Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 08:22 AM EDT

PDB ID	:	1RQC
Title	:	Crystals of peptide deformylase from Plasmodium falciparum with ten subunits per asymmetric unit reveal critical characteristics of the active site for drug design
Authors	:	Robien, M.A.; Nguyen, K.T.; Kumar, A.; Hirsh, I.; Turley, S.; Pei, D.; Hol, W.G.
Deposited on	:	2003-12-04
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

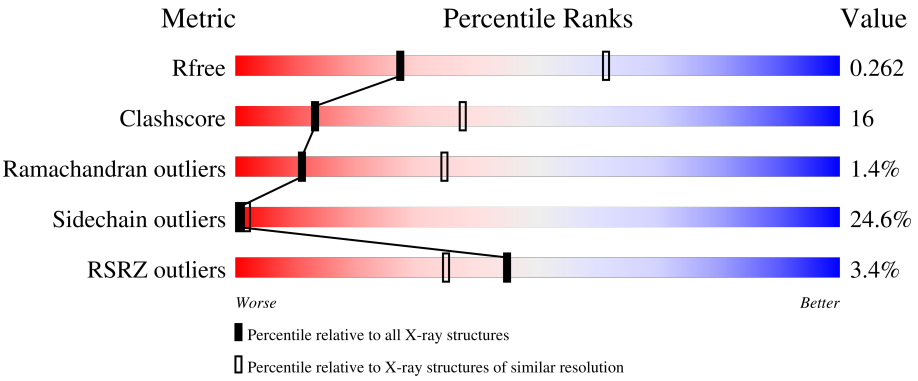
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	185	6% 48% 38% 10%
1	B	185	5% 49% 34% 13%
1	C	185	2% 48% 35% 8% 9%
1	D	185	2% 46% 37% 9% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	185	4% 47% 35% 11% • 5%
1	F	185	2% 53% 32% 8% • 7%
1	G	185	% 52% 30% 9% • 8%
1	H	185	4% 55% 28% 9% • 6%
1	I	185	2% 47% 33% 11% • 8%
1	J	185	3% 46% 36% 10% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14498 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 formylmethionine deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	Se	3	0	0
			1478	948	262	264	1	3			
1	B	178	Total	C	N	O	S	Se	3	0	0
			1478	948	262	264	1	3			
1	C	168	Total	C	N	O	S	Se	3	0	0
			1393	897	246	246	1	3			
1	D	173	Total	C	N	O	S	Se	3	0	0
			1434	920	253	257	1	3			
1	E	175	Total	C	N	O	S	Se	3	0	0
			1449	931	255	259	1	3			
1	F	172	Total	C	N	O	S	Se	3	0	0
			1425	915	252	254	1	3			
1	G	171	Total	C	N	O	S	Se	3	0	0
			1416	910	251	251	1	3			
1	H	173	Total	C	N	O	S	Se	3	0	0
			1434	920	253	257	1	3			
1	I	171	Total	C	N	O	S	Se	3	0	0
			1416	910	251	251	1	3			
1	J	171	Total	C	N	O	S	Se	3	0	0
			1416	910	251	251	1	3			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	240	LEU	-	EXPRESSION TAG	UNP Q8I372
A	241	GLU	-	EXPRESSION TAG	UNP Q8I372
A	242	HIS	-	EXPRESSION TAG	UNP Q8I372
A	243	HIS	-	EXPRESSION TAG	UNP Q8I372
A	244	HIS	-	EXPRESSION TAG	UNP Q8I372
A	245	HIS	-	EXPRESSION TAG	UNP Q8I372

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	HIS	-	EXPRESSION TAG	UNP Q8I372
A	247	HIS	-	EXPRESSION TAG	UNP Q8I372
B	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	240	LEU	-	EXPRESSION TAG	UNP Q8I372
B	241	GLU	-	EXPRESSION TAG	UNP Q8I372
B	242	HIS	-	EXPRESSION TAG	UNP Q8I372
B	243	HIS	-	EXPRESSION TAG	UNP Q8I372
B	244	HIS	-	EXPRESSION TAG	UNP Q8I372
B	245	HIS	-	EXPRESSION TAG	UNP Q8I372
B	246	HIS	-	EXPRESSION TAG	UNP Q8I372
B	247	HIS	-	EXPRESSION TAG	UNP Q8I372
C	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	240	LEU	-	EXPRESSION TAG	UNP Q8I372
C	241	GLU	-	EXPRESSION TAG	UNP Q8I372
C	242	HIS	-	EXPRESSION TAG	UNP Q8I372
C	243	HIS	-	EXPRESSION TAG	UNP Q8I372
C	244	HIS	-	EXPRESSION TAG	UNP Q8I372
C	245	HIS	-	EXPRESSION TAG	UNP Q8I372
C	246	HIS	-	EXPRESSION TAG	UNP Q8I372
C	247	HIS	-	EXPRESSION TAG	UNP Q8I372
D	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	240	LEU	-	EXPRESSION TAG	UNP Q8I372
D	241	GLU	-	EXPRESSION TAG	UNP Q8I372
D	242	HIS	-	EXPRESSION TAG	UNP Q8I372
D	243	HIS	-	EXPRESSION TAG	UNP Q8I372
D	244	HIS	-	EXPRESSION TAG	UNP Q8I372
D	245	HIS	-	EXPRESSION TAG	UNP Q8I372
D	246	HIS	-	EXPRESSION TAG	UNP Q8I372
D	247	HIS	-	EXPRESSION TAG	UNP Q8I372
E	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	240	LEU	-	EXPRESSION TAG	UNP Q8I372
E	241	GLU	-	EXPRESSION TAG	UNP Q8I372
E	242	HIS	-	EXPRESSION TAG	UNP Q8I372
E	243	HIS	-	EXPRESSION TAG	UNP Q8I372

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	244	HIS	-	EXPRESSION TAG	UNP Q8I372
E	245	HIS	-	EXPRESSION TAG	UNP Q8I372
E	246	HIS	-	EXPRESSION TAG	UNP Q8I372
E	247	HIS	-	EXPRESSION TAG	UNP Q8I372
F	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	240	LEU	-	EXPRESSION TAG	UNP Q8I372
F	241	GLU	-	EXPRESSION TAG	UNP Q8I372
F	242	HIS	-	EXPRESSION TAG	UNP Q8I372
F	243	HIS	-	EXPRESSION TAG	UNP Q8I372
F	244	HIS	-	EXPRESSION TAG	UNP Q8I372
F	245	HIS	-	EXPRESSION TAG	UNP Q8I372
F	246	HIS	-	EXPRESSION TAG	UNP Q8I372
F	247	HIS	-	EXPRESSION TAG	UNP Q8I372
G	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	240	LEU	-	EXPRESSION TAG	UNP Q8I372
G	241	GLU	-	EXPRESSION TAG	UNP Q8I372
G	242	HIS	-	EXPRESSION TAG	UNP Q8I372
G	243	HIS	-	EXPRESSION TAG	UNP Q8I372
G	244	HIS	-	EXPRESSION TAG	UNP Q8I372
G	245	HIS	-	EXPRESSION TAG	UNP Q8I372
G	246	HIS	-	EXPRESSION TAG	UNP Q8I372
G	247	HIS	-	EXPRESSION TAG	UNP Q8I372
H	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	240	LEU	-	EXPRESSION TAG	UNP Q8I372
H	241	GLU	-	EXPRESSION TAG	UNP Q8I372
H	242	HIS	-	EXPRESSION TAG	UNP Q8I372
H	243	HIS	-	EXPRESSION TAG	UNP Q8I372
H	244	HIS	-	EXPRESSION TAG	UNP Q8I372
H	245	HIS	-	EXPRESSION TAG	UNP Q8I372
H	246	HIS	-	EXPRESSION TAG	UNP Q8I372
H	247	HIS	-	EXPRESSION TAG	UNP Q8I372
I	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	240	LEU	-	EXPRESSION TAG	UNP Q8I372
I	241	GLU	-	EXPRESSION TAG	UNP Q8I372

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	242	HIS	-	EXPRESSION TAG	UNP Q8I372
I	243	HIS	-	EXPRESSION TAG	UNP Q8I372
I	244	HIS	-	EXPRESSION TAG	UNP Q8I372
I	245	HIS	-	EXPRESSION TAG	UNP Q8I372
I	246	HIS	-	EXPRESSION TAG	UNP Q8I372
I	247	HIS	-	EXPRESSION TAG	UNP Q8I372
J	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	240	LEU	-	EXPRESSION TAG	UNP Q8I372
J	241	GLU	-	EXPRESSION TAG	UNP Q8I372
J	242	HIS	-	EXPRESSION TAG	UNP Q8I372
J	243	HIS	-	EXPRESSION TAG	UNP Q8I372
J	244	HIS	-	EXPRESSION TAG	UNP Q8I372
J	245	HIS	-	EXPRESSION TAG	UNP Q8I372
J	246	HIS	-	EXPRESSION TAG	UNP Q8I372
J	247	HIS	-	EXPRESSION TAG	UNP Q8I372

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	B	1	Total Co 1 1	0	0
2	C	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	F	1	Total Co 1 1	0	0
2	G	1	Total Co 1 1	0	0
2	H	1	Total Co 1 1	0	0
2	I	1	Total Co 1 1	0	0
2	J	1	Total Co 1 1	0	0

- Molecule 3 is water.

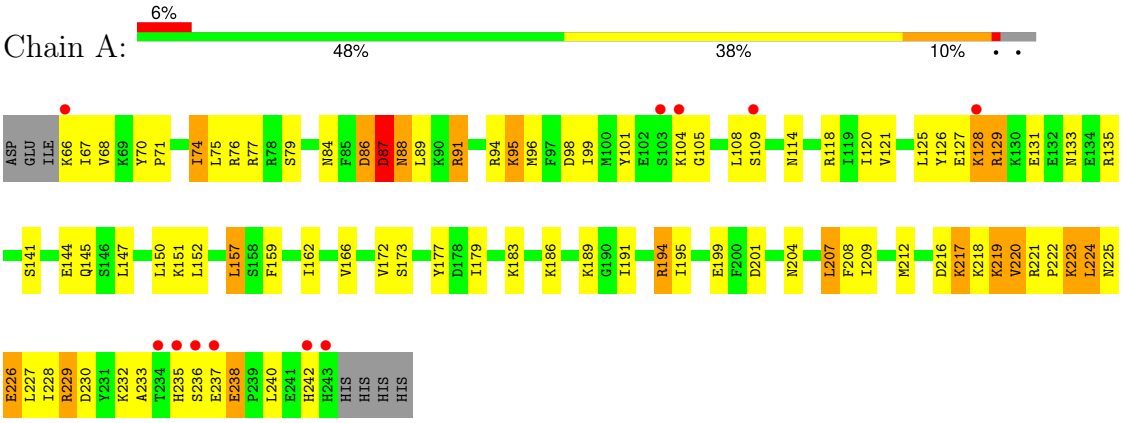
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	20	Total O 20 20	0	0
3	B	18	Total O 18 18	0	0
3	C	12	Total O 12 12	0	0
3	D	14	Total O 14 14	0	0
3	E	12	Total O 12 12	0	0
3	F	27	Total O 27 27	0	0
3	G	9	Total O 9 9	0	0
3	H	9	Total O 9 9	0	0
3	I	14	Total O 14 14	0	0
3	J	14	Total O 14 14	0	0

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.

