Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 01:04 AM EDT

PDB ID	:	1JYM
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	:	Kumar, A.; Nguyen, K.T.; Srivathsan, S.; Ornstein, B.; Turley, S.; Hirsh, I.; Pei, D.; Hol, W.G.J.
Deposited on	:	2001-09-12
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:

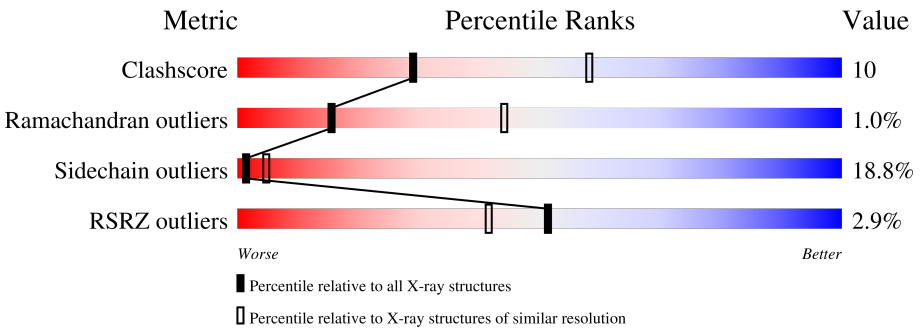
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (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))
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	183	2%, 58%, 35%, 5% •
1	B	183	3%, 60%, 30%, 7% • •
1	C	183	2%, 61%, 25%, 7%, 8%
1	D	183	2%, 64%, 26%, •, 5%
1	E	183	4%, 56%, 34%, 5%, •
1	F	183	%, 60%, 28%, • •, 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	183	3% 61% 27% 6% 6%
1	H	183	2% 57% 32% 5% 5%
1	I	183	4% 55% 32% 8% 6%
1	J	183	3% 58% 26% 10% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14584 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 Peptide Deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	179	1487	953	263	267	1	3	0	0	0
1	B	179	1487	953	263	267	1	3	0	0	0
1	C	168	1394	898	246	246	1	3	0	0	0
1	D	173	1435	921	253	257	1	3	0	0	0
1	E	176	1458	936	256	262	1	3	0	0	0
1	F	172	1426	916	252	254	1	3	0	0	0
1	G	172	1425	915	252	254	1	3	0	0	0
1	H	173	1435	921	253	257	1	3	0	0	0
1	I	172	1425	915	252	254	1	3	0	0	0
1	J	172	1425	915	252	254	1	3	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

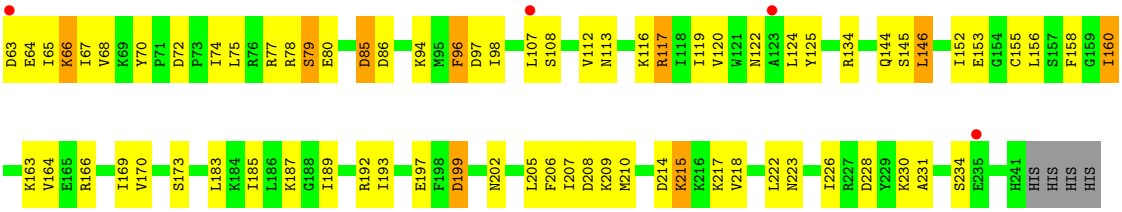
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	22	22	22	0	0
3	B	17	17	17	0	0
3	C	17	17	17	0	0
3	D	16	16	16	0	0
3	E	19	19	19	0	0
3	F	26	26	26	0	0
3	G	13	13	13	0	0
3	H	15	15	15	0	0
3	I	16	16	16	0	0
3	J	16	16	16	0	0

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.

