



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 AM UTC

PDB ID : 2PP3 / pdb_00002pp3
Title : Crystal structure of L-talarate/galactarate dehydratase mutant K197A liganded with Mg and L-glucarate
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2007-04-27
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

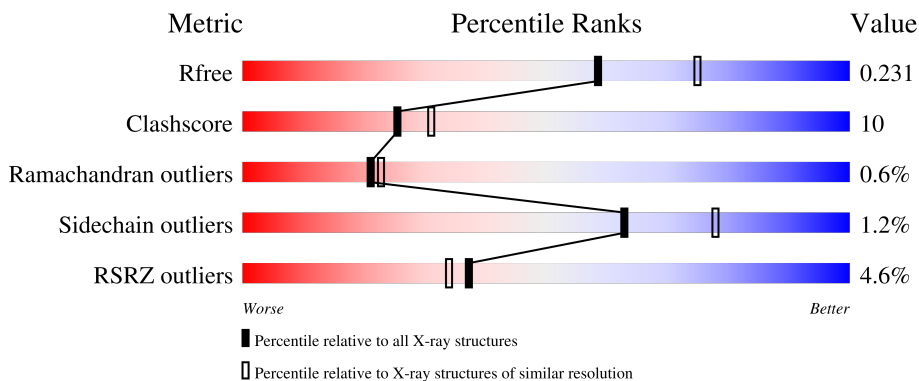
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

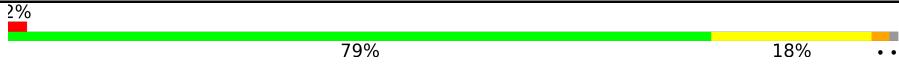
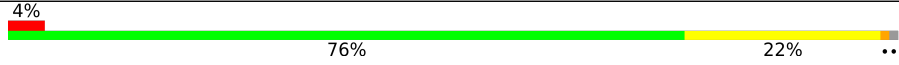

The reported resolution of this entry is 2.20 Å.

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	398	
1	B	398	
1	C	398	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9579 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 L-talarate/galactarate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3077	1948	547	570	12	0	0	0
1	B	395	3077	1948	547	570	12	0	0	0
1	C	395	3077	1948	547	570	12	0	0	0

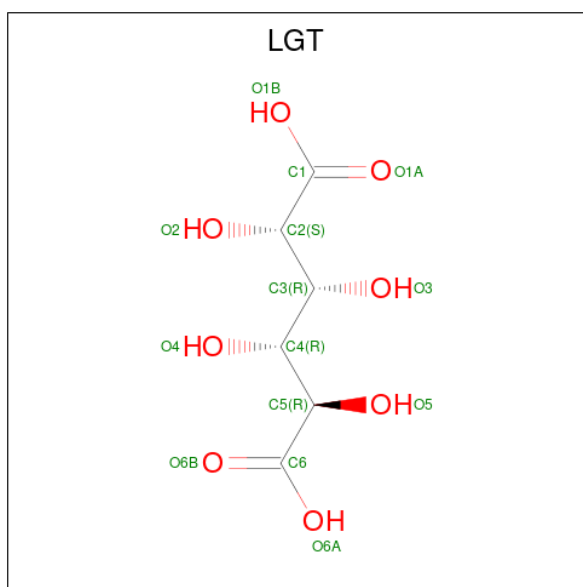
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	ALA	LYS	engineered mutation	UNP Q8ZL58
B	197	ALA	LYS	engineered mutation	UNP Q8ZL58
C	197	ALA	LYS	engineered mutation	UNP Q8ZL58

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

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

- Molecule 3 is L-GLUCARIC ACID (CCD ID: LGT) (formula: C₆H₁₀O₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 6 8	0	0
3	B	1	Total C O 14 6 8	0	0
3	C	1	Total C O 14 6 8	0	0

