WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 12:57 PM EDT

PDB ID	:	3PWQ
Title	:	The Phenylacetyl-CoA monooxygenase PaaAC subcomplex
Authors	:	Cygler, M.; Grishin, A.M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2010-12-08
Resolution	:	2.65 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

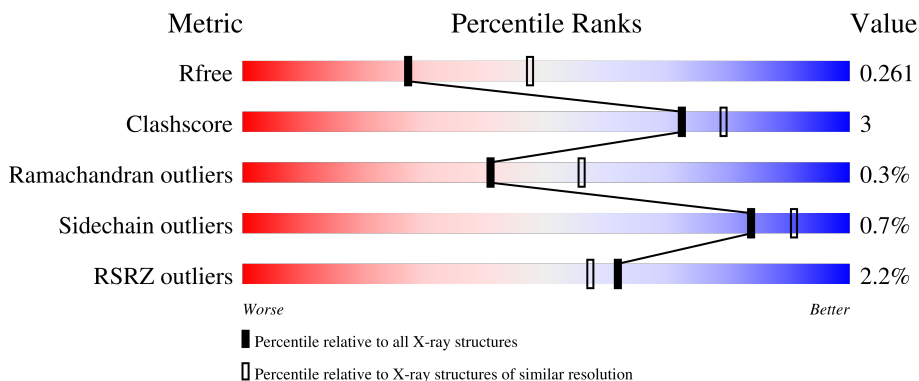|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.65 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		0.7%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	259	92% · ·
1	B	259	92% · ·
1	E	259	91% 5% ·
1	G	259	92% · ·
1	I	259	85% 6% · 8%

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Mol	Chain	Length	Quality of chain
1	J	259	7% / 86% / 6% / 8%
1	K	259	6% / 81% / 9% / 10%
1	R	259	4% / 83% / 8% / 8%
2	C	311	87% / 8% / 5%
2	D	311	4% / 89% / 6% / 5%
2	F	311	2% / 87% / 9%
2	H	311	% / 87% / 7% / 5%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 24804 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 Phenylacetic acid degradation protein paaC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1948	1229	346	367	6			
1	B	248	Total	C	N	O	S	0	0	0
			1952	1231	348	367	6			
1	E	248	Total	C	N	O	S	0	0	0
			1950	1229	344	371	6			
1	G	248	Total	C	N	O	S	0	0	0
			1935	1221	339	369	6			
1	I	238	Total	C	N	O	S	0	0	0
			1850	1165	328	351	6			
1	J	238	Total	C	N	O	S	0	0	0
			1831	1154	322	349	6			
1	K	234	Total	C	N	O	S	0	0	0
			1776	1123	315	332	6			
1	R	238	Total	C	N	O	S	0	0	0
			1850	1165	328	351	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P76079
A	-9	GLY	-	expression tag	UNP P76079
A	-8	SER	-	expression tag	UNP P76079
A	-7	SER	-	expression tag	UNP P76079
A	-6	HIS	-	expression tag	UNP P76079
A	-5	HIS	-	expression tag	UNP P76079
A	-4	HIS	-	expression tag	UNP P76079
A	-3	HIS	-	expression tag	UNP P76079
A	-2	HIS	-	expression tag	UNP P76079
A	-1	HIS	-	expression tag	UNP P76079
A	0	GLY	-	expression tag	UNP P76079
A	1	SER	-	expression tag	UNP P76079
B	-10	MET	-	expression tag	UNP P76079

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP P76079
B	-8	SER	-	expression tag	UNP P76079
B	-7	SER	-	expression tag	UNP P76079
B	-6	HIS	-	expression tag	UNP P76079
B	-5	HIS	-	expression tag	UNP P76079
B	-4	HIS	-	expression tag	UNP P76079
B	-3	HIS	-	expression tag	UNP P76079
B	-2	HIS	-	expression tag	UNP P76079
B	-1	HIS	-	expression tag	UNP P76079
B	0	GLY	-	expression tag	UNP P76079
B	1	SER	-	expression tag	UNP P76079
E	-10	MET	-	expression tag	UNP P76079
E	-9	GLY	-	expression tag	UNP P76079
E	-8	SER	-	expression tag	UNP P76079
E	-7	SER	-	expression tag	UNP P76079
E	-6	HIS	-	expression tag	UNP P76079
E	-5	HIS	-	expression tag	UNP P76079
E	-4	HIS	-	expression tag	UNP P76079
E	-3	HIS	-	expression tag	UNP P76079
E	-2	HIS	-	expression tag	UNP P76079
E	-1	HIS	-	expression tag	UNP P76079
E	0	GLY	-	expression tag	UNP P76079
E	1	SER	-	expression tag	UNP P76079
G	-10	MET	-	expression tag	UNP P76079
G	-9	GLY	-	expression tag	UNP P76079
G	-8	SER	-	expression tag	UNP P76079
G	-7	SER	-	expression tag	UNP P76079
G	-6	HIS	-	expression tag	UNP P76079
G	-5	HIS	-	expression tag	UNP P76079
G	-4	HIS	-	expression tag	UNP P76079
G	-3	HIS	-	expression tag	UNP P76079
G	-2	HIS	-	expression tag	UNP P76079
G	-1	HIS	-	expression tag	UNP P76079
G	0	GLY	-	expression tag	UNP P76079
G	1	SER	-	expression tag	UNP P76079
I	-10	MET	-	expression tag	UNP P76079
I	-9	GLY	-	expression tag	UNP P76079
I	-8	SER	-	expression tag	UNP P76079
I	-7	SER	-	expression tag	UNP P76079
I	-6	HIS	-	expression tag	UNP P76079
I	-5	HIS	-	expression tag	UNP P76079
I	-4	HIS	-	expression tag	UNP P76079

