



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:20 PM UTC

PDB ID : 6KTJ / pdb_00006ktj
Title : Crystal structure of scyllo-inositol dehydrogenase R178A mutant, apo-form, from *Paracoccus laeviglucosivorans*
Authors : Suzuki, M.; Koubara, K.; Takenoya, M.; Fukano, K.; Ito, S.; Sasaki, Y.; Nakamura, A.; Yajima, S.
Deposited on : 2019-08-28
Resolution : 2.10 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

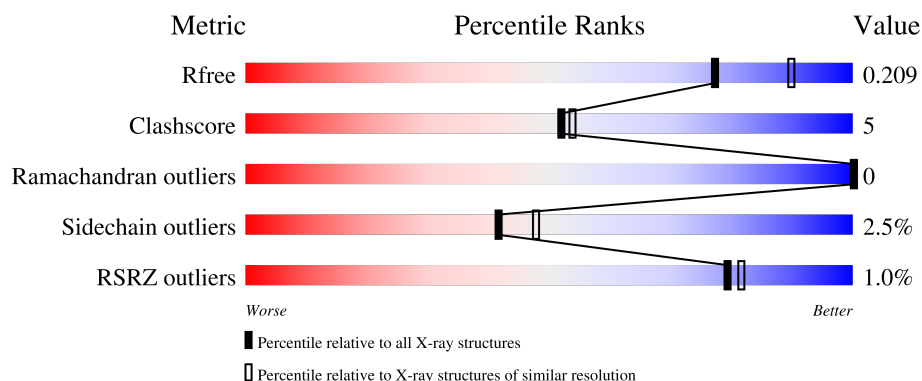
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	380	% 86% 10% ..
1	B	380	2% 84% 12% ..
1	C	380	% 89% 8% ..
1	D	380	% 87% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11585 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 Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2788	1747	509	514	18			
1	B	366	Total	C	N	O	S	0	0	0
			2779	1741	507	513	18			
1	C	368	Total	C	N	O	S	0	0	0
			2796	1753	510	515	18			
1	D	368	Total	C	N	O	S	0	1	0
			2802	1756	511	516	19			

There are 40 discrepancies between the modelled and reference sequences:

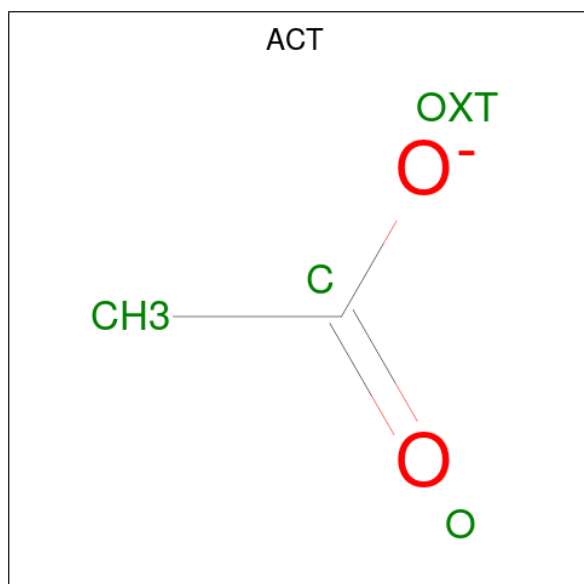
Chain	Residue	Modelled	Actual	Comment	Reference
A	72	SER	ASN	See sequence details	UNP K7ZP76
A	178	ALA	ARG	engineered mutation	UNP K7ZP76
A	373	LEU	-	expression tag	UNP K7ZP76
A	374	GLU	-	expression tag	UNP K7ZP76
A	375	HIS	-	expression tag	UNP K7ZP76
A	376	HIS	-	expression tag	UNP K7ZP76
A	377	HIS	-	expression tag	UNP K7ZP76
A	378	HIS	-	expression tag	UNP K7ZP76
A	379	HIS	-	expression tag	UNP K7ZP76
A	380	HIS	-	expression tag	UNP K7ZP76
B	72	SER	ASN	See sequence details	UNP K7ZP76
B	178	ALA	ARG	engineered mutation	UNP K7ZP76
B	373	LEU	-	expression tag	UNP K7ZP76
B	374	GLU	-	expression tag	UNP K7ZP76
B	375	HIS	-	expression tag	UNP K7ZP76
B	376	HIS	-	expression tag	UNP K7ZP76
B	377	HIS	-	expression tag	UNP K7ZP76
B	378	HIS	-	expression tag	UNP K7ZP76
B	379	HIS	-	expression tag	UNP K7ZP76
B	380	HIS	-	expression tag	UNP K7ZP76