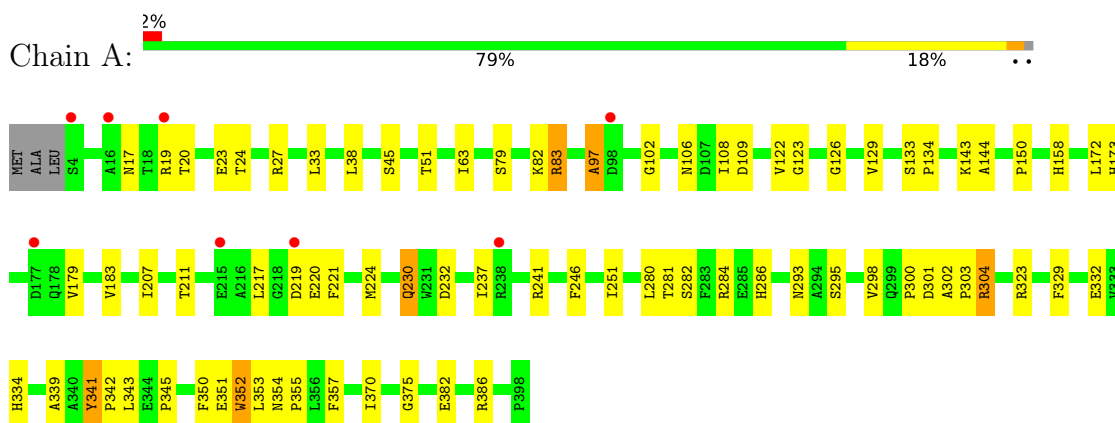
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	152	Total O 152 152	0	0
4	B	78	Total O 78 78	0	0
4	C	73	Total O 73 73	0	0

3 Residue-property plots [i](#)

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

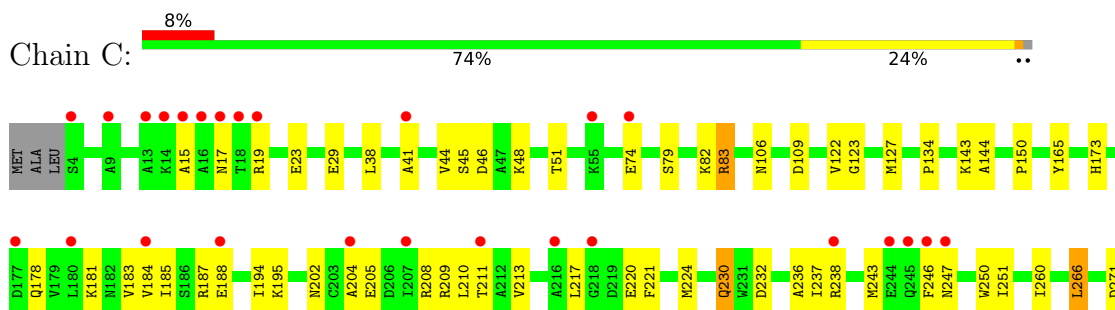
- Molecule 1: L-talarate/galactarate dehydratase