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	HIS	-	expression tag	UNP P76079
I	-2	HIS	-	expression tag	UNP P76079
I	-1	HIS	-	expression tag	UNP P76079
I	0	GLY	-	expression tag	UNP P76079
I	1	SER	-	expression tag	UNP P76079
J	-10	MET	-	expression tag	UNP P76079
J	-9	GLY	-	expression tag	UNP P76079
J	-8	SER	-	expression tag	UNP P76079
J	-7	SER	-	expression tag	UNP P76079
J	-6	HIS	-	expression tag	UNP P76079
J	-5	HIS	-	expression tag	UNP P76079
J	-4	HIS	-	expression tag	UNP P76079
J	-3	HIS	-	expression tag	UNP P76079
J	-2	HIS	-	expression tag	UNP P76079
J	-1	HIS	-	expression tag	UNP P76079
J	0	GLY	-	expression tag	UNP P76079
J	1	SER	-	expression tag	UNP P76079
K	-10	MET	-	expression tag	UNP P76079
K	-9	GLY	-	expression tag	UNP P76079
K	-8	SER	-	expression tag	UNP P76079
K	-7	SER	-	expression tag	UNP P76079
K	-6	HIS	-	expression tag	UNP P76079
K	-5	HIS	-	expression tag	UNP P76079
K	-4	HIS	-	expression tag	UNP P76079
K	-3	HIS	-	expression tag	UNP P76079
K	-2	HIS	-	expression tag	UNP P76079
K	-1	HIS	-	expression tag	UNP P76079
K	0	GLY	-	expression tag	UNP P76079
K	1	SER	-	expression tag	UNP P76079
R	-10	MET	-	expression tag	UNP P76079
R	-9	GLY	-	expression tag	UNP P76079
R	-8	SER	-	expression tag	UNP P76079
R	-7	SER	-	expression tag	UNP P76079
R	-6	HIS	-	expression tag	UNP P76079
R	-5	HIS	-	expression tag	UNP P76079
R	-4	HIS	-	expression tag	UNP P76079
R	-3	HIS	-	expression tag	UNP P76079
R	-2	HIS	-	expression tag	UNP P76079
R	-1	HIS	-	expression tag	UNP P76079
R	0	GLY	-	expression tag	UNP P76079
R	1	SER	-	expression tag	UNP P76079

- Molecule 2 is a protein called Phenylacetic acid degradation protein paaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	296	Total 2359	C 1490	N 423	O 430	S 16	0	0	0
2	D	297	Total 2379	C 1499	N 427	O 437	S 16	0	0	0
2	F	301	Total 2385	C 1504	N 423	O 442	S 16	0	0	0
2	H	295	Total 2372	C 1498	N 424	O 434	S 16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP P76077
C	0	ARG	-	expression tag	UNP P76077
C	1	SER	-	expression tag	UNP P76077
D	-1	MET	-	expression tag	UNP P76077
D	0	ARG	-	expression tag	UNP P76077
D	1	SER	-	expression tag	UNP P76077
F	-1	MET	-	expression tag	UNP P76077
F	0	ARG	-	expression tag	UNP P76077
F	1	SER	-	expression tag	UNP P76077
H	-1	MET	-	expression tag	UNP P76077
H	0	ARG	-	expression tag	UNP P76077
H	1	SER	-	expression tag	UNP P76077

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	C	29	Total 29	O 29	0	0
3	B	21	Total 21	O 21	0	0
3	D	15	Total 15	O 15	0	0
3	E	16	Total 16	O 16	0	0
3	F	19	Total 19	O 19	0	0
3	G	31	Total 31	O 31	0	0
3	H	16	Total 16	O 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total 11	O 11	0	0
3	J	12	Total 12	O 12	0	0
3	K	9	Total 9	O 9	0	0
3	R	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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: Phenylacetic acid degradation protein paaC

Chain A:

• Molecule 1: Phenylacetic acid degradation protein paaC
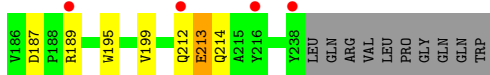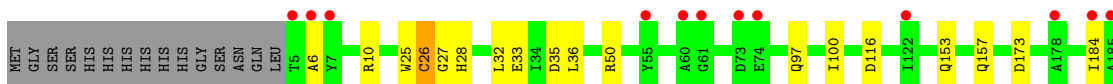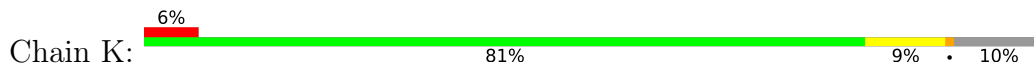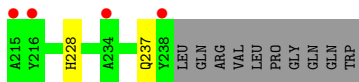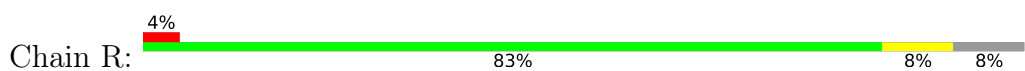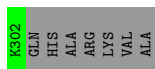
Chain B:

• Molecule 1: Phenylacetic acid degradation protein paaC

Chain E:

• Molecule 1: Phenylacetic acid degradation protein paaC
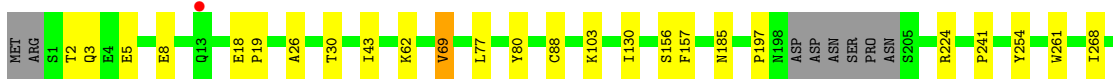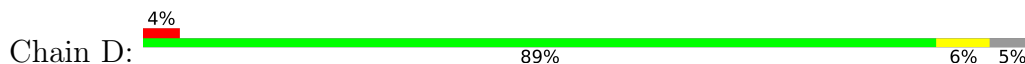
Chain G:

• Molecule 1: Phenylacetic acid degradation protein paaC

Chain I:

• Molecule 1: Phenylacetic acid degradation protein paaC

Chain J:

Chain J sequence bar:
MET GLY SER SER HIS HIS HIS HIS HIS GLY S1 L4 T8 L32 E33 I34 D35 L43 Y55 G61 E74 Q97 I100 D101 F108 L111 P117 Y132 W163 A167 E174 L179 S180 E181 E182 G183 I184 W195 V199

P211 Q212 E213 Q214 A215 Y216 E227 L233 Q237 Y238 LEU GLN ARG VAL LEU PRO GLY GLN GLN TRP

• Molecule 1: Phenylacetic acid degradation protein paaC

Chain K:

Chain K sequence bar:
MET GLY SER SER HIS HIS HIS HIS HIS GLY SER ASN GLN LEU T5 A6 Y7 R10 W25 C26 G27 H28 L32 E33 I34 D35 L36 R50 Y55 A60 G61 D73 E74 Q97 I100 D116 I122 Q153 Q157 D173 A178 I184 A185

V186 D187 P188 R189 W195 V199 Q212 E213 Q214 A215 Y216 Y238 LEU GLN ARG VAL LEU PRO GLY GLN GLN TRP

• Molecule 1: Phenylacetic acid degradation protein paaC

Chain R:

Chain R sequence bar:
MET GLY SER SER HIS HIS HIS HIS HIS GLY S1 E31 I34 N40 L43 F70 L80 V83 P86 Q97 I100 I127 R131 V150 E174 I175 D176 I177 A178 L179 I184 W195 V199 N204 E205 A206 T207 Q212 E213 Q214

A215 Y216 H228 A234 Q237 Y238 LEU GLN ARG VAL LEU PRO GLY GLN GLN TRP

• Molecule 2: Phenylacetic acid degradation protein paaA

Chain C:

Chain C sequence bar:
MET ARG S1 T2 Q3 E4 E5 E8 Q13 E18 P19 A26 T30 I43 K62 V69 L77 Y80 C88 K103 I130 S156 F157 N185 P197 N198 ASP ASP ASN SER PRO ASN S205 R224 P241 Y254 W261 I268

K302 GLN HIS ALA ARG LYS VAL ALA

• Molecule 2: Phenylacetic acid degradation protein paaA

Chain D:

Chain D sequence bar:
MET ARG S1 E18 P19 I43 E49 K62 V69 L77 Y80 E91 D99 K103 G122 D126 A129 R138 C152 E155 S156 F157 H158 Q159 R160 Q161 N185 N198 ASP ASP ASN SER PRO N204 R207 T210 F216 R224
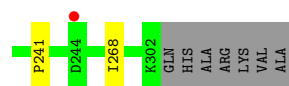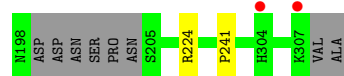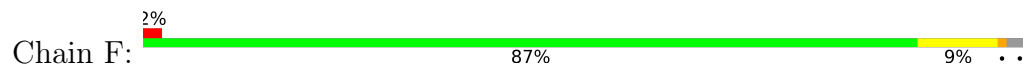
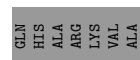• Molecule 2: Phenylacetic acid degradation protein paaA