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Chain	Residue	Modelled	Actual	Comment	Reference
C	72	SER	ASN	See sequence details	UNP K7ZP76
C	178	ALA	ARG	engineered mutation	UNP K7ZP76
C	373	LEU	-	expression tag	UNP K7ZP76
C	374	GLU	-	expression tag	UNP K7ZP76
C	375	HIS	-	expression tag	UNP K7ZP76
C	376	HIS	-	expression tag	UNP K7ZP76
C	377	HIS	-	expression tag	UNP K7ZP76
C	378	HIS	-	expression tag	UNP K7ZP76
C	379	HIS	-	expression tag	UNP K7ZP76
C	380	HIS	-	expression tag	UNP K7ZP76
D	72	SER	ASN	See sequence details	UNP K7ZP76
D	178	ALA	ARG	engineered mutation	UNP K7ZP76
D	373	LEU	-	expression tag	UNP K7ZP76
D	374	GLU	-	expression tag	UNP K7ZP76
D	375	HIS	-	expression tag	UNP K7ZP76
D	376	HIS	-	expression tag	UNP K7ZP76
D	377	HIS	-	expression tag	UNP K7ZP76
D	378	HIS	-	expression tag	UNP K7ZP76
D	379	HIS	-	expression tag	UNP K7ZP76
D	380	HIS	-	expression tag	UNP K7ZP76

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

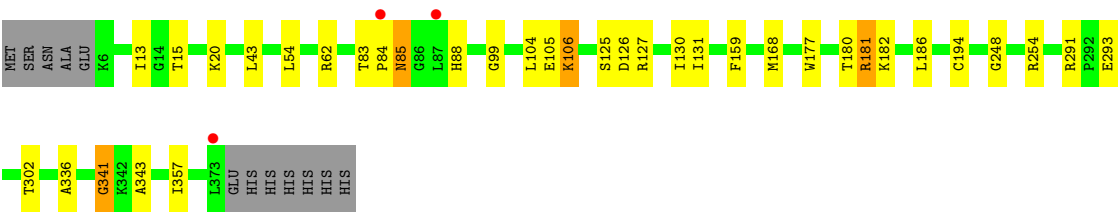
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	86	Total	O	0	0
			86	86		
3	C	101	Total	O	0	0
			101	101		
3	D	112	Total	O	0	0
			112	112		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.66Å 128.78Å 138.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.10 49.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.20-2.10) 99.3 (49.20-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.181 , 0.207 0.186 , 0.209	Depositor DCC
R_{free} test set	4758 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11585	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: ACT

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	0.97	0/2854	1.30	0/3869
1	B	0.98	0/2845	1.33	0/3858
1	C	0.98	0/2862	1.33	0/3880
1	D	0.96	0/2868	1.30	4/3888 (0.1%)
All	All	0.97	0/11429	1.32	4/15495 (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	D	62	ARG	CA-C-N	6.09	126.38	122.18
1	D	62	ARG	C-N-CA	6.09	126.38	122.18
1	D	341	GLY	CA-C-N	5.33	128.44	120.87
1	D	341	GLY	C-N-CA	5.33	128.44	120.87