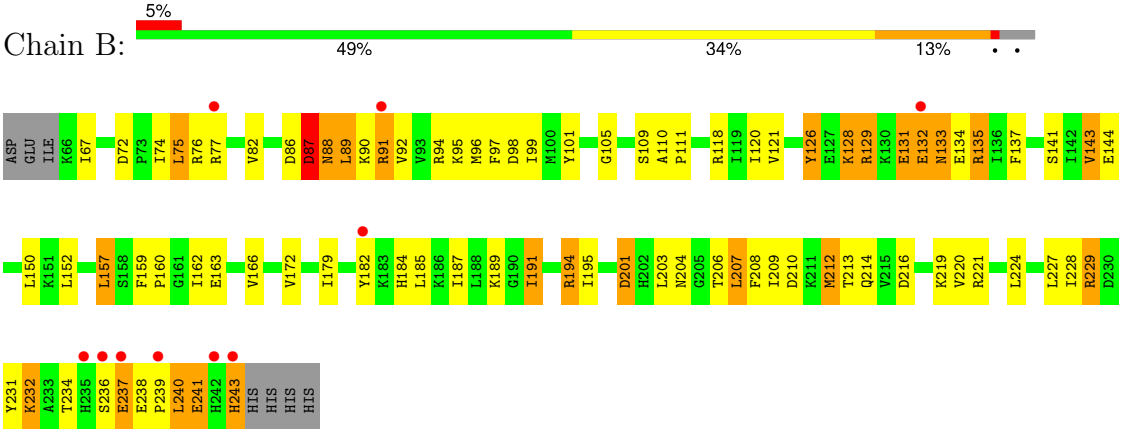
• Molecule 1: formylmethionine deformylase

Chain A:



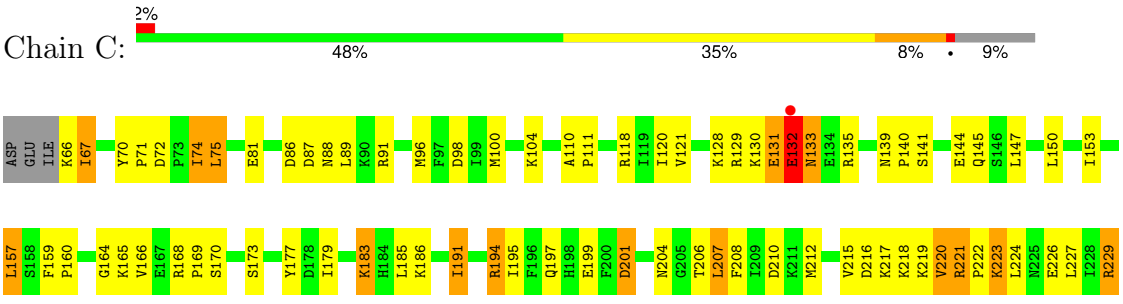
• Molecule 1: formylmethionine deformylase

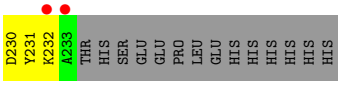
Chain B:



• Molecule 1: formylmethionine deformylase

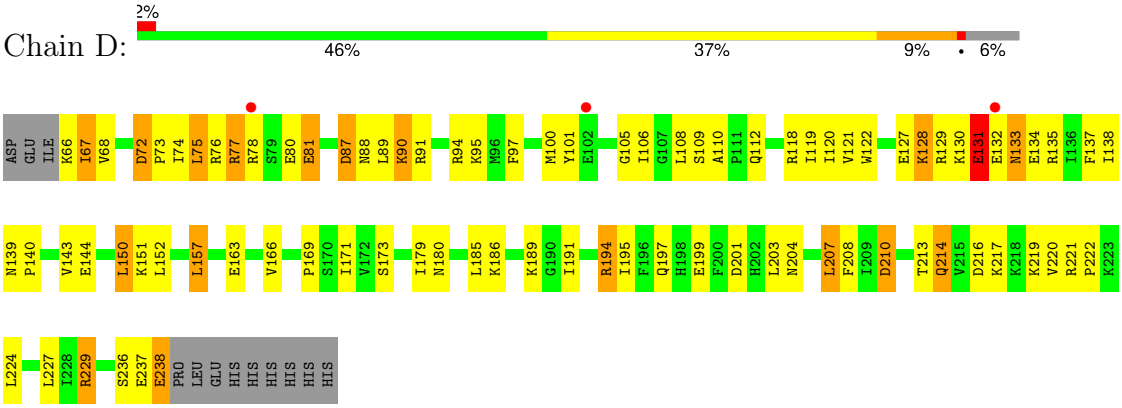
Chain C:





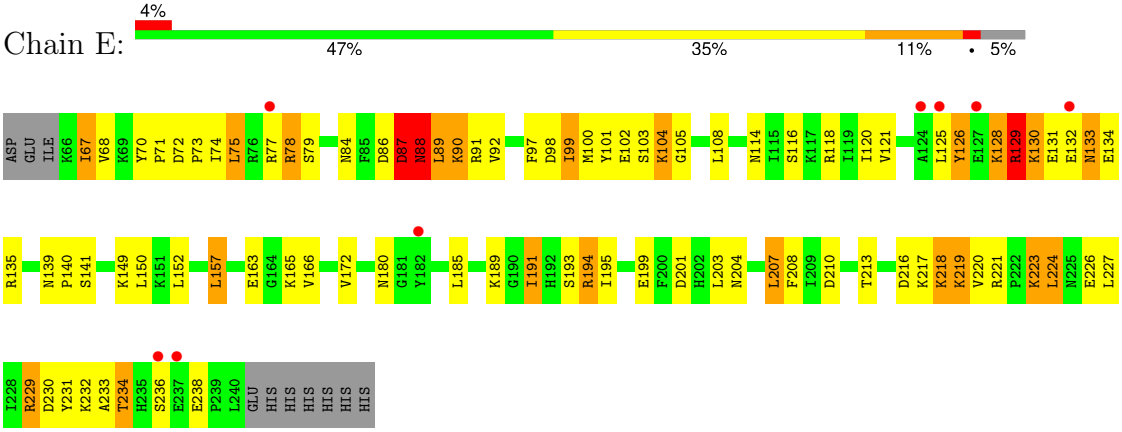
• Molecule 1: formylmethionine deformylase

Chain D:



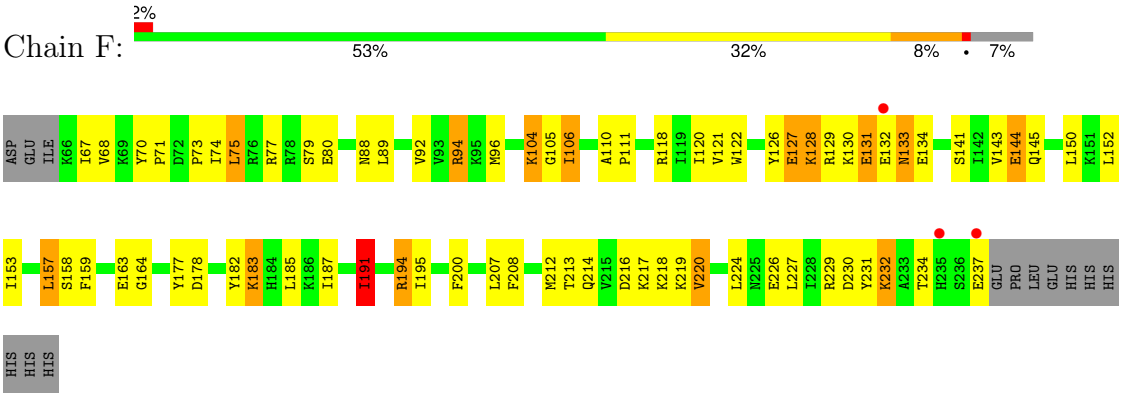
• Molecule 1: formylmethionine deformylase

Chain E:



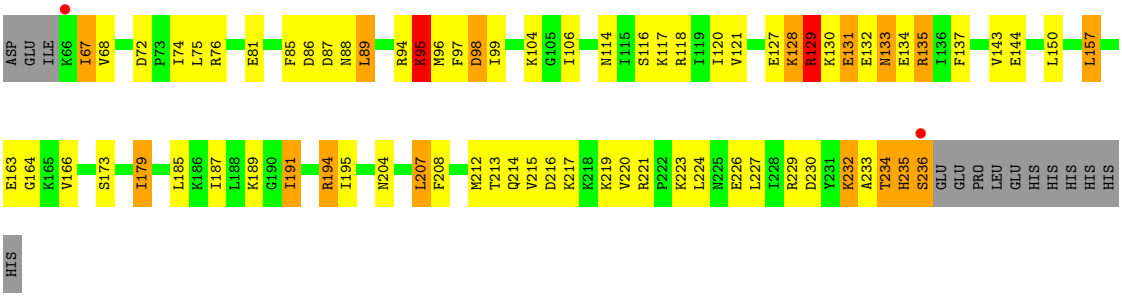
• Molecule 1: formylmethionine deformylase

Chain F:



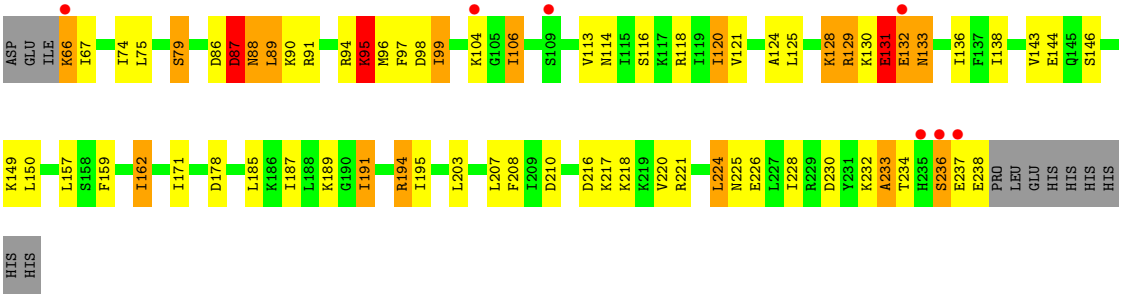
• Molecule 1: formylmethionine deformylase