- Molecule 1: L-talarate/galactarate dehydratase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.23Å 174.23Å 123.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.20 24.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.1 (24.94-2.20) 87.0 (24.94-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.231 0.204 , 0.231	Depositor DCC
R_{free} test set	5977 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.199	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: LGT, 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	0.42	0/3145	0.95	19/4262 (0.4%)
1	B	0.38	0/3145	0.89	12/4262 (0.3%)
1	C	0.38	0/3145	0.90	12/4262 (0.3%)
All	All	0.39	0/9435	0.91	43/12786 (0.3%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLN	N-CA-C	7.44	122.38	113.16
1	B	122	VAL	N-CA-C	7.14	118.26	111.91
1	B	150	PRO	N-CA-C	-7.09	100.11	111.38
1	C	150	PRO	N-CA-C	-6.80	100.56	111.38
1	A	341	TYR	CA-C-N	6.75	125.99	118.97
1	A	341	TYR	C-N-CA	6.75	125.99	118.97
1	A	350	PHE	N-CA-C	-6.58	99.03	109.23
1	B	230	GLN	N-CA-C	6.39	120.93	113.20
1	A	150	PRO	N-CA-C	-6.33	101.31	111.38
1	C	123	GLY	N-CA-C	6.26	123.48	112.83
1	C	122	VAL	N-CA-C	6.24	118.15	112.29
1	C	220	GLU	N-CA-C	6.17	119.28	111.69
1	C	230	GLN	N-CA-C	6.09	120.33	113.02
1	A	232	ASP	N-CA-C	-6.06	101.80	110.59
1	C	349	HIS	N-CA-C	5.99	118.66	108.90
1	B	123	GLY	N-CA-C	5.96	122.96	112.83
1	B	232	ASP	N-CA-C	-5.89	101.74	110.46
1	A	122	VAL	N-CA-C	5.80	117.07	111.91
1	A	295	SER	N-CA-C	5.76	117.82	109.07
1	A	219	ASP	N-CA-C	5.62	118.33	111.82
1	A	172	LEU	N-CA-C	5.55	119.67	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	GLU	N-CA-C	5.54	120.16	112.90
1	C	232	ASP	N-CA-C	-5.53	102.57	110.59
1	B	349	HIS	N-CA-C	5.50	117.92	109.07
1	B	295	SER	N-CA-C	5.48	117.41	109.07
1	A	97	ALA	N-CA-C	5.46	117.93	111.33
1	A	123	GLY	N-CA-C	5.43	122.06	112.83
1	A	220	GLU	N-CA-C	5.42	118.35	111.69
1	A	108	ILE	N-CA-C	5.37	115.57	110.42
1	C	351	GLU	N-CA-C	-5.36	106.76	113.72
1	C	271	ASP	N-CA-C	-5.34	105.54	111.36
1	C	350	PHE	N-CA-C	-5.28	101.27	109.24
1	A	304	ARG	N-CA-C	5.27	117.93	111.82
1	C	127	MET	N-CA-C	5.25	117.41	111.11
1	C	251	ILE	N-CA-C	-5.18	100.19	107.75
1	A	251	ILE	N-CA-C	-5.18	100.19	107.75
1	B	304	ARG	N-CA-C	5.12	117.76	111.82
1	B	158	HIS	N-CA-C	-5.12	107.06	113.72
1	A	221	PHE	N-CA-C	5.12	116.85	109.48
1	A	352	TRP	N-CA-C	5.10	117.50	111.33
1	B	108	ILE	N-CA-C	5.06	115.28	110.42
1	A	158	HIS	N-CA-C	-5.01	107.56	113.97
1	B	271	ASP	N-CA-C	-5.01	106.34	112.90