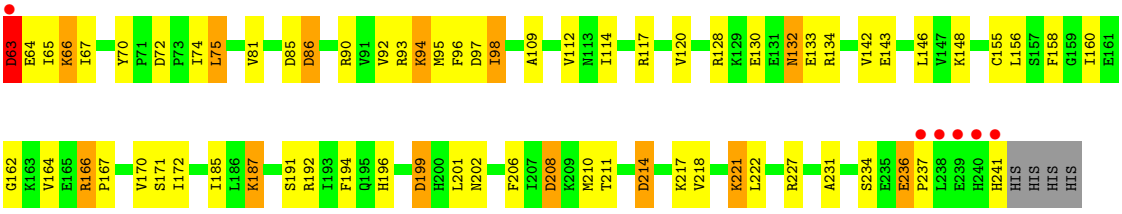
• Molecule 1: Peptide Deformylase

Chain A:



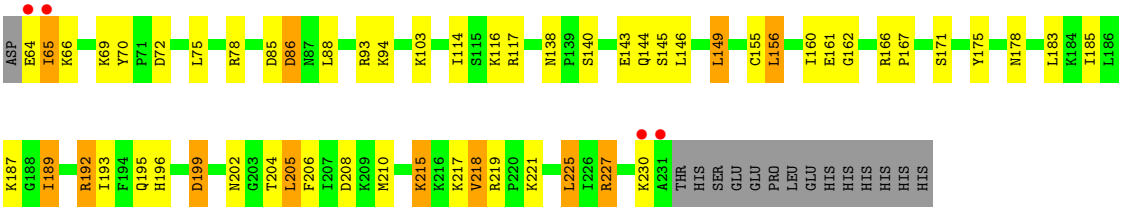
• Molecule 1: Peptide Deformylase

Chain B:



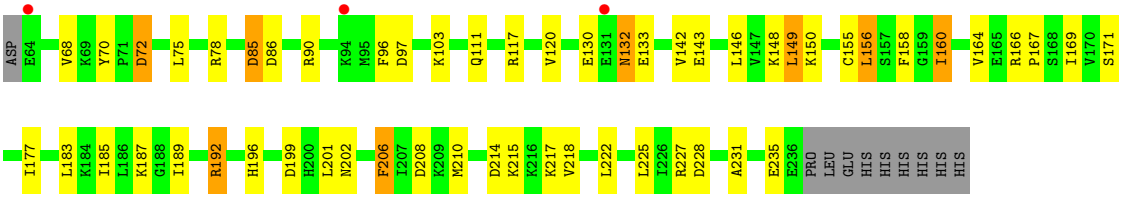
• Molecule 1: Peptide Deformylase

Chain C:



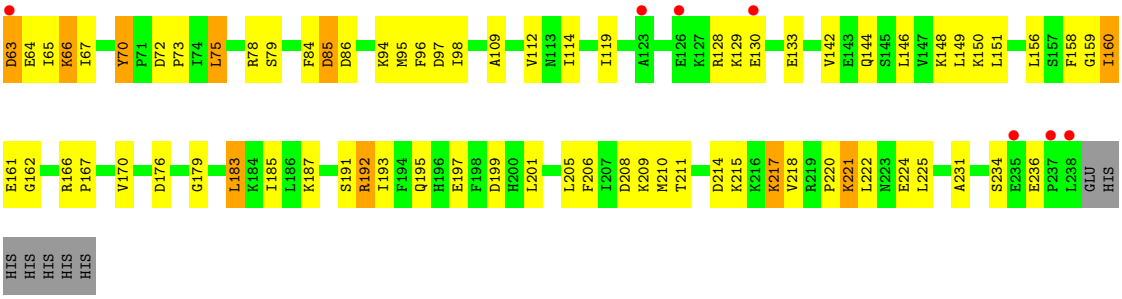
• Molecule 1: Peptide Deformylase

Chain D:



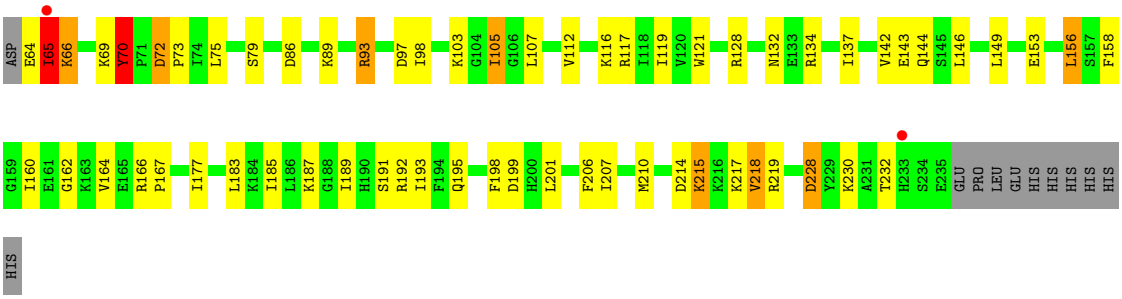
- Molecule 1: Peptide Deformylase

Chain E:



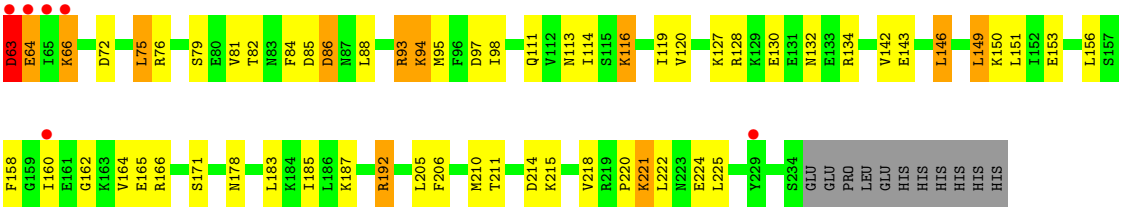
- Molecule 1: Peptide Deformylase

Chain F:



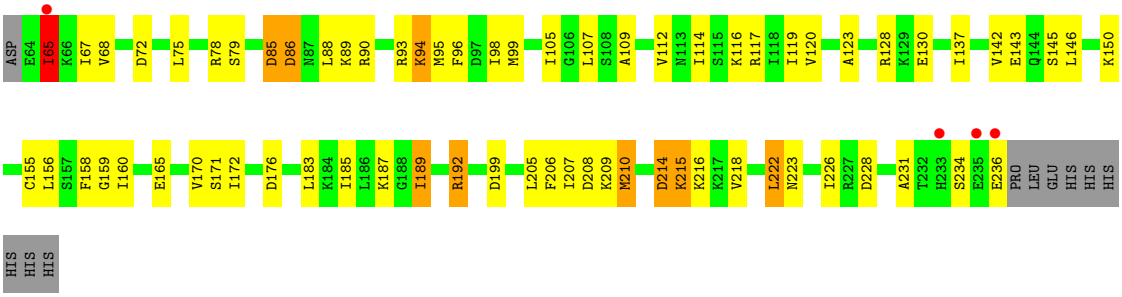
- Molecule 1: Peptide Deformylase

Chain G:



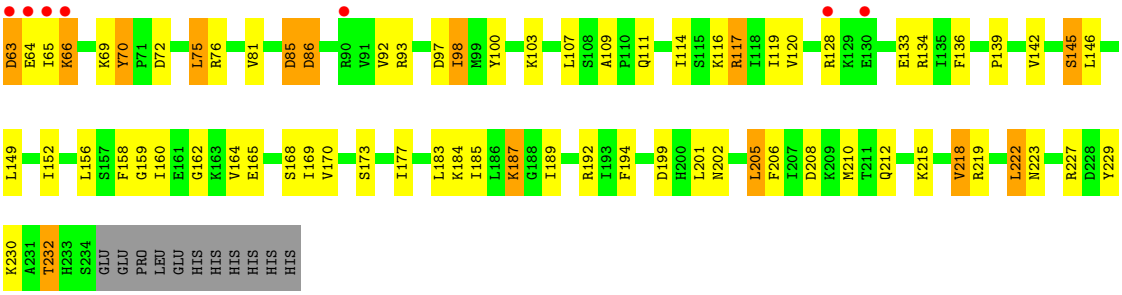
- Molecule 1: Peptide Deformylase

Chain H:



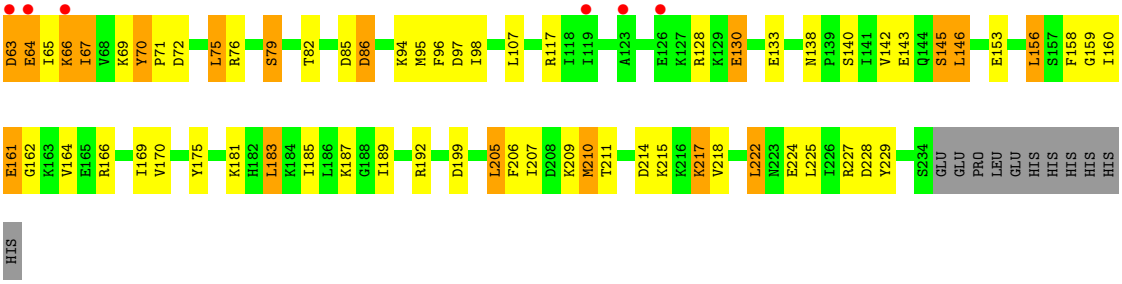
- Molecule 1: Peptide Deformylase

Chain I:



- Molecule 1: Peptide 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)	30.00 – 2.80 29.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (30.00-2.80) 82.5 (29.41-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.231 , 0.296 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.052 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14584	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 (i)

5.1 Standard geometry (i)

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	0.50	0/1513	0.87	5/2026 (0.2%)
1	B	0.54	0/1513	0.91	8/2026 (0.4%)
1	C	0.63	0/1416	0.92	5/1893 (0.3%)
1	D	0.53	0/1458	0.86	6/1950 (0.3%)
1	E	0.59	0/1482	0.91	5/1984 (0.3%)
1	F	0.71	0/1449	0.97	4/1938 (0.2%)
1	G	0.59	0/1448	0.92	6/1937 (0.3%)
1	H	0.63	0/1458	0.94	8/1950 (0.4%)
1	I	0.55	0/1448	0.91	8/1937 (0.4%)
1	J	0.60	0/1448	0.94	5/1937 (0.3%)
All	All	0.59	0/14633	0.91	60/19578 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	199	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	208	ASP	CB-CG-OD2	7.07	124.67	118.30
1	B	214	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	85	ASP	CB-CG-OD2	6.95	124.56	118.30
1	D	214	ASP	CB-CG-OD2	6.53	124.18	118.30
1	J	214	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	199	ASP	CB-CG-OD2	6.46	124.11	118.30
1	E	85	ASP	CB-CG-OD2	6.36	124.02	118.30
1	I	199	ASP	CB-CG-OD2	6.30	123.97	118.30
1	I	97	ASP	CB-CG-OD2	6.29	123.96	118.30
1	J	72	ASP	CB-CG-OD2	6.21	123.89	118.30
1	E	97	ASP	CB-CG-OD2	6.17	123.85	118.30
1	H	85	ASP	CB-CG-OD2	6.05	123.75	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	63	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	97	ASP	CB-CG-OD2	6.03	123.73	118.30
1	F	97	ASP	CB-CG-OD2	6.01	123.71	118.30
1	G	97	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	214	ASP	CB-CG-OD2	5.96	123.67	118.30
1	G	72	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	63	ASP	CB-CG-OD2	5.87	123.58	118.30
1	J	97	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	85	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	208	ASP	CB-CG-OD2	5.76	123.49	118.30
1	D	72	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	85	ASP	CB-CG-OD2	5.73	123.46	118.30
1	G	63	ASP	CB-CG-OD2	5.72	123.45	118.30
1	E	214	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	72	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	199	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	85	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	72	ASP	CB-CG-OD2	5.57	123.31	118.30
1	I	86	ASP	CB-CG-OD2	5.57	123.31	118.30
1	H	176	ASP	CB-CG-OD2	5.50	123.25	118.30
1	I	85	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	97	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	97	ASP	CB-CG-OD2	5.49	123.24	118.30
1	I	117	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	I	63	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	189	ILE	N-CA-C	-5.46	96.27	111.00
1	E	63	ASP	CB-CG-OD2	5.45	123.20	118.30
1	H	228	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	86	ASP	CB-CG-OD2	5.38	123.14	118.30
1	J	86	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	214	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	86	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	72	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	214	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	214	ASP	CB-CG-OD2	5.26	123.03	118.30
1	I	72	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	70	TYR	N-CA-C	5.24	125.14	111.00
1	I	208	ASP	CB-CG-OD2	5.23	123.01	118.30
1	H	86	ASP	CB-CG-OD2	5.23	123.01	118.30
1	F	72	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	208	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	228	ASP	CB-CG-OD2	5.13	122.92	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	228	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	208	ASP	CB-CG-OD2	5.05	122.85	118.30
1	G	85	ASP	CB-CG-OD2	5.04	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	1487	0	1533	34	0
1	B	1487	0	1533	34	0
1	C	1394	0	1460	26	0
1	D	1435	0	1491	22	0
1	E	1458	0	1513	29	0
1	F	1426	0	1485	26	0
1	G	1425	0	1483	26	0
1	H	1435	0	1491	29	0
1	I	1425	0	1483	35	0
1	J	1425	0	1483	36	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
3	A	22	0	0	0	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	16	0	0	0	0
3	E	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	26	0	0	1	0
3	G	13	0	0	0	0
3	H	15	0	0	1	0
3	I	16	0	0	1	0
3	J	16	0	0	0	0
All	All	14584	0	14955	283	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 10.

