



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 AM UTC

PDB ID : 3PFB / pdb_00003pfb
Title : Crystal structure of the Lactobacillus johnsonii cinnamoyl esterase LJ0536 S106A mutant in complex with ethylferulate
Authors : Stogios, P.J.; Lai, K.K.; Vu, C.; Xu, X.; Cui, H.; Molloy, S.; Gonzalez, C.F.; Yakunin, A.; Savchenko, A.
Deposited on : 2010-10-28
Resolution : 1.58 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

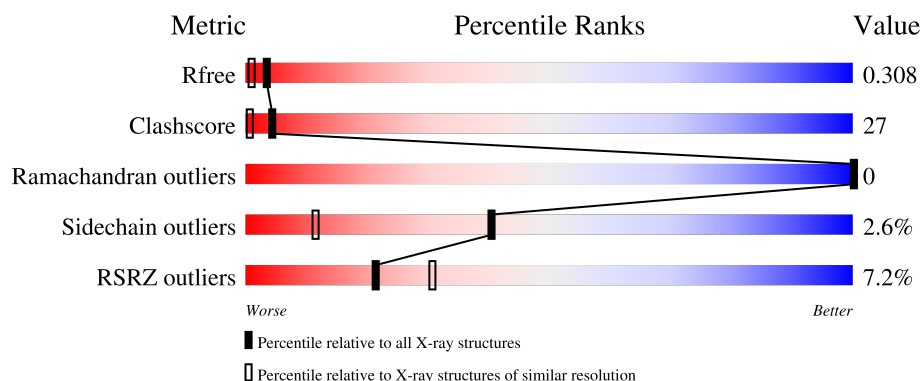
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	270	
1	B	270	

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	NH4	A	252	-	-	X	-
2	NH4	A	253	-	-	X	-
2	NH4	B	258	-	-	X	-
4	ZYC	A	256	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4898 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 Cinnamoyl esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	2	0
			1965	1246	332	381	6			
1	B	250	Total	C	N	O	S	0	4	0
			1974	1253	331	384	6			

There are 44 discrepancies between the modelled and reference sequences:

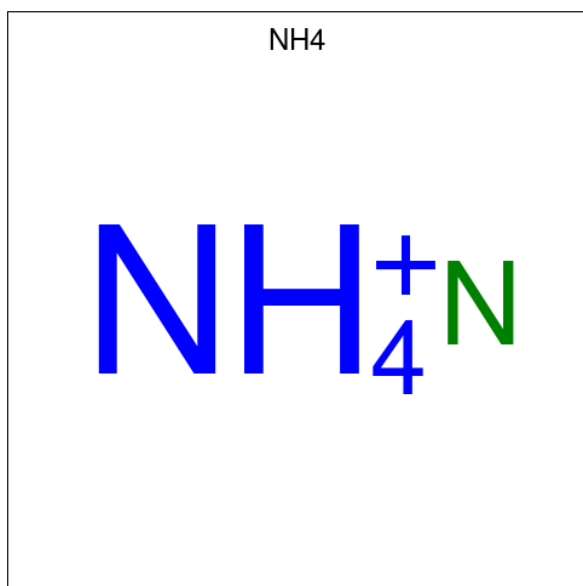
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP D3YEX6
A	-19	GLY	-	expression tag	UNP D3YEX6
A	-18	SER	-	expression tag	UNP D3YEX6
A	-17	SER	-	expression tag	UNP D3YEX6
A	-16	HIS	-	expression tag	UNP D3YEX6
A	-15	HIS	-	expression tag	UNP D3YEX6
A	-14	HIS	-	expression tag	UNP D3YEX6
A	-13	HIS	-	expression tag	UNP D3YEX6
A	-12	HIS	-	expression tag	UNP D3YEX6
A	-11	HIS	-	expression tag	UNP D3YEX6
A	-10	SER	-	expression tag	UNP D3YEX6
A	-9	SER	-	expression tag	UNP D3YEX6
A	-8	GLY	-	expression tag	UNP D3YEX6
A	-7	ARG	-	expression tag	UNP D3YEX6
A	-6	GLU	-	expression tag	UNP D3YEX6
A	-5	ASN	-	expression tag	UNP D3YEX6
A	-4	LEU	-	expression tag	UNP D3YEX6
A	-3	TYR	-	expression tag	UNP D3YEX6
A	-2	PHE	-	expression tag	UNP D3YEX6
A	-1	GLN	-	expression tag	UNP D3YEX6
A	0	GLY	-	expression tag	UNP D3YEX6
A	106	ALA	SER	engineered mutation	UNP D3YEX6
B	-20	MET	-	expression tag	UNP D3YEX6
B	-19	GLY	-	expression tag	UNP D3YEX6
B	-18	SER	-	expression tag	UNP D3YEX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP D3YEX6
B	-16	HIS	-	expression tag	UNP D3YEX6
B	-15	HIS	-	expression tag	UNP D3YEX6
B	-14	HIS	-	expression tag	UNP D3YEX6
B	-13	HIS	-	expression tag	UNP D3YEX6
B	-12	HIS	-	expression tag	UNP D3YEX6
B	-11	HIS	-	expression tag	UNP D3YEX6
B	-10	SER	-	expression tag	UNP D3YEX6
B	-9	SER	-	expression tag	UNP D3YEX6
B	-8	GLY	-	expression tag	UNP D3YEX6
B	-7	ARG	-	expression tag	UNP D3YEX6
B	-6	GLU	-	expression tag	UNP D3YEX6
B	-5	ASN	-	expression tag	UNP D3YEX6
B	-4	LEU	-	expression tag	UNP D3YEX6
B	-3	TYR	-	expression tag	UNP D3YEX6
B	-2	PHE	-	expression tag	UNP D3YEX6
B	-1	GLN	-	expression tag	UNP D3YEX6
B	0	GLY	-	expression tag	UNP D3YEX6
B	106	ALA	SER	engineered mutation	UNP D3YEX6

