



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:53 AM UTC

PDB ID : 1O5Q / pdb_00001o5q
Title : Crystal Structure of Pyruvate and Mg²⁺ bound 2-methylisocitrate lyase (PrpB) from Salmonella typhimurium
Authors : Simanshu, D.K.; Murthy, M.R.N.
Deposited on : 2003-10-04
Resolution : 2.30 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

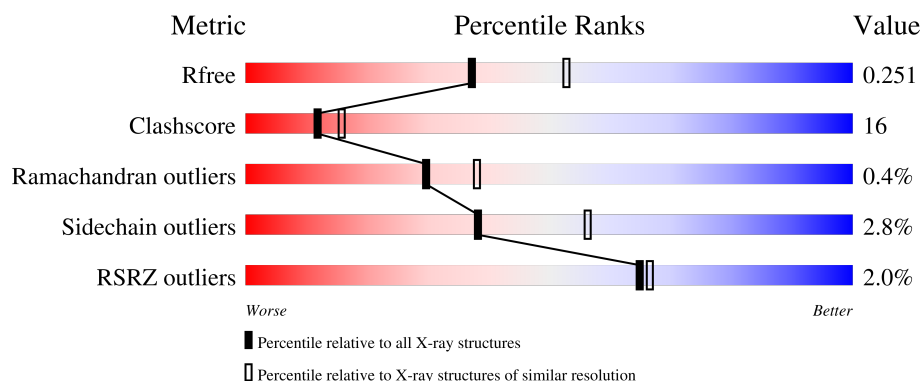
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	305	 2% 69% 17% • 11%
1	B	305	 % 69% 18% • 12%
1	C	305	 2% 62% 26% • 10%
1	D	305	 2% 58% 27% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8773 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 Probable methylisocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2056	1297	356	395	8			
1	B	268	Total	C	N	O	S	0	0	0
			2030	1280	352	390	8			
1	C	275	Total	C	N	O	S	0	0	0
			2081	1312	360	401	8			
1	D	268	Total	C	N	O	S	0	0	0
			2025	1277	352	388	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q56062
A	0	ALA	-	cloning artifact	UNP Q56062
A	1	SER	-	cloning artifact	UNP Q56062
A	296	LEU	-	expression tag	UNP Q56062
A	297	GLU	-	expression tag	UNP Q56062
A	298	HIS	-	expression tag	UNP Q56062
A	299	HIS	-	expression tag	UNP Q56062
A	300	HIS	-	expression tag	UNP Q56062
A	301	HIS	-	expression tag	UNP Q56062
A	302	HIS	-	expression tag	UNP Q56062
A	303	HIS	-	expression tag	UNP Q56062
B	-1	MET	-	cloning artifact	UNP Q56062
B	0	ALA	-	cloning artifact	UNP Q56062
B	1	SER	-	cloning artifact	UNP Q56062
B	296	LEU	-	expression tag	UNP Q56062
B	297	GLU	-	expression tag	UNP Q56062
B	298	HIS	-	expression tag	UNP Q56062
B	299	HIS	-	expression tag	UNP Q56062
B	300	HIS	-	expression tag	UNP Q56062
B	301	HIS	-	expression tag	UNP Q56062
B	302	HIS	-	expression tag	UNP Q56062

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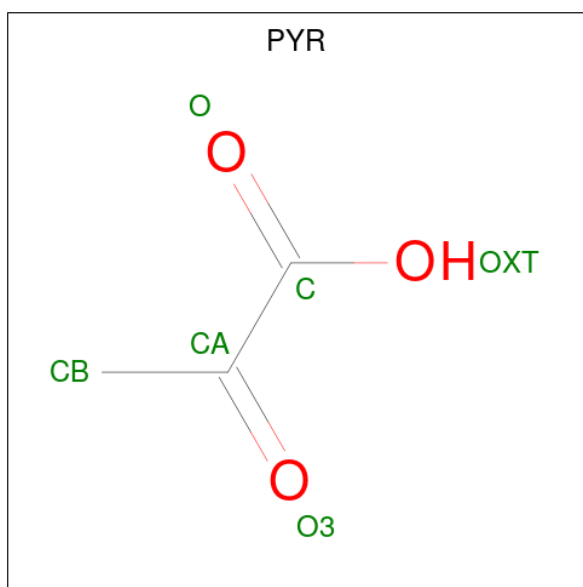
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Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP Q56062
C	-1	MET	-	cloning artifact	UNP Q56062
C	0	ALA	-	cloning artifact	UNP Q56062
C	1	SER	-	cloning artifact	UNP Q56062
C	296	LEU	-	expression tag	UNP Q56062
C	297	GLU	-	expression tag	UNP Q56062
C	298	HIS	-	expression tag	UNP Q56062
C	299	HIS	-	expression tag	UNP Q56062
C	300	HIS	-	expression tag	UNP Q56062
C	301	HIS	-	expression tag	UNP Q56062
C	302	HIS	-	expression tag	UNP Q56062
C	303	HIS	-	expression tag	UNP Q56062
D	-1	MET	-	cloning artifact	UNP Q56062
D	0	ALA	-	cloning artifact	UNP Q56062
D	1	SER	-	cloning artifact	UNP Q56062
D	296	LEU	-	expression tag	UNP Q56062
D	297	GLU	-	expression tag	UNP Q56062
D	298	HIS	-	expression tag	UNP Q56062
D	299	HIS	-	expression tag	UNP Q56062
D	300	HIS	-	expression tag	UNP Q56062
D	301	HIS	-	expression tag	UNP Q56062
D	302	HIS	-	expression tag	UNP Q56062
D	303	HIS	-	expression tag	UNP Q56062