All (283) 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:J:164:VAL:O	1:J:192:ARG:NH2	2.05	0.90
1:I:65:ILE:HA	1:I:98:ILE:HD12	1.57	0.86
1:D:117:ARG:HH22	1:D:202:ASN:HD21	1.26	0.84
1:F:65:ILE:HA	1:F:98:ILE:HD11	1.63	0.80
1:A:231:ALA:HA	1:A:234:SER:HB3	1.64	0.80
1:F:160:ILE:HG23	1:F:218:VAL:HG21	1.66	0.78
1:E:231:ALA:HA	1:E:234:SER:HB3	1.65	0.77
1:B:164:VAL:O	1:B:192:ARG:NH2	2.16	0.76
1:C:117:ARG:HH21	1:C:202:ASN:HD21	1.31	0.76
1:F:167:PRO:HD2	1:F:195:GLN:OE1	1.86	0.75
1:H:231:ALA:HA	1:H:234:SER:HB3	1.68	0.73
1:F:65:ILE:O	1:F:65:ILE:HG13	1.89	0.72
1:C:185:ILE:HG12	1:D:185:ILE:HG12	1.72	0.72
1:A:94:LYS:O	1:A:98:ILE:HG12	1.91	0.71
1:D:164:VAL:O	1:D:192:ARG:NH2	2.23	0.70
1:I:164:VAL:O	1:I:192:ARG:NH2	2.26	0.69
1:G:162:GLY:HA3	1:G:210:MSE:HE2	1.76	0.68
1:B:117:ARG:HH22	1:B:202:ASN:ND2	1.92	0.68
1:A:68:VAL:HG21	1:A:75:LEU:HD11	1.75	0.67
1:F:164:VAL:O	1:F:192:ARG:NH2	2.27	0.67
1:H:94:LYS:O	1:H:98:ILE:HG12	1.94	0.67
1:I:119:ILE:HD12	1:I:139:PRO:HG3	1.75	0.67
1:D:117:ARG:NH2	1:D:202:ASN:HD21	1.93	0.66
1:A:199:ASP:OD2	1:A:209:LYS:NZ	2.25	0.66
1:A:155:CYS:HB3	1:A:158:PHE:HD1	1.60	0.66
1:B:117:ARG:HA	1:B:201:LEU:HD22	1.78	0.65
1:F:158:PHE:O	3:F:5305:HOH:O	2.14	0.65
1:B:158:PHE:HB3	1:B:160:ILE:HB	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:TYR:OH	1:I:133:GLU:OE2	2.15	0.65
1:B:65:ILE:HA	1:B:98:ILE:HD12	1.77	0.64
1:I:134:ARG:HH21	1:I:136:PHE:HZ	1.45	0.64
1:J:158:PHE:C	1:J:160:ILE:H	1.99	0.64
1:D:117:ARG:HA	1:D:201:LEU:HD22	1.80	0.63
1:F:185:ILE:HG12	1:H:185:ILE:HG12	1.79	0.63
1:H:90:ARG:HA	1:H:93:ARG:HB2	1.81	0.63
1:E:166:ARG:NH2	1:E:199:ASP:OD2	2.33	0.62
1:D:158:PHE:HB3	1:D:160:ILE:HB	1.80	0.62
1:F:143:GLU:HG3	1:H:142:VAL:HG11	1.80	0.61
1:I:64:GLU:HB3	1:I:66:LYS:H	1.63	0.61
1:F:66:LYS:O	1:F:112:VAL:HA	2.00	0.60
