



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:22 AM UTC

PDB ID : 3V5C / pdb_00003v5c
Title : Crystal structure of the mutant E234A of Galacturonate Dehydratase from
GEOBACILLUS SP. complexed with Mg
Authors : Fedorov, A.A.; Fedorov, E.V.; Groninger-Poe, F.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2011-12-16
Resolution : 1.53 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

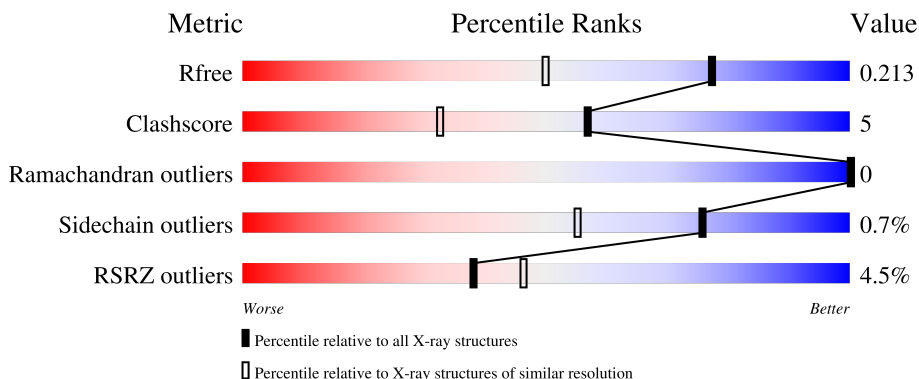
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	392	3% 90% 9% .
1	B	392	2% 88% 8% .
1	C	392	5% 88% 10% .
1	D	392	8% 83% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13728 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	7	0
			3100	1956	549	583	12			
1	B	376	Total	C	N	O	S	0	5	0
			3005	1900	526	568	11			
1	C	385	Total	C	N	O	S	0	5	0
			3072	1941	539	580	12			
1	D	376	Total	C	N	O	S	0	4	0
			3004	1900	528	565	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP D3EID5
A	3	LEU	-	expression tag	UNP D3EID5
A	234	ALA	GLU	engineered mutation	UNP D3EID5
A	385	GLU	-	expression tag	UNP D3EID5
A	386	GLY	-	expression tag	UNP D3EID5
A	387	HIS	-	expression tag	UNP D3EID5
A	388	HIS	-	expression tag	UNP D3EID5
A	389	HIS	-	expression tag	UNP D3EID5
A	390	HIS	-	expression tag	UNP D3EID5
A	391	HIS	-	expression tag	UNP D3EID5
A	392	HIS	-	expression tag	UNP D3EID5
B	2	SER	-	expression tag	UNP D3EID5
B	3	LEU	-	expression tag	UNP D3EID5
B	234	ALA	GLU	engineered mutation	UNP D3EID5
B	385	GLU	-	expression tag	UNP D3EID5
B	386	GLY	-	expression tag	UNP D3EID5
B	387	HIS	-	expression tag	UNP D3EID5