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	3077	0	3056	49	0
1	B	3077	0	3056	58	1
1	C	3077	0	3056	72	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	14	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	7	0	0
3	C	14	0	8	0	0
4	A	152	0	0	1	0
4	B	78	0	0	1	0
4	C	73	0	0	2	0
All	All	9579	0	9190	177	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (177) 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:302:ALA:H	1:A:334:HIS:HE1	1.22	0.86
1:B:302:ALA:H	1:B:334:HIS:HE1	1.26	0.84
1:C:45:SER:H	1:C:173:HIS:HD2	1.26	0.83
1:B:50:LEU:HD22	1:B:172:LEU:HD13	1.62	0.80
1:C:302:ALA:H	1:C:334:HIS:HE1	1.34	0.76
1:B:45:SER:H	1:B:173:HIS:HD2	1.33	0.76
1:C:45:SER:H	1:C:173:HIS:CD2	2.06	0.73
1:C:19:ARG:HG2	1:C:19:ARG:HH11	1.55	0.72
1:A:293:ASN:HD22	1:A:323:ARG:HH21	1.38	0.71
1:A:302:ALA:H	1:A:334:HIS:CE1	2.06	0.71
1:A:207:ILE:O	1:A:211:THR:HG23	1.90	0.71
1:B:301:ASP:OD1	1:B:303:PRO:HD2	1.92	0.70
1:C:45:SER:HB2	1:C:173:HIS:HB3	1.74	0.69
1:C:165:TYR:CE1	1:C:195:LYS:HE3	2.27	0.69
1:C:301:ASP:OD1	1:C:303:PRO:HD2	1.93	0.68
1:C:79:SER:HB2	1:C:134:PRO:HD3	1.73	0.68
1:C:236:ALA:HB1	1:C:266:LEU:HD21	1.75	0.68
1:C:298:VAL:HG12	1:C:300:PRO:HD3	1.76	0.68
1:A:298:VAL:HG12	1:A:300:PRO:HD3	1.73	0.68
1:B:298:VAL:HG12	1:B:300:PRO:HD3	1.77	0.66
1:B:302:ALA:H	1:B:334:HIS:CE1	2.09	0.66
1:C:297:PHE:CZ	1:C:324:LYS:HD3	2.30	0.66
1:C:202:ASN:HD21	1:C:204:ALA:HB3	1.62	0.65
1:C:293:ASN:HD22	1:C:323:ARG:HH21	1.43	0.65
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.62	0.64
1:A:329:PHE:O	1:A:334:HIS:HD2	1.81	0.63
1:C:165:TYR:HE1	1:C:195:LYS:HE3	1.63	0.63
1:A:211:THR:HG22	1:A:246:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:HB3	1:A:303:PRO:HD3	1.80	0.62
1:A:211:THR:HG22	1:A:246:PHE:HZ	1.65	0.61
1:B:45:SER:H	1:B:173:HIS:CD2	2.18	0.60
1:C:260:ILE:HG12	1:C:289:LEU:HD22	1.85	0.59
1:B:82:LYS:O	1:B:83:ARG:HB2	2.02	0.59
1:C:184:VAL:O	1:C:188:GLU:HG2	2.03	0.59
1:C:210:LEU:HD22	1:C:243:MET:HE2	1.85	0.59
1:B:332:GLU:HG2	1:B:357:PHE:CE2	2.38	0.58
1:C:82:LYS:O	1:C:83:ARG:HB2	2.03	0.58
1:A:45:SER:H	1:A:173:HIS:CD2	2.22	0.57
1:B:223:LEU:CA	1:B:224:MET:HE2	2.35	0.57
1:C:202:ASN:C	1:C:202:ASN:HD22	2.13	0.57
1:C:302:ALA:HB3	1:C:303:PRO:HD3	1.86	0.56
1:A:301:ASP:OD1	1:A:303:PRO:HD2	2.04	0.56
1:B:207:ILE:O	1:B:211:THR:HG23	2.05	0.56
1:C:329:PHE:O	1:C:334:HIS:HD2	1.88	0.56
1:B:133:SER:HB2	1:B:134:PRO:HD3	1.87	0.56
1:A:332:GLU:HG2	1:A:357:PHE:CE2	2.41	0.56
1:B:302:ALA:HB3	1:B:303:PRO:HD3	1.88	0.55
1:C:280:LEU:HD11	1:C:289:LEU:HG	1.88	0.55
1:C:178:GLN:NE2	1:C:181:LYS:HD2	2.22	0.55
1:B:329:PHE:O	1:B:334:HIS:HD2	1.90	0.55
1:B:63:ILE:HD12	1:B:63:ILE:N	2.22	0.55
1:A:82:LYS:O	1:A:83:ARG:HB2	2.07	0.54
1:B:19:ARG:HA	1:B:23:GLU:OE1	2.08	0.54
