



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:47 AM EDT

PDB ID : 2QQC
Title : E109Q mutant of Pyruvoyl-dependent Arginine Decarboxylase from Methanococcus jannashii
Authors : Ealick, S.E.; Soriano, E.S.
Deposited on : 2007-07-26
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

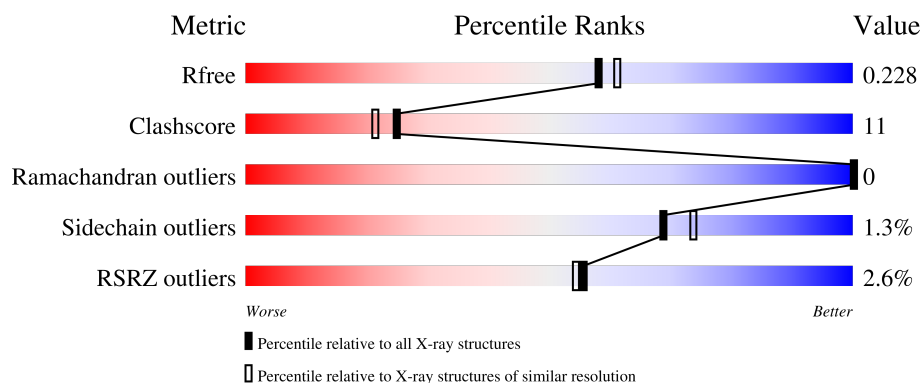
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	53	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>13%</div> </div> </div>
1	C	53	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>11%</div> </div> </div>
1	E	53	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	G	53	<div> <div></div> <div> <div></div> <div>62%</div> <div>13%</div> <div>25%</div> </div> </div>
1	I	53	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>9%</div> <div>•</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	53	<div><div></div><div>4%</div><div>57%</div><div>19%</div><div>25%</div></div>
2	B	112	<div><div></div><div>3%</div><div>79%</div><div>21%</div></div>
2	D	112	<div><div></div><div>4%</div><div>75%</div><div>24%</div><div>.</div></div>
2	F	112	<div><div></div><div>%</div><div>79%</div><div>21%</div></div>
2	H	112	<div><div></div><div>4%</div><div>77%</div><div>23%</div></div>
2	J	112	<div><div></div><div></div><div>71%</div><div>26%</div><div>.</div></div>
2	L	112	<div><div></div><div>3%</div><div>79%</div><div>21%</div><div>.</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7630 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 Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	0	0	0
			336	214	57	65			
1	C	47	Total	C	N	O	0	0	0
			344	218	59	67			
1	E	50	Total	C	N	O	0	0	0
			366	232	62	72			
1	G	40	Total	C	N	O	0	0	0
			283	176	49	58			
1	I	40	Total	C	N	O	0	0	0
			283	176	49	58			
1	K	40	Total	C	N	O	0	0	0
			283	176	49	58			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q57764
C	0	HIS	-	expression tag	UNP Q57764
E	0	HIS	-	expression tag	UNP Q57764
G	0	HIS	-	expression tag	UNP Q57764
I	0	HIS	-	expression tag	UNP Q57764
K	0	HIS	-	expression tag	UNP Q57764

- Molecule 2 is a protein called Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			
2	D	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			

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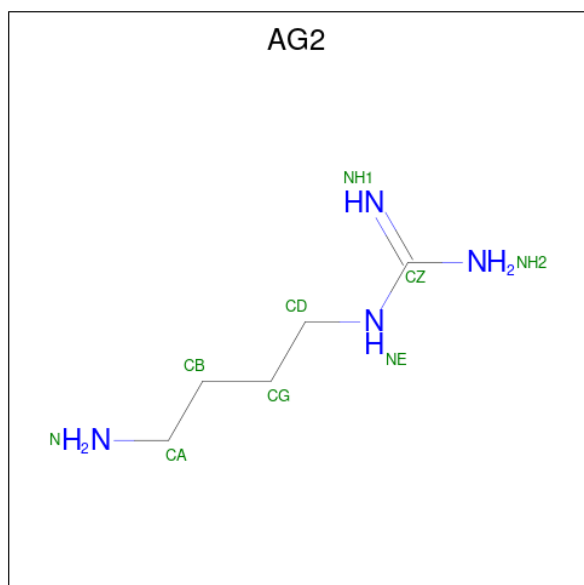
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			
2	H	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			
2	J	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			
2	L	112	Total	C	N	O	S	0	0	0
			853	552	136	157	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	GLN	GLU	engineered mutation	UNP Q57764
D	109	GLN	GLU	engineered mutation	UNP Q57764
F	109	GLN	GLU	engineered mutation	UNP Q57764
H	109	GLN	GLU	engineered mutation	UNP Q57764
J	109	GLN	GLU	engineered mutation	UNP Q57764
L	109	GLN	GLU	engineered mutation	UNP Q57764

- Molecule 3 is AGMATINE (three-letter code: AG2) (formula: C₅H₁₄N₄).



