



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:36 AM UTC

PDB ID : 4WXZ / pdb_00004wxz
Title : PdxS (G. stearothermophilus) co-crystallized with R5P
Authors : Smith, J.L.; Smith, A.M.
Deposited on : 2014-11-14
Resolution : 2.70 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

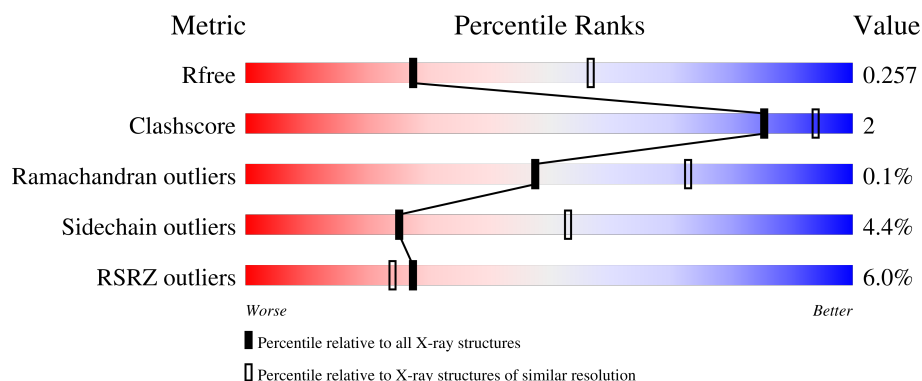
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	304	7% 73% 7% 20%
1	B	304	7% 74% 6% 20%
1	C	304	2% 76% 8% 16%
1	D	304	3% 74% 6% 19%
1	E	304	7% 73% 6% 20%

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Mol	Chain	Length	Quality of chain
1	F	304	15% 74% 6% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11422 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 Pyridoxal biosynthesis lyase PdxS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	P	S	0	0	0
			1864	1161	327	362	2	12			
1	B	243	Total	C	N	O	P	S	0	0	0
			1855	1155	325	361	2	12			
1	C	256	Total	C	N	O	P	S	0	0	0
			1953	1213	344	380	2	14			
1	D	245	Total	C	N	O	P	S	0	0	0
			1862	1160	324	363	2	13			
1	E	242	Total	C	N	O	P	S	0	0	0
			1845	1150	321	360	2	12			
1	F	244	Total	C	N	O	P	S	0	0	0
			1853	1154	323	362	2	12			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLU	-	expression tag	UNP Q5L3Y2
A	-8	ASN	-	expression tag	UNP Q5L3Y2
A	-7	LEU	-	expression tag	UNP Q5L3Y2
A	-6	THR	-	expression tag	UNP Q5L3Y2
A	-5	PRO	-	expression tag	UNP Q5L3Y2
A	-4	GLN	-	expression tag	UNP Q5L3Y2
A	-3	HIS	-	expression tag	UNP Q5L3Y2
A	-2	MET	-	expression tag	UNP Q5L3Y2
A	-1	ALA	-	expression tag	UNP Q5L3Y2
A	0	SER	-	expression tag	UNP Q5L3Y2
A	216	THR	ALA	conflict	UNP Q5L3Y2
B	-9	GLU	-	expression tag	UNP Q5L3Y2
B	-8	ASN	-	expression tag	UNP Q5L3Y2
B	-7	LEU	-	expression tag	UNP Q5L3Y2
B	-6	THR	-	expression tag	UNP Q5L3Y2
B	-5	PRO	-	expression tag	UNP Q5L3Y2
B	-4	GLN	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q5L3Y2
B	-2	MET	-	expression tag	UNP Q5L3Y2
B	-1	ALA	-	expression tag	UNP Q5L3Y2
B	0	SER	-	expression tag	UNP Q5L3Y2
B	216	THR	ALA	conflict	UNP Q5L3Y2
C	-9	GLU	-	expression tag	UNP Q5L3Y2
C	-8	ASN	-	expression tag	UNP Q5L3Y2
C	-7	LEU	-	expression tag	UNP Q5L3Y2
C	-6	THR	-	expression tag	UNP Q5L3Y2
C	-5	PRO	-	expression tag	UNP Q5L3Y2
C	-4	GLN	-	expression tag	UNP Q5L3Y2
C	-3	HIS	-	expression tag	UNP Q5L3Y2
C	-2	MET	-	expression tag	UNP Q5L3Y2
C	-1	ALA	-	expression tag	UNP Q5L3Y2
C	0	SER	-	expression tag	UNP Q5L3Y2
C	216	THR	ALA	conflict	UNP Q5L3Y2
D	-9	GLU	-	expression tag	UNP Q5L3Y2
D	-8	ASN	-	expression tag	UNP Q5L3Y2
D	-7	LEU	-	expression tag	UNP Q5L3Y2
D	-6	THR	-	expression tag	UNP Q5L3Y2
D	-5	PRO	-	expression tag	UNP Q5L3Y2
D	-4	GLN	-	expression tag	UNP Q5L3Y2
D	-3	HIS	-	expression tag	UNP Q5L3Y2
D	-2	MET	-	expression tag	UNP Q5L3Y2
D	-1	ALA	-	expression tag	UNP Q5L3Y2
D	0	SER	-	expression tag	UNP Q5L3Y2
D	216	THR	ALA	conflict	UNP Q5L3Y2
E	-9	GLU	-	expression tag	UNP Q5L3Y2
E	-8	ASN	-	expression tag	UNP Q5L3Y2
E	-7	LEU	-	expression tag	UNP Q5L3Y2
E	-6	THR	-	expression tag	UNP Q5L3Y2
E	-5	PRO	-	expression tag	UNP Q5L3Y2
E	-4	GLN	-	expression tag	UNP Q5L3Y2
E	-3	HIS	-	expression tag	UNP Q5L3Y2
E	-2	MET	-	expression tag	UNP Q5L3Y2
E	-1	ALA	-	expression tag	UNP Q5L3Y2
E	0	SER	-	expression tag	UNP Q5L3Y2
E	216	THR	ALA	conflict	UNP Q5L3Y2
F	-9	GLU	-	expression tag	UNP Q5L3Y2
F	-8	ASN	-	expression tag	UNP Q5L3Y2
F	-7	LEU	-	expression tag	UNP Q5L3Y2
F	-6	THR	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	PRO	-	expression tag	UNP Q5L3Y2
F	-4	GLN	-	expression tag	UNP Q5L3Y2
F	-3	HIS	-	expression tag	UNP Q5L3Y2
F	-2	MET	-	expression tag	UNP Q5L3Y2
F	-1	ALA	-	expression tag	UNP Q5L3Y2
F	0	SER	-	expression tag	UNP Q5L3Y2
F	216	THR	ALA	conflict	UNP Q5L3Y2