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0

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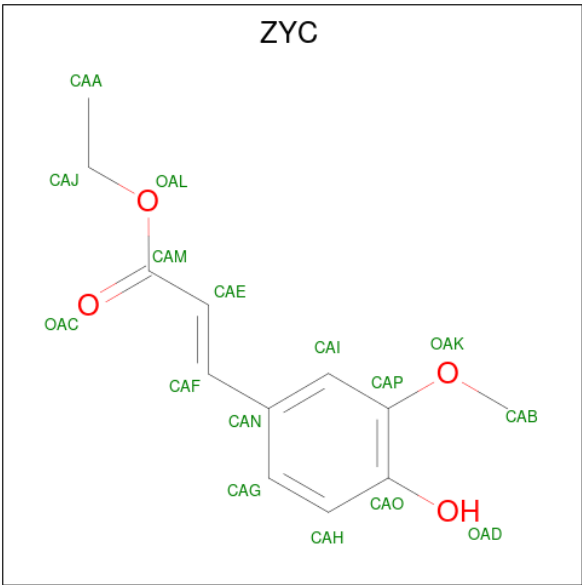
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ethyl (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate (CCD ID: ZYC) (formula: C₁₂H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	12	4		
4	B	1	Total	C	O	0	0
			16	12	4		

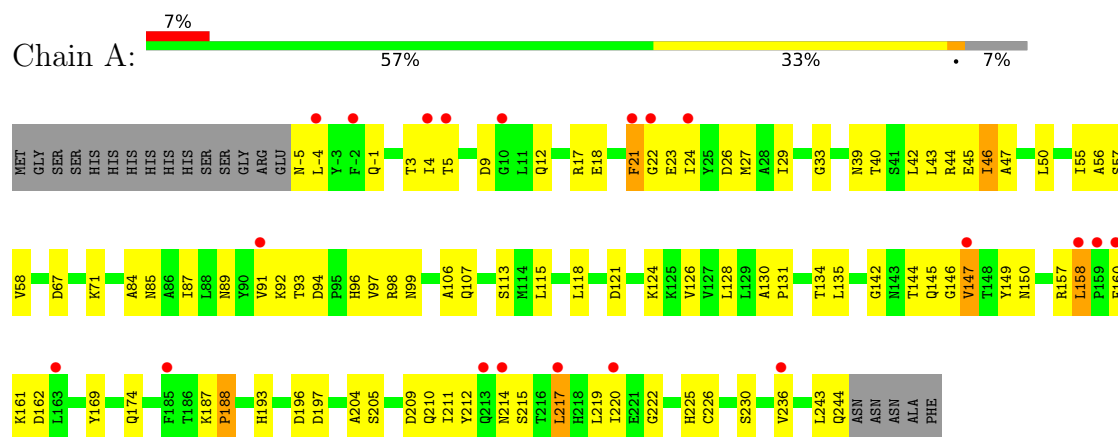
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	449	Total	O	0	0
			449	449		
5	B	458	Total	O	0	0
			458	458		