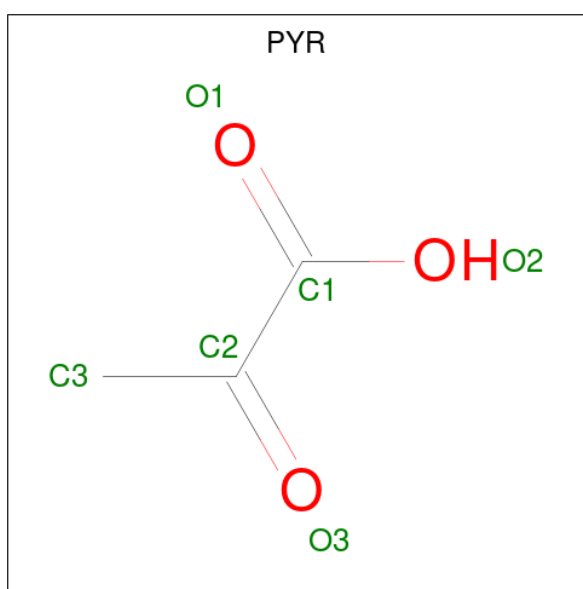
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	5	4		
3	A	1	Total	C	N	0	0
			9	5	4		

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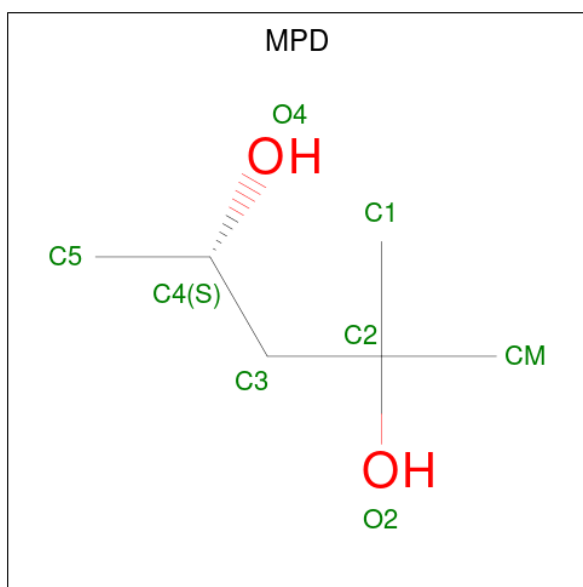
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	N	0	0
			9	5	4		
3	I	1	Total	C	N	0	0
			9	5	4		
3	I	1	Total	C	N	0	0
			9	5	4		
3	K	1	Total	C	N	0	0
			9	5	4		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			5	3	2		
4	D	1	Total	C	O	0	0
			5	3	2		
4	F	1	Total	C	O	0	0
			5	3	2		
4	H	1	Total	C	O	0	0
			5	3	2		
4	J	1	Total	C	O	0	0
			5	3	2		
4	L	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	60	Total	O	0	0
			60	60		
6	C	37	Total	O	0	0
			37	37		
6	D	48	Total	O	0	0
			48	48		
6	E	49	Total	O	0	0
			49	49		
6	F	69	Total	O	0	0
			69	69		
6	G	23	Total	O	0	0
			23	23		
6	H	39	Total	O	0	0
			39	39		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	18	Total 18	O 18	0	0
6	J	50	Total 50	O 50	0	0
6	K	25	Total 25	O 25	0	0
6	L	48	Total 48	O 48	0	0

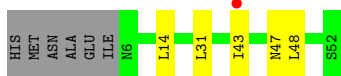
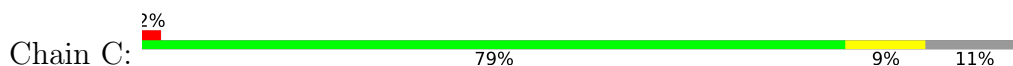
3 Residue-property plots [i](#)

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.