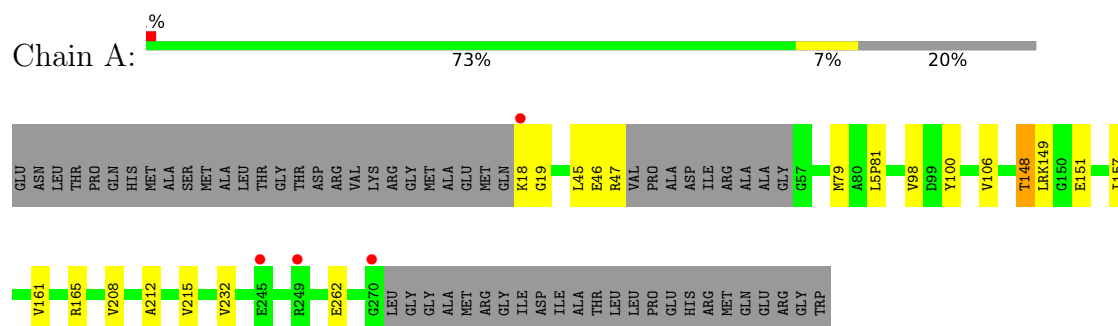
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	47	Total O 47 47	0	0
2	C	31	Total O 31 31	0	0
2	D	15	Total O 15 15	0	0
2	E	23	Total O 23 23	0	0
2	F	9	Total O 9 9	0	0

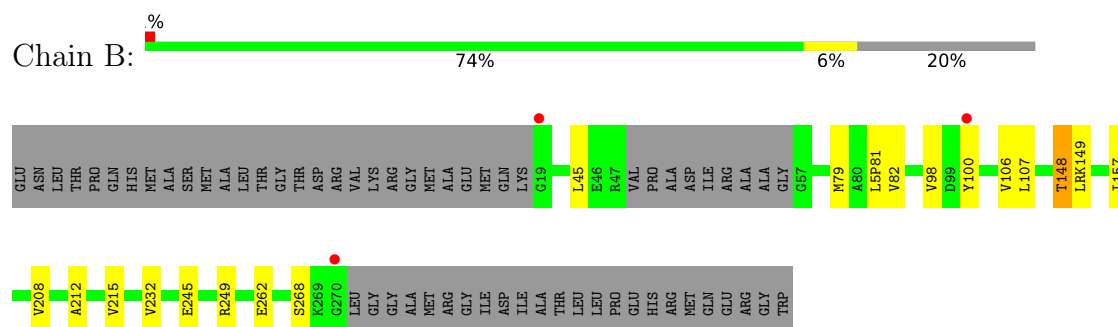
3 Residue-property plots [i](#)

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.