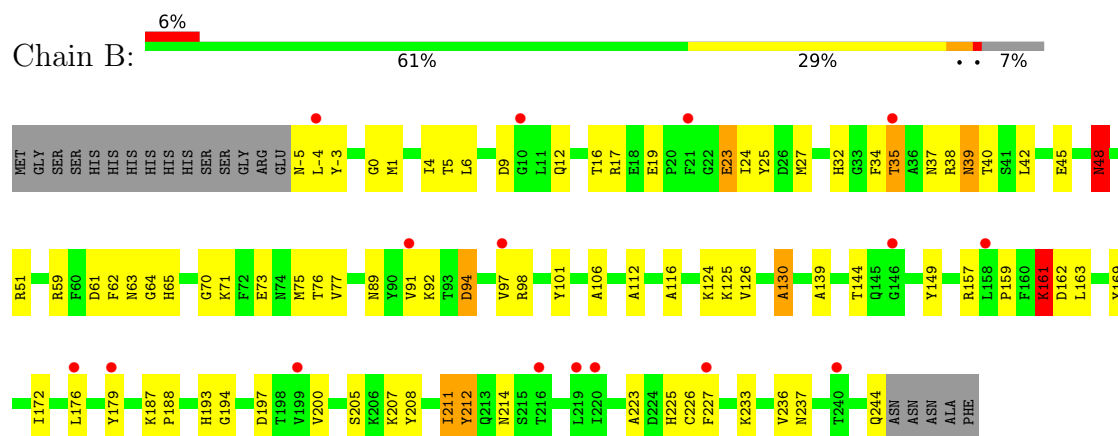
3 Residue-property plots [i](#)

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: Cinnamoyl esterase



• Molecule 1: Cinnamoyl esterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.26Å 83.89Å 88.95Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	44.20 – 1.58 44.20 – 1.58	Depositor EDS
% Data completeness (in resolution range)	73.1 (44.20-1.58) 73.0 (44.20-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.304 0.218 , 0.308	Depositor DCC
R_{free} test set	2673 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4898	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 21.99 % 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 6.2515e-03.*

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: NH4, ZYC, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	4/2011 (0.2%)	1.17	3/2732 (0.1%)
1	B	1.28	4/2026 (0.2%)	1.25	6/2753 (0.2%)
All	All	1.27	8/4037 (0.2%)	1.21	9/5485 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	ALA	C-O	9.30	1.28	1.23
1	B	130	ALA	CA-CB	9.21	1.60	1.52
1	B	116	ALA	CA-CB	-7.43	1.41	1.53
1	A	46	ILE	CA-CB	7.00	1.61	1.54
1	A	84	ALA	CA-CB	-6.05	1.43	1.53
1	A	220	ILE	CA-CB	5.81	1.60	1.53
1	A	58	VAL	C-O	5.61	1.29	1.24
1	B	211	ILE	CA-CB	5.20	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	THR	N-CA-CB	-8.48	104.50	114.17
1	B	161	LYS	N-CA-C	7.52	120.42	111.02
1	B	94	ASP	CA-C-N	6.32	125.94	119.56
1	B	94	ASP	C-N-CA	6.32	125.94	119.56
1	A	94	ASP	CA-C-N	-6.18	114.52	120.83
1	A	94	ASP	C-N-CA	-6.18	114.52	120.83
1	B	48	ASN	N-CA-C	5.99	117.47	111.07
1	B	212	TYR	N-CA-C	5.92	119.56	110.20
1	A	188	PRO	N-CA-C	5.11	118.90	111.03

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	1965	0	1926	103	0
1	B	1974	0	1937	106	0
2	A	5	0	0	6	0
2	B	11	0	0	2	0
3	A	1	0	0	0	0
3	B	3	0	0	2	0
4	A	16	0	13	13	0
4	B	16	0	13	3	0
5	A	449	0	0	39	0
5	B	458	0	0	43	0
All	All	4898	0	3889	210	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 27.