1:C:332:GLU:H	1:C:332:GLU:CD	2.16	0.54
1:C:332:GLU:HG2	1:C:357:PHE:CE2	2.44	0.53
1:A:20:THR:H	1:A:23:GLU:CD	2.18	0.53
1:A:183:VAL:CG1	1:A:217:LEU:HD21	2.39	0.52
1:C:19:ARG:HG2	1:C:19:ARG:NH1	2.20	0.52
1:C:302:ALA:H	1:C:334:HIS:CE1	2.20	0.52
1:A:38:LEU:HD21	1:A:352:TRP:O	2.09	0.52
1:A:339:ALA:HB2	1:A:370:ILE:HD11	1.90	0.52
1:C:280:LEU:HB2	1:C:286:HIS:CE1	2.45	0.52
1:A:237:ILE:O	1:A:241:ARG:HG2	2.10	0.52
1:C:247:ASN:HD22	1:C:247:ASN:N	2.08	0.52
1:C:38:LEU:CD2	1:C:353:LEU:HD23	2.40	0.51
1:A:79:SER:HA	1:A:303:PRO:HB3	1.92	0.51
1:B:286:HIS:HE1	4:B:903:HOH:O	1.92	0.51
1:C:274:ILE:O	1:C:295:SER:HB2	2.10	0.51
1:C:284:ARG:HG3	4:C:959:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:HA	1:C:23:GLU:OE1	2.11	0.51
1:B:301:ASP:HB3	1:B:304:ARG:HB2	1.93	0.51
1:B:354:ASN:N	1:B:355:PRO:HD2	2.26	0.51
1:B:79:SER:HA	1:B:303:PRO:HB3	1.92	0.50
1:B:223:LEU:HA	1:B:224:MET:HE2	1.94	0.50
1:B:38:LEU:HD12	1:B:387:TRP:CZ3	2.46	0.50
1:B:223:LEU:C	1:B:224:MET:HE2	2.37	0.49
1:C:106:ASN:HD22	1:C:143:LYS:HE2	1.77	0.49
1:A:38:LEU:CD2	1:A:353:LEU:HD23	2.42	0.49
1:A:106:ASN:HD22	1:A:143:LYS:HE2	1.76	0.49
1:C:194:ILE:HG12	1:C:221:PHE:HE2	1.77	0.49
1:B:194:ILE:O	1:B:224:MET:HE3	2.12	0.49
1:C:29:GLU:HB2	1:C:398:PRO:HG3	1.95	0.48
1:A:126:GLY:O	1:A:129:VAL:HG22	2.13	0.48
1:A:144:ALA:HB3	1:A:375:GLY:HA2	1.96	0.48
1:C:44:VAL:HA	1:C:173:HIS:CD2	2.49	0.48
1:C:354:ASN:N	1:C:355:PRO:HD2	2.29	0.48
1:A:293:ASN:HD22	1:A:323:ARG:NH2	2.08	0.47
1:B:211:THR:HG22	1:B:246:PHE:CZ	2.50	0.47
1:C:184:VAL:HG13	1:C:185:ILE:N	2.30	0.47
1:C:144:ALA:HB3	1:C:375:GLY:HA2	1.97	0.46
1:A:183:VAL:HG13	1:A:217:LEU:HD21	1.98	0.46
1:A:301:ASP:HB3	1:A:304:ARG:HB2	1.97	0.46
1:C:51:THR:HG21	1:C:230:GLN:HE21	1.81	0.46
1:A:63:ILE:HD12	1:A:63:ILE:N	2.31	0.45
1:A:20:THR:OG1	1:A:23:GLU:HG2	2.17	0.45
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.28	0.45
1:A:339:ALA:CB	1:A:370:ILE:HD11	2.45	0.45
1:B:38:LEU:HD21	1:B:352:TRP:O	2.16	0.45
1:C:205:GLU:OE2	1:C:205:GLU:HA	2.16	0.45
1:B:185:ILE:O	1:B:189:ASN:ND2	2.50	0.45
1:A:45:SER:H	1:A:173:HIS:HD2	1.63	0.45
1:A:179:VAL:O	1:A:183:VAL:HG23	2.17	0.45
1:A:382:GLU:HG3	1:A:386:ARG:NH1	2.32	0.44
1:C:358:ASN:HD21	1:C:381:SER:HA	1.82	0.44
1:B:248:LEU:HD12	1:B:251:ILE:HD11	2.00	0.44
1:A:354:ASN:N	1:A:355:PRO:HD2	2.33	0.44
1:B:64:ILE:HG21	1:B:380:LEU:HD11	1.99	0.44
1:C:205:GLU:OE2	1:C:208:ARG:HD3	2.18	0.44
1:C:281:THR:O	1:C:282:SER:HB3	2.18	0.44
1:B:33:LEU:HD11	1:B:97:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HD22	1:B:243:MET:HE2	2.00	0.44
1:A:343:LEU:O	1:A:345:PRO:HD3	2.18	0.44
1:A:33:LEU:HD11	1:A:97:ALA:HB2	2.00	0.43
1:B:45:SER:OG	1:B:173:HIS:HB3	2.18	0.43
1:C:38:LEU:HD21	1:C:353:LEU:HD23	1.99	0.43