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

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

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



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

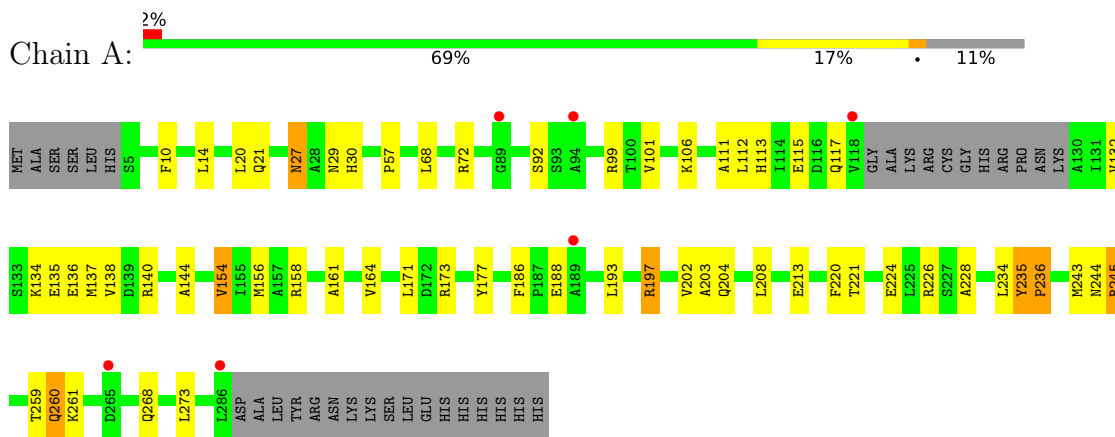
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	182	Total	O	0	0
			182	182		
4	C	113	Total	O	0	0
			113	113		
4	D	91	Total	O	0	0
			91	91		

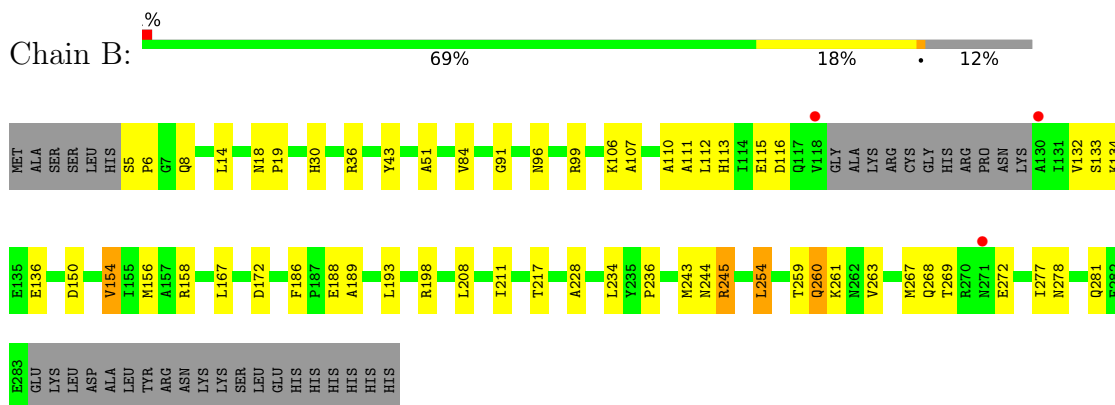
3 Residue-property plots [i](#)

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.

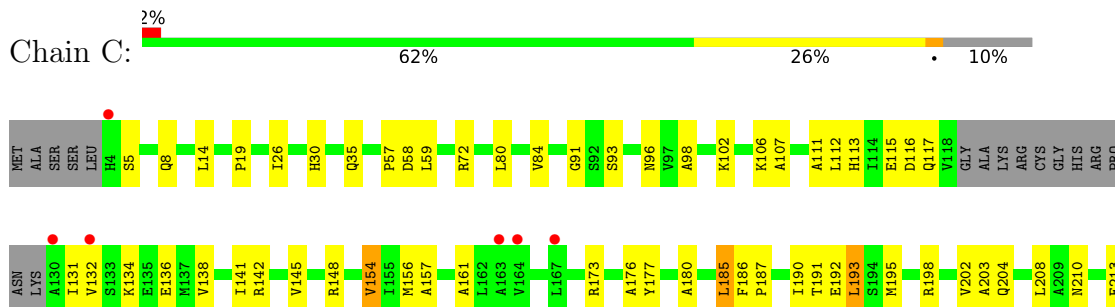
- Molecule 1: Probable methylisocitrate lyase