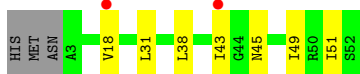
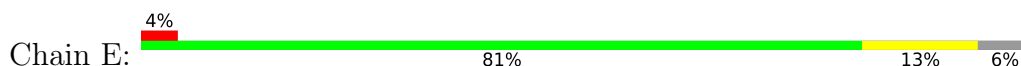
- Molecule 1: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



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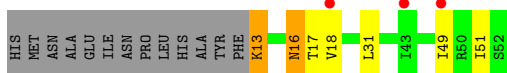
- Molecule 1: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



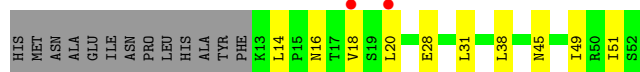
- Molecule 1: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



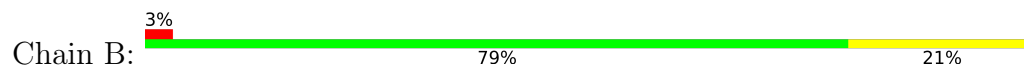
- Molecule 1: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



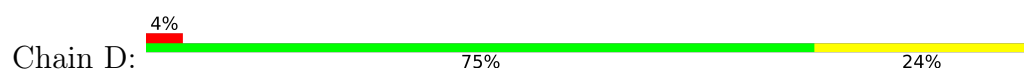
- Molecule 1: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



- Molecule 2: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



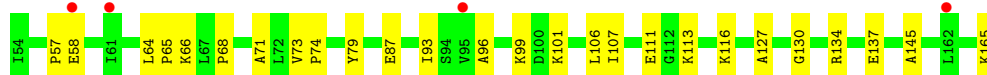
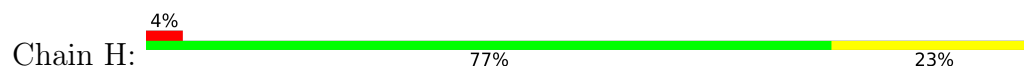
- Molecule 2: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



- Molecule 2: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



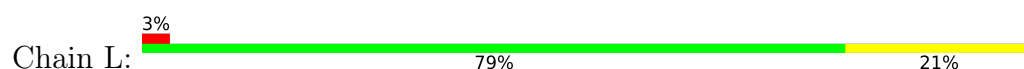
- Molecule 2: Pyruvoyl-dependent arginine decarboxylase (EC 4.1.1.19) (PvlArgDC)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.11Å 92.81Å 85.71Å 90.00° 95.11° 90.00°	Depositor
Resolution (Å)	44.03 – 2.00 49.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.03-2.00) 97.7 (49.11-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.09 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.194 , 0.237 0.186 , 0.228	Depositor DCC
R_{free} test set	6076 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.6	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	7630	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: AG2, MPD, PYR

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	0.35	0/342	0.63	0/464
1	C	0.35	0/350	0.60	0/476
1	E	0.35	0/372	0.59	0/506
1	G	0.31	0/285	0.61	0/386
1	I	0.34	0/285	0.59	0/386
1	K	0.34	0/285	0.61	0/386
2	B	0.31	0/871	0.60	0/1178
2	D	0.30	0/871	0.60	0/1178
2	F	0.30	0/871	0.63	0/1178
2	H	0.30	0/871	0.58	0/1178
2	J	0.28	0/871	0.58	0/1178
2	L	0.30	0/871	0.61	0/1178
All	All	0.31	0/7145	0.60	0/9672

There are no bond length outliers.

There are no bond angle outliers.

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	336	0	338	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	344	0	343	5	0
1	E	366	0	365	14	0
1	G	283	0	289	9	0
1	I	283	0	289	22	0
1	K	283	0	289	18	0
2	B	853	0	881	16	0
2	D	853	0	881	19	0
2	F	853	0	881	17	0
2	H	853	0	881	18	0
2	J	853	0	881	31	0
2	L	853	0	881	21	0
3	A	18	0	26	4	0
3	E	9	0	13	2	0
3	I	18	0	26	5	0
3	K	9	0	13	2	0
4	B	5	0	3	1	0
4	D	5	0	3	0	0
4	F	5	0	3	1	0
4	H	5	0	3	0	0
4	J	5	0	3	0	0
4	L	5	0	3	0	0
5	B	8	0	14	0	0
5	C	8	0	14	0	0
5	E	8	0	14	0	0
5	I	8	0	14	1	0
6	A	35	0	0	0	0
6	B	60	0	0	0	0
6	C	37	0	0	1	0
6	D	48	0	0	0	0
6	E	49	0	0	0	0
6	F	69	0	0	0	0
6	G	23	0	0	0	0
6	H	39	0	0	1	0
6	I	18	0	0	0	0
6	J	50	0	0	0	0
6	K	25	0	0	1	0
6	L	48	0	0	1	0
All	All	7630	0	7351	157	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 11.

