRO:O	1:C:230:ILE:HG13	2.21	0.41
1:B:108:LEU:HD21	1:B:154:VAL:HG11	2.03	0.41
1:B:88:GLU:HG3	1:C:43:ASN:O	2.20	0.41
1:D:35:GLU:HG3	1:D:64:MET:HG3	2.03	0.41
1:D:255:VAL:O	1:D:259:VAL:HG22	2.20	0.41
1:A:75:PHE:CZ	1:A:90:VAL:HG21	2.56	0.41
1:C:181:LYS:HB3	1:C:206:LYS:O	2.21	0.41
1:A:117:PRO:HB3	1:A:121:MET:CE	2.51	0.41
1:C:125:ARG:HG2	4:C:659:HOH:O	2.21	0.41
1:A:66:SER:HA	1:A:106:ALA:O	2.20	0.41
1:D:74:ASP:HB3	1:D:77:SER:HB2	2.04	0.40
1:D:270:THR:OG1	1:D:273:GLU:HG3	2.22	0.40
1:D:276:GLU:HA	1:D:276:GLU:OE2	2.20	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	292/300 (97%)	280 (96%)	11 (4%)	1 (0%)	36	42
1	B	288/300 (96%)	277 (96%)	9 (3%)	2 (1%)	18	19
1	C	295/300 (98%)	278 (94%)	17 (6%)	0	100	100
1	D	290/300 (97%)	280 (97%)	10 (3%)	0	100	100
All	All	1165/1200 (97%)	1115 (96%)	47 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	MET
1	B	121	MET
1	B	122	LYS

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	243/249 (98%)	238 (98%)	5 (2%)	47	63
1	B	240/249 (96%)	232 (97%)	8 (3%)	33	45
1	C	246/249 (99%)	246 (100%)	0	100	100
1	D	241/249 (97%)	238 (99%)	3 (1%)	63	78
All	All	970/996 (97%)	954 (98%)	16 (2%)	55	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	32	ASP
1	A	120	ASP
1	A	218	LEU
1	A	272	GLU
1	B	1	MET
1	B	46	ASP
1	B	79	ASP
1	B	114	PRO
1	B	122	LYS
1	B	159	GLN
1	B	218	LEU
1	B	272	GLU
1	D	108	LEU
1	D	218	LEU
1	D	222	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	267	ASN
1	B	43	ASN
1	B	163	ASN
1	C	190	ASN
1	C	267	ASN
1	C	283	GLN
1	C	295	HIS
1	D	98	HIS
1	D	190	ASN
1	D	283	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
3	LER	B	402	2	7,7,7	0.76	0	6,8,8	0.66	0
3	LER	C	403	-	7,7,7	0.69	0	6,8,8	0.61	0
3	LER	D	402	2	7,7,7	0.64	0	6,8,8	0.68	0
3	LER	A	403	-	7,7,7	0.66	0	6,8,8	0.60	0
3	LER	C	402	2	7,7,7	0.89	0	6,8,8	0.59	0
3	LER	A	402	2	7,7,7	0.80	0	6,8,8	0.62	0
3	LER	D	403	-	7,7,7	0.63	0	6,8,8	0.63	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
3	LER	B	402	2	-	2/8/8/8	-
3	LER	C	403	-	-	2/8/8/8	-
3	LER	D	402	2	-	4/8/8/8	-
3	LER	A	403	-	-	3/8/8/8	-
3	LER	C	402	2	-	2/8/8/8	-
3	LER	A	402	2	-	0/8/8/8	-
3	LER	D	403	-	-	2/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	LER	O1-C1-C2-O2
3	B	402	LER	C2-C3-C4-O4
3	B	402	LER	O3-C3-C4-O4
3	C	402	LER	C2-C3-C4-O4
3	C	402	LER	O3-C3-C4-O4
3	C	403	LER	O1-C1-C2-O2
3	C	403	LER	O1-C1-C2-C3
3	D	402	LER	O1-C1-C2-O2
3	D	402	LER	O1-C1-C2-C3
3	D	402	LER	O3-C3-C4-O4
3	D	403	LER	O1-C1-C2-O2
3	D	403	LER	O1-C1-C2-C3
3	D	402	LER	C2-C3-C4-O4
3	A	403	LER	O2-C2-C3-O3
3	A	403	LER	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	LER	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	294/300 (98%)	-0.19	1 (0%) 90 88	22, 29, 40, 64	0
1	B	290/300 (96%)	-0.17	2 (0%) 84 82	18, 28, 42, 62	0
1	C	297/300 (99%)	-0.19	1 (0%) 90 88	21, 30, 43, 64	0
1	D	292/300 (97%)	0.03	1 (0%) 90 88	23, 34, 50, 73	0
All	All	1173/1200 (97%)	-0.13	5 (0%) 88 87	18, 30, 44, 73	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	LEU	2.3
1	B	290	ALA	2.1
1	B	1	MET	2.1
1	A	294	SER	2.1
1	C	296	HIS	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 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
3	LER	A	402	8/8	0.73	0.16	48,54,57,59	0
3	LER	D	403	8/8	0.73	0.13	57,59,59,59	0
3	LER	C	403	8/8	0.74	0.15	66,68,69,69	0
3	LER	D	402	8/8	0.78	0.15	55,57,59,60	0
3	LER	B	402	8/8	0.81	0.13	39,46,48,49	0
3	LER	C	402	8/8	0.82	0.12	40,45,47,48	0
3	LER	A	403	8/8	0.87	0.11	54,56,57,60	0
2	MN	B	401	1/1	0.96	0.08	53,53,53,53	0
2	MN	D	401	1/1	0.98	0.02	39,39,39,39	0
2	MN	C	401	1/1	0.98	0.03	47,47,47,47	0
2	MN	A	401	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.