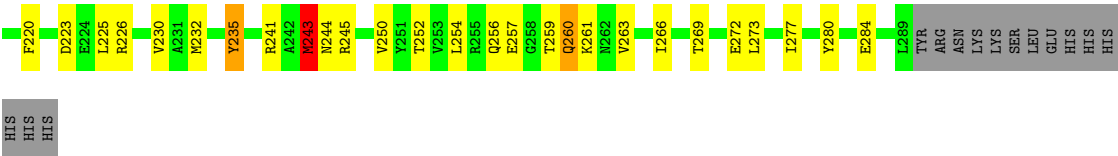


- Molecule 1: Probable methylisocitrate lyase

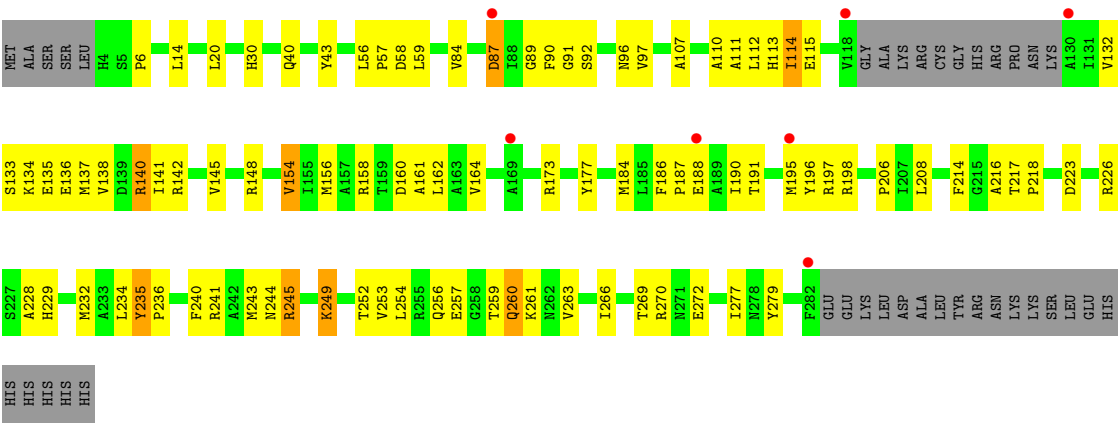


- Molecule 1: Probable methylisocitrate lyase





● Molecule 1: Probable methylisocitrate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.95Å 99.68Å 202.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.30 19.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.4 (19.90-2.30) 91.3 (19.90-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.251 0.200 , 0.251	Depositor DCC
R_{free} test set	2653 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	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	0.94	EDS
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, 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	0.37	0/2086	0.86	5/2832 (0.2%)
1	B	0.42	0/2060	0.88	5/2798 (0.2%)
1	C	0.38	1/2111 (0.0%)	0.83	3/2866 (0.1%)
1	D	0.35	0/2055	0.85	5/2791 (0.2%)
All	All	0.38	1/8312 (0.0%)	0.85	18/11287 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	MET	SD-CE	-5.64	1.65	1.79

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	PRO	N-CA-C	6.97	123.22	113.53
1	B	236	PRO	N-CA-C	6.66	123.68	113.75
1	B	154	VAL	N-CA-C	6.54	117.52	108.89
1	C	235	TYR	CA-C-N	6.01	125.50	119.24
1	C	235	TYR	C-N-CA	6.01	125.50	119.24
1	D	235	TYR	CA-C-N	6.00	125.48	119.24
1	D	235	TYR	C-N-CA	6.00	125.48	119.24
1	D	154	VAL	N-CA-C	5.91	117.09	108.58
1	A	235	TYR	CA-C-N	5.91	125.60	119.05
1	A	235	TYR	C-N-CA	5.91	125.60	119.05
1	C	154	VAL	N-CA-C	5.84	117.00	108.58
1	B	189	ALA	N-CA-C	5.64	120.11	113.23
1	B	84	VAL	N-CA-C	5.64	116.70	108.53
1	D	87	ASP	CB-CA-C	-5.58	110.13	116.54
1	D	257	GLU	N-CA-C	5.14	119.55	113.28
1	B	268	GLN	N-CA-C	-5.12	102.28	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	GLN	N-CA-C	-5.11	102.30	109.96
1	A	154	VAL	N-CA-C	5.07	116.58	108.87

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	2056	0	2062	54	0
1	B	2030	0	2032	49	0
1	C	2081	0	2083	93	0
1	D	2025	0	2027	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	1	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	167	0	0	3	0
4	B	182	0	0	8	0
4	C	113	0	0	7	0
4	D	91	0	0	1	0
All	All	8773	0	8204	259	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 16.