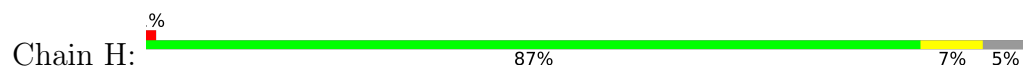• Molecule 2: Phenylacetic acid degradation protein paaA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.26Å 109.06Å 305.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.65 49.20 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.20-2.65) 99.9 (49.20-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.11 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.267 0.229 , 0.261	Depositor DCC
R_{free} test set	5363 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.8	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24804	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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 ⓘ

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	0.46	0/1987	0.54	0/2693
1	B	0.44	0/1991	0.54	0/2698
1	E	0.45	0/1989	0.54	0/2697
1	G	0.54	0/1974	0.54	0/2679
1	I	0.41	0/1885	0.55	0/2555
1	J	0.48	0/1866	0.55	0/2532
1	K	0.46	1/1811 (0.1%)	0.52	0/2461
1	R	0.45	0/1885	0.53	0/2555
2	C	0.46	0/2415	0.55	0/3269
2	D	0.46	0/2435	0.54	0/3294
2	F	0.49	0/2441	0.58	1/3307 (0.0%)
2	H	0.46	0/2428	0.54	0/3283
All	All	0.46	1/25107 (0.0%)	0.54	1/34023 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	26	CYS	CB-SG	-5.45	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	20	GLN	CB-CA-C	-7.51	95.38	110.40

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	1948	0	1894	13	0
1	B	1952	0	1902	13	0
1	E	1950	0	1888	14	0
1	G	1935	0	1859	10	0
1	I	1850	0	1793	10	0
1	J	1831	0	1758	12	0
1	K	1776	0	1694	21	0
1	R	1850	0	1793	17	0
2	C	2359	0	2271	26	0
2	D	2379	0	2291	30	0
2	F	2385	0	2270	32	0
2	H	2372	0	2295	19	0
3	A	30	0	0	1	0
3	B	21	0	0	0	0
3	C	29	0	0	2	0
3	D	15	0	0	0	0
3	E	16	0	0	0	0
3	F	19	0	0	1	0
3	G	31	0	0	1	0
3	H	16	0	0	0	0
3	I	11	0	0	0	0
3	J	12	0	0	0	0
3	K	9	0	0	0	0
3	R	8	0	0	0	0
All	All	24804	0	23708	162	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 3.