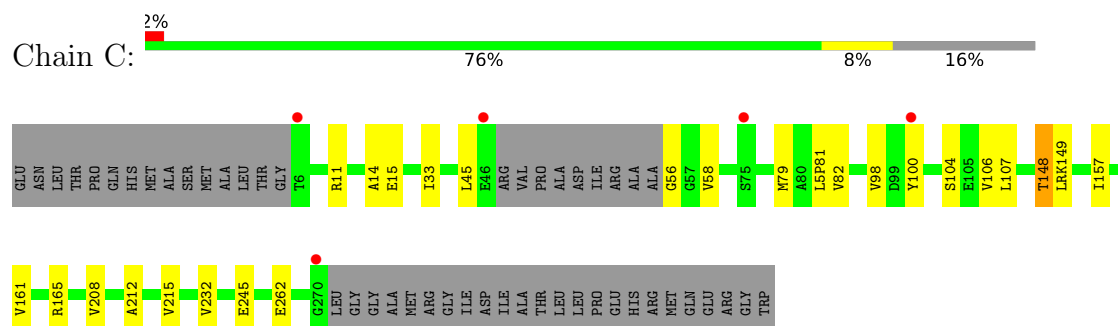
- Molecule 1: Pyridoxal biosynthesis lyase PdxS



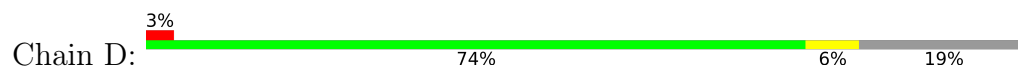
- Molecule 1: Pyridoxal biosynthesis lyase PdxS

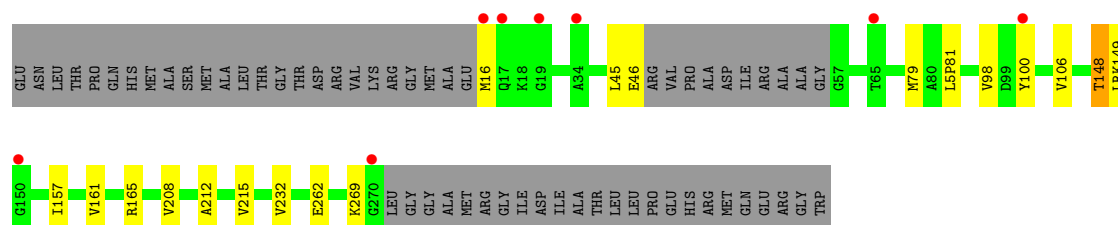


- Molecule 1: Pyridoxal biosynthesis lyase PdxS

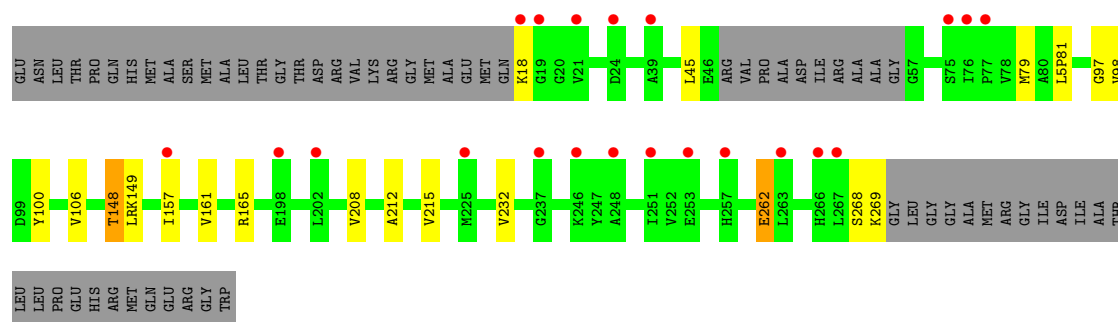
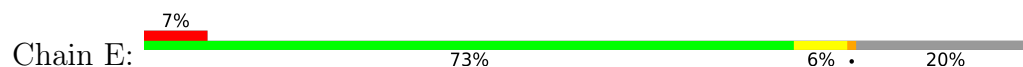


- Molecule 1: Pyridoxal biosynthesis lyase PdxS

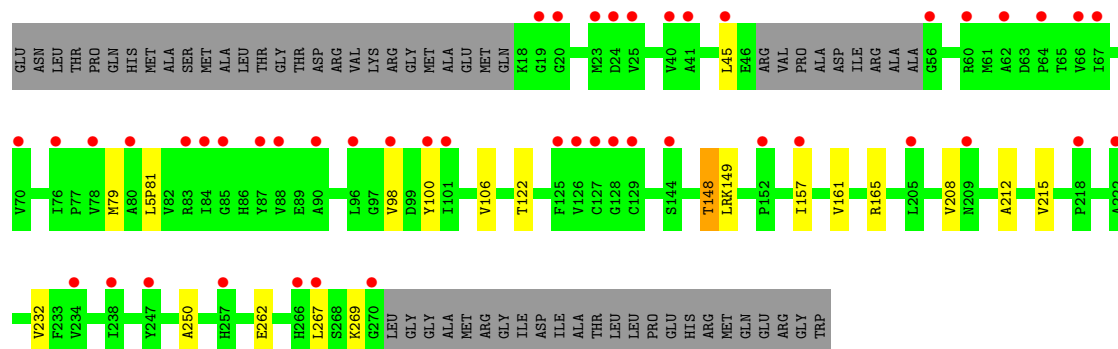
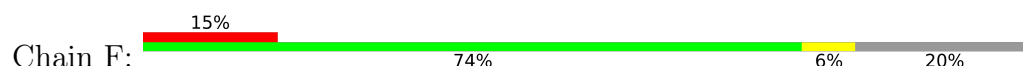