All (259) 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:30:HIS:NE2	1:C:243:MET:HE3	1.80	0.95
1:A:260:GLN:H	1:A:260:GLN:HE21	0.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:VAL:HG22	1:C:263:VAL:HG11	1.50	0.91
1:B:260:GLN:HE21	1:B:260:GLN:N	1.69	0.90
1:C:192:GLU:H	1:C:195:MET:HE3	1.37	0.89
1:C:192:GLU:N	1:C:195:MET:HE3	1.86	0.89
1:D:260:GLN:HE21	1:D:260:GLN:N	1.71	0.88
1:B:260:GLN:HE21	1:B:260:GLN:H	0.90	0.87
1:D:260:GLN:HE21	1:D:260:GLN:H	0.87	0.87
1:D:260:GLN:H	1:D:260:GLN:NE2	1.72	0.85
1:C:243:MET:HG3	1:D:243:MET:HB2	1.58	0.85
1:C:93:SER:HB3	1:C:96:ASN:ND2	1.92	0.84
1:D:249:LYS:HE3	1:D:249:LYS:HA	1.60	0.83
1:C:26:ILE:HG21	1:C:243:MET:HE1	1.60	0.83
1:C:243:MET:HE2	1:D:243:MET:HE3	1.58	0.83
1:C:260:GLN:H	1:C:260:GLN:HE21	1.27	0.82
1:A:132:VAL:HB	1:A:136:GLU:HG2	1.63	0.81
1:C:14:LEU:HD21	1:C:232:MET:HG2	1.62	0.80
1:C:243:MET:HE2	1:D:243:MET:CE	2.12	0.79
1:B:260:GLN:H	1:B:260:GLN:NE2	1.76	0.76
1:D:114:ILE:HD13	1:D:114:ILE:H	1.50	0.76
1:A:260:GLN:HE21	1:A:260:GLN:N	1.80	0.74
1:D:252:THR:O	1:D:256:GLN:HG3	1.89	0.72
1:C:250:VAL:HG22	1:C:263:VAL:CG1	2.19	0.72
1:A:260:GLN:H	1:A:260:GLN:NE2	1.82	0.71
1:A:112:LEU:C	1:A:112:LEU:HD12	2.16	0.71
1:C:57:PRO:HB2	1:C:59:LEU:HD13	1.72	0.70
1:D:91:GLY:HA3	1:D:96:ASN:HB3	1.73	0.70
1:D:249:LYS:HE2	1:D:253:VAL:HG23	1.73	0.69
1:D:190:ILE:HD12	1:D:196:TYR:CE1	2.28	0.69
1:B:5:SER:OG	1:B:8:GLN:HG3	1.93	0.69
1:D:187:PRO:HB2	1:D:190:ILE:HD11	1.75	0.68
1:A:137:MET:HE3	1:A:140:ARG:HB2	1.75	0.67
1:D:114:ILE:HG12	1:D:137:MET:HE1	1.78	0.65
1:B:259:THR:OG1	1:B:261:LYS:HG3	1.97	0.64
1:C:191:THR:OG1	1:C:195:MET:HE1	1.96	0.64
1:A:193:LEU:HD12	1:A:193:LEU:H	1.62	0.63
1:D:132:VAL:CG1	1:D:136:GLU:HB3	2.28	0.63
1:A:27:ASN:C	1:A:27:ASN:HD22	2.07	0.62
1:B:91:GLY:HA3	1:B:96:ASN:CB	2.29	0.62
1:C:260:GLN:H	1:C:260:GLN:NE2	1.97	0.62
1:C:208:LEU:HD23	1:C:208:LEU:C	2.24	0.62
1:C:112:LEU:C	1:C:112:LEU:HD12	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HG12	1:D:133:SER:N	2.14	0.62
1:D:134:LYS:O	1:D:138:VAL:HG23	2.00	0.62
1:D:197:ARG:HG2	1:D:229:HIS:CD2	2.35	0.62
1:C:223:ASP:HA	1:C:226:ARG:NH1	2.15	0.61
1:C:93:SER:H	1:C:96:ASN:HD22	1.47	0.61
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.66	0.61
1:D:223:ASP:HA	1:D:226:ARG:NH1	2.15	0.61
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.01	0.61
1:C:223:ASP:HA	1:C:226:ARG:HH12	1.65	0.60
1:B:112:LEU:HD12	1:B:112:LEU:C	2.26	0.60
1:D:112:LEU:HD12	1:D:112:LEU:C	2.27	0.60
1:D:111:ALA:CB	1:D:154:VAL:HB	2.32	0.60
1:C:26:ILE:CG2	1:C:243:MET:HE1	2.29	0.60
1:C:245:ARG:HD3	4:C:3330:HOH:O	2.02	0.59
1:C:208:LEU:HB2	1:C:232:MET:HE3	1.83	0.59
1:B:188:GLU:HG2	4:B:2354:HOH:O	2.02	0.59
1:A:30:HIS:HE1	1:B:244:ASN:ND2	2.00	0.59
1:A:30:HIS:HE1	1:B:244:ASN:HD22	1.51	0.59
1:C:14:LEU:HD21	1:C:232:MET:CG	2.31	0.59
1:A:259:THR:OG1	1:A:261:LYS:HG3	2.02	0.58
1:D:223:ASP:HA	1:D:226:ARG:HH12	1.68	0.58
1:C:138:VAL:O	1:C:142:ARG:HG3	2.03	0.58
1:D:111:ALA:HB2	1:D:154:VAL:HB	1.84	0.58
1:C:254:LEU:HD11	1:D:235:TYR:CE2	2.39	0.57
1:A:245:ARG:HD3	4:B:2355:HOH:O	2.04	0.57
1:C:58:ASP:C	1:C:59:LEU:HD12	2.30	0.57
1:A:208:LEU:C	1:A:208:LEU:HD23	2.28	0.57
1:A:244:ASN:ND2	1:B:30:HIS:HE1	2.04	0.56
1:B:99:ARG:HD3	4:B:2441:HOH:O	2.06	0.56
1:B:133:SER:OG	1:B:136:GLU:HG3	2.06	0.55
1:D:6:PRO:HB2	1:D:110:ALA:HB2	1.88	0.55
1:D:187:PRO:HB2	1:D:190:ILE:CD1	2.37	0.55
1:A:57:PRO:HA	1:B:277:ILE:HD12	1.88	0.55
1:A:193:LEU:HD12	1:A:193:LEU:N	2.21	0.55
1:B:106:LYS:HE2	1:C:107:ALA:O	2.05	0.55
4:A:1412:HOH:O	1:B:245:ARG:HD3	2.05	0.55
1:D:187:PRO:CB	1:D:190:ILE:HD11	2.37	0.55
1:C:5:SER:HB3	1:C:8:GLN:HG3	1.88	0.55
1:D:89:GLY:C	1:D:91:GLY:H	2.14	0.55
4:C:3309:HOH:O	1:D:241:ARG:HG2	2.07	0.55
1:B:208:LEU:C	1:B:208:LEU:HD23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASP:O	1:C:132:VAL:HG22	2.07	0.54
1:A:193:LEU:H	1:A:193:LEU:CD1	2.20	0.54
1:A:197:ARG:HD3	1:A:228:ALA:HA	1.88	0.54