Chain G:



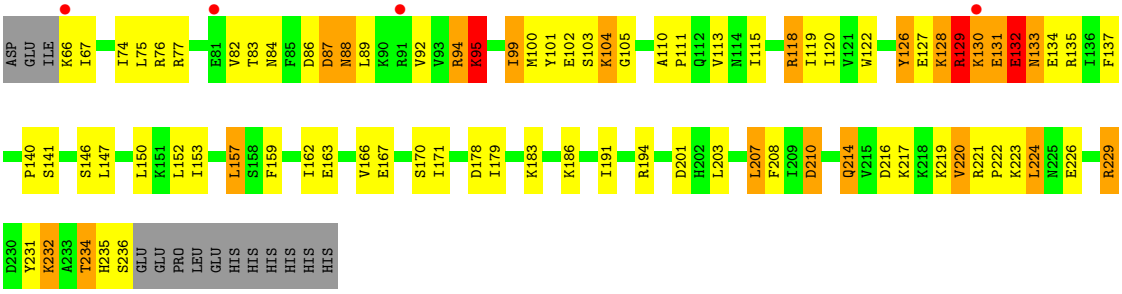
• Molecule 1: formylmethionine deformylase

Chain H:



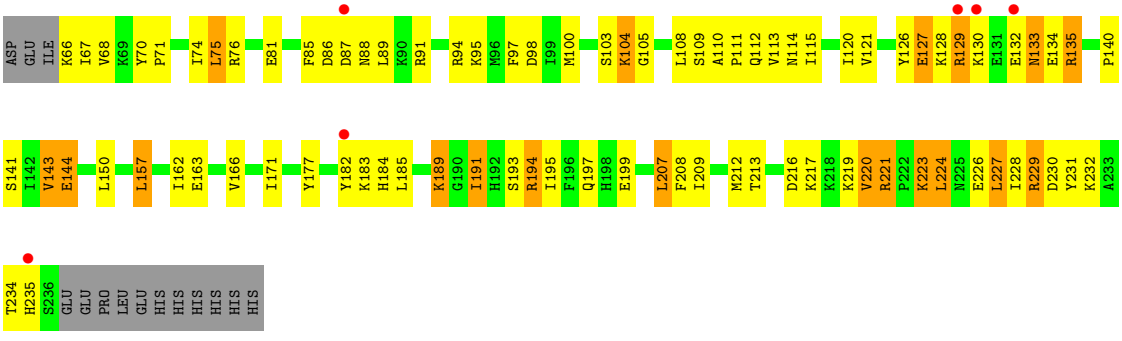
• Molecule 1: formylmethionine deformylase

Chain I:



• Molecule 1: formylmethionine deformylase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	121.26Å 121.26Å 177.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (20.00-2.80) 82.5 (19.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.225 , 0.277 0.213 , 0.262	Depositor DCC
R_{free} test set	5187 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: CO