All (162) 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:E:32:LEU:HD23	2:F:77:LEU:CD2	1.86	1.04
1:B:32:LEU:HD23	2:D:77:LEU:CD2	1.94	0.98
2:D:138:ARG:HH11	1:K:28:HIS:HA	1.32	0.95
1:R:212:GLN:HA	1:R:213:GLU:CB	2.01	0.90
1:A:32:LEU:HD23	2:C:77:LEU:CD2	2.06	0.86
1:G:32:LEU:HD23	2:H:77:LEU:CD2	2.09	0.83
2:C:224:ARG:HG2	1:J:32:LEU:CD2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:ARG:NH1	1:K:28:HIS:HA	1.94	0.81
2:H:249:THR:HG23	2:H:249:THR:O	1.79	0.78
1:E:32:LEU:HD23	2:F:77:LEU:HD23	1.64	0.78
1:E:32:LEU:HD23	2:F:77:LEU:HD21	1.67	0.77
1:E:32:LEU:HD21	2:F:77:LEU:HG	1.66	0.77
1:E:32:LEU:CD2	2:F:77:LEU:HG	2.15	0.77
1:A:20:GLN:OE1	2:C:62:LYS:HE2	1.85	0.77
1:B:32:LEU:HD23	2:D:77:LEU:HD23	1.65	0.77
2:D:216:PHE:CZ	1:K:32:LEU:HB2	2.20	0.76
1:B:32:LEU:CD2	2:D:77:LEU:HG	2.16	0.76
1:G:20:GLN:OE1	2:H:62:LYS:HE2	1.86	0.75
1:G:32:LEU:HD23	2:H:77:LEU:HD23	1.68	0.75
1:A:32:LEU:HD23	2:C:77:LEU:HD23	1.68	0.74
2:C:224:ARG:HG2	1:J:32:LEU:HD21	1.68	0.73
2:D:224:ARG:HG2	1:K:36:LEU:CD1	2.21	0.71
1:E:20:GLN:OE1	2:F:62:LYS:HE2	1.91	0.70
1:B:32:LEU:HD21	2:D:77:LEU:HG	1.75	0.69
1:R:206:ALA:O	1:R:207:THR:HG22	1.94	0.68
2:F:4:GLU:O	2:F:8:GLU:HG2	1.93	0.68
2:D:224:ARG:NH1	1:K:33:GLU:OE1	2.27	0.68
1:I:237:GLN:O	1:I:238:TYR:C	2.30	0.67
2:H:249:THR:O	2:H:249:THR:CG2	2.43	0.66
1:R:212:GLN:CA	1:R:213:GLU:CB	2.75	0.65
1:B:20:GLN:OE1	2:D:62:LYS:HE2	1.97	0.65
1:G:64:ASP:OD1	1:G:66:ASP:N	2.30	0.64
2:F:22:TRP:HA	3:F:311:HOH:O	1.97	0.63
1:R:70:PHE:O	1:R:237:GLN:HG2	1.98	0.62
1:B:244:PRO:O	1:B:246:GLN:HG2	1.99	0.62
1:E:86:PRO:HG3	1:E:228:HIS:CD2	2.35	0.62
2:F:28:ARG:HG3	2:F:86:LEU:HD22	1.82	0.61
2:C:224:ARG:HG2	1:J:32:LEU:HD23	1.81	0.61
1:J:163:TRP:CG	1:J:211:PRO:HG2	2.36	0.61
1:A:244:PRO:O	1:A:246:GLN:HG2	2.00	0.61
1:E:244:PRO:O	1:E:246:GLN:HG2	1.99	0.61
1:K:212:GLN:HA	1:K:213:GLU:CB	2.32	0.60
2:F:20:GLN:HG2	2:F:21:ASP:H	1.67	0.59
1:K:187:ASP:OD1	1:K:189:ARG:HG2	2.02	0.59
1:B:86:PRO:HG3	1:B:228:HIS:CD2	2.38	0.58
1:A:149:ASP:HB3	3:A:259:HOH:O	2.02	0.58
2:H:4:GLU:O	2:H:8:GLU:HG3	2.03	0.58
1:I:153:GLN:HG2	1:I:157:GLN:HE21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD23	2:D:77:LEU:HD21	1.83	0.58
2:C:254:TYR:OH	1:I:75:ARG:HB3	2.04	0.58
1:G:86:PRO:HG3	1:G:228:HIS:CD2	2.39	0.56
1:E:32:LEU:HD23	2:F:77:LEU:CG	2.36	0.56
1:J:163:TRP:CD2	1:J:211:PRO:HG2	2.41	0.56
1:I:212:GLN:HA	1:I:213:GLU:CB	2.36	0.56
1:A:32:LEU:CD2	2:C:77:LEU:HG	2.37	0.54
1:A:32:LEU:HD21	2:C:77:LEU:HG	1.89	0.54
1:G:64:ASP:OD1	1:G:64:ASP:C	2.46	0.54
1:E:32:LEU:CD2	2:F:77:LEU:CG	2.85	0.54
2:F:160:ARG:HB2	1:R:43:LEU:CD2	2.38	0.54
1:K:97:GLN:O	1:K:100:ILE:HG22	2.07	0.54
1:B:32:LEU:HD23	2:D:77:LEU:CG	2.38	0.54
2:D:224:ARG:HG2	1:K:36:LEU:HD11	1.89	0.54
1:R:195:TRP:CE2	1:R:199:VAL:HG21	2.44	0.54
1:G:32:LEU:CD2	2:H:77:LEU:HG	2.38	0.53
2:F:18:GLU:HB3	2:F:19:PRO:CD	2.38	0.53
1:J:195:TRP:CE2	1:J:199:VAL:HG21	2.44	0.53
2:D:18:GLU:HB3	2:D:19:PRO:CD	2.40	0.52
2:D:224:ARG:CG	1:K:36:LEU:CD1	2.86	0.52
2:F:224:ARG:O	2:F:224:ARG:HD3	2.10	0.52
2:C:88:CYS:HB2	3:C:319:HOH:O	2.10	0.52
2:C:3:GLN:C	2:C:5:GLU:H	2.13	0.52
1:I:195:TRP:CE2	1:I:199:VAL:HG21	2.45	0.52
1:J:233:LEU:O	1:J:237:GLN:HG3	2.11	0.51
2:F:28:ARG:HD3	2:F:86:LEU:O	2.11	0.51
1:K:195:TRP:CE2	1:K:199:VAL:HG21	2.46	0.51
1:J:97:GLN:O	1:J:100:ILE:HG22	2.11	0.51
2:F:43:ILE:CD1	2:F:80:TYR:HE2	2.24	0.50
2:C:197:PRO:HA	2:C:261:TRP:CH2	2.46	0.50
1:B:32:LEU:CD2	2:D:77:LEU:CG	2.89	0.50
2:D:43:ILE:HD11	2:D:80:TYR:HE2	1.76	0.50
1:J:213:GLU:O	1:J:214:GLN:O	2.30	0.50
2:F:25:ASP:OD2	2:F:25:ASP:O	2.30	0.50
1:A:32:LEU:HD23	2:C:77:LEU:HD21	1.93	0.49
1:G:32:LEU:HD21	2:H:77:LEU:HG	1.94	0.49
2:D:185:ASN:HA	2:D:241:PRO:HG3	1.95	0.49
1:R:97:GLN:O	1:R:100:ILE:HG22	2.13	0.49
2:D:138:ARG:NH1	1:K:27:GLY:O	2.45	0.49
2:F:130:ILE:HD11	2:F:156:SER:HA	1.95	0.48
2:H:7:PHE:CZ	2:H:11:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ILE:CD1	2:D:80:TYR:HE2	2.26	0.48