• Molecule 1: Pyridoxal biosynthesis lyase PdxS



• Molecule 1: Pyridoxal biosynthesis lyase PdxS



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.78Å 179.78Å 104.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 99.9 (50.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.216 , 0.259 0.217 , 0.257	Depositor DCC
R_{free} test set	2730 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11422	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: L5P, LRK

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	0.81	0/1842	0.88	0/2486
1	B	0.77	0/1833	0.86	0/2475
1	C	0.78	0/1931	0.91	2/2603 (0.1%)
1	D	0.65	0/1840	0.87	0/2485
1	E	0.60	0/1823	0.82	0/2463
1	F	0.55	0/1831	0.81	0/2473
All	All	0.70	0/11100	0.86	2/14985 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	VAL	N-CA-C	5.99	117.01	108.93
1	C	104	SER	N-CA-C	5.22	116.92	108.41

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	1864	0	1873	6	0
1	B	1855	0	1860	12	0
1	C	1953	0	1961	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1862	0	1860	5	0
1	E	1845	0	1845	8	0
1	F	1853	0	1852	7	0
2	A	65	0	0	2	0
2	B	47	0	0	8	0
2	C	31	0	0	3	0
2	D	15	0	0	1	0
2	E	23	0	0	4	0
2	F	9	0	0	2	0
All	All	11422	0	11251	49	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 2.

All (49) 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:249:ARG:CD	2:B:305:HOH:O	2.03	1.07
1:C:33:ILE:O	2:C:318:HOH:O	1.77	1.01
1:B:249:ARG:HD2	2:B:305:HOH:O	1.64	0.94
1:B:249:ARG:HD3	2:B:305:HOH:O	1.65	0.90
1:B:249:ARG:NH2	2:B:323:HOH:O	2.08	0.86
1:B:245:GLU:OE2	2:B:323:HOH:O	1.95	0.83
1:C:14:ALA:HB2	1:C:100:TYR:OH	1.79	0.82
1:D:46:GLU:C	2:D:306:HOH:O	2.34	0.69
1:B:249:ARG:NH1	2:B:301:HOH:O	2.23	0.68
1:B:157:ILE:HD11	1:B:215:VAL:HG22	1.85	0.59
1:C:11:ARG:O	1:C:15:GLU:HG2	2.04	0.57
1:A:157:ILE:HD11	1:A:215:VAL:HG22	1.85	0.56
1:D:79:MET:HG2	1:D:100:TYR:HB2	1.87	0.56
1:A:151:GLU:HG2	2:A:338:HOH:O	2.05	0.56
1:E:157:ILE:HD11	1:E:215:VAL:HG22	1.87	0.56
1:D:157:ILE:HD11	1:D:215:VAL:HG22	1.88	0.55
1:C:157:ILE:HD11	1:C:215:VAL:HG22	1.88	0.55
1:C:245:GLU:OE2	2:C:318:HOH:O	2.18	0.54
1:F:157:ILE:HD11	1:F:215:VAL:HG22	1.89	0.54
1:C:56:GLY:N	2:C:328:HOH:O	2.41	0.53
1:D:161:VAL:O	1:D:165:ARG:HG3	2.08	0.53
1:F:250:ALA:HA	1:F:267:LEU:HD22	1.91	0.53
1:B:79:MET:HG2	1:B:100:TYR:HB2	1.91	0.52
1:F:79:MET:HG2	1:F:100:TYR:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:HG2	1:A:100:TYR:HB2	1.92	0.52
1:A:47:ARG:HB2	2:A:365:HOH:O	2.10	0.51
1:A:161:VAL:O	1:A:165:ARG:HG3	2.11	0.50
1:E:148:THR:HG22	1:E:212:ALA:O	2.13	0.49
1:F:269:LYS:NZ	2:F:303:HOH:O	2.44	0.49
1:A:148:THR:HG22	1:A:212:ALA:O	2.13	0.49
1:F:148:THR:HG22	1:F:212:ALA:O	2.13	0.49
1:E:262:GLU:CG	2:E:317:HOH:O	2.60	0.49
1:D:148:THR:HG22	1:D:212:ALA:O	2.13	0.48
1:E:79:MET:HG2	1:E:100:TYR:HB2	1.95	0.48
1:B:245:GLU:HB2	2:B:343:HOH:O	2.14	0.48
1:C:148:THR:HG22	1:C:212:ALA:O	2.15	0.46
1:C:79:MET:HG2	1:C:100:TYR:HB2	1.97	0.46
1:B:249:ARG:CZ	2:B:323:HOH:O	2.57	0.46
1:C:14:ALA:CB	1:C:100:TYR:OH	2.58	0.45
1:F:122:THR:HA	2:F:305:HOH:O	2.17	0.45
1:F:161:VAL:O	1:F:165:ARG:HG3	2.17	0.44
1:E:97:GLY:HA2	2:E:310:HOH:O	2.16	0.44
1:C:161:VAL:O	1:C:165:ARG:HG3	2.18	0.44
1:E:18:LYS:N	2:E:321:HOH:O	2.52	0.42
1:E:161:VAL:O	1:E:165:ARG:HG3	2.18	0.42
1:B:148:THR:HG22	1:B:212:ALA:O	2.20	0.42
1:E:262:GLU:HG3	2:E:317:HOH:O	2.18	0.41
1:C:82:VAL:C	1:C:107:LEU:HD12	2.46	0.41
1:B:82:VAL:C	1:B:107:LEU:HD12	2.47	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	237/304 (78%)	233 (98%)	3 (1%)	1 (0%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	236/304 (78%)	233 (99%)	3 (1%)	0	100	100
1	C	249/304 (82%)	245 (98%)	4 (2%)	0	100	100
1	D	238/304 (78%)	231 (97%)	7 (3%)	0	100	100
1	E	235/304 (77%)	231 (98%)	4 (2%)	0	100	100
1	F	237/304 (78%)	233 (98%)	4 (2%)	0	100	100
All	All	1432/1824 (78%)	1406 (98%)	25 (2%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLY

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	187/232 (81%)	178 (95%)	9 (5%)	23	50
1	B	186/232 (80%)	178 (96%)	8 (4%)	26	54
1	C	196/232 (84%)	189 (96%)	7 (4%)	31	60
1	D	186/232 (80%)	177 (95%)	9 (5%)	23	50
1	E	185/232 (80%)	176 (95%)	9 (5%)	22	49
1	F	185/232 (80%)	178 (96%)	7 (4%)	29	58
All	All	1125/1392 (81%)	1076 (96%)	49 (4%)	25	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	45	LEU
1	A	46	GLU
1	A	98	VAL
1	A	106	VAL

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Mol	Chain	Res	Type
1	A	148	THR
1	A	208	VAL
1	A	232	VAL
1	A	262	GLU
1	B	45	LEU
1	B	98	VAL
1	B	106	VAL
1	B	148	THR
1	B	208	VAL
1	B	232	VAL
1	B	262	GLU
1	B	268	SER
1	C	45	LEU
1	C	98	VAL
1	C	106	VAL
1	C	148	THR
1	C	208	VAL
1	C	232	VAL
1	C	262	GLU
1	D	16	MET
1	D	45	LEU
1	D	98	VAL
1	D	106	VAL
1	D	148	THR
1	D	208	VAL
1	D	232	VAL
1	D	262	GLU
1	D	269	LYS
1	E	45	LEU
1	E	98	VAL
1	E	106	VAL
1	E	148	THR
1	E	208	VAL
1	E	232	VAL
1	E	262	GLU
1	E	268	SER
1	E	269	LYS
1	F	45	LEU
1	F	98	VAL
1	F	106	VAL
1	F	148	THR
1	F	208	VAL

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Mol	Chain	Res	Type
1	F	232	VAL
1	F	262	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	B	115	HIS
1	B	209	ASN
1	C	209	ASN
1	C	266	HIS
1	D	209	ASN
1	E	209	ASN
1	F	266	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
1	L5P	B	81	1	20,21,22	1.08	1 (5%)	16,27,29	2.28	3 (18%)
1	LRK	D	149	1	19,21,22	1.36	2 (10%)	15,27,29	0.82	0
1	L5P	C	81	1	20,21,22	1.09	1 (5%)	16,27,29	1.55	4 (25%)
1	LRK	C	149	1	19,21,22	1.42	2 (10%)	15,27,29	0.92	0
1	LRK	B	149	1	19,21,22	1.45	2 (10%)	15,27,29	0.91	1 (6%)
1	L5P	A	81	1	20,21,22	1.10	1 (5%)	16,27,29	1.25	3 (18%)
1	LRK	A	149	1	19,21,22	1.31	2 (10%)	15,27,29	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	L5P	E	81	1	20,21,22	1.30	2 (10%)	16,27,29	1.17	2 (12%)
1	LRK	E	149	1	19,21,22	1.46	2 (10%)	15,27,29	1.01	1 (6%)
1	L5P	D	81	1	20,21,22	1.23	1 (5%)	16,27,29	1.47	3 (18%)
1	LRK	F	149	1	19,21,22	1.30	2 (10%)	15,27,29	1.06	2 (13%)
1	L5P	F	81	1	20,21,22	0.99	0	16,27,29	1.04	1 (6%)