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	0.74	1/1505 (0.1%)	0.91	7/2016 (0.3%)
1	B	0.66	1/1505 (0.1%)	0.88	7/2016 (0.3%)
1	C	0.68	0/1416	0.87	5/1894 (0.3%)
1	D	0.64	1/1458 (0.1%)	0.98	8/1951 (0.4%)
1	E	0.64	0/1474	0.85	6/1974 (0.3%)
1	F	0.70	0/1449	0.85	2/1939 (0.1%)
1	G	1.01	1/1440 (0.1%)	0.88	5/1927 (0.3%)
1	H	0.68	0/1458	0.91	9/1951 (0.5%)
1	I	0.62	0/1440	0.89	6/1927 (0.3%)
1	J	0.66	0/1440	0.87	3/1927 (0.2%)
All	All	0.71	4/14585 (0.0%)	0.89	58/19522 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	95	LYS	CG-CD	29.21	2.51	1.52
1	A	95	LYS	CG-CD	-16.42	0.96	1.52
1	B	95	LYS	CG-CD	8.23	1.80	1.52
1	D	95	LYS	CG-CD	5.42	1.70	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	95	LYS	CG-CD-CE	-18.45	56.55	111.90
1	B	95	LYS	CG-CD-CE	-14.63	68.02	111.90
1	A	95	LYS	CB-CG-CD	14.04	148.11	111.60
1	A	95	LYS	CG-CD-CE	-12.87	73.30	111.90
1	G	95	LYS	CG-CD-CE	-12.82	73.45	111.90
1	F	191	ILE	CG1-CB-CG2	-11.76	85.52	111.40
1	I	95	LYS	CG-CD-CE	-11.44	77.59	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	95	LYS	CB-CG-CD	-9.57	86.72	111.60
1	H	95	LYS	CG-CD-CE	-8.82	85.43	111.90
1	H	98	ASP	CB-CG-OD2	7.67	125.20	118.30
1	C	210	ASP	CB-CG-OD2	7.32	124.88	118.30
1	B	201	ASP	CB-CG-OD2	6.96	124.56	118.30
1	H	210	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	201	ASP	CB-CG-OD2	6.89	124.50	118.30
1	E	210	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	216	ASP	CB-CG-OD2	6.51	124.16	118.30
1	H	216	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	216	ASP	CB-CG-OD2	6.46	124.12	118.30
1	D	201	ASP	CB-CG-OD2	6.42	124.07	118.30
1	F	216	ASP	CB-CG-OD2	6.40	124.06	118.30
1	I	178	ASP	CB-CG-OD2	6.31	123.98	118.30
1	H	95	LYS	CB-CG-CD	6.28	127.93	111.60
1	D	150	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	B	210	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	216	ASP	CB-CG-OD2	6.08	123.77	118.30
1	E	216	ASP	CB-CG-OD2	6.07	123.77	118.30
1	H	191	ILE	CG1-CB-CG2	-6.04	98.12	111.40
1	H	178	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	98	ASP	CB-CG-OD2	5.90	123.61	118.30
1	I	201	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	87	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	201	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	87	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	72	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	216	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	98	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	230	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	72	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	201	ASP	CB-CG-OD2	5.49	123.24	118.30
1	I	216	ASP	CB-CG-OD2	5.49	123.24	118.30
1	H	230	ASP	CB-CG-OD2	5.46	123.21	118.30
1	J	87	ASP	CB-CG-OD2	5.41	123.16	118.30
1	G	230	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	98	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	210	ASP	CB-CG-OD2	5.37	123.14	118.30
1	E	87	ASP	CB-CG-OD2	5.37	123.13	118.30
1	H	87	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	98	ASP	CB-CG-OD2	5.28	123.05	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	87	ASP	CB-CG-OD2	5.27	123.05	118.30
1	J	216	ASP	CB-CG-OD2	5.26	123.03	118.30
1	I	210	ASP	CB-CG-OD2	5.26	123.03	118.30
1	G	216	ASP	CB-CG-OD2	5.20	122.98	118.30
1	I	87	ASP	CB-CG-OD2	5.17	122.96	118.30
1	J	230	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	98	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	230	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	72	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1478	0	1525	57	0
1	B	1478	0	1525	50	1
1	C	1393	0	1456	40	0
1	D	1434	0	1487	60	0
1	E	1449	0	1505	51	1
1	F	1425	0	1481	47	0
1	G	1416	0	1475	32	0
1	H	1434	0	1487	40	0
1	I	1416	0	1475	64	0
1	J	1416	0	1475	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	0	1	0
3	B	18	0	0	0	0
3	C	12	0	0	1	0
3	D	14	0	0	4	0
3	E	12	0	0	1	0
3	F	27	0	0	1	0
3	G	9	0	0	1	0
3	H	9	0	0	1	0
3	I	14	0	0	1	0
3	J	14	0	0	0	0
All	All	14498	0	14891	475	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:MSE:SE	1:C:100:MSE:CE	2.14	1.43
1:G:164:GLY:HA3	1:G:212:MSE:HE2	1.22	1.14
1:F:164:GLY:HA3	1:F:212:MSE:HE2	1.27	1.09
1:I:131:GLU:O	1:I:133:ASN:N	1.88	1.06
1:I:229:ARG:HG3	1:I:229:ARG:HH11	1.18	1.06
1:E:233:ALA:HA	1:E:236:SER:HB3	1.35	1.04
1:I:221:ARG:HH12	1:J:163:GLU:CD	1.66	0.97
1:E:78:ARG:HG2	1:E:78:ARG:HH11	1.28	0.95
1:I:231:TYR:O	1:I:234:THR:HB	1.67	0.95
1:E:126:TYR:HD1	1:E:126:TYR:H	1.14	0.94
1:I:229:ARG:HH11	1:I:229:ARG:CG	1.78	0.94
1:J:234:THR:HG22	1:J:235:HIS:CD2	2.02	0.93
1:J:234:THR:HG22	1:J:235:HIS:HD2	1.32	0.93
1:D:229:ARG:HH11	1:D:229:ARG:HG2	1.35	0.89
1:E:100:MSE:HG3	1:E:108:LEU:HB2	1.55	0.88
1:J:231:TYR:O	1:J:234:THR:HB	1.73	0.88
1:A:233:ALA:HA	1:A:236:SER:HB3	1.55	0.87
1:G:128:LYS:O	1:G:129:ARG:O	1.92	0.87
1:B:209:ILE:HA	1:B:212:MSE:HE3	1.59	0.85
1:C:164:GLY:HA3	1:C:212:MSE:HE2	1.58	0.84
1:A:229:ARG:HH11	1:A:229:ARG:CG	1.91	0.84
1:B:131:GLU:O	1:B:133:ASN:N	2.10	0.83
1:E:78:ARG:HH11	1:E:78:ARG:CG	1.92	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:GLY:CA	1:G:212:MSE:HE2	2.08	0.82
1:D:87:ASP:O	3:D:708:HOH:O	1.97	0.82
1:E:131:GLU:O	1:E:133:ASN:N	2.12	0.81
1:C:131:GLU:O	1:C:133:ASN:N	2.14	0.80
1:D:229:ARG:HG2	1:D:229:ARG:NH1	1.93	0.80
1:I:221:ARG:NH1	1:J:163:GLU:CD	2.36	0.79
1:I:167:GLU:OE2	3:I:1204:HOH:O	2.01	0.78
1:A:233:ALA:HA	1:A:236:SER:CB	2.13	0.78
1:J:166:VAL:O	1:J:194:ARG:NH2	2.17	0.77
1:B:166:VAL:O	1:B:194:ARG:NH2	2.18	0.77
1:D:229:ARG:HH11	1:D:229:ARG:CG	1.99	0.76
1:I:127:GLU:HB2	1:I:128:LYS:HD3	1.69	0.74
1:B:131:GLU:C	1:B:133:ASN:H	1.90	0.74
1:B:105:GLY:HA3	1:B:157:LEU:HD21	1.68	0.74
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.54	0.73
1:I:221:ARG:HG3	1:I:221:ARG:HH11	1.54	0.72
1:C:201:ASP:HB3	1:C:206:THR:HB	1.73	0.71
1:F:73:PRO:HB2	3:F:912:HOH:O	1.91	0.71
1:D:131:GLU:O	1:D:133:ASN:N	2.22	0.71
1:I:229:ARG:HG3	1:I:229:ARG:NH1	1.96	0.70
1:J:229:ARG:HG2	1:J:229:ARG:HH11	1.54	0.70
1:D:131:GLU:C	1:D:133:ASN:H	1.93	0.69
1:E:231:TYR:O	1:E:234:THR:HB	1.93	0.69
1:I:221:ARG:HB3	1:I:222:PRO:HD3	1.74	0.68
1:I:221:ARG:NH1	1:J:163:GLU:OE1	2.25	0.68
1:J:177:TYR:CZ	1:J:183:LYS:HD2	2.29	0.68
1:J:229:ARG:HH11	1:J:229:ARG:CG	2.05	0.68
1:F:131:GLU:C	1:F:133:ASN:H	1.97	0.68
1:A:152:LEU:HD12	1:A:194:ARG:HG2	1.76	0.67
1:C:131:GLU:C	1:C:133:ASN:H	1.97	0.67
1:F:226:GLU:OE2	1:F:229:ARG:NH1	2.28	0.67
1:D:221:ARG:HB3	1:D:222:PRO:HD3	1.75	0.66
1:G:118:ARG:NH2	1:G:204:ASN:OD1	2.28	0.66
1:A:223:LYS:O	1:A:226:GLU:HB2	1.95	0.66
1:F:164:GLY:CA	1:F:212:MSE:HE2	2.16	0.66
1:A:96:MSE:HE2	1:A:121:VAL:HG22	1.78	0.66
1:D:236:SER:O	1:D:237:GLU:HB2	1.96	0.66
1:B:232:LYS:HZ3	1:B:232:LYS:HB3	1.61	0.65
1:I:126:TYR:HD1	1:I:126:TYR:H	1.44	0.65
1:J:191:ILE:O	1:J:195:ILE:HG12	1.96	0.65
1:J:100:MSE:HE3	1:J:105:GLY:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:ARG:HG3	1:J:221:ARG:HH11	1.63	0.64
1:E:118:ARG:NH2	1:E:204:ASN:OD1	2.30	0.64
1:F:104:LYS:NZ	1:F:104:LYS:HB3	2.12	0.64
1:E:88:ASN:O	1:E:92:VAL:HG23	1.97	0.64
1:I:220:VAL:HG13	1:I:224:LEU:HD22	1.79	0.64
1:F:105:GLY:HA3	1:F:157:LEU:HD21	1.79	0.64
1:A:67:ILE:HD11	1:A:157:LEU:HB3	1.79	0.63
1:G:127:GLU:HG3	3:G:1008:HOH:O	1.96	0.63
1:H:218:LYS:NZ	1:I:104:LYS:O	2.28	0.63
1:I:229:ARG:CG	1:I:229:ARG:NH1	2.50	0.63
1:F:231:TYR:O	1:F:234:THR:HB	1.99	0.63
1:F:152:LEU:HD12	1:F:194:ARG:HG2	1.80	0.63
1:A:147:LEU:HD22	1:E:130:LYS:HE2	1.80	0.62
1:E:84:ASN:HB3	1:E:86:ASP:OD1	1.98	0.62
1:B:232:LYS:HB3	1:B:232:LYS:NZ	2.13	0.62
1:D:157:LEU:HB2	3:D:701:HOH:O	2.00	0.62
1:C:191:ILE:O	1:C:195:ILE:HG12	2.00	0.62
1:I:131:GLU:C	1:I:133:ASN:H	2.01	0.62
1:B:126:TYR:HD1	1:B:126:TYR:H	1.48	0.61
1:H:97:PHE:CZ	1:H:121:VAL:HB	2.35	0.61
1:I:221:ARG:HH12	1:J:163:GLU:CG	2.13	0.61
1:D:80:GLU:HG2	3:D:710:HOH:O	2.00	0.61
1:I:101:TYR:OH	1:I:134:GLU:OE2	2.17	0.61
1:F:67:ILE:HD11	1:F:157:LEU:HB3	1.82	0.61
1:J:67:ILE:HD11	1:J:157:LEU:HB3	1.83	0.60
1:J:162:ILE:HG23	1:J:220:VAL:HG21	1.83	0.60
1:E:166:VAL:O	1:E:194:ARG:NH2	2.34	0.60
1:J:220:VAL:HG23	1:J:223:LYS:HE3	1.83	0.60
1:D:128:LYS:H	1:D:128:LYS:HD3	1.67	0.60
1:F:164:GLY:HA3	1:F:212:MSE:CE	2.18	0.59
1:H:106:ILE:HD11	1:H:124:ALA:HA	1.83	0.59
1:D:72:ASP:OD1	1:D:73:PRO:HD2	2.03	0.59