1:R:206:ALA:O	1:R:207:THR:CG2	2.61	0.48
2:F:43:ILE:HD11	2:F:80:TYR:HE2	1.78	0.47
2:D:224:ARG:HG2	1:K:36:LEU:HD12	1.95	0.47
1:A:135:ARG:NE	1:R:204:ASN:ND2	2.62	0.47
2:C:26:ALA:O	2:C:30:THR:HG23	2.14	0.47
2:C:185:ASN:HA	2:C:241:PRO:HG3	1.96	0.47
2:D:224:ARG:CG	1:K:36:LEU:HD12	2.44	0.47
2:H:185:ASN:HA	2:H:241:PRO:HG3	1.97	0.47
2:C:43:ILE:HD11	2:C:80:TYR:HE2	1.80	0.46
2:F:185:ASN:HA	2:F:241:PRO:HG3	1.97	0.46
2:F:18:GLU:HA	2:F:18:GLU:OE1	2.15	0.46
2:C:157:PHE:HA	1:J:43:LEU:HD21	1.97	0.46
1:I:97:GLN:O	1:I:100:ILE:HG22	2.15	0.46
2:F:157:PHE:HA	1:R:43:LEU:HD21	1.96	0.46
1:A:135:ARG:CZ	1:R:204:ASN:ND2	2.79	0.46
2:C:43:ILE:CD1	2:C:80:TYR:HE2	2.29	0.45
2:D:103:LYS:HE2	2:D:268:ILE:O	2.17	0.45
2:H:4:GLU:OE1	2:H:22:TRP:CH2	2.69	0.45
1:J:233:LEU:O	1:J:237:GLN:HB2	2.16	0.45
1:B:32:LEU:HD23	2:D:77:LEU:HG	1.94	0.45
2:F:224:ARG:HA	2:F:224:ARG:HE	1.82	0.45
2:D:18:GLU:HB3	2:D:19:PRO:HD2	2.00	0.44
2:F:4:GLU:O	2:F:7:PHE:HB3	2.17	0.44
1:I:209:ASN:O	1:I:211:PRO:HD3	2.18	0.44
1:G:145:GLY:HA2	1:G:152:GLY:HA2	2.00	0.44
2:F:160:ARG:HB2	1:R:43:LEU:HD22	1.99	0.44
1:B:81:LEU:O	1:B:84:GLU:HG2	2.17	0.43
2:F:224:ARG:HA	2:F:224:ARG:NE	2.33	0.43
2:H:4:GLU:OE1	2:H:24:PRO:HG3	2.17	0.43
2:C:130:ILE:HD11	2:C:156:SER:HA	2.00	0.43
1:E:32:LEU:CD2	2:F:77:LEU:CD2	2.75	0.43
2:H:43:ILE:CD1	2:H:80:TYR:HE2	2.31	0.43
2:H:43:ILE:HD11	2:H:80:TYR:HE2	1.83	0.43
1:A:20:GLN:OE1	2:C:62:LYS:CE	2.61	0.43
2:C:18:GLU:HB3	2:C:19:PRO:HD2	1.99	0.43
2:F:122:GLY:O	2:F:126:ASP:HB2	2.18	0.43
2:C:103:LYS:HE2	2:C:268:ILE:O	2.18	0.43
1:K:153:GLN:HG2	1:K:157:GLN:HE21	1.84	0.43
2:D:161:GLN:OE1	1:K:50:ARG:NH1	2.49	0.43
1:I:236:MET:O	1:I:237:GLN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:ALA:HB2	1:J:216:TYR:CD2	2.53	0.43
2:H:33:ARG:O	2:H:37:GLN:HG3	2.19	0.42
1:E:81:LEU:O	1:E:84:GLU:HG2	2.20	0.42
2:F:33:ARG:O	2:F:37:GLN:HG3	2.19	0.42
2:H:14:GLU:OE2	2:H:212:LYS:NZ	2.51	0.42
1:K:25:TRP:O	1:K:26:CYS:C	2.56	0.42
1:A:26:CYS:SG	2:C:69:VAL:HG11	2.59	0.42
1:I:236:MET:O	1:I:238:TYR:N	2.52	0.42
1:E:145:GLY:HA2	1:E:152:GLY:HA2	2.02	0.42
2:D:216:PHE:CE1	1:K:32:LEU:HB2	2.55	0.42
1:I:10:ARG:NH2	1:I:173:ASP:OD2	2.52	0.42
1:G:246:GLN:HG3	3:G:277:HOH:O	2.19	0.42
2:C:18:GLU:HB3	2:C:19:PRO:CD	2.49	0.41
2:F:160:ARG:CB	1:R:43:LEU:HD23	2.50	0.41
2:H:103:LYS:HE2	2:H:268:ILE:O	2.19	0.41
1:A:81:LEU:O	1:A:84:GLU:HG2	2.21	0.41
1:B:26:CYS:SG	2:D:69:VAL:HG11	2.61	0.41
2:D:91:GLU:H	2:D:91:GLU:CD	2.23	0.41
2:C:62:LYS:NZ	3:C:338:HOH:O	2.54	0.41
1:K:116:ASP:HB2	1:K:184:ILE:HG23	2.03	0.41
2:C:3:GLN:C	2:C:5:GLU:N	2.74	0.41
2:D:122:GLY:O	2:D:126:ASP:HB2	2.20	0.41
2:H:27:TYR:HA	2:H:30:THR:HG22	2.02	0.41
2:H:91:GLU:H	2:H:91:GLU:CD	2.24	0.41
1:K:10:ARG:NH2	1:K:173:ASP:OD2	2.54	0.41
1:R:80:LEU:O	1:R:83:VAL:HG22	2.21	0.41
1:R:86:PRO:HG3	1:R:228:HIS:CD2	2.55	0.41
1:E:85:GLN:HE22	1:E:226:THR:HG21	1.85	0.40
2:F:10:ARG:HB3	2:F:15:THR:HB	2.03	0.40
1:R:31:GLU:HB2	1:R:34:ILE:HD12	2.03	0.40
1:K:6:ALA:O	1:K:10:ARG:HG3	2.20	0.40
1:R:127:ILE:O	1:R:131:ARG:HG3	2.22	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	246/259 (95%)	240 (98%)	6 (2%)	0	100	100
1	B	246/259 (95%)	243 (99%)	3 (1%)	0	100	100
1	E	246/259 (95%)	242 (98%)	4 (2%)	0	100	100
1	G	246/259 (95%)	242 (98%)	4 (2%)	0	100	100
1	I	236/259 (91%)	227 (96%)	6 (2%)	3 (1%)	12	18
1	J	236/259 (91%)	231 (98%)	4 (2%)	1 (0%)	34	48
1	K	232/259 (90%)	225 (97%)	5 (2%)	2 (1%)	17	26
1	R	236/259 (91%)	230 (98%)	4 (2%)	2 (1%)	19	29
2	C	292/311 (94%)	289 (99%)	3 (1%)	0	100	100
2	D	293/311 (94%)	293 (100%)	0	0	100	100
2	F	297/311 (96%)	286 (96%)	11 (4%)	0	100	100
2	H	291/311 (94%)	288 (99%)	2 (1%)	1 (0%)	41	56
All	All	3097/3316 (93%)	3036 (98%)	52 (2%)	9 (0%)	41	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	250	GLU
1	I	214	GLN
1	J	214	GLN
1	R	213	GLU
1	R	214	GLN
1	I	213	GLU
1	K	213	GLU
1	K	214	GLN
1	I	237	GLN