All (157) 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)
2:H:134:ARG:HE	1:K:45:ASN:HD21	1.18	0.90
2:L:115:SER:OG	2:L:118:GLU:HG2	1.84	0.77
2:D:134:ARG:HE	1:E:45:ASN:HD21	1.30	0.77
2:H:134:ARG:HE	1:K:45:ASN:ND2	1.86	0.73
1:E:31:LEU:HD11	3:E:671:AG2:HA1	1.70	0.73
1:I:16:ASN:HD21	2:J:165:LYS:H	1.40	0.70
1:I:18:VAL:HG22	2:J:162:LEU:HD22	1.76	0.68
1:I:17:THR:HG22	2:J:165:LYS:HD2	1.75	0.67
2:H:116:LYS:HE2	2:H:145:ALA:O	1.94	0.67
2:D:134:ARG:HE	1:E:45:ASN:ND2	1.94	0.66
1:A:52:SER:HB2	1:C:48:LEU:HB2	1.77	0.65
2:D:60:GLU:HG3	2:D:62:VAL:HG13	1.78	0.65
3:A:671:AG2:HA1	1:C:31:LEU:HD21	1.79	0.65
1:E:18:VAL:HB	2:F:61:ILE:HD13	1.80	0.64
1:G:49:ILE:CD1	1:I:51:ILE:HG22	2.27	0.64
1:G:49:ILE:HD13	1:I:51:ILE:HG22	1.79	0.64
2:L:93:ILE:HG22	2:L:144:ILE:HG22	1.80	0.63
1:E:18:VAL:HG22	2:F:162:LEU:CD2	2.29	0.63
1:I:49:ILE:CD1	1:K:51:ILE:HG22	2.27	0.63
2:L:93:ILE:HG22	2:L:144:ILE:CG2	2.30	0.61
1:E:18:VAL:HG22	2:F:162:LEU:HD23	1.81	0.61
1:A:18:VAL:HG21	2:B:55:MET:HG3	1.81	0.60
1:G:51:ILE:HG22	1:K:49:ILE:CD1	2.32	0.59
1:I:49:ILE:HD13	1:K:51:ILE:HG22	1.85	0.58
2:J:83:ASP:O	2:J:85:PRO:HD3	2.03	0.58
2:F:116:LYS:HE2	2:F:145:ALA:O	2.03	0.58
1:I:17:THR:HG21	2:J:165:LYS:HB3	1.87	0.56
1:G:51:ILE:HG22	1:K:49:ILE:HD13	1.88	0.56
2:J:128:LYS:O	2:J:132:GLU:HG3	2.05	0.56
1:K:20:LEU:N	1:K:20:LEU:HD22	2.20	0.56
2:H:99:LYS:HD3	2:H:137:GLU:OE2	2.06	0.56
2:L:128:LYS:O	2:L:132:GLU:HG3	2.05	0.56
1:G:31:LEU:HD11	3:I:671:AG2:HA2	1.88	0.55
2:J:165:LYS:HB2	2:J:165:LYS:NZ	2.21	0.55
2:H:57:PRO:O	2:H:58:GLU:HB2	2.06	0.55
2:L:93:ILE:CG2	2:L:144:ILE:HG22	2.36	0.55
1:I:18:VAL:HG22	2:J:162:LEU:CD2	2.36	0.55
2:F:60:GLU:HG2	2:F:62:VAL:CG1	2.37	0.55
2:B:60:GLU:HG2	2:B:62:VAL:HG13	1.88	0.55
2:D:94:SER:HB3	2:D:123:VAL:HG13	1.88	0.55
1:E:18:VAL:HG21	2:F:55:MET:HG3	1.90	0.54
1:I:16:ASN:HD21	2:J:165:LYS:N	2.03	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:733:HOH:O	2:D:152:LYS:HD3	2.06	0.54
2:F:83:ASP:HB3	2:F:153:LEU:HD13	1.90	0.54
1:I:16:ASN:ND2	2:J:164:TYR:HA	2.23	0.54
2:H:68:PRO:HG2	2:H:71:ALA:HB2	1.91	0.53
2:B:116:LYS:HB2	2:B:147:GLU:HB3	1.89	0.53
2:B:128:LYS:O	2:B:132:GLU:HG3	2.08	0.53
2:J:61:ILE:CD1	2:J:97:ILE:HD11	2.39	0.53
2:L:60:GLU:HG3	2:L:62:VAL:HG13	1.89	0.53
2:F:60:GLU:HG2	2:F:62:VAL:HG13	1.89	0.53
2:J:96:ALA:HB2	2:J:127:ALA:HB1	1.91	0.52
2:L:87:GLU:OE2	2:L:113:LYS:HD3	2.09	0.52
2:D:128:LYS:O	2:D:132:GLU:HG3	2.09	0.52
1:I:31:LEU:HD11	3:I:672:AG2:HA1	1.91	0.52
2:D:83:ASP:HB3	2:D:153:LEU:HD13	1.90	0.52
1:K:28:GLU:HG3	6:K:678:HOH:O	2.09	0.52
2:B:87:GLU:OE2	2:B:113:LYS:HD3	2.11	0.51
2:D:115:SER:OG	2:D:118:GLU:HG3	2.10	0.51
2:H:106:LEU:CD2	2:H:130:GLY:HA3	2.41	0.51
2:D:60:GLU:HG3	2:D:62:VAL:CG1	2.41	0.51
2:H:134:ARG:NE	1:K:45:ASN:HD21	1.99	0.51
2:H:116:LYS:HG2	6:H:174:HOH:O	2.10	0.50
2:B:81:ILE:HG12	2:B:155:CYS:HB2	1.93	0.50
2:D:152:LYS:N	2:D:152:LYS:HD2	2.26	0.50
1:K:31:LEU:HD11	3:K:671:AG2:HA1	1.94	0.50
1:A:49:ILE:CD1	1:E:51:ILE:HG22	2.41	0.50
2:D:96:ALA:HB2	2:D:127:ALA:HB1	1.93	0.49
1:A:31:LEU:HD11	3:A:672:AG2:CA	2.43	0.49
1:I:17:THR:CG2	2:J:165:LYS:HD2	2.41	0.49
1:A:31:LEU:HD11	3:A:672:AG2:HA1	1.94	0.49
2:L:134:ARG:HH11	2:L:134:ARG:HG3	1.78	0.49
1:I:16:ASN:H	1:I:16:ASN:HD22	1.60	0.48
2:F:106:LEU:HD21	2:F:108:MET:HE3	1.94	0.48
1:I:13:LYS:N	1:I:13:LYS:HD2	2.29	0.48
3:A:671:AG2:HA2	2:B:107:ILE:O	2.13	0.48
2:D:106:LEU:CD2	2:D:130:GLY:HA3	2.44	0.48
2:F:128:LYS:O	2:F:132:GLU:HG3	2.13	0.48
2:J:116:LYS:HE3	2:J:145:ALA:O	2.13	0.48
1:E:49:ILE:HD11	2:F:72:LEU:HB3	1.94	0.48
1:I:31:LEU:HD11	3:I:672:AG2:CA	2.43	0.48
2:J:61:ILE:HD12	2:J:97:ILE:HD11	1.96	0.47
2:D:77:TYR:HB3	2:D:159:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ALA:HB2	2:B:127:ALA:HB1	1.95	0.47
2:J:165:LYS:HB2	2:J:165:LYS:HZ2	1.79	0.47
2:F:106:LEU:CD2	2:F:130:GLY:HA3	2.45	0.47
1:A:51:ILE:HG21	4:B:53:PYR:H32	1.96	0.46
2:B:61:ILE:CD1	2:B:142:GLU:HG3	2.45	0.46
2:D:134:ARG:NE	1:E:45:ASN:HD21	2.06	0.46
2:D:68:PRO:HG2	2:D:71:ALA:HB2	1.96	0.46
2:L:99:LYS:HE3	2:L:99:LYS:HB2	1.79	0.46
2:D:61:ILE:HD12	2:D:142:GLU:OE2	2.16	0.46
1:K:18:VAL:O	2:L:61:ILE:HA	2.16	0.46
2:L:79:TYR:O	2:L:111:GLU:HG3	2.15	0.46
2:H:87:GLU:OE2	2:H:113:LYS:HD3	2.15	0.45
2:J:79:TYR:O	2:J:111:GLU:HG3	2.16	0.45