1:F:92:VAL:O	1:F:96:MSE:HG3	2.03	0.59
1:H:128:LYS:O	1:H:130:LYS:HB2	2.02	0.59
1:C:118:ARG:NH2	1:C:204:ASN:OD1	2.35	0.59
1:H:89:LEU:HD23	1:H:89:LEU:O	2.03	0.59
1:A:238:GLU:HG2	1:A:238:GLU:O	2.02	0.59
1:B:201:ASP:HB3	1:B:206:THR:HB	1.84	0.59
1:E:87:ASP:O	1:E:90:LYS:N	2.35	0.59
1:E:120:ILE:HG13	1:E:203:LEU:HD11	1.85	0.59
1:A:242:HIS:CE1	1:D:189:LYS:HD3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:VAL:O	1:I:194:ARG:NH2	2.36	0.58
1:C:67:ILE:HD11	1:C:157:LEU:HB3	1.86	0.58
1:H:146:SER:HB3	1:H:171:ILE:HB	1.86	0.58
1:A:74:ILE:HD12	1:A:77:ARG:NH1	2.19	0.58
1:B:105:GLY:HA3	1:B:157:LEU:CD2	2.33	0.58
1:B:209:ILE:HG22	1:B:212:MSE:HE3	1.85	0.57
1:B:231:TYR:O	1:B:234:THR:HB	2.04	0.57
1:C:81:GLU:N	1:C:81:GLU:OE2	2.32	0.57
1:H:74:ILE:HD13	1:H:114:ASN:ND2	2.19	0.57
1:I:118:ARG:HA	1:I:203:LEU:HD22	1.86	0.57
1:I:82:VAL:HG11	1:I:89:LEU:HD11	1.85	0.57
1:J:209:ILE:HA	1:J:212:MSE:HE3	1.86	0.57
1:E:131:GLU:C	1:E:133:ASN:H	2.04	0.57
1:D:138:ILE:N	1:D:138:ILE:HD12	2.19	0.57
1:E:97:PHE:CZ	1:E:121:VAL:HB	2.40	0.57
1:F:67:ILE:HG23	1:F:67:ILE:O	2.02	0.57
1:A:84:ASN:HB3	1:A:86:ASP:OD1	2.05	0.57
1:D:108:LEU:HD12	1:D:109:SER:H	1.69	0.57
1:C:177:TYR:CZ	1:C:183:LYS:HD2	2.40	0.56
1:B:120:ILE:HG13	1:B:203:LEU:HD11	1.85	0.56
1:H:131:GLU:O	1:H:132:GLU:HB2	2.04	0.56
1:B:209:ILE:HG22	1:B:212:MSE:CE	2.34	0.56
1:G:67:ILE:HD11	1:G:157:LEU:HB3	1.87	0.56
1:G:128:LYS:O	1:G:129:ARG:C	2.43	0.56
1:C:72:ASP:OD1	1:C:74:ILE:HG22	2.04	0.56
1:B:182:TYR:O	1:B:184:HIS:HD2	1.88	0.56
1:E:72:ASP:OD1	1:E:73:PRO:HD2	2.06	0.56
1:A:105:GLY:HA3	1:A:157:LEU:HD21	1.87	0.56
1:I:76:ARG:CZ	1:I:207:LEU:HD22	2.35	0.56
1:I:214:GLN:O	1:I:214:GLN:HG2	2.04	0.56
1:B:74:ILE:HD12	1:B:77:ARG:HH11	1.70	0.56
1:H:171:ILE:HG12	1:H:189:LYS:HG2	1.88	0.55
1:H:191:ILE:HG22	1:H:195:ILE:HG12	1.88	0.55
1:D:67:ILE:HG23	1:D:67:ILE:O	2.05	0.55
1:D:108:LEU:HD12	1:D:109:SER:N	2.22	0.55
1:D:221:ARG:NH1	1:E:163:GLU:HG2	2.22	0.55
1:F:153:ILE:CG2	1:F:163:GLU:HG2	2.37	0.55
1:F:187:ILE:HG12	1:H:187:ILE:HG12	1.87	0.55
1:E:87:ASP:O	1:E:88:ASN:C	2.45	0.55
1:E:221:ARG:HG3	1:E:221:ARG:HH11	1.71	0.55
1:I:67:ILE:HD11	1:I:157:LEU:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:TYR:CD1	1:E:126:TYR:N	2.63	0.55
1:G:173:SER:HA	1:G:187:ILE:HD13	1.87	0.54
1:G:191:ILE:O	1:G:195:ILE:HG12	2.08	0.54
1:D:97:PHE:CZ	1:D:121:VAL:HB	2.43	0.54
1:C:221:ARG:N	1:C:222:PRO:HD2	2.23	0.54
1:B:131:GLU:C	1:B:133:ASN:N	2.58	0.54
1:B:143:VAL:O	1:B:144:GLU:HG2	2.07	0.54
1:I:100:MSE:HE3	1:I:105:GLY:O	2.08	0.54
1:J:113:VAL:HG23	1:J:115:ILE:HD12	1.90	0.54
1:A:177:TYR:CZ	1:A:183:LYS:HD2	2.43	0.54
1:A:240:LEU:N	1:A:240:LEU:HD23	2.23	0.54
1:G:96:MSE:HE2	1:G:121:VAL:HG22	1.89	0.54
1:C:169:PRO:HD2	1:C:197:GLN:OE1	2.07	0.54
1:A:162:ILE:HD13	1:A:224:LEU:HD13	1.89	0.53
1:I:221:ARG:CZ	1:J:163:GLU:OE1	2.56	0.53
1:D:118:ARG:NH2	1:D:204:ASN:OD1	2.41	0.53
1:E:100:MSE:HG3	1:E:108:LEU:CB	2.33	0.53
1:A:118:ARG:NH2	1:A:204:ASN:OD1	2.42	0.53
1:E:218:LYS:C	1:E:220:VAL:H	2.11	0.53
1:C:164:GLY:CA	1:C:212:MSE:HE2	2.34	0.53
1:F:131:GLU:O	1:F:133:ASN:N	2.41	0.53
1:I:126:TYR:CD1	1:I:126:TYR:N	2.73	0.53
1:E:78:ARG:CG	1:E:78:ARG:NH1	2.61	0.53
1:D:152:LEU:HD12	1:D:194:ARG:HG2	1.91	0.53
1:F:159:PHE:HZ	1:F:207:LEU:HD23	1.73	0.53
1:I:221:ARG:NH1	1:I:221:ARG:HG3	2.22	0.53
1:J:143:VAL:O	1:J:144:GLU:HG2	2.09	0.53
1:D:128:LYS:HD3	1:D:128:LYS:N	2.24	0.53
1:D:76:ARG:CZ	1:D:207:LEU:HD22	2.39	0.52
1:E:105:GLY:HA3	1:E:157:LEU:HD21	1.90	0.52
1:F:178:ASP:OD2	1:F:182:TYR:HB2	2.09	0.52
1:E:78:ARG:HG2	1:E:78:ARG:NH1	2.09	0.52
1:E:229:ARG:NH2	3:E:419:HOH:O	2.25	0.52
1:G:97:PHE:CZ	1:G:121:VAL:HB	2.45	0.52
1:J:97:PHE:CZ	1:J:134:GLU:HB3	2.44	0.52
1:H:226:GLU:OE1	3:H:1110:HOH:O	2.19	0.52
1:B:118:ARG:NH2	1:B:204:ASN:OD1	2.39	0.51
1:B:228:ILE:O	1:B:232:LYS:HG2	2.09	0.51
1:B:229:ARG:HG2	1:B:243:HIS:ND1	2.25	0.51
1:H:232:LYS:C	1:H:234:THR:H	2.13	0.51
1:I:120:ILE:HD12	1:I:140:PRO:HG3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:105:GLY:HA3	1:J:157:LEU:HD21	1.91	0.51
1:B:97:PHE:CZ	1:B:134:GLU:HB3	2.46	0.51
1:D:100:MSE:HG3	1:D:108:LEU:HB2	1.91	0.51
1:D:144:GLU:HB2	1:D:173:SER:HB3	1.91	0.51
1:B:221:ARG:HD2	1:C:153:ILE:O	2.10	0.51
1:J:110:ALA:N	1:J:111:PRO:CD	2.73	0.51
1:B:76:ARG:CZ	1:B:207:LEU:HD22	2.41	0.51
1:D:221:ARG:HG3	1:D:221:ARG:HH11	1.75	0.51
1:A:127:GLU:HB2	1:A:128:LYS:HD2	1.92	0.51
1:B:82:VAL:HG11	1:B:89:LEU:HD11	1.92	0.51
1:D:100:MSE:HE3	1:D:105:GLY:O	2.10	0.51
1:D:166:VAL:O	1:D:194:ARG:NH2	2.44	0.51
1:J:97:PHE:CZ	1:J:121:VAL:HB	2.46	0.51
1:A:238:GLU:HG3	1:A:240:LEU:HG	1.92	0.51
1:B:135:ARG:HB2	1:B:137:PHE:HE1	1.76	0.51
1:C:199:GLU:OE1	1:C:199:GLU:HA	2.11	0.51
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.76	0.51
1:E:104:LYS:O	1:E:126:TYR:HE2	1.94	0.50
1:C:230:ASP:O	1:C:231:TYR:C	2.49	0.50
1:A:131:GLU:C	1:A:133:ASN:H	2.15	0.50
1:J:74:ILE:HD13	1:J:114:ASN:HD22	1.76	0.50
1:B:152:LEU:HD12	1:B:194:ARG:HG2	1.94	0.50
1:C:144:GLU:HB2	1:C:173:SER:HB3	1.94	0.50
1:D:195:ILE:HD13	1:D:195:ILE:N	2.25	0.50
1:B:159:PHE:O	1:B:160:PRO:C	2.48	0.50
1:D:118:ARG:HA	1:D:203:LEU:HD22	1.92	0.50
1:D:108:LEU:HD11	1:D:112:GLN:HB2	1.94	0.50
1:H:96:MSE:HG2	1:H:113:VAL:HG21	1.94	0.50
1:B:159:PHE:HB3	1:B:162:ILE:HB	1.94	0.50
1:I:223:LYS:O	1:I:226:GLU:HB2	2.12	0.50
1:A:221:ARG:NH1	1:D:163:GLU:OE1	2.45	0.49
1:I:131:GLU:O	1:I:132:GLU:C	2.43	0.49
1:H:191:ILE:O	1:H:195:ILE:HG12	2.12	0.49
1:I:74:ILE:HD12	1:I:77:ARG:HH11	1.77	0.49
1:C:130:LYS:C	1:C:131:GLU:O	2.49	0.49
1:A:88:ASN:HA	1:A:91:ARG:NH1	2.28	0.49
1:E:128:LYS:O	1:E:130:LYS:HE3	2.13	0.49
1:I:88:ASN:O	1:I:92:VAL:HG23	2.12	0.49
1:D:81:GLU:HG3	1:D:139:ASN:OD1	2.12	0.49
1:J:71:PRO:HG3	1:J:228:ILE:HG12	1.93	0.49
1:A:126:TYR:HD1	1:A:126:TYR:H	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ILE:O	1:E:67:ILE:CG2	2.59	0.49
1:H:130:LYS:O	1:H:131:GLU:C	2.52	0.48
1:I:159:PHE:HB3	1:I:162:ILE:HB	1.94	0.48
1:I:221:ARG:HB3	1:I:222:PRO:CD	2.42	0.48
1:B:118:ARG:HA	1:B:203:LEU:HD22	1.96	0.48
1:F:104:LYS:HB3	1:F:104:LYS:HZ2	1.78	0.48
1:G:87:ASP:O	1:G:88:ASN:C	2.51	0.48
1:H:221:ARG:HD3	1:I:153:ILE:HG22	1.95	0.48
1:I:221:ARG:NH2	1:J:163:GLU:OE1	2.46	0.48
1:D:110:ALA:HB2	1:D:119:ILE:HB	1.94	0.48
1:I:101:TYR:CE1	1:I:129:ARG:HB3	2.48	0.48
1:A:87:ASP:O	1:A:88:ASN:C	2.52	0.48
1:F:106:ILE:O	1:F:122:TRP:HB2	2.12	0.48
1:F:144:GLU:HG3	1:H:143:VAL:HG11	1.95	0.48
1:B:239:PRO:C	1:B:241:GLU:H	2.17	0.48
1:C:139:ASN:N	1:C:140:PRO:CD	2.76	0.48
1:D:108:LEU:CD1	1:D:112:GLN:HB2	2.44	0.48
1:B:88:ASN:O	1:B:92:VAL:HG23	2.13	0.48
1:F:67:ILE:O	1:F:67:ILE:CG2	2.61	0.48
1:A:220:VAL:O	1:A:220:VAL:HG13	2.14	0.48
1:C:166:VAL:O	1:C:194:ARG:NH2	2.47	0.48
1:J:109:SER:OG	1:J:112:GLN:HG3	2.14	0.48
1:F:94:ARG:HE	1:F:94:ARG:HA	1.79	0.47
1:F:131:GLU:C	1:F:133:ASN:N	2.63	0.47
1:J:100:MSE:HG3	1:J:108:LEU:HB2	1.95	0.47
1:B:239:PRO:HD2	1:B:240:LEU:HD12	1.96	0.47
1:G:133:ASN:HD22	1:G:133:ASN:HA	1.50	0.47
1:H:89:LEU:O	1:H:89:LEU:CD2	2.62	0.47
1:A:88:ASN:HA	1:A:91:ARG:CZ	2.45	0.47
1:A:209:ILE:O	1:A:217:LYS:HE3	2.15	0.47
1:E:220:VAL:HG13	1:E:224:LEU:HD22	1.95	0.47
1:A:76:ARG:CZ	1:A:207:LEU:HD22	2.45	0.47
1:C:220:VAL:HG22	1:C:223:LYS:HD3	1.96	0.47
1:D:122:TRP:CH2	1:D:137:PHE:CE1	3.03	0.47
1:E:75:LEU:HD12	1:E:75:LEU:HA	1.43	0.47
1:F:94:ARG:NH2	1:F:134:GLU:OE1	2.46	0.47
1:G:233:ALA:O	1:G:234:THR:OG1	2.32	0.47
1:H:120:ILE:HG13	1:H:203:LEU:HD11	1.96	0.47
1:I:147:LEU:HD23	1:I:147:LEU:HA	1.67	0.47
1:J:133:ASN:HD22	1:J:133:ASN:HA	1.52	0.47
1:A:224:LEU:O	1:A:228:ILE:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HH11	1:A:229:ARG:HG3	1.73	0.47
1:F:128:LYS:O	1:F:130:LYS:N	2.48	0.47
1:C:75:LEU:HD12	1:C:75:LEU:HA	1.68	0.46
1:D:169:PRO:HG2	1:D:197:GLN:OE1	2.15	0.46
1:E:67:ILE:O	1:E:67:ILE:HG22	2.14	0.46
1:F:74:ILE:HA	1:F:77:ARG:HH11	1.80	0.46
1:I:232:LYS:HD2	1:I:232:LYS:HA	1.64	0.46
1:J:95:LYS:O	1:J:98:ASP:HB2	2.15	0.46
1:B:135:ARG:HE	1:B:135:ARG:HB3	1.53	0.46
1:G:94:ARG:HH22	1:G:134:GLU:CD	2.18	0.46
1:J:127:GLU:H	1:J:127:GLU:HG2	1.43	0.46
1:A:68:VAL:HG21	1:A:75:LEU:HD11	1.98	0.46
1:C:120:ILE:HG12	1:C:199:GLU:HB3	1.98	0.46
1:F:191:ILE:HG23	1:F:191:ILE:HD13	0.91	0.46
1:F:105:GLY:HA3	1:F:157:LEU:CD2	2.46	0.46
1:I:110:ALA:N	1:I:111:PRO:CD	2.79	0.46
1:B:92:VAL:O	1:B:96:MSE:HG3	2.16	0.46
1:J:85:PHE:CD1	1:J:85:PHE:N	2.83	0.46