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	2788	0	2707	30	0
1	B	2779	0	2694	37	0
1	C	2796	0	2718	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2802	0	2722	27	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	105	0	0	0	0
3	B	86	0	0	0	0
3	C	101	0	0	0	0
3	D	112	0	0	1	0
All	All	11585	0	10853	113	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 (113) 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:C:15:THR:HB	1:C:54:LEU:HD23	1.24	1.10
1:B:47:PRO:O	1:B:50:LYS:HB3	1.56	1.05
1:A:168:MET:HE1	1:A:179:LEU:HD21	1.47	0.95
1:B:168:MET:HA	1:B:168:MET:HE2	1.51	0.90
1:D:194[B]:CYS:SG	1:D:357:ILE:HD13	2.12	0.90
1:B:15:THR:HG22	1:B:43:LEU:HD11	1.55	0.89
1:C:15:THR:HG22	1:C:43:LEU:HD11	1.54	0.88
1:B:220:ASP:HB3	1:B:227:THR:HG23	1.57	0.86
1:C:15:THR:OG1	1:C:50:LYS:HE2	1.74	0.86
1:C:15:THR:HG23	1:C:45:ASP:HB2	1.61	0.83
1:D:106:LYS:HD2	1:D:194[A]:CYS:SG	2.21	0.80
1:C:15:THR:HB	1:C:54:LEU:CD2	2.12	0.77
1:C:15:THR:CB	1:C:54:LEU:HD23	2.12	0.72
1:B:169:ALA:HB1	1:B:257:ARG:HD3	1.72	0.72
1:A:39:ARG:NH2	1:A:41:GLU:OE2	2.23	0.71
1:D:336:ALA:HA	1:D:341:GLY:O	1.92	0.69
1:D:83:THR:HB	1:D:84:PRO:CD	2.23	0.69
1:D:106:LYS:HE2	1:D:106:LYS:C	2.19	0.68
1:B:62:ARG:NH1	1:B:69:GLU:OE2	2.25	0.68
1:B:168:MET:HG3	1:B:254:ARG:HD2	1.77	0.65
1:B:220:ASP:HB3	1:B:227:THR:CG2	2.26	0.65
1:C:66:ASP:O	1:C:69:GLU:HB3	1.98	0.63
1:B:106:LYS:HD2	1:B:106:LYS:C	2.24	0.62
1:C:15:THR:HG23	1:C:45:ASP:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HD12	1:D:357:ILE:HD12	1.82	0.61
1:C:336:ALA:HA	1:C:341:GLY:O	2.01	0.61
1:D:181:ARG:CG	1:D:181:ARG:HH11	2.13	0.60
1:A:18:MET:CE	1:A:326:LYS:HE2	2.32	0.59
1:B:68:ARG:NH1	1:B:90:GLU:OE2	2.35	0.59
1:D:83:THR:HB	1:D:84:PRO:HD2	1.84	0.59
1:B:209:ARG:HG3	1:B:371:ASN:OD1	2.02	0.59
1:B:71:VAL:HG13	1:B:95:ALA:HA	1.85	0.58
1:B:175:TRP:CG	1:B:228:ALA:HB3	2.41	0.56
1:A:83:THR:HB	1:A:84:PRO:HD2	1.87	0.55
1:A:106:LYS:HD2	1:A:106:LYS:C	2.32	0.55
1:B:99:GLY:O	1:B:127:ARG:HD2	2.07	0.55
1:B:169:ALA:CB	1:B:257:ARG:HD3	2.37	0.55
1:D:194[B]:CYS:HG	1:D:357:ILE:HD13	1.72	0.55
1:A:168:MET:CE	1:A:179:LEU:HD21	2.30	0.54
1:C:15:THR:CG2	1:C:45:ASP:HB2	2.33	0.54
1:B:168:MET:HA	1:B:168:MET:CE	2.32	0.53
1:A:168:MET:HG3	1:A:254:ARG:HD2	1.90	0.53
1:B:336:ALA:HA	1:B:341:GLY:O	2.09	0.52
1:D:15:THR:HB	1:D:54:LEU:HD13	1.92	0.51
1:A:106:LYS:HE2	1:A:195:HIS:NE2	2.27	0.50
1:B:99:GLY:C	1:B:127:ARG:HD2	2.35	0.50
1:B:177:TRP:CE3	1:B:180:THR:HG21	2.46	0.50
1:B:175:TRP:CZ2	1:B:180:THR:HG22	2.47	0.50
1:A:71:VAL:HG13	1:A:95:ALA:HA	1.93	0.50
1:D:194[B]:CYS:SG	1:D:357:ILE:CD1	2.93	0.50
1:B:44:ALA:HA	1:B:64:THR:O	2.13	0.49
1:D:168:MET:HG3	1:D:254:ARG:HD2	1.94	0.49
1:D:177:TRP:O	1:D:180:THR:OG1	2.31	0.49
1:A:223:HIS:C	1:A:224:GLN:HG2	2.38	0.48
1:A:106:LYS:HD2	1:A:106:LYS:O	2.14	0.48
1:A:128:ARG:HD3	1:A:128:ARG:HA	1.62	0.48
1:A:106:LYS:HD3	1:A:194:CYS:SG	2.53	0.48
1:B:46:MET:HA	1:B:47:PRO:C	2.38	0.47
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.80	0.47
1:B:166:ASP:HB3	1:B:256:ALA:O	2.15	0.47
1:B:219:THR:HB	1:B:229:ARG:HH11	1.78	0.47
1:D:181:ARG:HH11	1:D:181:ARG:HG2	1.80	0.47
1:A:108:MET:O	1:A:118:MET:HE1	2.15	0.47