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
1	L5P	B	81	1	-	5/23/25/27	-
1	LRK	D	149	1	-	11/24/26/28	-
1	L5P	C	81	1	-	8/23/25/27	-
1	LRK	C	149	1	-	10/24/26/28	-
1	LRK	B	149	1	-	10/24/26/28	-
1	L5P	A	81	1	-	13/23/25/27	-
1	LRK	A	149	1	-	10/24/26/28	-
1	L5P	E	81	1	-	3/23/25/27	-
1	LRK	E	149	1	-	10/24/26/28	-
1	L5P	D	81	1	-	12/23/25/27	-
1	LRK	F	149	1	-	11/24/26/28	-
1	L5P	F	81	1	-	11/23/25/27	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	LRK	P9-O10	4.21	1.63	1.50
1	E	149	LRK	C6-C5	-3.99	1.49	1.53
1	D	81	L5P	P9-O11	3.96	1.62	1.50
1	C	149	LRK	P9-O10	3.78	1.62	1.50
1	D	149	LRK	C6-C5	-3.76	1.50	1.53
1	F	149	LRK	P9-O10	3.76	1.62	1.50
1	C	81	L5P	P9-O11	3.65	1.61	1.50
1	E	81	L5P	P9-O11	3.62	1.61	1.50
1	C	149	LRK	C6-C5	-3.58	1.50	1.53
1	E	149	LRK	P9-O10	3.56	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	LRK	P9-O10	3.48	1.61	1.50
1	D	149	LRK	P9-O10	3.46	1.61	1.50
1	A	81	L5P	P9-O11	3.37	1.61	1.50
1	B	81	L5P	P9-O11	3.19	1.60	1.50
1	A	149	LRK	C6-C5	-3.18	1.50	1.53
1	B	149	LRK	C6-C5	-3.12	1.50	1.53
1	F	149	LRK	C6-C5	-2.69	1.50	1.53
1	E	81	L5P	P9-O10	2.11	1.62	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	L5P	C2-C3-C5	7.50	128.72	116.43
1	D	81	L5P	C2-C3-C5	3.98	122.95	116.43
1	C	81	L5P	C2-C3-C5	3.85	122.74	116.43
1	B	81	L5P	O4-C3-C2	-3.11	117.07	121.23
1	E	81	L5P	C2-C3-C5	3.07	121.47	116.43
1	B	81	L5P	O10-P9-O8	2.53	113.27	106.67
1	F	81	L5P	O12-P9-O8	2.41	112.96	106.67
1	D	81	L5P	O12-P9-O8	2.34	112.77	106.67
1	C	81	L5P	O10-P9-O8	2.30	112.68	106.67
1	B	149	LRK	C5-C3-NZ	-2.29	106.26	110.28
1	D	81	L5P	O8-P9-O11	2.26	112.54	106.44
1	A	81	L5P	C2-C3-C5	2.24	120.10	116.43
1	E	81	L5P	O8-P9-O11	2.24	112.49	106.44
1	A	81	L5P	O10-P9-O8	2.21	112.44	106.67
1	C	81	L5P	O12-P9-O8	2.18	112.36	106.67
1	A	149	LRK	C5-C3-NZ	-2.16	106.49	110.28
1	A	81	L5P	O10-P9-O11	-2.12	102.59	110.83
1	E	149	LRK	C5-C3-NZ	-2.11	106.57	110.28
1	F	149	LRK	O8-P9-O10	2.07	112.03	106.44
1	C	81	L5P	O13-C5-C6	2.04	114.66	109.46
1	F	149	LRK	C5-C3-NZ	-2.02	106.74	110.28