B	388	HIS	-	expression tag	UNP D3EID5
B	389	HIS	-	expression tag	UNP D3EID5
B	390	HIS	-	expression tag	UNP D3EID5
B	391	HIS	-	expression tag	UNP D3EID5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP D3EID5
C	2	SER	-	expression tag	UNP D3EID5
C	3	LEU	-	expression tag	UNP D3EID5
C	234	ALA	GLU	engineered mutation	UNP D3EID5
C	385	GLU	-	expression tag	UNP D3EID5
C	386	GLY	-	expression tag	UNP D3EID5
C	387	HIS	-	expression tag	UNP D3EID5
C	388	HIS	-	expression tag	UNP D3EID5
C	389	HIS	-	expression tag	UNP D3EID5
C	390	HIS	-	expression tag	UNP D3EID5
C	391	HIS	-	expression tag	UNP D3EID5
C	392	HIS	-	expression tag	UNP D3EID5
D	2	SER	-	expression tag	UNP D3EID5
D	3	LEU	-	expression tag	UNP D3EID5
D	234	ALA	GLU	engineered mutation	UNP D3EID5
D	385	GLU	-	expression tag	UNP D3EID5
D	386	GLY	-	expression tag	UNP D3EID5
D	387	HIS	-	expression tag	UNP D3EID5
D	388	HIS	-	expression tag	UNP D3EID5
D	389	HIS	-	expression tag	UNP D3EID5
D	390	HIS	-	expression tag	UNP D3EID5
D	391	HIS	-	expression tag	UNP D3EID5
D	392	HIS	-	expression tag	UNP D3EID5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	3	Total Mg 3 3	0	0
2	C	1	Total Mg 1 1	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

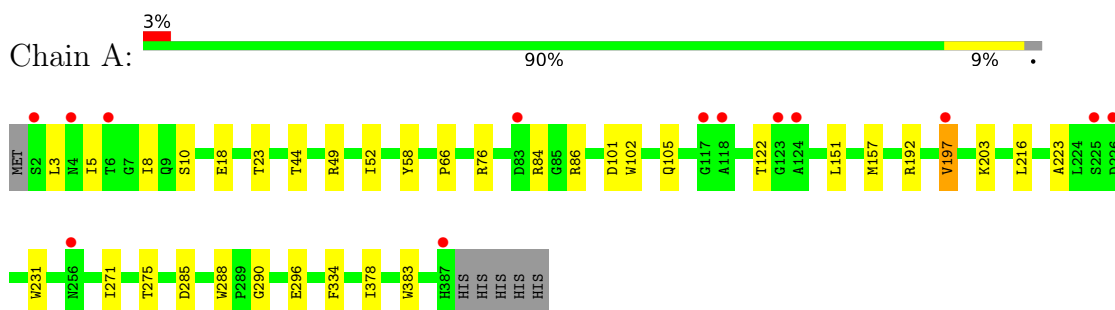
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	487	Total	O	0	0
			487	487		
4	B	387	Total	O	0	0
			387	387		
4	C	385	Total	O	0	0
			385	385		
4	D	239	Total	O	0	0
			239	239		

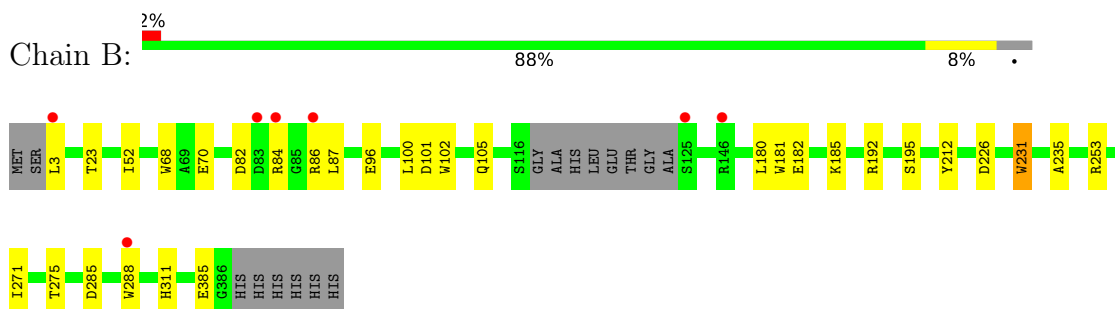
3 Residue-property plots [i](#)

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.