2:J:95:VAL:HG22	2:J:107:ILE:HG12	1.97	0.45
1:G:17:THR:CG2	2:H:165:LYS:HG2	2.46	0.45
2:F:96:ALA:HB2	2:F:127:ALA:HB1	1.99	0.45
1:G:39:LEU:HD23	1:G:44:GLY:HA3	1.98	0.45
1:A:17:THR:CG2	2:B:165:LYS:HG3	2.47	0.45
2:J:87:GLU:OE2	2:J:113:LYS:HD3	2.17	0.45
1:K:20:LEU:HD12	2:L:93:ILE:HG21	1.99	0.45
2:L:100:ASP:HB3	2:L:103:LEU:HD12	1.99	0.45
1:I:16:ASN:HD21	2:J:164:TYR:HA	1.80	0.45
2:J:106:LEU:HD21	2:J:108:MET:HE3	1.99	0.45
2:L:99:LYS:HD2	2:L:137:GLU:OE1	2.17	0.45
1:G:13:LYS:O	1:G:13:LYS:HG3	2.17	0.44
2:J:55:MET:O	2:J:104:CYS:HB2	2.17	0.44
1:A:49:ILE:HD13	1:E:51:ILE:HG22	1.99	0.44
1:A:51:ILE:HG21	1:C:47:ASN:OD1	2.17	0.44
3:I:671:AG2:HN2	2:J:109:GLN:NE2	2.16	0.44
2:L:57:PRO:O	2:L:58:GLU:HB2	2.17	0.44
1:I:16:ASN:ND2	1:I:16:ASN:H	2.16	0.44
2:B:94:SER:HB3	2:B:123:VAL:HG13	2.00	0.43
2:J:165:LYS:NZ	2:J:165:LYS:CB	2.81	0.43
1:K:20:LEU:HD12	2:L:93:ILE:CG2	2.48	0.43
2:J:106:LEU:CD2	2:J:130:GLY:HA3	2.48	0.43
2:B:61:ILE:HD12	2:B:142:GLU:HG3	2.01	0.43
2:H:93:ILE:HD11	2:H:107:ILE:CG2	2.48	0.43
3:I:671:AG2:HN2	2:J:109:GLN:HE21	1.67	0.43
1:K:51:ILE:HG12	2:L:75:THR:C	2.38	0.43
2:B:120:GLU:OE1	2:H:66:LYS:HE2	2.19	0.43
2:F:163:TRP:CG	2:F:164:TYR:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HG23	1:C:47:ASN:HB3	2.02	0.42
2:D:57:PRO:O	2:D:58:GLU:HB2	2.19	0.42
1:I:49:ILE:HD11	1:K:51:ILE:HG22	1.99	0.42
1:C:43:ILE:O	1:C:43:ILE:HG23	2.20	0.42
2:H:96:ALA:HB2	2:H:127:ALA:HB1	2.02	0.42
2:J:64:LEU:HA	2:J:65:PRO:HD3	1.87	0.42
1:A:43:ILE:HD11	2:B:157:PHE:CE2	2.55	0.42
1:I:31:LEU:HD13	5:I:700:MPD:HM2	2.01	0.42
1:G:49:ILE:HD11	1:I:51:ILE:HG22	2.00	0.41
2:J:163:TRP:CG	2:J:164:TYR:N	2.87	0.41
1:K:38:LEU:HD12	3:K:671:AG2:CZ	2.50	0.41
2:L:58:GLU:OE2	2:L:58:GLU:HA	2.21	0.41
1:A:18:VAL:CG2	2:B:55:MET:HG3	2.48	0.41
1:A:24:SER:HB2	2:B:148:HIS:HB2	2.03	0.41
1:E:43:ILE:O	1:E:43:ILE:HG23	2.21	0.41
1:E:51:ILE:HD12	4:F:53:PYR:H33	2.02	0.41
2:J:71:ALA:HA	1:K:14:LEU:HD22	2.02	0.41
2:L:99:LYS:HE2	6:L:204:HOH:O	2.20	0.41
1:E:38:LEU:HD12	3:E:671:AG2:CZ	2.51	0.41
2:F:94:SER:HB3	2:F:123:VAL:HG13	2.03	0.41
2:F:116:LYS:HB2	2:F:147:GLU:HG2	2.02	0.41
2:H:64:LEU:HA	2:H:65:PRO:HD3	1.92	0.41
2:H:73:VAL:HA	2:H:74:PRO:HD3	1.97	0.41
2:H:79:TYR:O	2:H:111:GLU:HG3	2.21	0.41
2:H:101:LYS:HA	2:H:101:LYS:HD3	1.90	0.41
1:K:16:ASN:OD1	2:L:165:LYS:HG3	2.20	0.41
2:J:77:TYR:HB3	2:J:159:ALA:HB2	2.01	0.40
2:J:97:ILE:O	2:J:139:ASP:HB3	2.22	0.40
1:A:31:LEU:HB3	2:F:126:MET:CE	2.52	0.40
2:D:99:LYS:HG3	2:D:137:GLU:CD	2.41	0.40
1:I:16:ASN:HD22	1:I:16:ASN:N	2.17	0.40
2:D:151:GLU:C	2:D:152:LYS:HD2	2.42	0.40
2:L:83:ASP:O	2:L:85:PRO:HD3	2.22	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	44/53 (83%)	42 (96%)	2 (4%)	0	100	100
1	C	45/53 (85%)	43 (96%)	2 (4%)	0	100	100
1	E	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
1	G	38/53 (72%)	37 (97%)	1 (3%)	0	100	100
1	I	38/53 (72%)	36 (95%)	2 (5%)	0	100	100
1	K	38/53 (72%)	37 (97%)	1 (3%)	0	100	100
2	B	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
2	D	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	F	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
2	H	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
2	J	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	L	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
All	All	911/990 (92%)	878 (96%)	33 (4%)	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	36/42 (86%)	36 (100%)	0	100	100
1	C	37/42 (88%)	36 (97%)	1 (3%)	44	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	39/42 (93%)	39 (100%)	0	100	100
1	G	31/42 (74%)	31 (100%)	0	100	100
1	I	31/42 (74%)	29 (94%)	2 (6%)	17	12
1	K	31/42 (74%)	31 (100%)	0	100	100
2	B	90/90 (100%)	89 (99%)	1 (1%)	73	78
2	D	90/90 (100%)	88 (98%)	2 (2%)	52	55
2	F	90/90 (100%)	90 (100%)	0	100	100
2	H	90/90 (100%)	90 (100%)	0	100	100
2	J	90/90 (100%)	87 (97%)	3 (3%)	38	37
2	L	90/90 (100%)	89 (99%)	1 (1%)	73	78
All	All	745/792 (94%)	735 (99%)	10 (1%)	69	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	111	GLU
1	C	14	LEU
2	D	109	GLN
2	D	152	LYS
1	I	13	LYS
1	I	16	ASN
2	J	109	GLN
2	J	111	GLU
2	J	165	LYS
2	L	111	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
2	D	109	GLN
1	E	32	ASN
1	E	45	ASN
1	G	32	ASN
1	I	16	ASN
1	I	32	ASN
2	J	109	GLN