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81	L5P	O-C1-CA-CB
1	A	81	L5P	C3-C2-NZ-CE
1	A	81	L5P	C3-C5-C6-O14
1	A	81	L5P	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
1	A	81	L5P	O13-C5-C6-O14
1	A	81	L5P	O13-C5-C6-C7
1	A	81	L5P	C5-C6-C7-O8
1	A	81	L5P	O14-C6-C7-O8
1	A	81	L5P	C7-O8-P9-O12
1	A	81	L5P	C7-O8-P9-O11
1	A	81	L5P	C7-O8-P9-O10
1	A	149	LRK	C-CA-CB-CG
1	A	149	LRK	N-CA-CB-CG
1	A	149	LRK	C5-C3-NZ-CE
1	B	81	L5P	O4-C3-C5-O13
1	B	81	L5P	O4-C3-C5-C6
1	B	81	L5P	C2-C3-C5-C6
1	B	149	LRK	C-CA-CB-CG
1	B	149	LRK	N-CA-CB-CG
1	B	149	LRK	C5-C3-NZ-CE
1	C	81	L5P	O4-C3-C5-O13
1	C	81	L5P	C2-C3-C5-O13
1	C	81	L5P	C3-C5-C6-O14
1	C	149	LRK	C-CA-CB-CG
1	C	149	LRK	N-CA-CB-CG
1	C	149	LRK	C5-C3-NZ-CE
1	D	81	L5P	C3-C2-NZ-CE
1	D	81	L5P	O4-C3-C5-O13
1	D	81	L5P	C3-C5-C6-O14
1	D	81	L5P	C3-C5-C6-C7
1	D	81	L5P	O13-C5-C6-O14
1	D	81	L5P	O13-C5-C6-C7
1	D	149	LRK	C-CA-CB-CG
1	D	149	LRK	N-CA-CB-CG
1	D	149	LRK	C5-C3-NZ-CE
1	E	149	LRK	C-CA-CB-CG
1	E	149	LRK	N-CA-CB-CG
1	E	149	LRK	C5-C3-NZ-CE
1	F	81	L5P	O4-C3-C5-O13
1	F	81	L5P	C5-C6-C7-O8
1	F	81	L5P	O14-C6-C7-O8
1	F	81	L5P	C7-O8-P9-O12
1	F	81	L5P	C7-O8-P9-O11
1	F	81	L5P	C7-O8-P9-O10
1	F	149	LRK	C-CA-CB-CG
1	F	149	LRK	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	F	149	LRK	C5-C3-NZ-CE
1	B	81	L5P	CG-CD-CE-NZ
1	E	81	L5P	CG-CD-CE-NZ
1	A	81	L5P	CG-CD-CE-NZ
1	D	81	L5P	CG-CD-CE-NZ
1	F	81	L5P	CD-CE-NZ-C2
1	C	81	L5P	CG-CD-CE-NZ
1	C	81	L5P	CE-CD-CG-CB
1	D	81	L5P	C5-C6-C7-O8
1	D	149	LRK	CG-CD-CE-NZ
1	C	149	LRK	CG-CD-CE-NZ
1	B	149	LRK	CG-CD-CE-NZ
1	F	149	LRK	CG-CD-CE-NZ
1	E	149	LRK	CG-CD-CE-NZ
1	A	149	LRK	CG-CD-CE-NZ
1	F	149	LRK	C7-O8-P9-O10
1	D	81	L5P	NZ-C2-C3-O4
1	A	149	LRK	C6-C7-O8-P9
1	D	81	L5P	C6-C7-O8-P9
1	F	81	L5P	O13-C5-C6-O14
1	F	81	L5P	NZ-C2-C3-O4
1	C	81	L5P	CD-CE-NZ-C2
1	D	149	LRK	C6-C7-O8-P9
1	E	81	L5P	C6-C7-O8-P9
1	E	149	LRK	C6-C7-O8-P9
1	A	81	L5P	CD-CE-NZ-C2
1	D	81	L5P	CD-CE-NZ-C2
1	F	81	L5P	CG-CD-CE-NZ
1	E	81	L5P	C1-CA-CB-CG
1	D	81	L5P	O14-C6-C7-O8
1	A	149	LRK	C3-C5-C6-O14
1	B	149	LRK	C3-C5-C6-O14
1	C	149	LRK	C3-C5-C6-O14
1	D	149	LRK	C3-C5-C6-O14
1	E	149	LRK	C3-C5-C6-O14
1	F	81	L5P	O4-C3-C5-C6
1	F	149	LRK	C3-C5-C6-O14
1	B	149	LRK	C6-C7-O8-P9
1	C	149	LRK	C6-C7-O8-P9
1	F	149	LRK	C6-C7-O8-P9
1	C	149	LRK	C7-O8-P9-O10
1	D	149	LRK	C7-O8-P9-O10

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Mol	Chain	Res	Type	Atoms
1	A	149	LRK	CA-CB-CG-CD
1	D	149	LRK	CA-CB-CG-CD
1	F	149	LRK	CA-CB-CG-CD
1	C	149	LRK	CA-CB-CG-CD
1	B	81	L5P	NZ-C2-C3-O4
1	E	149	LRK	CA-CB-CG-CD
1	B	149	LRK	CA-CB-CG-CD
1	C	81	L5P	O13-C5-C6-O14
1	C	81	L5P	O13-C5-C6-C7
1	A	149	LRK	C2-C3-NZ-CE
1	B	149	LRK	C2-C3-NZ-CE
1	C	149	LRK	C2-C3-NZ-CE
1	D	149	LRK	C2-C3-NZ-CE
1	E	149	LRK	C2-C3-NZ-CE
1	F	149	LRK	C2-C3-NZ-CE
1	A	149	LRK	C2-C3-C5-O13
1	B	149	LRK	C2-C3-C5-O13
1	D	149	LRK	C2-C3-C5-O13
1	E	149	LRK	C2-C3-C5-O13
1	F	149	LRK	C2-C3-C5-O13
1	A	149	LRK	NZ-C3-C5-O13
1	B	149	LRK	NZ-C3-C5-O13
1	C	149	LRK	NZ-C3-C5-O13
1	D	149	LRK	NZ-C3-C5-O13
1	E	149	LRK	NZ-C3-C5-O13
1	F	149	LRK	NZ-C3-C5-O13