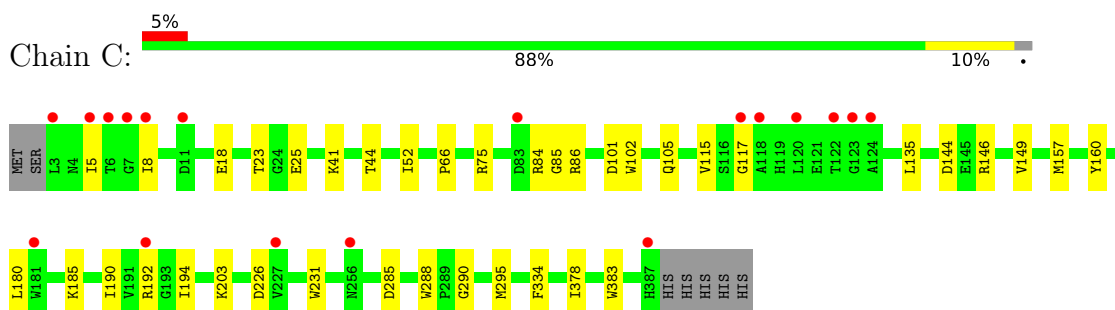
- Molecule 1: Mandelate racemase/muconate lactonizing protein



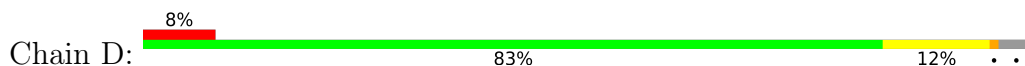
- Molecule 1: Mandelate racemase/muconate lactonizing protein

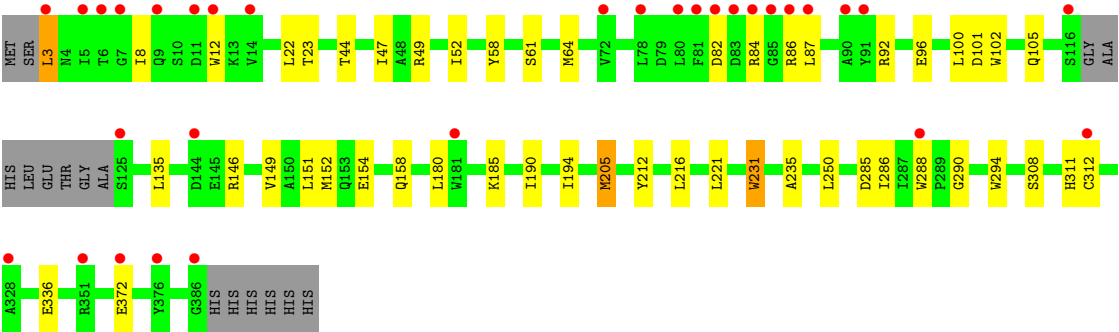


- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.27Å 65.86Å 151.22Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	40.47 – 1.53 40.47 – 1.53	Depositor EDS
% Data completeness (in resolution range)	87.6 (40.47-1.53) 87.6 (40.47-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.53Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.185 , 0.216 0.182 , 0.213	Depositor DCC
R_{free} test set	10061 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13728	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 63.92 % 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 8.9722e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, MG

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	0/3171	0.75	2/4295 (0.0%)
1	B	0.43	0/3073	0.73	0/4163
1	C	0.41	0/3143	0.72	2/4259 (0.0%)
1	D	0.37	0/3072	0.71	0/4161
All	All	0.42	0/12459	0.73	4/16878 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	VAL	CB-CA-C	-5.88	104.44	111.97
1	C	290	GLY	N-CA-C	5.27	119.55	112.17
1	C	117	GLY	N-CA-C	-5.24	107.75	115.30
1	A	290	GLY	N-CA-C	5.10	119.31	112.17

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	3100	0	2989	23	0
1	B	3005	0	2898	22	0
1	C	3072	0	2958	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3004	0	2902	40	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	10	0	0
3	B	14	0	20	1	0
3	C	21	0	30	3	0
4	A	487	0	0	5	0
4	B	387	0	0	4	0
4	C	385	0	0	3	0
4	D	239	0	0	3	0
All	All	13728	0	11807	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (110) 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:84:ARG:HD3	1:A:86:ARG:HH21	1.17	1.08
1:C:84:ARG:HD3	1:C:86:ARG:HH21	1.35	0.91
1:A:157:MET:SD	1:A:197:VAL:HG13	2.15	0.86
1:D:84:ARG:HD3	1:D:86:ARG:HH21	1.45	0.80
1:B:84:ARG:HD3	1:B:86:ARG:HH21	1.46	0.79
1:A:84:ARG:HD3	1:A:86:ARG:NH2	1.95	0.76