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Mol	Chain	Res	Type
1	K	45	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
3	AG2	K	671	-	8,8,8	0.46	0	7,8,8	0.26	0
4	PYR	D	53	2	4,4,5	0.77	0	3,4,6	3.95	3 (100%)
3	AG2	I	672	-	8,8,8	0.45	0	7,8,8	0.26	0
4	PYR	F	53	2	4,4,5	0.88	0	3,4,6	3.95	3 (100%)
3	AG2	I	671	-	8,8,8	0.38	0	7,8,8	0.18	0
4	PYR	H	53	2	4,4,5	0.69	0	3,4,6	3.93	3 (100%)
5	MPD	I	700	-	7,7,7	0.52	0	9,10,10	0.60	0
3	AG2	A	672	-	8,8,8	0.53	0	7,8,8	0.35	0
5	MPD	E	700	-	7,7,7	0.52	0	9,10,10	0.56	0
3	AG2	E	671	-	8,8,8	0.49	0	7,8,8	0.19	0
4	PYR	L	53	2	4,4,5	0.90	0	3,4,6	3.79	3 (100%)
3	AG2	A	671	-	8,8,8	0.37	0	7,8,8	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	B	700	-	7,7,7	0.52	0	9,10,10	0.55	0
4	PYR	J	53	2	4,4,5	0.77	0	3,4,6	3.82	3 (100%)
5	MPD	C	700	-	7,7,7	0.53	0	9,10,10	0.56	0
4	PYR	B	53	2	4,4,5	0.95	0	3,4,6	3.66	3 (100%)

