



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:52 PM GMT

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)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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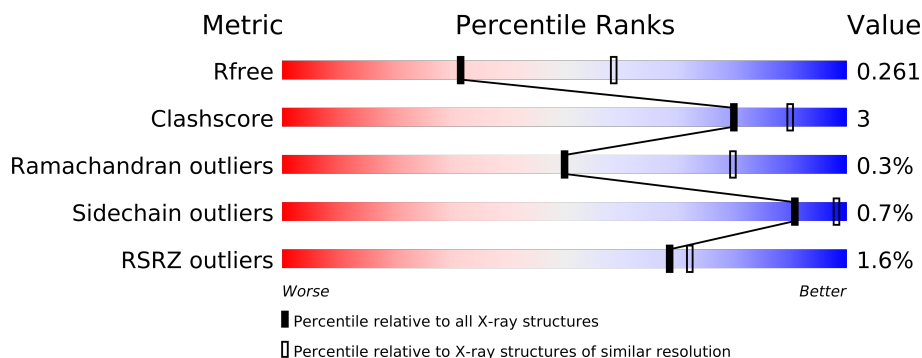
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	E	259	
1	G	259	
1	I	259	
1	J	259	
1	K	259	
1	R	259	
2	C	311	
2	D	311	
2	F	311	
2	H	311	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24804 atoms, of which 0 are hydrogen and 0 are deuterium.

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	C	N	O	S	0	0	0
			2359	1490	423	430	16			
2	D	297	Total	C	N	O	S	0	0	0
			2379	1499	427	437	16			
2	F	301	Total	C	N	O	S	0	0	0
			2385	1504	423	442	16			
2	H	295	Total	C	N	O	S	0	0	0
			2372	1498	424	434	16			

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	O	0	0
			30	30		
3	C	29	Total	O	0	0
			29	29		
3	B	21	Total	O	0	0
			21	21		
3	D	15	Total	O	0	0
			15	15		
3	E	16	Total	O	0	0
			16	16		
3	F	19	Total	O	0	0
			19	19		
3	G	31	Total	O	0	0
			31	31		
3	H	16	Total	O	0	0
			16	16		

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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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

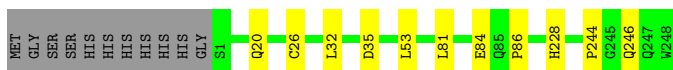
- Molecule 1: Phenylacetic acid degradation protein paaC

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: 

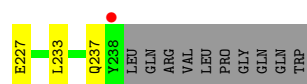


- Molecule 1: Phenylacetic acid degradation protein paaC

Chain J: 

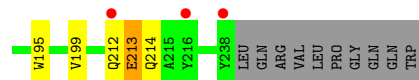
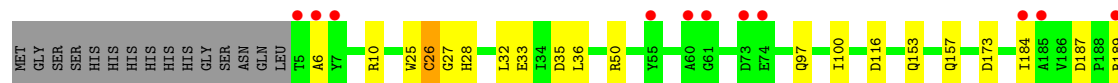






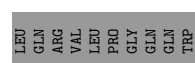
- Molecule 1: Phenylacetic acid degradation protein paaC

Chain K:



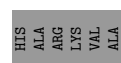
- Molecule 1: Phenylacetic acid degradation protein paaC

Chain R:



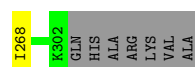
- Molecule 2: Phenylacetic acid degradation protein paaA

Chain C:



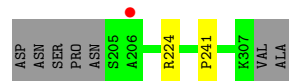
- Molecule 2: Phenylacetic acid degradation protein paaA

Chain D:



- Molecule 2: Phenylacetic acid degradation protein paaA

Chain F:



● Molecule 2: Phenylacetic acid degradation protein paaA

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.234 , 0.267 0.230 , 0.261	Depositor DCC
$R_{free}$ test set	5363 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 21.4	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 107560 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (162) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:D:138:ARG:NH1	1:K:28:HIS:HA	1.94	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:249:THR:O	2:H:249:THR:HG23	1.79	0.78
1:E:32:LEU:HD23	2:F:77:LEU:HD23	1.64	0.78
1:E:32:LEU:HD21	2:F:77:LEU:HG	1.66	0.77
1:E:32:LEU:HD23	2:F:77:LEU:HD21	1.67	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:32:LEU:HD23	2:H:77:LEU:HD23	1.68	0.75
1:G:20:GLN:OE1	2:H:62:LYS:HE2	1.86	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:O	2:F:25:ASP:OD2	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
1:R:206:ALA:O	1:R:207:THR:CG2	2.61	0.48
2:D:43:ILE:CD1	2:D:80:TYR:HE2	2.26	0.48
2:F:43:ILE:HD11	2:F:80:TYR:HE2	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:185:ASN:HA	2:C:241:PRO:HG3	1.96	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:H:4:GLU:OE1	2:H:22:TRP:CH2	2.69	0.45
2:D:103:LYS:HE2	2:D:268:ILE:O	2.17	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:HE	2:F:224:ARG:HA	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
2:H:4:GLU:OE1	2:H:24:PRO:HG3	2.17	0.43
2:F:224:ARG:HA	2:F:224:ARG:NE	2.33	0.43
1:B:81:LEU:O	1:B:84:GLU:HG2	2.17	0.43
1:E:32:LEU:CD2	2:F:77:LEU:CD2	2.75	0.43
2:C:130:ILE:HD11	2:C:156:SER:HA	2.00	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
1:I:236:MET:O	1:I:237:GLN:C	2.56	0.43
1:J:167:ALA:HB2	1:J:216:TYR:CD2	2.53	0.43
2:D:161:GLN:OE1	1:K:50:ARG:NH1	2.49	0.43
2:H:33:ARG:O	2:H:37:GLN:HG3	2.19	0.42
1:K:25:TRP:O	1:K:26:CYS:C	2.56	0.42
2:F:33:ARG:O	2:F:37:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:14:GLU:OE2	2:H:212:LYS:NZ	2.51	0.42
1:E:81:LEU:O	1:E:84:GLU:HG2	2.20	0.42
1:I:236:MET:O	1:I:238:TYR:N	2.52	0.42
1:A:26:CYS:SG	2:C:69:VAL:HG11	2.59	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:F:160:ARG:CB	1:R:43:LEU:HD23	2.50	0.41
2:C:18:GLU:HB3	2:C:19:PRO:CD	2.49	0.41
2:H:103:LYS:HE2	2:H:268:ILE:O	2.19	0.41
1:B:26:CYS:SG	2:D:69:VAL:HG11	2.61	0.41
1:A:81:LEU:O	1:A:84:GLU:HG2	2.21	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
2:F:10:ARG:HB3	2:F:15:THR:HB	2.03	0.40
1:E:85:GLN:HE22	1:E:226:THR:HG21	1.85	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