1:A:29:ASN:HB2	1:B:51:ALA:O	2.07	0.54
1:C:257:GLU:O	1:C:259:THR:HG22	2.08	0.54
1:D:186:PHE:CD2	1:D:186:PHE:C	2.86	0.54
1:C:192:GLU:HG3	4:C:3415:HOH:O	2.08	0.54
1:C:30:HIS:HE1	1:D:244:ASN:HD22	1.56	0.54
1:D:132:VAL:HG12	1:D:136:GLU:HB3	1.90	0.54
1:C:145:VAL:HG13	1:C:148:ARG:NH2	2.23	0.53
1:D:14:LEU:HD21	1:D:232:MET:SD	2.48	0.53
1:D:208:LEU:C	1:D:208:LEU:HD23	2.33	0.53
1:C:111:ALA:HB2	1:C:154:VAL:HB	1.91	0.53
1:A:115:GLU:HA	1:A:158:ARG:O	2.09	0.53
1:C:134:LYS:O	1:C:138:VAL:HG23	2.08	0.53
1:A:203:ALA:O	1:A:204:GLN:HB2	2.09	0.52
1:C:213:GLU:CD	1:C:213:GLU:H	2.17	0.52
1:D:161:ALA:CB	1:D:173:ARG:HD2	2.39	0.52
1:C:186:PHE:C	1:C:186:PHE:CD2	2.87	0.52
1:C:30:HIS:HE1	1:D:244:ASN:ND2	2.06	0.52
1:A:221:THR:OG1	1:A:224:GLU:HG3	2.09	0.52
1:A:193:LEU:HD11	1:A:220:PHE:CE2	2.45	0.52
1:A:135:GLU:CD	1:A:135:GLU:H	2.18	0.52
1:B:91:GLY:HA3	1:B:96:ASN:HB3	1.92	0.52
1:A:113:HIS:HA	1:A:156:MET:O	2.10	0.52
1:C:30:HIS:HD2	4:C:3349:HOH:O	1.92	0.52
1:D:259:THR:OG1	1:D:261:LYS:HG3	2.11	0.51
1:C:111:ALA:CB	1:C:154:VAL:HB	2.40	0.51
1:B:99:ARG:NH2	1:D:56:LEU:HD11	2.26	0.51
1:D:137:MET:O	1:D:141:ILE:HG13	2.11	0.51
1:A:113:HIS:HB3	1:A:156:MET:HB3	1.93	0.51
1:D:263:VAL:O	1:D:266:ILE:HG12	2.10	0.51
1:A:14:LEU:HD22	1:A:20:LEU:CD2	2.41	0.50
1:B:269:THR:OG1	1:B:272:GLU:HG3	2.11	0.50
1:D:132:VAL:HG11	1:D:136:GLU:HB3	1.93	0.50
1:A:30:HIS:HD2	4:A:1389:HOH:O	1.93	0.50
1:C:252:THR:CG2	1:C:256:GLN:HE21	2.24	0.50
1:B:111:ALA:CB	1:B:154:VAL:HB	2.41	0.50
1:C:141:ILE:O	1:C:145:VAL:HG23	2.11	0.50
1:D:138:VAL:O	1:D:142:ARG:HG3	2.12	0.50
1:D:186:PHE:C	1:D:186:PHE:HD2	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:TYR:CE2	1:D:254:LEU:HD11	2.47	0.50
1:C:261:LYS:HD2	4:C:3360:HOH:O	2.12	0.49
1:B:99:ARG:NH1	4:B:2484:HOH:O	2.44	0.49
1:D:197:ARG:HG2	1:D:229:HIS:HD2	1.74	0.49
1:D:240:PHE:O	1:D:243:MET:HG2	2.13	0.49
1:B:134:LYS:HE2	1:B:172:ASP:OD2	2.13	0.49
1:C:254:LEU:HD21	1:D:235:TYR:CG	2.47	0.49
1:C:244:ASN:HD22	1:D:30:HIS:HE1	1.61	0.49
1:D:145:VAL:HG13	1:D:148:ARG:NH2	2.27	0.49
1:D:158:ARG:HH21	1:D:188:GLU:CD	2.21	0.49
1:C:186:PHE:C	1:C:186:PHE:HD2	2.20	0.49
1:C:5:SER:HB3	1:C:8:GLN:CG	2.43	0.49
1:A:27:ASN:ND2	1:A:30:HIS:H	2.10	0.49
1:C:30:HIS:NE2	1:C:243:MET:CE	2.65	0.49
1:C:30:HIS:CD2	1:C:243:MET:HE3	2.47	0.48
1:D:20:LEU:HD11	1:D:40:GLN:HB2	1.95	0.48
1:B:211:ILE:HG22	1:B:211:ILE:O	2.14	0.48
1:A:226:ARG:HA	4:A:1469:HOH:O	2.13	0.48
1:C:243:MET:CG	1:D:243:MET:HB2	2.38	0.48
1:D:184:MET:HG2	1:D:206:PRO:HB2	1.94	0.48
1:B:193:LEU:HB3	1:B:228:ALA:HB2	1.96	0.48
1:A:112:LEU:C	1:A:112:LEU:CD1	2.87	0.48
1:C:132:VAL:HB	1:C:136:GLU:HG2	1.95	0.48
1:D:132:VAL:HG11	1:D:136:GLU:CD	2.39	0.48
1:C:203:ALA:O	1:C:204:GLN:HB2	2.13	0.47
1:B:116:ASP:O	1:B:132:VAL:HG22	2.14	0.47
1:D:114:ILE:HD13	1:D:156:MET:O	2.15	0.47
1:D:162:LEU:HD13	1:D:162:LEU:C	2.39	0.47
1:B:158:ARG:NH1	3:B:2302:PYR:O3	2.47	0.47
1:B:158:ARG:NH2	1:B:188:GLU:OE2	2.46	0.47
1:C:254:LEU:HD13	1:C:260:GLN:HB3	1.97	0.47
1:A:171:LEU:HD22	1:A:202:VAL:HG21	1.97	0.46
1:A:161:ALA:HB2	1:A:173:ARG:HD2	1.97	0.46
1:D:135:GLU:CD	1:D:135:GLU:H	2.23	0.46
1:D:214:PHE:HE2	1:D:241:ARG:HD3	1.80	0.46
1:D:228:ALA:O	1:D:229:HIS:HB2	2.14	0.46
1:D:87:ASP:O	1:D:114:ILE:HA	2.15	0.46
1:B:107:ALA:O	1:C:106:LYS:HE2	2.15	0.46
1:C:35:GLN:HA	1:C:80:LEU:HD11	1.98	0.46
1:C:243:MET:CE	1:D:243:MET:HE3	2.37	0.46
1:B:36:ARG:HG3	4:B:2430:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HD13	1:C:220:PHE:CE2	2.51	0.46
1:A:21:GLN:NE2	1:B:254:LEU:HD22	2.31	0.45
1:A:132:VAL:HB	1:A:136:GLU:CG	2.39	0.45
1:C:84:VAL:O	1:C:112:LEU:HA	2.16	0.45
1:B:18:ASN:HA	1:B:19:PRO:HA	1.86	0.45
1:C:225:LEU:HB3	1:C:230:VAL:HB	1.98	0.45
1:C:244:ASN:ND2	1:D:30:HIS:HE1	2.14	0.45
1:D:160:ASP:O	1:D:164:VAL:HG23	2.17	0.45
1:C:57:PRO:HA	1:D:277:ILE:HD12	1.98	0.45
1:C:243:MET:HE2	1:D:243:MET:SD	2.56	0.45
1:A:111:ALA:HB2	1:A:154:VAL:HB	1.98	0.45