All (210) 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:6:LEU:HG	5:B:1785:HOH:O	1.42	1.19
2:B:258:NH4:N	3:B:261:CL:CL	2.28	1.02
1:A:26:ASP:HA	5:A:2076:HOH:O	1.60	1.01
1:B:161:LYS:O	1:B:161:LYS:HG2	1.57	1.00
1:B:65:HIS:HB3	5:B:1620:HOH:O	1.63	0.99
1:B:94:ASP:HB2	5:B:1545:HOH:O	1.63	0.97
1:A:225:HIS:HE1	4:A:256:ZYC:CAJ	1.77	0.96
1:B:42:LEU:HD12	5:B:2005:HOH:O	1.65	0.96
1:B:193:HIS:HB2	5:B:775:HOH:O	1.68	0.93
1:B:214:ASN:HB2	5:B:923:HOH:O	1.68	0.93
1:B:5:THR:HG23	5:B:1019:HOH:O	1.65	0.93
1:A:126:VAL:HG11	5:A:1846:HOH:O	1.70	0.92
1:B:45:GLU:HG3	1:B:236:VAL:HG21	1.50	0.92
1:A:226:CYS:SG	5:A:2014:HOH:O	2.26	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:CD1	5:A:1103:HOH:O	2.19	0.89
1:B:233:LYS:HE3	1:B:237:ASN:HD21	1.35	0.89
1:A:225:HIS:HE1	4:A:256:ZYC:HAJ	1.40	0.85
1:A:29:ILE:HD13	5:A:1687:HOH:O	1.76	0.85
1:B:161:LYS:O	1:B:162:ASP:HB2	1.77	0.83
1:B:4:ILE:HG22	5:B:1785:HOH:O	1.78	0.83
1:A:225:HIS:CE1	4:A:256:ZYC:HAJ	2.16	0.81
1:B:34:PHE:O	1:B:35:THR:HB	1.80	0.78
1:B:23:GLU:C	1:B:24:ILE:HD12	2.09	0.78
4:A:256:ZYC:HAAA	5:A:2055:HOH:O	1.83	0.77
1:B:71:LYS:HD2	1:B:73[B]:GLU:OE2	1.86	0.76
1:B:244:GLN:HB3	5:B:863:HOH:O	1.83	0.76
1:B:126:VAL:HG13	5:B:312:HOH:O	1.86	0.75
1:B:233:LYS:HD2	5:B:649:HOH:O	1.85	0.75
1:A:225:HIS:CE1	4:A:256:ZYC:CAJ	2.66	0.74
1:B:24:ILE:HG22	5:B:845:HOH:O	1.88	0.74
1:B:161:LYS:O	1:B:161:LYS:CG	2.34	0.73
1:A:99:ASN:N	5:A:2076:HOH:O	2.22	0.72
1:B:35:THR:H	1:B:65:HIS:HE1	1.36	0.72
1:B:233:LYS:HE3	1:B:237:ASN:ND2	2.05	0.71
1:A:161:LYS:HG3	1:A:162:ASP:H	1.55	0.71
1:A:39:ASN:ND2	1:A:44:ARG:HH11	1.89	0.71
1:B:91:VAL:HG12	5:B:1708:HOH:O	1.91	0.70
1:A:9:ASP:O	1:B:9:ASP:O	2.10	0.70
1:A:113:SER:HA	5:A:1846:HOH:O	1.91	0.70
1:B:161:LYS:O	1:B:162:ASP:CB	2.40	0.70
1:B:233:LYS:CE	1:B:237:ASN:HD21	2.04	0.70
1:A:161:LYS:HG3	1:A:162:ASP:N	2.06	0.70
1:B:32:HIS:CE1	1:B:62:PHE:H	2.10	0.70
1:A:106:ALA:CB	4:A:256:ZYC:HAJA	2.22	0.69
1:B:187:LYS:HB3	1:B:188:PRO:CD	2.22	0.69
1:A:115:LEU:HB2	5:A:1157:HOH:O	1.94	0.68
1:A:193:HIS:HD2	1:A:205:SER:OG	1.76	0.68
1:B:179:TYR:CZ	1:B:207:LYS:HG2	2.31	0.66
1:B:1:MET:HE1	5:B:1857:HOH:O	1.96	0.66
1:B:159:PRO:HG3	5:B:1438:HOH:O	1.94	0.66
1:A:150:ASN:OD1	2:A:254:NH4:N	2.29	0.66
1:A:217:LEU:HD21	1:A:219:LEU:HG	1.77	0.66
1:B:12:GLN:HG2	5:B:854:HOH:O	1.98	0.63
1:B:77:VAL:HG11	1:B:176:LEU:HD21	1.79	0.63
1:A:161:LYS:CG	1:A:162:ASP:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLU:HG3	1:A:47:ALA:HB1	1.80	0.63
1:A:5:THR:HG21	5:A:530:HOH:O	1.99	0.62
1:A:85:ASN:HB2	5:A:1103:HOH:O	1.99	0.62
1:A:5:THR:OG1	1:A:12:GLN:NE2	2.27	0.62
1:A:118:LEU:HD22	5:B:1125:HOH:O	1.99	0.62
1:A:144:THR:CG2	4:A:256:ZYC:HABB	2.30	0.62
1:A:57:SER:HB3	5:A:1633:HOH:O	2.00	0.62
1:B:24:ILE:HG13	5:B:579:HOH:O	2.00	0.61
1:B:32:HIS:HE1	1:B:61:ASP:HA	1.64	0.61
1:A:225:HIS:HE1	4:A:256:ZYC:HAJA	1.63	0.61
1:A:-5:ASN:HA	1:A:22:GLY:O	2.00	0.61
1:B:161:LYS:O	1:B:161:LYS:NZ	2.30	0.61
1:B:193:HIS:HD2	1:B:205:SER:OG	1.84	0.61
1:A:93:THR:HG22	5:B:1786:HOH:O	2.00	0.61
1:B:244:GLN:OE1	5:B:1685:HOH:O	2.16	0.61
1:A:115:LEU:HD13	5:A:1103:HOH:O	1.94	0.60
1:A:50:LEU:HD13	5:A:1633:HOH:O	2.01	0.60