1:A:284:ARG:HG3	4:A:1046:HOH:O	2.17	0.43
1:C:301:ASP:HB3	1:C:304:ARG:HB2	2.00	0.43
1:B:4:SER:HB2	1:C:41:ALA:HB2	2.00	0.43
1:B:177:ASP:OD2	1:B:178:GLN:N	2.51	0.43
1:C:209:ARG:O	1:C:213:VAL:HG23	2.18	0.43
1:C:293:ASN:ND2	1:C:323:ARG:HH21	2.11	0.43
1:A:280:LEU:HB2	1:A:286:HIS:CE1	2.54	0.43
1:B:37:PHE:O	1:B:39:PRO:HD3	2.17	0.43
1:B:300:PRO:HG2	1:B:311:PHE:CE1	2.54	0.43
1:B:74:GLU:CD	1:B:74:GLU:C	2.86	0.43
1:A:17:ASN:OD1	1:A:19:ARG:HB2	2.18	0.43
1:A:281:THR:O	1:A:282:SER:HB3	2.19	0.43
1:C:181:LYS:O	1:C:184:VAL:HG12	2.19	0.43
1:A:45:SER:HB2	1:A:173:HIS:HB3	2.01	0.43
1:B:339:ALA:HB2	1:B:370:ILE:HD11	2.00	0.43
1:C:247:ASN:N	1:C:247:ASN:ND2	2.67	0.43
1:C:286:HIS:HE1	4:C:906:HOH:O	2.01	0.42
1:C:338:SER:O	1:C:345:PRO:HG3	2.19	0.42
1:B:179:VAL:O	1:B:183:VAL:HG23	2.20	0.42
1:A:133:SER:N	1:A:134:PRO:HD2	2.34	0.42
1:B:85:GLY:O	1:B:89:ILE:HG13	2.20	0.42
1:B:224:MET:HE2	1:B:224:MET:N	2.34	0.42
1:B:280:LEU:HB2	1:B:286:HIS:CE1	2.55	0.42
1:B:331:MET:HE3	1:B:361:LEU:HD12	2.00	0.42
1:C:293:ASN:HD22	1:C:323:ARG:NH2	2.15	0.42
1:C:332:GLU:CD	1:C:332:GLU:N	2.78	0.42
1:C:359:GLU:OE1	1:C:359:GLU:N	2.52	0.42
1:A:341:TYR:HA	1:A:342:PRO:HD3	1.88	0.42
1:C:183:VAL:O	1:C:187:ARG:HG3	2.20	0.42
1:C:202:ASN:C	1:C:202:ASN:ND2	2.77	0.42
1:B:360:GLN:O	1:C:15:ALA:HB2	2.20	0.42
1:C:211:THR:HG22	1:C:246:PHE:CZ	2.54	0.41
1:B:183:VAL:HG13	1:B:217:LEU:HD21	2.02	0.41
1:B:214:ARG:NH2	1:B:223:LEU:HB3	2.34	0.41
1:B:30:TRP:CH2	1:B:32:LYS:HB2	2.55	0.41
1:A:51:THR:HG21	1:A:230:GLN:HE21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:VAL:HA	1:B:173:HIS:CD2	2.54	0.41
1:B:38:LEU:HD21	1:B:352:TRP:C	2.46	0.41
1:C:46:ASP:CG	1:C:48:LYS:HZ2	2.29	0.41
1:C:79:SER:HA	1:C:303:PRO:HB3	2.03	0.41
1:C:183:VAL:HG13	1:C:217:LEU:HD21	2.03	0.41
1:B:293:ASN:ND2	1:B:323:ARG:HH21	2.18	0.41
1:B:293:ASN:HD22	1:B:323:ARG:HH21	1.69	0.41
1:B:341:TYR:CD1	1:B:342:PRO:HD2	2.56	0.41
1:A:27:ARG:HD2	1:A:102:GLY:O	2.20	0.41
1:B:211:THR:HG22	1:B:246:PHE:HZ	1.86	0.41
1:C:315:MET:HE3	1:C:341:TYR:HD1	1.86	0.41
1:C:339:ALA:HB2	1:C:370:ILE:HD11	2.02	0.41
1:A:351:GLU:OE1	1:A:351:GLU:N	2.46	0.41
1:C:351:GLU:OE1	1:C:351:GLU:N	2.53	0.41
1:C:237:ILE:HG23	1:C:238:ARG:N	2.36	0.40
1:B:106:ASN:HD22	1:B:143:LYS:HE2	1.86	0.40
1:B:274:ILE:O	1:B:295:SER:HB2	2.22	0.40
1:A:20:THR:O	1:A:23:GLU:HG2	2.21	0.40
1:C:250:TRP:CD1	1:C:250:TRP:C	2.99	0.40
1:C:339:ALA:CB	1:C:370:ILE:HD11	2.52	0.40
1:C:397:ARG:HG3	1:C:397:ARG:HH11	1.86	0.40
1:A:23:GLU:HG3	1:A:24:THR:HG23	2.03	0.40
1:C:217:LEU:HB3	1:C:221:PHE:HB3	2.02	0.40
1:B:48:LYS:HB2	1:B:48:LYS:NZ	2.37	0.40
1:B:82:LYS:O	1:B:83:ARG:CB	2.66	0.40
1:B:250:TRP:CD1	1:B:250:TRP:C	2.99	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:MET:CE	1:B:127:MET:CE[2_565]	2.03	0.17