1:C:280:TYR:O	1:C:284:GLU:HG3	2.16	0.45
1:A:134:LYS:O	1:A:138:VAL:HG23	2.17	0.45
1:D:132:VAL:CG1	1:D:133:SER:N	2.78	0.45
1:A:235:TYR:CG	1:B:254:LEU:HD11	2.52	0.45
1:C:138:VAL:HG13	1:C:180:ALA:HB2	1.97	0.45
1:A:101:VAL:HG21	1:A:144:ALA:HA	1.98	0.45
1:A:106:LYS:HE2	1:D:107:ALA:O	2.17	0.44
1:C:235:TYR:CG	1:D:254:LEU:HD21	2.52	0.44
1:D:84:VAL:O	1:D:112:LEU:HA	2.18	0.44
1:D:115:GLU:HA	1:D:158:ARG:O	2.17	0.44
1:A:132:VAL:CB	1:A:136:GLU:HG2	2.42	0.44
1:C:190:ILE:HG23	1:C:195:MET:HB2	1.99	0.44
1:C:213:GLU:HG2	1:C:241:ARG:NE	2.33	0.44
1:D:135:GLU:O	1:D:138:VAL:HB	2.17	0.44
1:A:10:PHE:O	1:A:14:LEU:HD23	2.17	0.44
1:B:278:ASN:ND2	4:B:2469:HOH:O	2.51	0.44
1:C:213:GLU:HG2	1:C:241:ARG:HE	1.82	0.44
1:D:113:HIS:HB3	1:D:156:MET:HB3	1.99	0.44
1:A:115:GLU:HG3	1:A:117:GLN:HB2	2.00	0.43
1:D:89:GLY:C	1:D:91:GLY:N	2.75	0.43
1:A:14:LEU:HD22	1:A:20:LEU:HD22	2.00	0.43
1:C:134:LYS:HD3	1:C:176:ALA:HB2	2.00	0.43
1:D:195:MET:HE2	1:D:198:ARG:NH1	2.33	0.43
1:D:195:MET:HE2	1:D:198:ARG:HH11	1.83	0.43
1:A:158:ARG:HH21	1:A:188:GLU:CD	2.26	0.43
1:A:137:MET:HG2	1:A:177:TYR:CZ	2.53	0.43
1:D:132:VAL:HG12	1:D:133:SER:H	1.83	0.43
1:D:158:ARG:HA	1:D:186:PHE:HB3	2.00	0.43
1:B:30:HIS:HD2	4:B:2317:HOH:O	2.01	0.43
1:C:157:ALA:O	1:C:185:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HA	1:B:186:PHE:HB3	2.01	0.43
1:C:5:SER:HB3	1:C:8:GLN:OE1	2.19	0.43
1:C:131:ILE:HD13	1:C:161:ALA:HA	2.00	0.43
1:B:43:TYR:CG	1:B:234:LEU:HD11	2.54	0.42
1:C:277:ILE:HD12	1:D:57:PRO:HA	2.01	0.42
1:C:91:GLY:HA3	1:C:96:ASN:CB	2.49	0.42
1:C:173:ARG:HB3	1:C:177:TYR:CZ	2.54	0.42
1:C:187:PRO:HB2	1:C:190:ILE:CD1	2.49	0.42
1:D:191:THR:HG22	1:D:216:ALA:O	2.19	0.42
1:A:186:PHE:C	1:A:186:PHE:CD2	2.97	0.42
1:B:263:VAL:O	1:B:267:MET:HG3	2.20	0.42
1:C:5:SER:HB3	1:C:8:GLN:CD	2.44	0.42
1:C:263:VAL:HG13	1:C:266:ILE:HD11	2.00	0.42
1:B:6:PRO:HB2	1:B:110:ALA:HB2	2.01	0.42
1:C:263:VAL:O	1:C:263:VAL:HG12	2.20	0.42
1:D:269:THR:OG1	1:D:272:GLU:HG3	2.19	0.42
1:C:19:PRO:HD3	1:C:226:ARG:HB2	2.02	0.42
1:C:98:ALA:O	1:C:102:LYS:HE2	2.20	0.42
1:B:111:ALA:HB1	1:B:154:VAL:HB	2.02	0.42
1:B:111:ALA:HB2	1:B:154:VAL:HB	2.02	0.42
1:C:113:HIS:HA	1:C:156:MET:O	2.20	0.42
4:C:3361:HOH:O	1:D:245:ARG:HD3	2.19	0.42
1:D:249:LYS:HE3	1:D:249:LYS:CA	2.42	0.42
1:D:270:ARG:NH2	4:D:4350:HOH:O	2.52	0.42
1:A:158:ARG:HA	1:A:186:PHE:HB3	2.01	0.41
1:C:72:ARG:HD2	4:C:3331:HOH:O	2.20	0.41
1:D:114:ILE:HD13	1:D:114:ILE:N	2.26	0.41
1:D:173:ARG:HB3	1:D:177:TYR:CZ	2.56	0.41
1:D:234:LEU:HG	1:D:236:PRO:HD3	2.02	0.41
1:D:217:THR:HA	1:D:218:PRO:HD3	1.92	0.41
1:A:213:GLU:CD	1:A:213:GLU:H	2.27	0.41
1:B:115:GLU:HB3	1:B:158:ARG:HB3	2.01	0.41
1:B:217:THR:HB	4:B:2359:HOH:O	2.19	0.41
1:C:186:PHE:CE2	1:C:210:ASN:HB2	2.56	0.41
1:B:150:ASP:OD1	1:B:150:ASP:C	2.63	0.41
1:A:111:ALA:CB	1:A:154:VAL:HB	2.49	0.41
1:C:198:ARG:O	1:C:202:VAL:HG23	2.20	0.41
1:D:43:TYR:CG	1:D:234:LEU:HD11	2.56	0.41
1:D:58:ASP:O	1:D:59:LEU:HD12	2.19	0.41
1:A:27:ASN:C	1:A:27:ASN:ND2	2.78	0.41
1:D:97:VAL:HG21	1:D:140:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LYS:HD3	1:C:176:ALA:CB	2.51	0.41
1:C:192:GLU:HB2	1:C:195:MET:HG3	2.03	0.41
1:C:59:LEU:HD11	1:D:279:TYR:CE1	2.56	0.41
1:B:113:HIS:HA	1:B:156:MET:O	2.20	0.41
1:B:113:HIS:HB3	1:B:156:MET:HB3	2.03	0.40
1:B:186:PHE:C	1:B:186:PHE:CD2	2.99	0.40
1:B:278:ASN:HB3	1:B:281:GLN:CD	2.46	0.40
1:C:115:GLU:OE2	1:C:117:GLN:NE2	2.55	0.40
1:A:68:LEU:O	1:A:72:ARG:HG3	2.20	0.40
1:C:191:THR:H	1:C:195:MET:CE	2.33	0.40
1:A:234:LEU:HG	1:A:236:PRO:HD3	2.04	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	267/305 (88%)	257 (96%)	8 (3%)	2 (1%)	18	23
1	B	264/305 (87%)	258 (98%)	6 (2%)	0	100	100
1	C	271/305 (89%)	262 (97%)	9 (3%)	0	100	100
1	D	264/305 (87%)	255 (97%)	7 (3%)	2 (1%)	16	20
All	All	1066/1220 (87%)	1032 (97%)	30 (3%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	164	VAL
1	D	90	PHE
1	D	92	SER