1:A:147:VAL:HG21	1:A:160:PHE:CD1	2.37	0.59
1:B:32:HIS:CE1	1:B:61:ASP:HA	2.38	0.59
1:A:39:ASN:ND2	1:A:44:ARG:NH1	2.51	0.58
1:A:144:THR:CG2	4:A:256:ZYC:CAB	2.81	0.58
1:A:236:VAL:HG12	5:A:878:HOH:O	2.03	0.58
1:B:225:HIS:HE1	4:B:264:ZYC:OAL	1.86	0.58
1:B:17:ARG:HG3	5:B:387:HOH:O	2.02	0.58
1:B:35:THR:H	1:B:65:HIS:CE1	2.19	0.58
1:A:33:GLY:HA3	4:A:256:ZYC:HAAB	1.85	0.58
1:A:71[A]:LYS:NZ	5:A:1392:HOH:O	2.36	0.58
1:A:210:GLN:HA	5:A:1885:HOH:O	2.02	0.58
1:B:124:LYS:HG3	5:B:1327:HOH:O	2.04	0.57
1:A:5:THR:HB	5:A:1598:HOH:O	2.02	0.57
1:A:174:GLN:HB3	5:A:1561:HOH:O	2.04	0.56
1:B:32:HIS:HE1	1:B:62:PHE:H	1.51	0.56
1:B:112:ALA:HB1	5:B:312:HOH:O	2.05	0.56
1:B:193:HIS:HE1	1:B:200:VAL:O	1.89	0.55
1:B:25:TYR:CA	5:B:845:HOH:O	2.54	0.55
1:A:215:SER:OG	2:A:252:NH4:N	2.39	0.55
1:B:106:ALA:HA	1:B:130:ALA:O	2.07	0.55
1:B:76:THR:HG22	1:B:169:TYR:HA	1.89	0.54
1:A:24:ILE:HD11	5:A:2100:HOH:O	2.06	0.54
1:A:98:ARG:HB3	5:A:2076:HOH:O	2.07	0.54
1:B:38:ARG:HD2	1:B:59:ARG:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CD2	5:A:1662:HOH:O	2.59	0.54
1:B:48:ASN:ND2	5:B:1626:HOH:O	2.36	0.54
1:A:67:ASP:HA	5:A:1773:HOH:O	2.06	0.53
1:A:115:LEU:HD11	5:A:1103:HOH:O	1.95	0.53
1:A:50:LEU:HD21	1:A:243:LEU:HD12	1.90	0.53
1:A:187:LYS:HB3	1:A:188:PRO:CD	2.38	0.53
1:A:225:HIS:CE1	4:A:256:ZYC:HAJA	2.41	0.53
1:B:37:ASN:HA	5:B:1620:HOH:O	2.07	0.53
1:B:24:ILE:HD11	5:B:1803:HOH:O	2.07	0.53
1:B:159:PRO:CG	5:B:1438:HOH:O	2.55	0.53
1:B:161:LYS:HZ2	1:B:162:ASP:HB2	1.72	0.53
1:A:196[A]:ASP:OD2	1:A:222:GLY:HA2	2.08	0.52
1:B:187:LYS:HB3	1:B:188:PRO:HD3	1.92	0.52
1:A:4:ILE:HD13	1:A:17:ARG:HB2	1.91	0.52
1:B:226:CYS:HA	5:B:717:HOH:O	2.08	0.52
1:B:179:TYR:CD2	1:B:207:LYS:HE2	2.44	0.52
1:A:39:ASN:HD22	1:A:44:ARG:HH11	1.55	0.51
1:A:107:GLN:HB2	4:A:256:ZYC:HAF	1.91	0.51
1:A:24:ILE:HG13	5:A:1684:HOH:O	2.10	0.51
1:B:39:ASN:HD21	1:B:59:ARG:HH21	1.58	0.51
1:A:45:GLU:HG2	1:A:236:VAL:HG11	1.91	0.51
1:B:214:ASN:CB	5:B:923:HOH:O	2.42	0.51
1:A:89:ASN:HD22	1:A:92:LYS:HE2	1.76	0.51
1:B:63:ASN:HD21	1:B:75:MET:HA	1.76	0.51
1:B:40:THR:HB	2:B:258:NH4:N	2.25	0.51
1:A:-4:LEU:HD12	2:A:253:NH4:N	2.25	0.50
1:A:3:THR:OG1	5:A:1560:HOH:O	2.18	0.50
1:A:29:ILE:HD11	1:A:91:VAL:HG21	1.93	0.50
1:A:27:MET:HE3	1:A:56:ALA:HB1	1.94	0.50
1:B:179:TYR:CE1	1:B:207:LYS:HG2	2.46	0.50
1:A:-1:GLN:O	5:A:275:HOH:O	2.19	0.50
1:A:17:ARG:CZ	1:A:27:MET:HE1	2.43	0.49
1:A:142:GLY:HA2	1:A:149:TYR:CE1	2.47	0.49
1:B:12:GLN:CG	5:B:854:HOH:O	2.59	0.49
1:A:149:TYR:CD2	1:A:158:LEU:HD11	2.47	0.49
1:B:25:TYR:C	5:B:845:HOH:O	2.55	0.49
1:A:98:ARG:HG3	5:A:779:HOH:O	2.12	0.49
1:A:124:LYS:NZ	5:A:1738:HOH:O	2.33	0.49
1:A:98:ARG:N	5:A:2076:HOH:O	2.39	0.49
1:B:124:LYS:NZ	5:B:1077:HOH:O	2.45	0.49
1:A:146:GLY:HA2	5:A:2041:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLN:HB3	5:A:1825:HOH:O	2.12	0.49
1:A:212:TYR:O	2:A:252:NH4:N	2.46	0.49
1:A:4:ILE:HD13	1:A:17:ARG:CB	2.43	0.49
1:A:106:ALA:HA	1:A:130:ALA:O	2.14	0.48
1:B:-3:TYR:HA	5:B:1717:HOH:O	2.13	0.48
1:A:197:ASP:OD2	1:A:225:HIS:HD2	1.96	0.48
1:B:98:ARG:HB2	5:B:845:HOH:O	2.13	0.48
1:A:27:MET:HE3	1:A:56:ALA:CB	2.43	0.48