1:C:117:ARG:NH2	1:C:202:ASN:HD21	1.98	0.59
1:B:231:ALA:HA	1:B:234:SER:HB3	1.83	0.59
1:A:164:VAL:O	1:A:192:ARG:NH2	2.36	0.58
1:I:158:PHE:HB3	1:I:160:ILE:HB	1.84	0.58
1:G:220:PRO:O	1:G:224:GLU:HG3	2.03	0.58
1:B:227:ARG:HB3	1:B:241:HIS:CE1	2.39	0.58
1:A:74:ILE:HD12	1:A:77:ARG:HH11	1.68	0.58
1:E:149:LEU:O	1:E:192:ARG:NH2	2.27	0.58
1:C:117:ARG:HH21	1:C:202:ASN:ND2	2.02	0.57
1:H:199:ASP:OD2	1:H:209:LYS:NZ	2.26	0.57
1:I:64:GLU:HB3	1:I:66:LYS:HB2	1.86	0.57
1:D:68:VAL:HG22	1:D:111:GLN:HA	1.87	0.57
1:I:117:ARG:HH22	1:I:202:ASN:ND2	2.02	0.57
1:H:105:ILE:HD11	1:H:123:ALA:HA	1.87	0.56
1:C:114:ILE:HG22	1:C:116:LYS:HB2	1.86	0.56
1:J:199:ASP:OD2	1:J:209:LYS:NZ	2.30	0.56
1:C:143:GLU:HB2	1:C:171:SER:HB2	1.87	0.56
1:G:164:VAL:O	1:G:192:ARG:NH2	2.39	0.56
1:D:143:GLU:HB2	1:D:171:SER:HB3	1.88	0.55
1:E:148:LYS:HA	1:E:167:PRO:HA	1.89	0.55
1:I:145:SER:HB3	1:I:169:ILE:HB	1.90	0.55
1:J:67:ILE:HD11	1:J:156:LEU:HB3	1.88	0.54
1:B:63:ASP:O	1:B:94:LYS:HD3	2.08	0.54
1:A:117:ARG:NH2	1:A:202:ASN:OD1	2.35	0.54
1:J:71:PRO:HG2	1:J:229:TYR:HB2	1.90	0.54
1:B:162:GLY:HA3	1:B:210:MSE:HE3	1.90	0.54
1:E:70:TYR:CD1	1:E:70:TYR:C	2.81	0.54
1:I:229:TYR:O	1:I:232:THR:HB	2.07	0.54
1:D:169:ILE:HG12	1:D:187:LYS:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:158:PHE:HB3	1:J:160:ILE:HB	1.90	0.53
1:E:167:PRO:HD2	1:E:195:GLN:OE1	2.09	0.53
1:F:105:ILE:O	1:F:121:TRP:HB2	2.09	0.53
1:I:219:ARG:NH1	1:J:161:GLU:OE2	2.41	0.53
1:E:185:ILE:HG12	1:J:185:ILE:HG12	1.92	0.52
1:E:158:PHE:O	1:E:160:ILE:N	2.32	0.52
1:G:114:ILE:HG22	1:G:116:LYS:HB2	1.91	0.52
1:B:96:PHE:CZ	1:B:133:GLU:HB3	2.45	0.52
1:C:210:MSE:HB3	1:C:215:LYS:HG2	1.92	0.52
1:J:153:GLU:OE2	1:J:166:ARG:NH1	2.43	0.52
1:I:117:ARG:HH22	1:I:202:ASN:HD21	1.58	0.51
1:B:95:MSE:HG2	1:B:112:VAL:HG21	1.92	0.51
1:A:185:ILE:HG12	1:B:185:ILE:HG12	1.93	0.51