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	210/239 (88%)	204 (97%)	6 (3%)	37	55
1	B	207/239 (87%)	200 (97%)	7 (3%)	32	49
1	C	212/239 (89%)	207 (98%)	5 (2%)	43	62
1	D	206/239 (86%)	201 (98%)	5 (2%)	43	62
All	All	835/956 (87%)	812 (97%)	23 (3%)	38	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	197	ARG
1	A	243	MET
1	A	245	ARG
1	A	260	GLN
1	A	273	LEU
1	B	14	LEU
1	B	167	LEU
1	B	198	ARG
1	B	243	MET
1	B	245	ARG
1	B	254	LEU
1	B	260	GLN
1	C	185	LEU
1	C	193	LEU
1	C	243	MET
1	C	260	GLN
1	C	273	LEU
1	D	114	ILE
1	D	140	ARG
1	D	245	ARG
1	D	249	LYS
1	D	260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	27	ASN
1	A	30	HIS
1	A	35	GLN
1	A	40	GLN
1	A	244	ASN
1	A	260	GLN
1	A	281	GLN
1	B	30	HIS
1	B	35	GLN
1	B	40	GLN
1	B	117	GLN
1	B	204	GLN
1	B	244	ASN
1	B	260	GLN
1	B	281	GLN
1	C	30	HIS
1	C	35	GLN
1	C	96	ASN
1	C	117	GLN
1	C	175	GLN
1	C	229	HIS
1	C	244	ASN
1	C	256	GLN
1	C	260	GLN
1	C	281	GLN
1	D	30	HIS
1	D	35	GLN
1	D	96	ASN
1	D	204	GLN
1	D	229	HIS
1	D	244	ASN
1	D	260	GLN
1	D	271	ASN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PYR	D	4302	2	5,5,5	1.47	2 (40%)	3,6,6	2.79	2 (66%)
3	PYR	A	1302	2	5,5,5	1.52	1 (20%)	3,6,6	2.75	2 (66%)
3	PYR	C	3302	2	5,5,5	1.45	1 (20%)	3,6,6	2.75	2 (66%)
3	PYR	B	2302	2	5,5,5	1.45	2 (40%)	3,6,6	2.76	2 (66%)