1:B:237:GLU:OE2	1:B:237:GLU:HA	2.16	0.46
1:C:131:GLU:C	1:C:133:ASN:N	2.62	0.46
1:I:82:VAL:HG11	1:I:89:LEU:CD1	2.44	0.46
1:I:101:TYR:CZ	1:I:129:ARG:HB3	2.51	0.46
1:I:110:ALA:HB2	1:I:119:ILE:HB	1.98	0.46
1:D:120:ILE:HD12	1:D:140:PRO:HG3	1.97	0.46
1:D:157:LEU:HA	1:D:157:LEU:HD12	1.50	0.46
1:F:214:GLN:O	1:F:214:GLN:HG2	2.15	0.46
1:D:77:ARG:HG3	1:D:77:ARG:NH1	2.31	0.46
1:H:233:ALA:HA	1:H:236:SER:CB	2.46	0.46
1:D:97:PHE:CZ	1:D:134:GLU:HB3	2.51	0.45
1:E:101:TYR:CE1	1:E:129:ARG:HB3	2.51	0.45
1:F:232:LYS:HA	1:F:232:LYS:HD3	1.59	0.45
1:A:151:LYS:HA	1:A:166:VAL:O	2.16	0.45
1:C:132:GLU:HA	3:C:612:HOH:O	2.15	0.45
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.71	0.45
1:H:125:LEU:HD22	1:H:128:LYS:HE2	1.98	0.45
1:A:68:VAL:CG2	1:A:75:LEU:HD11	2.46	0.45
1:E:74:ILE:HA	1:E:77:ARG:HH11	1.81	0.45
1:G:191:ILE:H	1:G:191:ILE:HG12	1.34	0.45
1:I:128:LYS:HD3	1:I:128:LYS:N	2.30	0.45
1:B:238:GLU:HA	1:B:239:PRO:HD3	1.84	0.45
1:D:214:GLN:HE22	1:E:223:LYS:NZ	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ILE:O	1:F:195:ILE:HG12	2.16	0.45
1:G:166:VAL:O	1:G:194:ARG:NH2	2.50	0.45
1:A:218:LYS:C	1:A:220:VAL:H	2.19	0.45
1:B:74:ILE:HD12	1:B:77:ARG:NH1	2.32	0.45
1:B:110:ALA:N	1:B:111:PRO:CD	2.79	0.45
1:C:218:LYS:O	1:C:220:VAL:N	2.50	0.45
1:D:74:ILE:HG23	1:D:75:LEU:HD13	1.98	0.45
1:D:90:LYS:HB2	3:D:708:HOH:O	2.16	0.45
1:D:131:GLU:C	1:D:133:ASN:N	2.60	0.45
1:I:89:LEU:O	1:I:89:LEU:HD23	2.16	0.45
1:J:74:ILE:HD13	1:J:114:ASN:ND2	2.30	0.45
1:D:194:ARG:HD3	1:D:194:ARG:HA	1.61	0.45
1:E:74:ILE:HD12	1:E:77:ARG:HH11	1.81	0.45
1:F:143:VAL:O	1:F:144:GLU:HG2	2.17	0.45
1:I:95:LYS:O	1:I:99:ILE:HG13	2.17	0.45
1:C:191:ILE:H	1:C:191:ILE:HG12	1.35	0.45
1:I:162:ILE:HG23	1:I:220:VAL:HG21	1.98	0.45
1:F:75:LEU:HD12	1:F:75:LEU:HA	1.74	0.45
1:H:87:ASP:O	1:H:88:ASN:C	2.55	0.45
1:E:218:LYS:O	1:E:220:VAL:N	2.50	0.45
1:J:130:LYS:O	1:J:134:GLU:HG2	2.17	0.44
1:H:130:LYS:C	1:H:131:GLU:O	2.54	0.44
1:I:122:TRP:CH2	1:I:137:PHE:CE1	3.05	0.44
1:D:221:ARG:HB3	1:D:222:PRO:CD	2.45	0.44
1:H:225:ASN:HA	1:H:228:ILE:HD12	1.99	0.44
1:E:99:ILE:O	1:E:102:GLU:HB3	2.18	0.44
1:E:223:LYS:HZ2	1:E:223:LYS:HG2	1.45	0.44
1:H:191:ILE:HG21	1:H:191:ILE:HD12	1.57	0.44
1:A:225:ASN:OD1	1:D:152:LEU:HB3	2.18	0.44
1:E:99:ILE:H	1:E:99:ILE:HG12	1.55	0.44
1:H:79:SER:HB3	1:H:118:ARG:HG2	2.00	0.44
1:J:193:SER:O	1:J:197:GLN:HG3	2.17	0.44
1:A:195:ILE:O	1:A:199:GLU:HG2	2.17	0.44
1:B:191:ILE:O	1:B:195:ILE:HG12	2.18	0.44
1:F:110:ALA:N	1:F:111:PRO:CD	2.81	0.44
1:F:194:ARG:HA	1:F:194:ARG:HD3	1.66	0.44
1:H:194:ARG:HA	1:H:194:ARG:HD3	1.67	0.44
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.78	0.44
1:E:207:LEU:HD12	1:E:207:LEU:HA	1.82	0.44
1:H:66:LYS:HA	1:H:66:LYS:HD2	1.54	0.44
1:A:233:ALA:HA	1:A:236:SER:HB2	1.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ASN:HA	1:B:91:ARG:NH1	2.33	0.43
1:D:97:PHE:O	1:D:101:TYR:CD2	2.71	0.43
1:D:138:ILE:N	1:D:138:ILE:CD1	2.81	0.43
1:I:94:ARG:NE	1:I:94:ARG:HA	2.33	0.43
1:J:227:LEU:HD12	1:J:227:LEU:HA	1.78	0.43
1:C:110:ALA:N	1:C:111:PRO:HD2	2.33	0.43
1:F:220:VAL:HG13	1:F:220:VAL:O	2.19	0.43
1:G:213:THR:O	1:G:215:VAL:N	2.51	0.43
1:J:191:ILE:H	1:J:191:ILE:HG12	1.38	0.43
1:C:74:ILE:HG13	1:C:74:ILE:O	2.19	0.43
1:E:194:ARG:HA	1:E:194:ARG:HD3	1.66	0.43
1:G:94:ARG:NH2	1:G:134:GLU:OE2	2.51	0.43
1:H:95:LYS:O	1:H:99:ILE:HG12	2.18	0.43
1:J:171:ILE:HG12	1:J:189:LYS:HB3	2.01	0.43
1:A:229:ARG:CG	1:A:229:ARG:NH1	2.61	0.43
1:F:191:ILE:HG21	1:F:191:ILE:HD12	1.19	0.43
1:D:195:ILE:O	1:D:199:GLU:HG2	2.19	0.43
1:D:221:ARG:CB	1:D:222:PRO:HD3	2.46	0.43
1:G:95:LYS:O	1:G:98:ASP:HB2	2.18	0.43
1:A:101:TYR:CE1	1:A:129:ARG:HB3	2.54	0.43
1:C:96:MSE:HE2	1:C:121:VAL:HG22	2.00	0.43
1:E:191:ILE:O	1:E:195:ILE:HG12	2.18	0.43
1:I:224:LEU:HD12	1:I:224:LEU:HA	1.77	0.43
1:A:68:VAL:HG21	1:A:75:LEU:CD1	2.49	0.43
1:D:237:GLU:C	1:D:238:GLU:HG2	2.38	0.43
1:H:130:LYS:O	1:H:131:GLU:O	2.36	0.43
1:I:234:THR:HG22	1:I:235:HIS:CD2	2.54	0.43
1:G:85:PHE:HA	1:G:89:LEU:HD12	2.01	0.43
1:H:89:LEU:CD2	1:H:89:LEU:C	2.88	0.43
1:G:97:PHE:CZ	1:G:134:GLU:HB3	2.53	0.42
1:G:235:HIS:O	1:G:236:SER:C	2.57	0.42
1:I:74:ILE:HD12	1:I:77:ARG:NH1	2.33	0.42
1:I:130:LYS:O	1:I:134:GLU:HG3	2.19	0.42
1:B:101:TYR:CE1	1:B:129:ARG:HB3	2.54	0.42
1:J:120:ILE:HD12	1:J:140:PRO:HG3	2.00	0.42
1:A:70:TYR:HA	1:A:71:PRO:HA	1.75	0.42
1:A:120:ILE:HD13	1:A:120:ILE:HG21	1.82	0.42
1:A:212:MSE:HB3	1:A:217:LYS:HG2	2.00	0.42
1:A:232:LYS:HD2	1:A:232:LYS:HA	1.75	0.42
1:C:226:GLU:O	1:C:229:ARG:HB3	2.19	0.42
1:E:87:ASP:O	1:E:89:LEU:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:TYR:HA	1:F:71:PRO:HA	1.86	0.42
1:G:135:ARG:HB2	1:G:137:PHE:HE1	1.84	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD12	1.68	0.42
1:C:70:TYR:HA	1:C:71:PRO:HA	1.84	0.42
1:F:121:VAL:O	1:F:122:TRP:HB3	2.19	0.42
1:C:231:TYR:CD1	1:C:232:LYS:HG2	2.54	0.42
1:E:218:LYS:C	1:E:220:VAL:N	2.72	0.42
1:G:76:ARG:CZ	1:G:207:LEU:HD22	2.50	0.42
1:G:86:ASP:HB2	1:G:87:ASP:H	1.55	0.42
1:H:191:ILE:HD13	1:H:191:ILE:HG23	1.47	0.42
1:I:95:LYS:O	1:I:99:ILE:CG1	2.68	0.42
1:J:130:LYS:O	1:J:134:GLU:CG	2.68	0.42
1:C:207:LEU:HD12	1:C:207:LEU:HA	1.81	0.42
1:G:76:ARG:NH1	1:G:207:LEU:HD22	2.35	0.42
1:G:131:GLU:C	1:G:133:ASN:H	2.22	0.42
1:A:86:ASP:HB2	1:A:87:ASP:H	1.74	0.42
1:H:125:LEU:HB2	1:H:133:ASN:OD1	2.18	0.42
1:J:94:ARG:HH22	1:J:134:GLU:CD	2.22	0.42
1:B:97:PHE:CZ	1:B:121:VAL:HB	2.55	0.42
1:I:130:LYS:C	1:I:131:GLU:O	2.56	0.42
1:J:70:TYR:HA	1:J:71:PRO:HA	1.85	0.42
1:J:182:TYR:O	1:J:184:HIS:HD2	2.03	0.42
1:C:168:ARG:HD2	1:C:194:ARG:NE	2.35	0.41
1:E:70:TYR:HA	1:E:71:PRO:HA	1.81	0.41
1:A:221:ARG:N	1:A:222:PRO:HD2	2.35	0.41
1:D:131:GLU:H	1:D:131:GLU:HG2	1.48	0.41
1:F:177:TYR:CZ	1:F:183:LYS:HD2	2.55	0.41
1:G:232:LYS:C	1:G:234:THR:H	2.23	0.41
1:I:146:SER:HB3	1:I:171:ILE:HB	2.00	0.41
1:B:194:ARG:HD3	1:B:194:ARG:HA	1.72	0.41
1:C:157:LEU:HD12	1:C:157:LEU:HA	1.57	0.41
1:H:224:LEU:HD23	1:I:153:ILE:HD13	2.02	0.41
1:I:129:ARG:H	1:I:129:ARG:HG3	1.54	0.41
1:F:80:GLU:C	1:F:118:ARG:HG3	2.40	0.41
1:G:120:ILE:O	1:G:120:ILE:HG22	2.19	0.41
1:G:179:ILE:HD12	1:G:179:ILE:HA	1.74	0.41
1:J:135:ARG:HE	1:J:135:ARG:HB3	1.73	0.41
1:C:218:LYS:C	1:C:220:VAL:H	2.23	0.41
1:E:133:ASN:HD22	1:E:133:ASN:HA	1.66	0.41
1:H:87:ASP:O	1:H:90:LYS:HB2	2.21	0.41
1:J:75:LEU:HA	1:J:75:LEU:HD12	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:ARG:CZ	1:J:207:LEU:HD22	2.51	0.41
1:A:166:VAL:O	1:A:194:ARG:NH2	2.54	0.41
1:A:235:HIS:HB2	3:A:410:HOH:O	2.21	0.41
1:B:182:TYR:O	1:B:184:HIS:CD2	2.70	0.41
1:F:120:ILE:HD11	1:F:200:PHE:HA	2.03	0.41
1:B:109:SER:OG	1:B:111:PRO:HD2	2.21	0.41
1:D:171:ILE:HG12	1:D:189:LYS:CG	2.51	0.41
1:E:139:ASN:N	1:E:140:PRO:HD3	2.36	0.41
1:H:120:ILE:HG21	1:H:120:ILE:HD13	1.77	0.41
1:I:152:LEU:H	1:I:194:ARG:NH2	2.18	0.41
1:A:88:ASN:HA	1:A:91:ARG:NH2	2.36	0.41
1:B:128:LYS:HB2	1:B:128:LYS:HE3	1.34	0.41
1:D:78:ARG:CZ	1:D:118:ARG:HH21	2.34	0.41
1:D:171:ILE:HG12	1:D:189:LYS:HG2	2.02	0.41
1:E:195:ILE:O	1:E:199:GLU:HG2	2.21	0.41
1:F:106:ILE:HB	1:F:126:TYR:CD1	2.55	0.41
1:J:195:ILE:O	1:J:199:GLU:HG2	2.21	0.41
1:J:229:ARG:CG	1:J:229:ARG:NH1	2.76	0.41
1:D:67:ILE:O	1:D:67:ILE:CG2	2.68	0.40
1:D:75:LEU:HA	1:D:75:LEU:HD12	1.52	0.40
1:H:128:LYS:O	1:H:129:ARG:C	2.60	0.40
1:I:103:SER:O	1:I:104:LYS:HB2	2.21	0.40
1:J:104:LYS:C	1:J:126:TYR:HE2	2.25	0.40
1:J:220:VAL:HG13	1:J:224:LEU:HD22	2.03	0.40
1:F:127:GLU:HB2	1:F:128:LYS:HD3	2.02	0.40
1:H:159:PHE:HB3	1:H:162:ILE:HB	2.03	0.40
1:I:127:GLU:H	1:I:127:GLU:HG2	1.74	0.40
1:A:108:LEU:HG	1:A:109:SER:N	2.35	0.40
1:A:131:GLU:O	1:A:133:ASN:N	2.54	0.40
1:E:152:LEU:O	1:E:165:LYS:HA	2.21	0.40
1:F:74:ILE:HG23	1:F:75:LEU:N	2.36	0.40
1:F:130:LYS:O	1:F:133:ASN:HB2	2.20	0.40
1:H:136:ILE:HG22	1:H:138:ILE:HD12	2.03	0.40
1:A:194:ARG:HD3	1:A:194:ARG:HA	1.59	0.40
1:C:159:PHE:N	1:C:160:PRO:HD3	2.36	0.40
1:I:113:VAL:HG23	1:I:115:ILE:HG13	2.01	0.40
1:A:67:ILE:HG23	1:A:67:ILE:O	2.21	0.40
1:A:159:PHE:HB3	1:A:162:ILE:HB	2.02	0.40
1:A:240:LEU:N	1:A:240:LEU:CD2	2.83	0.40
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.59	0.40
1:B:86:ASP:HB2	1:B:87:ASP:H	1.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ARG:H	1:G:129:ARG:HG3	1.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:OE1	1:E:221:ARG:NH1[4_564]	2.11	0.09