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	393/398 (99%)	383 (98%)	9 (2%)	1 (0%)	36	42
1	B	393/398 (99%)	379 (96%)	11 (3%)	3 (1%)	16	16
1	C	393/398 (99%)	380 (97%)	10 (2%)	3 (1%)	16	16
All	All	1179/1194 (99%)	1142 (97%)	30 (2%)	7 (1%)	21	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	B	83	ARG
1	C	83	ARG
1	C	330	ALA
1	B	330	ALA
1	C	17	ASN
1	B	17	ASN

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	317/319 (99%)	315 (99%)	2 (1%)	78	89
1	B	317/319 (99%)	313 (99%)	4 (1%)	61	76
1	C	317/319 (99%)	312 (98%)	5 (2%)	55	71
All	All	951/957 (99%)	940 (99%)	11 (1%)	63	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	A	224	MET
1	B	74	GLU

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Mol	Chain	Res	Type
1	B	98	ASP
1	B	188	GLU
1	B	224	MET
1	C	74	GLU
1	C	109	ASP
1	C	224	MET
1	C	266	LEU
1	C	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	106	ASN
1	A	163	GLN
1	A	173	HIS
1	A	230	GLN
1	A	247	ASN
1	A	263	HIS
1	A	286	HIS
1	A	293	ASN
1	A	334	HIS
1	B	17	ASN
1	B	99	ASN
1	B	106	ASN
1	B	163	GLN
1	B	173	HIS
1	B	230	GLN
1	B	247	ASN
1	B	263	HIS
1	B	286	HIS
1	B	293	ASN
1	B	334	HIS
1	B	358	ASN
1	C	99	ASN
1	C	106	ASN
1	C	163	GLN
1	C	173	HIS
1	C	178	GLN
1	C	202	ASN
1	C	230	GLN
1	C	247	ASN