1:F:105:ILE:HD11	1:F:193:ILE:HD11	1.92	0.51
1:F:162:GLY:HA3	1:F:210:MSE:HE2	1.92	0.51
1:G:63:ASP:O	1:G:94:LYS:HD3	2.10	0.51
1:B:155:CYS:HB2	1:B:196:HIS:CE1	2.46	0.51
1:I:117:ARG:HA	1:I:201:LEU:HD22	1.92	0.51
1:J:158:PHE:O	1:J:160:ILE:N	2.34	0.51
1:C:166:ARG:HG3	1:C:192:ARG:CZ	2.41	0.51
1:G:158:PHE:HB3	1:G:160:ILE:HB	1.92	0.50
1:A:74:ILE:HG21	1:A:113:ASN:ND2	2.27	0.50
1:E:149:LEU:HD23	1:E:151:LEU:HD11	1.93	0.50
1:I:165:GLU:OE1	3:I:8304:HOH:O	2.20	0.50
1:H:223:ASN:HA	1:H:226:ILE:HD12	1.93	0.50
1:F:107:LEU:HD13	1:F:156:LEU:HD23	1.93	0.50
1:J:218:VAL:HG13	1:J:222:LEU:HD22	1.94	0.50
1:E:66:LYS:O	1:E:112:VAL:HA	2.12	0.50
1:E:193:ILE:O	1:E:197:GLU:HG2	2.11	0.50
1:F:207:ILE:HB	1:F:215:LYS:HE2	1.94	0.50
1:B:70:TYR:HB2	1:B:158:PHE:CE2	2.47	0.49
1:E:158:PHE:C	1:E:160:ILE:H	2.15	0.49
1:B:210:MSE:HE3	1:B:214:ASP:HB3	1.94	0.49
1:D:96:PHE:CZ	1:D:133:GLU:HB3	2.46	0.49
1:G:95:MSE:HE2	1:G:120:VAL:HG22	1.93	0.49
1:A:230:LYS:HG3	1:D:149:LEU:HD11	1.94	0.49
1:J:70:TYR:HB2	1:J:158:PHE:CE2	2.47	0.49
1:B:142:VAL:HG22	1:B:171:SER:HB3	1.94	0.49
1:H:210:MSE:HE3	1:H:214:ASP:HB3	1.95	0.49
1:E:158:PHE:HB3	1:E:160:ILE:HB	1.95	0.49
1:G:153:GLU:OE2	1:G:166:ARG:NH1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:GLU:HB2	1:H:171:SER:HB3	1.94	0.49
1:E:65:ILE:O	1:E:65:ILE:HG13	2.12	0.49
1:E:160:ILE:HD11	1:E:221:LYS:HB2	1.94	0.48
1:I:70:TYR:C	1:I:70:TYR:CD2	2.86	0.48
1:A:65:ILE:HA	1:A:98:ILE:HD11	1.95	0.48
1:G:150:LYS:HG2	1:G:165:GLU:HB2	1.95	0.48
1:J:162:GLY:HA3	1:J:210:MSE:HE3	1.96	0.48
1:A:79:SER:HB3	1:A:117:ARG:HG2	1.96	0.48
1:B:148:LYS:HA	1:B:167:PRO:HA	1.94	0.48
1:A:122:ASN:HB3	1:A:125:TYR:HB3	1.95	0.48
1:J:70:TYR:C	1:J:70:TYR:CD2	2.86	0.48
1:A:226:ILE:O	1:A:230:LYS:HG2	2.13	0.47
1:J:95:MSE:HE2	1:J:95:MSE:HB3	1.79	0.47
1:J:96:PHE:CZ	1:J:133:GLU:HB3	2.49	0.47