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	176/185 (95%)	152 (86%)	23 (13%)	1 (1%)	25	56
1	B	176/185 (95%)	160 (91%)	13 (7%)	3 (2%)	9	29
1	C	166/185 (90%)	148 (89%)	14 (8%)	4 (2%)	6	20
1	D	171/185 (92%)	155 (91%)	14 (8%)	2 (1%)	13	39
1	E	173/185 (94%)	152 (88%)	17 (10%)	4 (2%)	6	21
1	F	170/185 (92%)	157 (92%)	11 (6%)	2 (1%)	13	39
1	G	169/185 (91%)	148 (88%)	19 (11%)	2 (1%)	13	39
1	H	171/185 (92%)	154 (90%)	15 (9%)	2 (1%)	13	39
1	I	169/185 (91%)	154 (91%)	12 (7%)	3 (2%)	8	28
1	J	169/185 (91%)	158 (94%)	10 (6%)	1 (1%)	25	56
All	All	1710/1850 (92%)	1538 (90%)	148 (9%)	24 (1%)	11	34

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	GLU
1	D	132	GLU
1	E	129	ARG
1	E	132	GLU
1	G	129	ARG
1	I	129	ARG
1	I	131	GLU
1	I	132	GLU
1	B	131	GLU
1	C	219	LYS
1	D	131	GLU
1	F	129	ARG
1	G	214	GLN
1	H	131	GLU
1	J	129	ARG
1	A	219	LYS
1	C	132	GLU
1	E	88	ASN
1	F	131	GLU
1	H	233	ALA
1	B	240	LEU
1	E	219	LYS
1	C	215	VAL