1:D:126:ASP:O	1:D:126:ASP:CG	2.57	0.47
1:A:167:TYR:CD1	1:A:168:MET:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HD3	1:B:27:ARG:O	2.15	0.46
1:C:106:LYS:HD2	1:C:106:LYS:C	2.40	0.46
1:B:15:THR:CG2	1:B:43:LEU:HD11	2.39	0.46
1:A:18:MET:HE3	1:A:326:LYS:HE2	1.97	0.46
1:D:291:ARG:HG2	3:D:696:HOH:O	2.15	0.46
1:A:131:ILE:N	1:A:131:ILE:HD13	2.31	0.46
1:C:83:THR:HB	1:C:84:PRO:CD	2.45	0.46
1:B:23:ALA:O	1:B:27:ARG:HG2	2.17	0.45
1:C:13:ILE:HG22	1:C:83:THR:CG2	2.46	0.45
1:C:25:ALA:HA	1:C:327:VAL:HG22	1.98	0.45
1:C:64:THR:OG1	1:C:69:GLU:OE1	2.31	0.45
1:B:17:PHE:CE2	1:B:18:MET:CE	3.00	0.45
1:B:27:ARG:CD	1:B:40:LEU:HD11	2.47	0.45
1:B:47:PRO:HG2	1:B:50:LYS:HB2	1.99	0.44
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.85	0.44
1:A:126:ASP:O	1:A:126:ASP:CG	2.60	0.44
1:B:199:VAL:HG11	1:B:265:TRP:CD1	2.53	0.44
1:A:126:ASP:O	1:A:128:ARG:NH2	2.51	0.44
1:B:106:LYS:C	1:B:106:LYS:CD	2.89	0.44
1:D:85:ASN:HA	1:D:88:HIS:CD2	2.53	0.43
1:C:194:CYS:HB3	1:C:357:ILE:HD13	2.00	0.43
1:A:43:LEU:O	1:A:63:GLY:HA2	2.19	0.43
1:A:46:MET:HE2	1:A:46:MET:HB2	1.70	0.43
1:C:31:THR:O	1:D:20:LYS:HE3	2.18	0.43
1:A:73:ASP:HA	1:A:74:PRO:HD3	1.93	0.42
1:C:166:ASP:HB3	1:C:256:ALA:O	2.19	0.42
1:A:83:THR:HB	1:A:84:PRO:CD	2.48	0.42
1:B:130:ILE:HD12	1:B:343:ALA:HB1	2.01	0.42
1:C:68:ARG:NH1	1:C:90:GLU:OE2	2.52	0.42
1:C:199:VAL:HG11	1:C:265:TRP:CD1	2.54	0.42
1:B:25:ALA:HA	1:B:327:VAL:HG22	2.02	0.42
1:A:150:GLU:OE1	1:D:293:GLU:OE2	2.38	0.42
1:A:8:LEU:HD12	1:A:334:ARG:HG3	2.02	0.41
1:D:130:ILE:HD12	1:D:343:ALA:HB1	2.02	0.41
1:A:11:ALA:HB2	1:A:76:VAL:HG21	2.02	0.41
1:B:13:ILE:HD11	1:B:71:VAL:HG23	2.01	0.41
1:D:15:THR:CG2	1:D:43:LEU:HD21	2.50	0.41
1:B:219:THR:O	1:B:229:ARG:HD3	2.21	0.41
1:C:15:THR:CB	1:C:54:LEU:CD2	2.86	0.41
1:D:85:ASN:OD1	1:D:85:ASN:N	2.53	0.41
1:D:99:GLY:O	1:D:127:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:131:ILE:HA	2.21	0.41
1:B:71:VAL:CG1	1:B:95:ALA:HA	2.51	0.41
1:D:159:PHE:O	1:D:248:GLY:HA2	2.21	0.41
1:D:43:LEU:C	1:D:43:LEU:HD23	2.47	0.40
1:C:43:LEU:HD23	1:C:55:ALA:CA	2.51	0.40
1:D:13:ILE:HG22	1:D:83:THR:HG21	2.02	0.40
1:D:104:LEU:O	1:D:131:ILE:HA	2.21	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	365/380 (96%)	359 (98%)	6 (2%)	0	100	100
1	B	364/380 (96%)	353 (97%)	11 (3%)	0	100	100
1	C	366/380 (96%)	359 (98%)	7 (2%)	0	100	100
1	D	367/380 (97%)	358 (98%)	9 (2%)	0	100	100
All	All	1462/1520 (96%)	1429 (98%)	33 (2%)	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	275/287 (96%)	265 (96%)	10 (4%)	31	34
1	B	274/287 (96%)	271 (99%)	3 (1%)	65	74
1	C	276/287 (96%)	269 (98%)	7 (2%)	42	48
1	D	277/287 (96%)	270 (98%)	7 (2%)	42	48
All	All	1102/1148 (96%)	1075 (98%)	27 (2%)	42	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	46	MET
1	A	50	LYS
1	A	113	GLU
1	A	116	GLN
1	A	128	ARG
1	A	134	ASN
1	A	173	LEU
1	A	227	THR
1	A	342	LYS
1	B	71	VAL
1	B	106	LYS
1	B	134	ASN
1	C	6	LYS
1	C	54	LEU
1	C	106	LYS
1	C	110	LEU
1	C	116	GLN
1	C	134	ASN
1	C	334	ARG
1	D	85	ASN
1	D	105	GLU
1	D	106	LYS
1	D	125	SER
1	D	181	ARG
1	D	182	LYS
1	D	302	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	195	HIS