1:A:97:VAL:O	5:A:1534:HOH:O	2.20	0.47
1:A:145:GLN:HE21	1:A:160:PHE:HZ	1.61	0.47
1:B:42:LEU:HA	5:B:2005:HOH:O	2.14	0.47
1:B:-4[A]:LEU:HA	3:B:263:CL:CL	2.52	0.47
1:B:194:GLY:HA3	1:B:223:ALA:HB3	1.97	0.46
1:A:27:MET:CE	1:A:56:ALA:HB1	2.44	0.46
1:A:87:ILE:HB	5:A:1687:HOH:O	2.14	0.46
1:B:89:ASN:HA	1:B:92:LYS:HE2	1.97	0.46
1:B:197:ASP:OD2	1:B:225:HIS:HD2	1.98	0.46
1:B:71:LYS:CD	1:B:73[B]:GLU:OE2	2.61	0.46
1:B:75:MET:HE3	1:B:75:MET:HB3	1.85	0.46
1:B:144:THR:HG23	1:B:149:TYR:OH	2.16	0.45
1:B:179:TYR:HD1	1:B:211:ILE:HD13	1.81	0.45
1:B:27:MET:HE2	5:B:387:HOH:O	2.16	0.45
1:B:139:ALA:HA	1:B:149:TYR:OH	2.17	0.45
1:B:144:THR:CG2	1:B:149:TYR:OH	2.65	0.45
1:B:227:PHE:HD2	5:B:717:HOH:O	1.99	0.45
1:A:161:LYS:CG	1:A:162:ASP:N	2.73	0.45
1:B:144:THR:HG23	1:B:149:TYR:CE2	2.52	0.45
1:B:0:GLY:HA2	1:B:51:ARG:HH22	1.82	0.45
1:A:21:PHE:HD2	1:A:21:PHE:H	1.65	0.44
1:A:29:ILE:HG21	5:A:1687:HOH:O	2.16	0.44
1:B:12:GLN:HB3	5:B:1019:HOH:O	2.18	0.44
1:A:193:HIS:CD2	1:A:205:SER:OG	2.64	0.44
1:A:42:LEU:O	1:A:46:ILE:HG13	2.18	0.43
1:B:76:THR:HG21	1:B:172:ILE:HD12	1.99	0.43
1:A:121:ASP:OD2	5:A:821:HOH:O	2.21	0.43
1:A:135:LEU:HD12	1:A:135:LEU:C	2.44	0.43
1:B:211:ILE:HG13	1:B:212:TYR:N	2.34	0.43
1:B:101:TYR:CD1	1:B:125:LYS:HB2	2.54	0.43
1:B:1:MET:HE3	1:B:16:THR:CG2	2.49	0.43
1:B:39:ASN:ND2	1:B:59:ARG:HH21	2.17	0.43
1:B:73[A]:GLU:OE2	1:B:157:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:CG1	5:A:1846:HOH:O	2.48	0.43
1:A:128:LEU:HB3	1:A:131:PRO:HG3	2.00	0.43
1:A:4:ILE:CD1	1:A:17:ARG:HB3	2.49	0.42
1:B:32:HIS:HE1	1:B:62:PHE:N	2.17	0.42
1:B:97:VAL:HG11	5:B:1708:HOH:O	2.18	0.42
1:A:134:THR:HG23	1:A:204:ALA:HB2	2.01	0.42
1:B:23:GLU:HB3	1:B:24:ILE:CD1	2.50	0.42
1:B:187:LYS:NZ	5:B:1570:HOH:O	2.51	0.42
1:B:24:ILE:HD12	1:B:24:ILE:N	2.34	0.42
1:A:209:ASP:O	2:A:252:NH4:N	2.52	0.42
1:B:-5:ASN:N	1:B:19:GLU:OE2	2.50	0.42
1:B:51:ARG:NE	5:B:1868:HOH:O	2.52	0.42
1:B:23:GLU:HB3	1:B:24:ILE:HD12	2.03	0.41
1:A:55:ILE:HD11	1:A:244:GLN:HG2	2.02	0.41
1:B:214:ASN:HB2	5:B:767:HOH:O	2.20	0.41
1:A:217:LEU:C	1:A:217:LEU:HD23	2.46	0.41
1:A:4:ILE:HD11	1:A:17:ARG:HB3	2.03	0.41
1:B:144:THR:HG23	1:B:149:TYR:HE2	1.86	0.41
1:A:40:THR:OG1	1:A:43:LEU:HG	2.21	0.41
1:A:-5:ASN:HB2	2:A:253:NH4:N	2.35	0.41
1:A:91:VAL:HA	5:A:1556:HOH:O	2.20	0.41
1:B:106:ALA:HB1	4:B:264:ZYC:CAM	2.50	0.41
1:B:208:TYR:HA	1:B:211:ILE:HG12	2.03	0.41
1:B:225:HIS:HE1	4:B:264:ZYC:CAJ	2.33	0.41
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.85	0.40
1:A:169:TYR:CD2	1:A:169:TYR:C	2.99	0.40
1:B:63:ASN:O	1:B:65:HIS:HD2	2.03	0.40
1:B:64:GLY:HA2	1:B:70:GLY:O	2.21	0.40
1:A:12:GLN:NE2	5:A:825:HOH:O	2.53	0.40
1:A:187:LYS:C	1:A:214:ASN:HD22	2.28	0.40
1:A:-4:LEU:HD11	1:A:23:GLU:HB2	2.04	0.40
1:A:106:ALA:HB1	4:A:256:ZYC:CAM	2.51	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	250/270 (93%)	240 (96%)	10 (4%)	0	100	100
1	B	252/270 (93%)	237 (94%)	15 (6%)	0	100	100
All	All	502/540 (93%)	477 (95%)	25 (5%)	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	214/229 (93%)	207 (97%)	7 (3%)	33	6
1	B	216/229 (94%)	212 (98%)	4 (2%)	50	21
All	All	430/458 (94%)	419 (97%)	11 (3%)	40	11