5.3.2 Protein sidechains (i)

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	167/171 (98%)	126 (75%)	41 (25%)	0 2
1	B	167/171 (98%)	126 (75%)	41 (25%)	0 2
1	C	157/171 (92%)	122 (78%)	35 (22%)	1 2
1	D	162/171 (95%)	121 (75%)	41 (25%)	0 1
1	E	164/171 (96%)	116 (71%)	48 (29%)	0 1
1	F	161/171 (94%)	128 (80%)	33 (20%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	160/171 (94%)	115 (72%)	45 (28%)	0 1
1	H	162/171 (95%)	126 (78%)	36 (22%)	1 2
1	I	160/171 (94%)	119 (74%)	41 (26%)	0 1
1	J	160/171 (94%)	122 (76%)	38 (24%)	0 2
All	All	1620/1710 (95%)	1221 (75%)	399 (25%)	0 2

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	74	ILE
1	A	79	SER
1	A	86	ASP
1	A	87	ASP
1	A	88	ASN
1	A	89	LEU
1	A	91	ARG
1	A	94	ARG
1	A	95	LYS
1	A	99	ILE
1	A	104	LYS
1	A	114	ASN
1	A	125	LEU
1	A	128	LYS
1	A	129	ARG
1	A	135	ARG
1	A	141	SER
1	A	144	GLU
1	A	145	GLN
1	A	150	LEU
1	A	157	LEU
1	A	172	VAL
1	A	173	SER
1	A	179	ILE
1	A	186	LYS
1	A	189	LYS
1	A	191	ILE
1	A	194	ARG
1	A	207	LEU
1	A	208	PHE
1	A	217	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	LYS
1	A	220	VAL
1	A	223	LYS
1	A	224	LEU
1	A	226	GLU
1	A	227	LEU
1	A	229	ARG
1	A	237	GLU
1	A	238	GLU
1	B	67	ILE
1	B	75	LEU
1	B	87	ASP
1	B	88	ASN
1	B	89	LEU
1	B	90	LYS
1	B	91	ARG
1	B	94	ARG
1	B	99	ILE
1	B	126	TYR
1	B	128	LYS
1	B	129	ARG
1	B	132	GLU
1	B	133	ASN
1	B	135	ARG
1	B	141	SER
1	B	143	VAL
1	B	150	LEU
1	B	157	LEU
1	B	172	VAL
1	B	179	ILE
1	B	185	LEU
1	B	187	ILE
1	B	189	LYS
1	B	191	ILE
1	B	194	ARG
1	B	207	LEU
1	B	208	PHE
1	B	212	MSE
1	B	213	THR
1	B	214	GLN
1	B	219	LYS
1	B	220	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	224	LEU
1	B	227	LEU
1	B	229	ARG
1	B	232	LYS
1	B	236	SER
1	B	237	GLU
1	B	241	GLU
1	B	243	HIS
1	C	66	LYS
1	C	67	ILE
1	C	74	ILE
1	C	75	LEU
1	C	86	ASP
1	C	88	ASN
1	C	89	LEU
1	C	91	ARG
1	C	104	LYS
1	C	128	LYS
1	C	129	ARG
1	C	132	GLU
1	C	133	ASN
1	C	135	ARG
1	C	141	SER
1	C	145	GLN
1	C	150	LEU
1	C	157	LEU
1	C	165	LYS
1	C	170	SER
1	C	179	ILE
1	C	183	LYS
1	C	185	LEU
1	C	186	LYS
1	C	191	ILE
1	C	194	ARG
1	C	207	LEU
1	C	208	PHE
1	C	217	LYS
1	C	220	VAL
1	C	221	ARG
1	C	223	LYS
1	C	224	LEU
1	C	227	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	229	ARG
1	D	66	LYS
1	D	67	ILE
1	D	68	VAL
1	D	75	LEU
1	D	77	ARG
1	D	81	GLU
1	D	88	ASN
1	D	89	LEU
1	D	90	LYS
1	D	91	ARG
1	D	94	ARG
1	D	106	ILE
1	D	127	GLU
1	D	128	LYS
1	D	129	ARG
1	D	130	LYS
1	D	131	GLU
1	D	133	ASN
1	D	135	ARG
1	D	143	VAL
1	D	150	LEU
1	D	151	LYS
1	D	157	LEU
1	D	179	ILE
1	D	180	ASN
1	D	185	LEU
1	D	186	LYS
1	D	191	ILE
1	D	194	ARG
1	D	207	LEU
1	D	208	PHE
1	D	210	ASP
1	D	213	THR
1	D	214	GLN
1	D	217	LYS
1	D	219	LYS
1	D	220	VAL
1	D	224	LEU
1	D	227	LEU
1	D	229	ARG
1	D	238	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	67	ILE
1	E	68	VAL
1	E	75	LEU
1	E	78	ARG
1	E	79	SER
1	E	87	ASP
1	E	88	ASN
1	E	89	LEU
1	E	90	LYS
1	E	91	ARG
1	E	99	ILE
1	E	103	SER
1	E	104	LYS
1	E	114	ASN
1	E	116	SER
1	E	125	LEU
1	E	126	TYR
1	E	128	LYS
1	E	129	ARG
1	E	130	LYS
1	E	133	ASN
1	E	134	GLU
1	E	135	ARG
1	E	141	SER
1	E	149	LYS
1	E	150	LEU
1	E	157	LEU
1	E	172	VAL
1	E	180	ASN
1	E	185	LEU
1	E	189	LYS
1	E	191	ILE
1	E	193	SER
1	E	194	ARG
1	E	207	LEU
1	E	208	PHE
1	E	213	THR
1	E	217	LYS
1	E	218	LYS
1	E	219	LYS
1	E	223	LYS
1	E	224	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	226	GLU
1	E	227	LEU
1	E	229	ARG
1	E	232	LYS
1	E	234	THR
1	E	238	GLU
1	F	68	VAL
1	F	75	LEU
1	F	79	SER
1	F	88	ASN
1	F	89	LEU
1	F	94	ARG
1	F	104	LYS
1	F	106	ILE
1	F	127	GLU
1	F	128	LYS
1	F	132	GLU
1	F	133	ASN
1	F	141	SER
1	F	144	GLU
1	F	145	GLN
1	F	150	LEU
1	F	157	LEU
1	F	158	SER
1	F	183	LYS
1	F	185	LEU
1	F	191	ILE
1	F	194	ARG
1	F	208	PHE
1	F	213	THR
1	F	217	LYS
1	F	218	LYS
1	F	219	LYS
1	F	220	VAL
1	F	224	LEU
1	F	227	LEU
1	F	230	ASP
1	F	232	LYS
1	F	237	GLU
1	G	67	ILE
1	G	68	VAL
1	G	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	75	LEU
1	G	81	GLU
1	G	89	LEU
1	G	95	LYS
1	G	99	ILE
1	G	104	LYS
1	G	106	ILE
1	G	114	ASN
1	G	116	SER
1	G	117	LYS
1	G	128	LYS
1	G	129	ARG
1	G	130	LYS
1	G	131	GLU
1	G	132	GLU
1	G	133	ASN
1	G	135	ARG
1	G	143	VAL
1	G	144	GLU
1	G	150	LEU
1	G	157	LEU
1	G	163	GLU
1	G	179	ILE
1	G	185	LEU
1	G	189	LYS
1	G	191	ILE
1	G	194	ARG
1	G	207	LEU
1	G	208	PHE
1	G	217	LYS
1	G	219	LYS
1	G	220	VAL
1	G	221	ARG
1	G	223	LYS
1	G	224	LEU
1	G	226	GLU
1	G	227	LEU
1	G	229	ARG
1	G	232	LYS
1	G	234	THR
1	G	235	HIS
1	G	236	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	66	LYS
1	H	67	ILE
1	H	75	LEU
1	H	79	SER
1	H	86	ASP
1	H	87	ASP
1	H	88	ASN
1	H	89	LEU
1	H	91	ARG
1	H	94	ARG
1	H	95	LYS
1	H	99	ILE
1	H	104	LYS
1	H	106	ILE
1	H	116	SER
1	H	120	ILE
1	H	128	LYS
1	H	129	ARG
1	H	131	GLU
1	H	132	GLU
1	H	133	ASN
1	H	144	GLU
1	H	149	LYS
1	H	150	LEU
1	H	157	LEU
1	H	162	ILE
1	H	185	LEU
1	H	194	ARG
1	H	207	LEU
1	H	208	PHE
1	H	217	LYS
1	H	220	VAL
1	H	224	LEU
1	H	236	SER
1	H	237	GLU
1	H	238	GLU
1	I	66	LYS
1	I	75	LEU
1	I	83	THR
1	I	84	ASN
1	I	86	ASP
1	I	87	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	88	ASN
1	I	94	ARG
1	I	95	LYS
1	I	99	ILE
1	I	102	GLU
1	I	104	LYS
1	I	118	ARG
1	I	126	TYR
1	I	128	LYS
1	I	129	ARG
1	I	130	LYS
1	I	132	GLU
1	I	133	ASN
1	I	135	ARG
1	I	141	SER
1	I	150	LEU
1	I	157	LEU
1	I	163	GLU
1	I	170	SER
1	I	179	ILE
1	I	183	LYS
1	I	186	LYS
1	I	191	ILE
1	I	207	LEU
1	I	208	PHE
1	I	210	ASP
1	I	214	GLN
1	I	217	LYS
1	I	219	LYS
1	I	220	VAL
1	I	224	LEU
1	I	229	ARG
1	I	232	LYS
1	I	234	THR
1	I	236	SER
1	J	66	LYS
1	J	68	VAL
1	J	75	LEU
1	J	81	GLU
1	J	86	ASP
1	J	88	ASN
1	J	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	91	ARG
1	J	103	SER
1	J	104	LYS
1	J	127	GLU
1	J	128	LYS
1	J	129	ARG
1	J	132	GLU
1	J	133	ASN
1	J	135	ARG
1	J	141	SER
1	J	143	VAL
1	J	144	GLU
1	J	150	LEU
1	J	157	LEU
1	J	185	LEU
1	J	189	LYS
1	J	191	ILE
1	J	194	ARG
1	J	207	LEU
1	J	208	PHE
1	J	213	THR
1	J	217	LYS
1	J	219	LYS
1	J	220	VAL
1	J	221	ARG
1	J	223	LYS
1	J	224	LEU
1	J	226	GLU
1	J	227	LEU
1	J	229	ARG
1	J	232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	114	ASN
1	A	184	HIS
1	A	242	HIS
1	B	133	ASN
1	B	184	HIS
1	B	214	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	114	ASN
1	C	133	ASN
1	D	214	GLN
1	E	114	ASN
1	E	180	ASN
1	E	184	HIS
1	F	114	ASN
1	F	133	ASN
1	F	180	ASN
1	G	114	ASN
1	G	133	ASN
1	H	112	GLN
1	H	114	ASN
1	H	180	ASN
1	H	214	GLN
1	I	114	ASN
1	I	214	GLN
1	I	235	HIS
1	J	114	ASN
1	J	133	ASN
1	J	235	HIS

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

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	175/185 (94%)	0.09	11 (6%)	20	12	23, 41, 86, 97	1 (0%)
1	B	175/185 (94%)	-0.03	10 (5%)	23	15	15, 36, 83, 101	1 (0%)
1	C	165/185 (89%)	-0.17	3 (1%)	68	61	12, 32, 65, 76	1 (0%)
1	D	170/185 (91%)	-0.22	3 (1%)	68	61	19, 38, 78, 91	1 (0%)
1	E	172/185 (92%)	0.01	8 (4%)	31	22	17, 36, 88, 97	1 (0%)
1	F	169/185 (91%)	-0.26	3 (1%)	68	61	8, 28, 71, 96	1 (0%)
1	G	168/185 (90%)	-0.19	2 (1%)	79	73	17, 35, 70, 89	1 (0%)
1	H	170/185 (91%)	-0.15	7 (4%)	37	27	12, 32, 78, 98	1 (0%)
1	I	168/185 (90%)	-0.15	4 (2%)	59	49	15, 35, 76, 88	1 (0%)
1	J	168/185 (90%)	-0.09	6 (3%)	42	32	18, 35, 74, 87	1 (0%)
All	All	1700/1850 (91%)	-0.11	57 (3%)	45	35	8, 35, 78, 101	10 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	8.1
1	E	237	GLU	6.3
1	A	243	HIS	5.7
1	G	236	SER	5.3
1	F	235	HIS	4.8
1	A	237	GLU	4.6
1	B	243	HIS	4.3
1	H	236	SER	4.2
1	H	235	HIS	3.9
1	B	239	PRO	3.7
1	J	129	ARG	3.6
1	G	66	LYS	3.6
1	B	235	HIS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	232	LYS	3.4
1	A	242	HIS	3.4
1	J	132	GLU	3.4
1	E	132	GLU	3.3
1	F	132	GLU	3.3
1	A	104	LYS	3.3
1	H	237	GLU	3.2
1	A	235	HIS	3.2
1	B	237	GLU	3.1
1	B	242	HIS	3.1
1	C	132	GLU	3.0
1	D	132	GLU	3.0
1	E	127	GLU	2.9
1	A	109	SER	2.9
1	A	128	LYS	2.8
1	B	236	SER	2.8
1	J	87	ASP	2.8
1	J	130	LYS	2.8
1	B	182	TYR	2.8
1	I	91	ARG	2.7
1	A	103	SER	2.6
1	I	130	LYS	2.6
1	H	66	LYS	2.6
1	A	234	THR	2.5
1	B	91	ARG	2.5
1	A	66	LYS	2.5
1	E	77	ARG	2.4
1	A	236	SER	2.4
1	E	236	SER	2.4
1	E	182	TYR	2.4
1	D	78	ARG	2.4
1	H	132	GLU	2.3
1	E	125	LEU	2.3
1	H	109	SER	2.2
1	J	182	TYR	2.2
1	J	235	HIS	2.2
1	D	102	GLU	2.2
1	B	132	GLU	2.2
1	B	77	ARG	2.1
1	F	237	GLU	2.1
1	I	66	LYS	2.1
1	E	124	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	104	LYS	2.0
1	I	81	GLU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO	C	321	1/1	0.98	0.11	27,27,27,27	0
2	CO	D	331	1/1	0.98	0.07	28,28,28,28	0
2	CO	A	301	1/1	0.99	0.07	34,34,34,34	0
2	CO	B	311	1/1	0.99	0.13	27,27,27,27	0
2	CO	F	351	1/1	0.99	0.13	18,18,18,18	0
2	CO	G	361	1/1	0.99	0.09	26,26,26,26	0
2	CO	H	371	1/1	0.99	0.11	27,27,27,27	0
2	CO	I	381	1/1	0.99	0.13	37,37,37,37	0
2	CO	E	341	1/1	1.00	0.07	29,29,29,29	0
2	CO	J	391	1/1	1.00	0.12	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.