1:C:75:ARG:HH12	3:C:396:PEG:H42	1.53	0.72
1:D:3:LEU:HD11	1:D:100:LEU:HD21	1.74	0.69
1:D:285:ASP:HB3	1:D:288:TRP:O	1.96	0.66
1:D:152:MET:HG3	1:D:190:ILE:HD12	1.77	0.66
1:D:205:MET:HG2	1:D:231:TRP:CD1	2.31	0.65
1:C:75:ARG:NH1	3:C:396:PEG:H42	2.14	0.63
1:B:311:HIS:HD2	4:B:1479:HOH:O	1.82	0.63
1:B:3:LEU:HD11	1:B:100:LEU:HD21	1.82	0.62
1:B:253:ARG:HD2	4:B:661:HOH:O	1.98	0.62
1:C:84:ARG:HD3	1:C:86:ARG:NH2	2.11	0.61
1:D:151:LEU:HD12	4:D:1484:HOH:O	1.99	0.61
1:D:149:VAL:HA	1:D:190:ILE:HD13	1.84	0.59
1:D:180:LEU:HD11	1:D:216:LEU:HD11	1.83	0.58
1:C:75:ARG:HH12	3:C:396:PEG:C4	2.17	0.58
1:D:205:MET:HG2	1:D:231:TRP:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HA	4:A:1153:HOH:O	2.03	0.58
1:D:372[A]:GLU:H	1:D:372[A]:GLU:CD	2.13	0.56
1:B:68:TRP:CD1	3:B:397:PEG:H32	2.41	0.56
1:A:86:ARG:HD2	1:A:296:GLU:OE2	2.07	0.55
1:D:152:MET:CG	1:D:190:ILE:HD12	2.36	0.55
1:B:192[B]:ARG:NH2	1:B:226:ASP:OD1	2.38	0.54
1:D:101:ASP:O	1:D:105:GLN:HG2	2.07	0.54
1:C:23:THR:HG23	4:C:1399:HOH:O	2.08	0.54
1:A:122:THR:HB	4:A:1529:HOH:O	2.09	0.53
1:B:23:THR:HG23	4:B:541:HOH:O	2.08	0.52
1:C:192[B]:ARG:HH22	1:C:226:ASP:CG	2.18	0.52
1:D:311:HIS:HD2	4:D:1114:HOH:O	1.92	0.52
1:C:101:ASP:O	1:C:105:GLN:HG2	2.10	0.51
1:C:285:ASP:HB3	1:C:288:TRP:O	2.10	0.51
1:A:192[A]:ARG:NH2	4:A:1471:HOH:O	2.43	0.51
1:A:66:PRO:HG3	1:A:383:TRP:CG	2.46	0.51
1:D:205:MET:HG2	1:D:231:TRP:CG	2.46	0.50
1:D:205:MET:HG2	1:D:231:TRP:NE1	2.27	0.49
1:B:285:ASP:HB3	1:B:288:TRP:O	2.13	0.49
1:A:192[B]:ARG:NH2	1:A:223:ALA:O	2.45	0.49
1:C:157:MET:HE1	1:C:160:TYR:CD1	2.48	0.48
1:C:180:LEU:HD22	1:D:216:LEU:HG	1.94	0.48
1:D:231:TRP:CD1	1:D:231:TRP:C	2.92	0.48
1:C:135:LEU:HD13	1:C:194:ILE:HD13	1.95	0.47
1:C:192[A]:ARG:NH2	4:C:1476:HOH:O	2.47	0.47
1:A:285:ASP:HB3	1:A:288:TRP:O	2.14	0.47
1:D:8:ILE:HA	1:D:12:TRP:CZ3	2.49	0.47
1:A:49:ARG:HD3	1:A:58:TYR:CZ	2.49	0.47
1:B:182[B]:GLU:OE1	4:B:1445:HOH:O	2.20	0.47
1:A:203:LYS:HD2	1:A:334:PHE:HZ	1.80	0.47
1:B:82:ASP:OD2	1:B:86:ARG:HB2	2.15	0.47
1:C:25:GLU:OE1	1:C:41:LYS:HE3	2.15	0.47
1:C:180:LEU:CD2	1:D:216:LEU:HG	2.45	0.47