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

Mol	Chain	Res	Type
1	A	21	PHE
1	A	147	VAL
1	A	157	ARG
1	A	158	LEU
1	A	211	ILE
1	A	217	LEU
1	A	230	SER
1	B	23	GLU
1	B	39	ASN
1	B	48	ASN
1	B	161	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	39	ASN
1	A	54	ASN
1	A	89	ASN
1	A	145	GLN
1	A	184	GLN
1	A	193	HIS
1	A	210	GLN
1	A	214	ASN
1	A	225	HIS
1	B	32	HIS
1	B	39	ASN
1	B	63	ASN
1	B	65	HIS
1	B	96	HIS
1	B	99	ASN
1	B	193	HIS
1	B	203	ASN
1	B	225	HIS
1	B	234	ASN
1	B	237	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 22 ligands modelled in this entry, 16 are modelled with single atom and 4 are monoatomic - leaving 2 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
4	ZYC	A	256	-	16,16,16	1.90	4 (25%)	20,20,20	3.38	10 (50%)
4	ZYC	B	264	-	16,16,16	1.58	4 (25%)	20,20,20	2.65	8 (40%)

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	ZYC	A	256	-	-	6/10/10/10	0/1/1/1
4	ZYC	B	264	-	-	5/10/10/10	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	256	ZYC	CAE-CAM	-5.17	1.36	1.48
4	B	264	ZYC	CAE-CAM	-4.00	1.39	1.48
4	A	256	ZYC	CAN-CAF	-3.99	1.36	1.47
4	B	264	ZYC	CAN-CAF	-2.79	1.39	1.47
4	A	256	ZYC	CAE-CAF	2.23	1.38	1.33
4	A	256	ZYC	OAL-CAM	2.14	1.39	1.34
4	B	264	ZYC	OAL-CAM	2.06	1.39	1.34
4	B	264	ZYC	CAE-CAF	2.00	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	256	ZYC	CAN-CAF-CAE	-9.94	105.21	126.92
4	B	264	ZYC	CAJ-OAL-CAM	6.44	129.14	116.38
4	A	256	ZYC	OAK-CAP-CAO	6.17	123.80	114.55
4	B	264	ZYC	OAL-CAJ-CAA	5.70	128.86	108.40
4	A	256	ZYC	CAB-OAK-CAP	-5.56	109.36	117.51
4	B	264	ZYC	OAK-CAP-CAO	4.86	121.84	114.55
4	A	256	ZYC	OAK-CAP-CAI	-4.33	116.62	124.08
4	B	264	ZYC	CAB-OAK-CAP	-3.18	112.85	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	256	ZYC	CAG-CAN-CAI	3.14	122.68	118.72
4	A	256	ZYC	OAC-CAM-CAE	-2.63	114.75	123.69
4	A	256	ZYC	OAL-CAM-CAE	2.48	117.68	111.55
4	B	264	ZYC	CAI-CAP-CAO	-2.44	117.58	120.04
4	A	256	ZYC	CAH-CAG-CAN	-2.37	118.15	121.22
4	B	264	ZYC	OAL-CAM-OAC	2.23	127.65	122.96
4	A	256	ZYC	CAI-CAN-CAF	-2.22	113.98	120.61
4	A	256	ZYC	OAL-CAM-OAC	2.19	127.57	122.96
4	B	264	ZYC	OAK-CAP-CAI	-2.03	120.57	124.08
4	B	264	ZYC	CAN-CAF-CAE	-2.03	122.49	126.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	264	ZYC	CAA-CAJ-OAL-CAM
4	A	256	ZYC	CAO-CAP-OAK-CAB
4	A	256	ZYC	CAE-CAF-CAN-CAI
4	A	256	ZYC	CAE-CAF-CAN-CAG
4	A	256	ZYC	CAI-CAP-OAK-CAB
4	A	256	ZYC	CAE-CAM-OAL-CAJ
4	B	264	ZYC	CAE-CAF-CAN-CAI
4	B	264	ZYC	CAE-CAF-CAN-CAG
4	A	256	ZYC	OAC-CAM-OAL-CAJ
4	B	264	ZYC	OAC-CAM-OAL-CAJ
4	B	264	ZYC	CAO-CAP-OAK-CAB