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	195/208 (94%)	194 (100%)	1 (0%)		88	94
1	B	196/208 (94%)	194 (99%)	2 (1%)		76	86
1	E	196/208 (94%)	195 (100%)	1 (0%)		88	94
1	G	192/208 (92%)	191 (100%)	1 (0%)		88	94
1	I	184/208 (88%)	183 (100%)	1 (0%)		88	94
1	J	180/208 (86%)	178 (99%)	2 (1%)		73	85
1	K	170/208 (82%)	169 (99%)	1 (1%)		86	92
1	R	184/208 (88%)	183 (100%)	1 (0%)		88	94
2	C	238/259 (92%)	235 (99%)	3 (1%)		69	82
2	D	242/259 (93%)	241 (100%)	1 (0%)		91	95
2	F	239/259 (92%)	235 (98%)	4 (2%)		60	77
2	H	242/259 (93%)	242 (100%)	0	100	100	
All	All	2458/2700 (91%)	2440 (99%)	18 (1%)		84	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
2	C	2	THR
2	C	8	GLU
2	C	69	VAL
1	B	35	ASP
1	B	53	LEU
2	D	49	GLU
1	E	35	ASP
2	F	4	GLU
2	F	14	GLU
2	F	30	THR
2	F	69	VAL
1	G	35	ASP
1	I	35	ASP
1	J	35	ASP
1	J	227	GLU
1	K	35	ASP
1	R	40	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	85	GLN
1	A	157	GLN
2	C	51	ASN
2	C	70	GLN
2	C	133	GLN
2	C	161	GLN
1	B	51	ASN
1	B	85	GLN
1	B	157	GLN
2	D	51	ASN
2	D	70	GLN
2	D	133	GLN
1	E	51	ASN
1	E	85	GLN
1	E	157	GLN
2	F	51	ASN
2	F	70	GLN
2	F	133	GLN
2	F	161	GLN
1	G	51	ASN
1	G	85	GLN
1	G	157	GLN
2	H	51	ASN
2	H	70	GLN
2	H	133	GLN
1	I	51	ASN
1	I	118	GLN
1	I	157	GLN
1	J	51	ASN
1	J	118	GLN
1	K	28	HIS
1	K	51	ASN
1	K	118	GLN
1	K	157	GLN
1	R	51	ASN
1	R	118	GLN
1	R	204	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 ⓘ