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Mol	Chain	Res	Type
1	C	368	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	500	-	3,3,3	1.17	0	3,3,3	0.76	0
2	ACT	D	500	-	3,3,3	0.96	0	3,3,3	0.83	0
2	ACT	A	500	-	3,3,3	1.10	0	3,3,3	0.86	0
2	ACT	C	500	-	3,3,3	0.97	0	3,3,3	0.78	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [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	367/380 (96%)	-0.16	3 (0%) 82 84	25, 33, 49, 64	0
1	B	366/380 (96%)	-0.04	6 (1%) 70 73	24, 35, 62, 85	0
1	C	368/380 (96%)	-0.13	3 (0%) 82 84	25, 33, 55, 77	0
1	D	368/380 (96%)	-0.15	3 (0%) 82 84	14, 32, 51, 75	1 (0%)
All	All	1469/1520 (96%)	-0.12	15 (1%) 79 81	14, 33, 55, 85	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	373	LEU	5.9
1	B	48	ALA	3.4
1	C	177	TRP	3.2
1	C	46	MET	2.3
1	B	47	PRO	2.3
1	B	7	ALA	2.3
1	A	173	LEU	2.3
1	A	177	TRP	2.2
1	B	184	GLY	2.1
1	D	87	LEU	2.1
1	B	342	LYS	2.1
1	C	209	ARG	2.1
1	B	177	TRP	2.1
1	A	6	LYS	2.1
1	D	84	PRO	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($\text{\AA}^2$)	Q<0.9
2	ACT	B	500	4/4	0.94	0.10	29,33,33,34	0
2	ACT	A	500	4/4	0.95	0.11	38,39,39,40	0
2	ACT	C	500	4/4	0.95	0.08	29,32,32,33	0
2	ACT	D	500	4/4	0.96	0.10	29,32,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.