1:D:49:ARG:HD3	1:D:58:TYR:CZ	2.50	0.47
1:D:154:GLU:OE1	1:D:158:GLN:NE2	2.47	0.47
1:B:192[B]:ARG:HH12	1:B:226:ASP:CG	2.23	0.46
1:D:185:LYS:HB3	1:D:185:LYS:HE2	1.66	0.46
1:D:205:MET:HG2	1:D:231:TRP:CD2	2.50	0.46
1:B:185:LYS:HB3	1:B:185:LYS:HE2	1.52	0.46
1:A:23:THR:HG22	1:A:44:THR:HG22	1.97	0.46
1:A:216:LEU:HG	1:B:180:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD22	1:D:96:GLU:HA	1.98	0.46
1:A:10:SER:O	1:A:76[A]:ARG:HD3	2.16	0.46
1:C:149:VAL:HA	1:C:190:ILE:HD13	1.98	0.46
1:A:18:GLU:HB3	1:A:378:ILE:HD13	1.99	0.45
1:D:312[B]:CYS:HB2	1:D:336:GLU:HB3	1.97	0.45
1:B:101:ASP:O	1:B:105:GLN:HG2	2.17	0.45
1:D:294:TRP:CZ3	1:D:308:SER:HB3	2.51	0.45
1:D:23:THR:HG22	1:D:44:THR:HG22	1.99	0.45
1:D:135:LEU:HD13	1:D:194:ILE:HD13	1.98	0.44
1:C:52:ILE:HB	1:C:102:TRP:CE2	2.52	0.44
1:D:82:ASP:OD2	1:D:86:ARG:HB2	2.17	0.44
1:B:70:GLU:HG2	1:B:385:GLU:OE1	2.18	0.44
1:B:212:TYR:HB2	1:B:235:ALA:O	2.18	0.44
1:C:23:THR:HG22	1:C:44:THR:HG22	1.99	0.44
1:D:311:HIS:CD2	4:D:1114:HOH:O	2.70	0.44
1:C:115:VAL:HB	1:C:295:MET:SD	2.59	0.43
1:C:144:ASP:OD1	1:C:146:ARG:HB2	2.17	0.43
1:B:181:TRP:CH2	1:B:185:LYS:HD3	2.53	0.43
1:D:92:ARG:HA	1:D:96:GLU:HB3	2.00	0.43
1:A:52:ILE:HB	1:A:102:TRP:CE2	2.54	0.43
1:A:157:MET:HE3	4:A:1458:HOH:O	2.18	0.43
1:C:157:MET:HE1	1:C:160:TYR:CG	2.53	0.43
1:A:192[A]:ARG:CZ	4:A:1471:HOH:O	2.67	0.43
1:D:212:TYR:HB2	1:D:235:ALA:O	2.19	0.42
1:D:61:SER:OG	1:D:64:MET:HE2	2.19	0.42
1:A:151:LEU:C	1:A:151:LEU:HD23	2.44	0.42
1:A:271:ILE:O	1:A:275:THR:HG23	2.19	0.42
1:B:231:TRP:CD1	1:B:231:TRP:C	2.97	0.42
1:D:22:LEU:HD22	1:D:47:ILE:HG13	2.01	0.42
1:B:52:ILE:HB	1:B:102:TRP:CE2	2.55	0.42
1:A:101:ASP:O	1:A:105:GLN:HG2	2.19	0.42
1:C:66:PRO:HG3	1:C:383:TRP:CG	2.55	0.42
1:B:192[B]:ARG:O	1:B:195:SER:HB3	2.20	0.41
1:C:18:GLU:HB3	1:C:378:ILE:HD13	2.01	0.41
1:C:5:ILE:HD13	1:C:85:GLY:HA2	2.01	0.41
1:C:157:MET:HE3	1:C:160:TYR:HB3	2.01	0.41
1:B:271:ILE:O	1:B:275:THR:HG23	2.21	0.41
1:C:5:ILE:HB	1:C:8:ILE:HD12	2.01	0.41
1:D:146:ARG:HD3	1:D:146:ARG:HA	1.73	0.41
1:C:203:LYS:HD2	1:C:334:PHE:HZ	1.85	0.41