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	AG2	K	671	-	-	1/6/6/6	-
4	PYR	D	53	2	-	0/0/2/4	-
3	AG2	I	672	-	-	2/6/6/6	-
4	PYR	F	53	2	-	0/0/2/4	-
3	AG2	I	671	-	-	0/6/6/6	-
4	PYR	H	53	2	-	0/0/2/4	-
5	MPD	I	700	-	-	0/5/5/5	-
3	AG2	A	672	-	-	1/6/6/6	-
5	MPD	E	700	-	-	0/5/5/5	-
3	AG2	E	671	-	-	1/6/6/6	-
4	PYR	L	53	2	-	0/0/2/4	-
3	AG2	A	671	-	-	0/6/6/6	-
5	MPD	B	700	-	-	1/5/5/5	-
4	PYR	J	53	2	-	0/0/2/4	-
5	MPD	C	700	-	-	0/5/5/5	-
4	PYR	B	53	2	-	0/0/2/4	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	53	PYR	C3-C2-C1	5.62	129.30	118.37
4	D	53	PYR	C3-C2-C1	5.62	129.29	118.37
4	H	53	PYR	C3-C2-C1	5.62	129.28	118.37
4	J	53	PYR	C3-C2-C1	5.45	128.95	118.37
4	L	53	PYR	C3-C2-C1	5.38	128.82	118.37
4	B	53	PYR	C3-C2-C1	5.21	128.49	118.37
4	D	53	PYR	O3-C2-C1	-3.22	116.90	122.75
4	F	53	PYR	O3-C2-C1	-3.12	117.07	122.75
4	L	53	PYR	O3-C2-C1	-3.07	117.17	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	PYR	O3-C2-C1	-3.07	117.17	122.75
4	J	53	PYR	O3-C2-C1	-3.04	117.22	122.75
4	B	53	PYR	O3-C2-C1	-2.91	117.47	122.75
4	H	53	PYR	O3-C2-C3	-2.34	113.55	119.17
4	F	53	PYR	O3-C2-C3	-2.31	113.62	119.17
4	D	53	PYR	O3-C2-C3	-2.23	113.81	119.17
4	J	53	PYR	O3-C2-C3	-2.22	113.83	119.17
4	B	53	PYR	O3-C2-C3	-2.16	113.99	119.17
4	L	53	PYR	O3-C2-C3	-2.16	113.99	119.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	671	AG2	CA-CB-CG-CD
3	I	672	AG2	CA-CB-CG-CD
3	K	671	AG2	CA-CB-CG-CD
3	A	672	AG2	CA-CB-CG-CD
5	B	700	MPD	O2-C2-C3-C4
3	I	672	AG2	NE-CD-CG-CB