### 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	246/259 (95%)	240 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	18	39
1	J	236/259 (91%)	231 (98%)	4 (2%)	1 (0%)	43	74
1	K	232/259 (90%)	225 (97%)	5 (2%)	2 (1%)	25	52
1	R	236/259 (91%)	230 (98%)	4 (2%)	2 (1%)	27	55
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%)	50	80
All	All	3097/3316 (93%)	3036 (98%)	52 (2%)	9 (0%)	50	80

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%)	94	99
1	B	196/208 (94%)	194 (99%)	2 (1%)	85	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	196/208 (94%)	195 (100%)	1 (0%)	94	99
1	G	192/208 (92%)	191 (100%)	1 (0%)	94	99
1	I	184/208 (88%)	183 (100%)	1 (0%)	94	99
1	J	180/208 (86%)	178 (99%)	2 (1%)	84	96
1	K	170/208 (82%)	169 (99%)	1 (1%)	92	98
1	R	184/208 (88%)	183 (100%)	1 (0%)	94	99
2	C	238/259 (92%)	235 (99%)	3 (1%)	80	95
2	D	242/259 (93%)	241 (100%)	1 (0%)	95	99
2	F	239/259 (92%)	235 (98%)	4 (2%)	73	93
2	H	242/259 (93%)	242 (100%)	0	100	100
All	All	2458/2700 (91%)	2440 (99%)	18 (1%)	91	98

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

Some 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 chains 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	248/259 (95%)	0.02	0 100 100	32, 46, 61, 67	0
1	B	248/259 (95%)	-0.11	0 100 100	32, 46, 61, 68	0
1	E	248/259 (95%)	-0.10	0 100 100	32, 46, 61, 66	0
1	G	248/259 (95%)	-0.14	0 100 100	32, 46, 61, 66	0
1	I	238/259 (91%)	0.06	2 (0%) 83 86	44, 68, 85, 94	0
1	J	238/259 (91%)	0.44	14 (5%) 22 22	37, 68, 85, 94	0
1	K	234/259 (90%)	0.30	14 (5%) 21 22	44, 68, 85, 94	0
1	R	238/259 (91%)	0.23	4 (1%) 67 71	44, 68, 85, 94	0
2	C	296/311 (95%)	0.02	1 (0%) 91 94	33, 51, 72, 93	0
2	D	297/311 (95%)	0.17	9 (3%) 48 51	33, 52, 68, 94	0
2	F	301/311 (96%)	0.06	4 (1%) 74 78	33, 52, 81, 95	0
2	H	295/311 (94%)	-0.07	1 (0%) 91 94	33, 51, 72, 93	0
All	All	3129/3316 (94%)	0.07	49 (1%) 68 72	32, 54, 82, 95	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	238	TYR	6.3
2	D	156	SER	4.4
1	K	60	ALA	4.2
1	J	1	SER	4.2
1	K	5	THR	4.2
1	K	6	ALA	4.2
1	K	185	ALA	4.1
1	K	7	TYR	4.1
2	D	155	GLU	3.9
1	J	238	TYR	3.8
2	D	129	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	152	CYS	3.6
1	R	184	ILE	3.4
2	F	23	MET	3.3
1	K	212	GLN	3.3
2	D	198	ASN	3.1
2	F	26	ALA	3.1
1	J	184	ILE	3.1
1	K	73	ASP	3.1
1	K	61	GLY	3.0
1	I	238	TYR	3.0
1	J	132	TYR	2.9
1	J	111	LEU	2.9
2	H	9	GLN	2.8
1	R	150	VAL	2.7
2	D	210	THR	2.6
1	J	55	TYR	2.6
2	D	158	HIS	2.5
1	R	175	ILE	2.5
1	J	108	PHE	2.5
1	J	4	LEU	2.5
1	K	74	GLU	2.5
1	K	238	TYR	2.5
2	C	198	ASN	2.5
1	J	74	GLU	2.4
1	J	183	GLY	2.4
1	J	117	PRO	2.4
1	J	174	GLU	2.4
1	I	149	ASP	2.3
1	K	184	ILE	2.2
2	F	78	TYR	2.2
1	K	55	TYR	2.2
1	K	216	TYR	2.2
1	K	189	ARG	2.2
2	D	157	PHE	2.1
2	D	207	ARG	2.1
1	J	11	LEU	2.1
2	F	206	ALA	2.1
1	J	33	GLU	2.1

## 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 carbohydrates 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.