1:D:154:GLU:O	1:D:158:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:HD3	1:D:86:ARG:NH2	2.23	0.41
1:D:221:LEU:HD13	1:D:250:LEU:HD21	2.03	0.41
1:D:52:ILE:HB	1:D:102:TRP:CE2	2.56	0.41
1:C:192[A]:ARG:CZ	4:C:1476:HOH:O	2.68	0.41
1:D:286:ILE:O	1:D:290:GLY:HA2	2.20	0.40
1:A:5:ILE:HB	1:A:8:ILE:HD12	2.02	0.40
1:B:87:LEU:HD22	1:B:96:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/392 (100%)	388 (99%)	3 (1%)	0	100	100
1	B	377/392 (96%)	373 (99%)	4 (1%)	0	100	100
1	C	388/392 (99%)	384 (99%)	4 (1%)	0	100	100
1	D	376/392 (96%)	372 (99%)	4 (1%)	0	100	100
All	All	1532/1568 (98%)	1517 (99%)	15 (1%)	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	316/315 (100%)	314 (99%)	2 (1%)	78	59
1	B	308/315 (98%)	307 (100%)	1 (0%)	86	74
1	C	313/315 (99%)	311 (99%)	2 (1%)	78	59
1	D	307/315 (98%)	304 (99%)	3 (1%)	68	42
All	All	1244/1260 (99%)	1236 (99%)	8 (1%)	76	59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	231	TRP
1	B	231	TRP
1	C	185	LYS
1	C	231	TRP
1	D	3	LEU
1	D	205	MET
1	D	231	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	B	209	ASN
1	B	269	HIS
1	C	304	HIS
1	D	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	PEG	C	394	-	6,6,6	0.47	0	5,5,5	0.27	0
3	PEG	B	396	-	6,6,6	0.53	0	5,5,5	0.09	0
3	PEG	C	396	-	6,6,6	0.45	0	5,5,5	0.20	0
3	PEG	C	395	-	6,6,6	0.44	0	5,5,5	0.25	0
3	PEG	A	394	-	6,6,6	0.41	0	5,5,5	0.31	0
3	PEG	B	397	-	6,6,6	0.42	0	5,5,5	0.33	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	PEG	C	394	-	-	2/4/4/4	-
3	PEG	B	396	-	-	1/4/4/4	-
3	PEG	C	396	-	-	2/4/4/4	-
3	PEG	C	395	-	-	1/4/4/4	-
3	PEG	A	394	-	-	2/4/4/4	-
3	PEG	B	397	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	394	PEG	O1-C1-C2-O2
3	A	394	PEG	O1-C1-C2-O2
3	C	396	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	396	PEG	C1-C2-O2-C3
3	B	397	PEG	O2-C3-C4-O4
3	A	394	PEG	C4-C3-O2-C2
3	C	396	PEG	C4-C3-O2-C2
3	C	394	PEG	O2-C3-C4-O4
3	C	395	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	396	PEG	3	0
3	B	397	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	386/392 (98%)	-0.16	13 (3%)	48 57	6, 15, 30, 54	7 (1%)