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	671	AG2	2	0
3	I	672	AG2	2	0
4	F	53	PYR	1	0
3	I	671	AG2	3	0
5	I	700	MPD	1	0
3	A	672	AG2	2	0
3	E	671	AG2	2	0
3	A	671	AG2	2	0
4	B	53	PYR	1	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	46/53 (86%)	-0.41	1 (2%) 62 60	14, 18, 29, 43	1 (2%)
1	C	47/53 (88%)	-0.31	1 (2%) 63 62	10, 17, 28, 43	1 (2%)
1	E	50/53 (94%)	-0.35	2 (4%) 38 37	6, 16, 25, 35	2 (4%)
1	G	40/53 (75%)	-0.45	0 100 100	16, 20, 28, 39	0
1	I	40/53 (75%)	0.09	3 (7%) 14 13	10, 22, 32, 38	3 (7%)
1	K	40/53 (75%)	-0.32	2 (5%) 28 28	4, 18, 33, 38	2 (5%)
2	B	112/112 (100%)	-0.29	3 (2%) 54 53	10, 20, 32, 37	4 (3%)
2	D	112/112 (100%)	-0.27	4 (3%) 42 42	10, 20, 33, 37	5 (4%)
2	F	112/112 (100%)	-0.35	1 (0%) 84 83	8, 17, 31, 35	3 (2%)
2	H	112/112 (100%)	-0.11	4 (3%) 42 42	8, 25, 40, 43	5 (4%)
2	J	112/112 (100%)	-0.28	0 100 100	15, 25, 39, 44	1 (0%)
2	L	112/112 (100%)	-0.26	3 (2%) 54 53	12, 23, 36, 39	2 (1%)
All	All	935/990 (94%)	-0.27	24 (2%) 56 54	4, 21, 35, 44	29 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	18	VAL	4.8
1	E	43	ILE	4.7
2	D	153	LEU	4.5
1	C	43	ILE	4.3
1	I	43	ILE	4.3
1	E	18	VAL	4.2
2	H	95	VAL	3.8
2	H	61	ILE	3.7
2	D	95	VAL	3.6
1	A	11	TYR	3.6
2	H	162	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	58	GLU	3.1
2	B	69	MET	3.1
1	I	49	ILE	3.0
2	L	144	ILE	3.0
1	K	20	LEU	3.0
2	L	69	MET	2.8
2	F	90	SER	2.7
2	D	90	SER	2.6
2	B	90	SER	2.5
1	K	18	VAL	2.4
2	B	55	MET	2.2
2	L	58	GLU	2.2
2	D	139	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
5	MPD	I	700	8/8	0.75	0.25	59,60,60,61	0
5	MPD	B	700	8/8	0.80	0.20	41,41,42,43	0
5	MPD	C	700	8/8	0.83	0.19	45,46,46,47	0
5	MPD	E	700	8/8	0.84	0.17	50,51,51,52	0
3	AG2	A	671	9/9	0.85	0.22	31,34,38,38	0
3	AG2	I	671	9/9	0.87	0.23	33,36,41,42	0
3	AG2	I	672	9/9	0.90	0.16	30,32,37,38	0
4	PYR	B	53	5/6	0.90	0.14	18,21,26,31	0
3	AG2	E	671	9/9	0.91	0.14	22,27,32,33	0
4	PYR	D	53	5/6	0.92	0.15	18,22,28,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PYR	F	53	5/6	0.92	0.14	15,19,26,30	0
3	AG2	A	672	9/9	0.93	0.11	23,25,30,31	0
4	PYR	J	53	5/6	0.94	0.13	25,26,30,32	0
4	PYR	L	53	5/6	0.94	0.13	22,22,26,31	0
4	PYR	H	53	5/6	0.94	0.13	21,23,30,31	0
3	AG2	K	671	9/9	0.96	0.13	21,23,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.