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Mol	Chain	Res	Type
1	C	263	HIS
1	C	286	HIS
1	C	293	ASN
1	C	334	HIS
1	C	358	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LGT	B	502	2	13,13,13	1.42	1 (7%)	16,18,18	0.85	0
3	LGT	C	503	2	13,13,13	1.28	1 (7%)	16,18,18	0.82	0
3	LGT	A	501	2	13,13,13	1.27	1 (7%)	16,18,18	0.84	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	LGT	B	502	2	-	6/20/20/20	-
3	LGT	C	503	2	-	4/20/20/20	-
3	LGT	A	501	2	-	6/20/20/20	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	LGT	C2-C1	3.55	1.57	1.52
3	C	503	LGT	C2-C1	2.83	1.56	1.52
3	A	501	LGT	C2-C1	2.68	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	LGT	O5-C5-C6-O6B
3	C	503	LGT	O5-C5-C6-O6A
3	B	502	LGT	O5-C5-C6-O6A
3	B	502	LGT	O5-C5-C6-O6B
3	C	503	LGT	O1A-C1-C2-C3
3	C	503	LGT	O1B-C1-C2-C3
3	A	501	LGT	O1A-C1-C2-C3
3	A	501	LGT	O5-C5-C6-O6A
3	A	501	LGT	O1B-C1-C2-C3
3	A	501	LGT	O5-C5-C6-O6B
3	A	501	LGT	C4-C5-C6-O6A
3	A	501	LGT	C4-C5-C6-O6B
3	B	502	LGT	O1A-C1-C2-C3
3	B	502	LGT	C4-C5-C6-O6B
3	B	502	LGT	O1B-C1-C2-C3
3	B	502	LGT	C4-C5-C6-O6A

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	395/398 (99%)	-0.19	8 (2%) 65 62	20, 27, 42, 56	0
1	B	395/398 (99%)	0.32	17 (4%) 40 36	24, 36, 58, 75	0
1	C	395/398 (99%)	0.40	30 (7%) 20 17	22, 35, 60, 74	0
All	All	1185/1194 (99%)	0.18	55 (4%) 37 34	20, 33, 57, 75	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	9.4
1	B	17	ASN	7.3
1	C	16	ALA	6.2
1	C	15	ALA	6.2
1	C	17	ASN	5.0
1	B	15	ALA	4.8
1	A	4	SER	4.4
1	C	13	ALA	4.0
1	C	177	ASP	3.6
1	C	14	LYS	3.6
1	B	177	ASP	3.6
1	B	14	LYS	3.5
1	C	18	THR	3.5
1	B	18	THR	3.4
1	C	218	GLY	3.4
1	C	188	GLU	3.1
1	A	177	ASP	3.1
1	C	398	PRO	3.0
1	C	204	ALA	2.9
1	C	180	LEU	2.9
1	A	238	ARG	2.9
1	B	386	ARG	2.8
1	B	19	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	238	ARG	2.7
1	C	207	ILE	2.7
1	B	98	ASP	2.6
1	C	4	SER	2.6
1	A	215	GLU	2.6
1	C	74	GLU	2.6
1	B	9	ALA	2.5
1	A	19	ARG	2.5
1	B	13	ALA	2.4
1	C	246	PHE	2.4
1	A	98	ASP	2.4
1	C	397	ARG	2.4
1	B	218	GLY	2.3
1	C	9	ALA	2.3
1	C	216	ALA	2.3
1	C	19	ARG	2.3
1	C	55	LYS	2.3
1	C	211	THR	2.3
1	C	184	VAL	2.3
1	B	11	THR	2.3
1	C	396	LYS	2.3
1	B	4	SER	2.2
1	C	364	ARG	2.2
1	C	244	GLU	2.2
1	B	10	VAL	2.2
1	C	245	GLN	2.2
1	B	397	ARG	2.1
1	C	41	ALA	2.1
1	C	247	ASN	2.1
1	B	378	PHE	2.1
1	A	16	ALA	2.1
1	A	219	ASP	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	LGT	C	503	14/14	0.84	0.12	42,45,47,48	0
3	LGT	B	502	14/14	0.86	0.11	37,40,45,45	0
2	MG	B	902	1/1	0.93	0.07	41,41,41,41	0
3	LGT	A	501	14/14	0.94	0.08	23,27,36,37	0
2	MG	C	903	1/1	0.96	0.06	50,50,50,50	0
2	MG	A	901	1/1	0.99	0.11	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.