There are no ligands in this entry.

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	248/259 (95%)	0.04	0	100	100	32, 46, 61, 67	0
1	B	248/259 (95%)	-0.09	0	100	100	32, 46, 61, 68	0
1	E	248/259 (95%)	-0.09	1 (0%)	92	93	32, 46, 61, 66	0
1	G	248/259 (95%)	-0.13	0	100	100	32, 46, 61, 66	0
1	I	238/259 (91%)	0.13	2 (0%)	86	85	44, 68, 85, 94	0
1	J	238/259 (91%)	0.49	19 (7%)	12	9	37, 68, 85, 94	0
1	K	234/259 (90%)	0.35	16 (6%)	17	14	44, 68, 85, 94	0
1	R	238/259 (91%)	0.26	11 (4%)	32	29	44, 68, 85, 94	0
2	C	296/311 (95%)	0.04	1 (0%)	94	95	33, 51, 72, 93	0
2	D	297/311 (95%)	0.19	12 (4%)	38	34	33, 52, 68, 94	0
2	F	301/311 (96%)	0.11	6 (1%)	65	60	33, 52, 81, 95	0
2	H	295/311 (94%)	-0.03	2 (0%)	87	87	33, 51, 72, 93	0
All	All	3129/3316 (94%)	0.10	70 (2%)	62	57	32, 54, 82, 95	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	238	TYR	6.5
1	K	185	ALA	4.8
2	D	156	SER	4.6
2	D	155	GLU	4.5
1	J	238	TYR	4.3
1	K	60	ALA	4.1
1	J	1	SER	4.1
1	K	6	ALA	4.0
1	J	55	TYR	3.6
1	R	175	ILE	3.5
2	D	152	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	198	ASN	3.4
1	R	184	ILE	3.4
2	D	129	ALA	3.3
1	K	7	TYR	3.3
1	K	5	THR	3.3
1	I	238	TYR	3.2
2	F	26	ALA	3.2
2	F	23	MET	3.2
2	H	9	GLN	3.0
1	R	150	VAL	3.0
2	D	158	HIS	2.9
1	K	238	TYR	2.9
1	J	216	TYR	2.9
1	J	184	ILE	2.9
1	K	55	TYR	2.9
2	D	210	THR	2.9
1	K	73	ASP	2.9
1	J	181	GLU	2.8
1	J	111	LEU	2.7
1	K	212	GLN	2.7
2	D	207	ARG	2.7
1	R	216	TYR	2.6
1	J	74	GLU	2.6
1	K	189	ARG	2.5
1	J	61	GLY	2.5
1	K	216	TYR	2.5
1	R	176	ASP	2.5
1	K	184	ILE	2.4
1	K	61	GLY	2.4
1	R	178	ALA	2.4
1	R	179	LEU	2.3
1	J	174	GLU	2.3
2	F	99	ASP	2.3
1	J	183	GLY	2.3
1	J	117	PRO	2.2
2	F	307	LYS	2.2
1	K	122	ILE	2.2
1	J	179	LEU	2.2
1	R	215	ALA	2.2
1	J	108	PHE	2.2
1	J	132	TYR	2.2
2	D	99	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	244	ASP	2.2
2	H	198	ASN	2.1
1	E	204	ASN	2.1
2	C	13	GLN	2.1
2	D	157	PHE	2.1
1	J	101	ASP	2.1
2	F	78	TYR	2.1
1	K	74	GLU	2.1
1	J	8	THR	2.1
1	K	178	ALA	2.1
1	I	149	ASP	2.0
1	J	4	LEU	2.0
2	F	304	HIS	2.0
1	R	234	ALA	2.0
1	J	33	GLU	2.0
1	R	174	GLU	2.0
2	D	160	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.