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	242/304 (79%)	-0.11	4 (1%) 69 67	28, 42, 73, 111	0
1	B	241/304 (79%)	-0.12	3 (1%) 76 75	30, 44, 77, 111	0
1	C	254/304 (83%)	0.20	5 (1%) 65 62	30, 47, 85, 124	0
1	D	243/304 (79%)	0.64	8 (3%) 49 45	40, 64, 94, 117	0
1	E	240/304 (78%)	0.94	21 (8%) 15 13	46, 75, 109, 140	0
1	F	242/304 (79%)	1.33	47 (19%) 3 2	63, 88, 122, 151	0
All	All	1462/1824 (80%)	0.48	88 (6%) 27 24	28, 61, 105, 151	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	GLY	4.1
1	F	40	VAL	3.8
1	B	19	GLY	3.8
1	C	100	TYR	3.4
1	A	249	ARG	3.3
1	C	6	THR	3.2
1	E	76	ILE	3.2
1	F	205	LEU	3.1
1	D	19	GLY	3.1
1	F	101	ILE	3.1
1	F	23	MET	3.1
1	F	129	CYS	3.1
1	A	270	GLY	3.0
1	F	96	LEU	3.0
1	F	88	VAL	3.0
1	F	70	VAL	2.9
1	F	56	GLY	2.8
1	D	17	GLN	2.7
1	E	19	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	85	GLY	2.7
1	E	225	MET	2.7
1	F	25	VAL	2.7
1	D	100	TYR	2.7
1	F	67	ILE	2.7
1	F	19	GLY	2.7
1	E	18	LYS	2.7
1	F	157	ILE	2.7
1	E	253	GLU	2.7
1	F	66	VAL	2.7
1	A	18	LYS	2.6
1	B	270	GLY	2.6
1	E	202	LEU	2.6
1	F	41	ALA	2.6
1	F	98	VAL	2.6
1	F	76	ILE	2.6
1	F	127	CYS	2.5
1	F	62	ALA	2.5
1	F	125	PHE	2.5
1	F	128	GLY	2.5
1	F	78	VAL	2.5
1	F	209	ASN	2.4
1	E	21	VAL	2.4
1	F	100	TYR	2.4
1	F	24	ASP	2.4
1	F	247	TYR	2.4
1	F	20	GLY	2.4
1	E	39	ALA	2.4
1	F	257	HIS	2.3
1	F	45	LEU	2.3
1	E	77	PRO	2.3
1	E	251	ILE	2.3
1	B	100	TYR	2.3
1	E	237	GLY	2.3
1	F	266	HIS	2.2
1	E	246	LYS	2.2
1	F	60	ARG	2.2
1	F	152	PRO	2.2
1	E	75	SER	2.2
1	F	80	ALA	2.2
1	F	267	LEU	2.2
1	F	218	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	263	LEU	2.2
1	E	157	ILE	2.2
1	F	270	GLY	2.2
1	E	24	ASP	2.2
1	F	84	ILE	2.2
1	F	126	VAL	2.2
1	F	238	ILE	2.2
1	F	90	ALA	2.1
1	D	270	GLY	2.1
1	A	245	GLU	2.1
1	F	234	VAL	2.1
1	F	144	SER	2.1
1	C	46	GLU	2.1
1	E	267	LEU	2.1
1	C	75	SER	2.1
1	E	198	GLU	2.1
1	F	87	TYR	2.1
1	D	34	ALA	2.0
1	D	150	GLY	2.0
1	E	248	ALA	2.0
1	F	222	ALA	2.0
1	D	16	MET	2.0
1	D	65	THR	2.0
1	F	64	PRO	2.0
1	E	257	HIS	2.0
1	E	266	HIS	2.0
1	F	83	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LRK	F	149	22/23	0.80	0.15	73,96,106,108	0
1	L5P	F	81	22/23	0.86	0.16	75,93,111,113	0
1	LRK	D	149	22/23	0.87	0.12	60,79,97,103	0
1	LRK	E	149	22/23	0.88	0.12	80,90,101,104	0
1	LRK	A	149	22/23	0.90	0.13	47,73,98,103	0
1	L5P	D	81	22/23	0.91	0.14	65,81,100,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LRK	B	149	22/23	0.91	0.11	56,72,91,95	0
1	L5P	E	81	22/23	0.91	0.12	53,78,93,98	0
1	LRK	C	149	22/23	0.92	0.10	41,72,85,89	0
1	L5P	C	81	22/23	0.94	0.12	37,63,94,109	0
1	L5P	B	81	22/23	0.94	0.12	40,59,78,89	0
1	L5P	A	81	22/23	0.95	0.10	39,53,79,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.