1	B	376/392 (95%)	-0.01	7 (1%)	66 76	8, 18, 33, 67	5 (1%)
1	C	385/392 (98%)	0.14	18 (4%)	36 44	8, 19, 38, 59	5 (1%)
1	D	376/392 (95%)	0.65	31 (8%)	17 22	13, 26, 51, 81	4 (1%)
All	All	1523/1568 (97%)	0.15	69 (4%)	38 46	6, 19, 39, 81	21 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	ALA	6.0
1	D	5	ILE	5.1
1	A	6	THR	4.2
1	C	6	THR	4.1
1	C	120	LEU	4.0
1	D	85	GLY	3.7
1	D	288	TRP	3.7
1	D	376	TYR	3.6
1	B	3	LEU	3.5
1	B	83	ASP	3.5
1	A	124	ALA	3.5
1	D	86	ARG	3.2
1	C	181	TRP	3.2
1	D	125	SER	3.1
1	D	78	LEU	3.1
1	C	387	HIS	3.1
1	D	12	TRP	3.0
1	C	118	ALA	2.9
1	D	351[A]	ARG	2.9
1	C	122	THR	2.9
1	D	144	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	288	TRP	2.8
1	D	87	LEU	2.8
1	A	225	SER	2.8
1	C	192[A]	ARG	2.8
1	A	83	ASP	2.7
1	C	83	ASP	2.7
1	D	6	THR	2.7
1	A	387	HIS	2.7
1	D	81	PHE	2.7
1	D	9	GLN	2.7
1	D	181	TRP	2.7
1	C	11	ASP	2.7
1	A	117	GLY	2.6
1	D	3	LEU	2.6
1	D	82	ASP	2.6
1	D	90	ALA	2.5
1	C	123	GLY	2.5
1	D	91	TYR	2.5
1	B	146	ARG	2.5
1	D	312[A]	CYS	2.5
1	D	116	SER	2.4
1	B	84	ARG	2.4
1	B	86	ARG	2.4
1	D	14	VAL	2.4
1	C	8	ILE	2.4
1	A	123	GLY	2.4
1	A	118	ALA	2.3
1	D	328	ALA	2.3
1	A	226	ASP	2.3
1	D	386	GLY	2.3
1	D	84	ARG	2.2
1	C	7	GLY	2.2
1	A	2	SER	2.2
1	D	7	GLY	2.2
1	D	11	ASP	2.2
1	C	5	ILE	2.2
1	D	372[A]	GLU	2.2
1	C	3	LEU	2.1
1	A	4	ASN	2.1
1	C	227	VAL	2.1
1	D	72	VAL	2.1
1	C	117	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	83	ASP	2.1
1	A	197	VAL	2.0
1	B	125	SER	2.0
1	C	256	ASN	2.0
1	D	80	LEU	2.0
1	A	256	ASN	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	PEG	C	394	7/7	0.76	0.14	30,32,41,52	0
3	PEG	B	396	7/7	0.78	0.15	33,37,41,42	0
3	PEG	C	395	7/7	0.82	0.14	33,36,39,44	0
3	PEG	A	394	7/7	0.85	0.10	29,35,42,43	0
3	PEG	B	397	7/7	0.85	0.11	36,37,39,41	0
3	PEG	C	396	7/7	0.85	0.09	33,36,43,43	0
2	MG	B	394	1/1	0.95	0.20	29,29,29,29	0
2	MG	B	395	1/1	0.97	0.08	29,29,29,29	0
2	MG	D	394	1/1	0.97	0.17	31,31,31,31	0
2	MG	D	393	1/1	0.98	0.04	18,18,18,18	0
2	MG	A	393	1/1	0.99	0.03	11,11,11,11	0
2	MG	B	393	1/1	0.99	0.02	13,13,13,13	0
2	MG	C	393	1/1	1.00	0.04	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.