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	256	ZYC	13	0
4	B	264	ZYC	3	0

5.7 Other polymers

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	250/270 (92%)	0.91	20 (8%) 18 27	14, 23, 33, 40	2 (0%)
1	B	250/270 (92%)	0.82	16 (6%) 25 34	14, 22, 29, 34	4 (1%)
All	All	500/540 (92%)	0.87	36 (7%) 21 31	14, 23, 32, 40	6 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	4.0
1	A	21	PHE	3.9
1	A	158	LEU	3.9
1	A	160	PHE	3.7
1	A	22	GLY	3.1
1	A	10	GLY	3.0
1	B	21	PHE	2.8
1	B	146	GLY	2.7
1	B	216	THR	2.6
1	B	176	LEU	2.5
1	B	91	VAL	2.4
1	A	24	ILE	2.4
1	A	185	PHE	2.4
1	B	10	GLY	2.4
1	A	163	LEU	2.4
1	A	214	ASN	2.3
1	B	219	LEU	2.3
1	B	220	ILE	2.3
1	A	236	VAL	2.2
1	B	97	VAL	2.2
1	B	199	VAL	2.2
1	A	-4	LEU	2.2
1	B	158	LEU	2.2
1	A	4	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	179	TYR	2.2
1	A	5	THR	2.2
1	B	35	THR	2.2
1	A	91	VAL	2.2
1	B	-4[A]	LEU	2.1
1	A	-2	PHE	2.1
1	B	227	PHE	2.1
1	A	220	ILE	2.1
1	A	213	GLN	2.1
1	A	159	PRO	2.1
1	B	240	THR	2.0
1	A	217	LEU	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
4	ZYC	A	256	16/16	0.76	0.19	20,39,45,45	16
2	NH4	B	258	1/1	0.79	0.17	26,26,26,26	0
4	ZYC	B	264	16/16	0.87	0.12	20,31,33,34	0
2	NH4	A	254	1/1	0.89	0.13	30,30,30,30	0
2	NH4	B	259	1/1	0.92	0.10	25,25,25,25	0
3	CL	B	261	1/1	0.93	0.12	48,48,48,48	0
3	CL	A	255	1/1	0.94	0.14	49,49,49,49	0
3	CL	B	263	1/1	0.94	0.08	53,53,53,53	0
3	CL	B	262	1/1	0.95	0.09	44,44,44,44	0
2	NH4	B	251	1/1	0.95	0.14	22,22,22,22	0
2	NH4	B	257	1/1	0.95	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NH4	A	253	1/1	0.95	0.07	17,17,17,17	0
2	NH4	B	254	1/1	0.96	0.08	14,14,14,14	0
2	NH4	A	252	1/1	0.96	0.15	15,15,15,15	0
2	NH4	A	251	1/1	0.97	0.11	15,15,15,15	0
2	NH4	B	253	1/1	0.97	0.06	16,16,16,16	0
2	NH4	A	250	1/1	0.97	0.11	14,14,14,14	0
2	NH4	B	260	1/1	0.97	0.07	26,26,26,26	0
2	NH4	B	256	1/1	0.97	0.05	22,22,22,22	0
2	NH4	B	255	1/1	0.98	0.07	17,17,17,17	0
2	NH4	B	250	1/1	0.98	0.12	20,20,20,20	0
2	NH4	B	252	1/1	0.98	0.09	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.