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	PYR	D	4302	2	-	0/4/4/4	-
3	PYR	A	1302	2	-	0/4/4/4	-
3	PYR	C	3302	2	-	0/4/4/4	-
3	PYR	B	2302	2	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	PYR	CB-CA	2.32	1.54	1.50
3	C	3302	PYR	CB-CA	2.30	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2302	PYR	CB-CA	2.25	1.54	1.50
3	D	4302	PYR	OXT-C	-2.08	1.24	1.30
3	D	4302	PYR	CB-CA	2.08	1.54	1.50
3	B	2302	PYR	OXT-C	-2.00	1.25	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4302	PYR	OXT-C-O	-3.80	114.86	123.90
3	B	2302	PYR	OXT-C-O	-3.77	114.91	123.90
3	C	3302	PYR	OXT-C-O	-3.73	115.01	123.90
3	A	1302	PYR	OXT-C-O	-3.73	115.03	123.90
3	C	3302	PYR	OXT-C-CA	2.61	120.82	113.59
3	A	1302	PYR	OXT-C-CA	2.60	120.80	113.59
3	D	4302	PYR	OXT-C-CA	2.58	120.74	113.59
3	B	2302	PYR	OXT-C-CA	2.56	120.70	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2302	PYR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	271/305 (88%)	-0.14	6 (2%) 62 64	21, 34, 63, 76	0
1	B	268/305 (87%)	-0.40	3 (1%) 78 79	20, 29, 46, 76	0
1	C	275/305 (90%)	0.13	6 (2%) 62 64	26, 44, 69, 85	0
1	D	268/305 (87%)	0.25	7 (2%) 57 59	26, 46, 72, 87	0
All	All	1082/1220 (88%)	-0.04	22 (2%) 65 66	20, 38, 67, 87	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	ALA	4.2
1	B	118	VAL	3.6
1	C	163	ALA	3.0
1	A	286	LEU	3.0
1	C	4	HIS	2.9
1	D	169	ALA	2.8
1	A	89	GLY	2.8
1	D	87	ASP	2.7
1	C	164	VAL	2.6
1	A	265	ASP	2.5
1	C	167	LEU	2.4
1	C	130	ALA	2.3
1	D	118	VAL	2.3
1	D	188	GLU	2.2
1	D	282	PHE	2.2
1	C	132	VAL	2.1
1	A	94	ALA	2.1
1	D	195	MET	2.1
1	B	271	ASN	2.1
1	A	189	ALA	2.0
1	B	130	ALA	2.0
1	A	118	VAL	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	MG	C	3301	1/1	0.84	0.09	49,49,49,49	1
3	PYR	D	4302	6/6	0.89	0.10	49,50,52,53	6
3	PYR	C	3302	6/6	0.91	0.08	36,39,41,43	6
2	MG	A	1301	1/1	0.93	0.06	33,33,33,33	1
3	PYR	A	1302	6/6	0.94	0.07	29,31,34,34	6
2	MG	D	4301	1/1	0.95	0.06	53,53,53,53	1
2	MG	B	2301	1/1	0.97	0.07	32,32,32,32	1
3	PYR	B	2302	6/6	0.97	0.07	27,31,33,34	6

6.5 Other polymers [i](#)

There are no such residues in this entry.