1:D:117:ARG:NH2	1:D:202:ASN:ND2	2.62	0.47
1:H:114:ILE:HG22	1:H:116:LYS:HB2	1.97	0.47
1:E:220:PRO:O	1:E:224:GLU:HG3	2.14	0.47
1:B:96:PHE:CZ	1:B:120:VAL:HB	2.49	0.47
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.59	0.47
1:B:109:ALA:HB1	1:B:114:ILE:HB	1.96	0.47
1:E:96:PHE:CZ	1:E:133:GLU:HB3	2.50	0.47
1:I:223:ASN:O	1:I:227:ARG:HG3	2.15	0.47
1:A:96:PHE:CZ	1:A:120:VAL:HB	2.50	0.47
1:C:167:PRO:HD2	1:C:195:GLN:OE1	2.13	0.47
1:C:162:GLY:HA3	1:C:210:MSE:HE2	1.96	0.47
1:J:79:SER:HB3	1:J:117:ARG:HG2	1.97	0.47
1:E:142:VAL:HG11	1:J:143:GLU:HG3	1.97	0.47
1:F:117:ARG:HA	1:F:201:LEU:HD22	1.96	0.47
1:J:107:LEU:HD12	1:J:107:LEU:HA	1.69	0.47
1:I:158:PHE:C	1:I:160:ILE:H	2.16	0.46
1:A:193:ILE:O	1:A:197:GLU:HG2	2.14	0.46
1:A:234:SER:O	1:A:234:SER:OG	2.31	0.46
1:E:192:ARG:HD3	1:E:192:ARG:HA	1.71	0.46
1:I:107:LEU:HD11	1:I:111:GLN:HB2	1.97	0.46
1:J:192:ARG:HD2	1:J:192:ARG:HA	1.68	0.46
1:D:231:ALA:O	1:D:235:GLU:HG3	2.16	0.46
1:B:132:ASN:HD22	1:B:132:ASN:HA	1.54	0.46
1:B:160:ILE:HG23	1:B:218:VAL:HG21	1.98	0.46
1:H:207:ILE:HB	1:H:215:LYS:HE2	1.96	0.46
1:J:75:LEU:HD12	1:J:75:LEU:HA	1.59	0.46
1:B:64:GLU:HB3	1:B:66:LYS:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ILE:HG13	1:E:201:LEU:HD11	1.97	0.46
1:F:119:ILE:HD13	1:F:119:ILE:HG21	1.60	0.46
1:G:158:PHE:C	1:G:160:ILE:H	2.18	0.46
1:I:66:LYS:HE2	1:I:66:LYS:HB3	1.77	0.46
1:A:153:GLU:OE2	1:A:166:ARG:NH1	2.49	0.46
1:B:187:LYS:HE2	1:B:187:LYS:HB3	1.78	0.46
1:H:95:MSE:HG2	1:H:112:VAL:HG21	1.98	0.46
1:A:183:LEU:HD21	1:B:143:GLU:HB3	1.98	0.46
1:D:206:PHE:H	1:D:206:PHE:HD2	1.64	0.46
1:H:65:ILE:HA	1:H:98:ILE:HD12	1.97	0.45
1:A:74:ILE:HG21	1:A:113:ASN:HD22	1.81	0.45
1:E:183:LEU:HB3	1:J:185:ILE:HD12	1.98	0.45
1:I:218:VAL:HG13	1:I:222:LEU:HD22	1.98	0.45
1:J:160:ILE:HG23	1:J:218:VAL:HG21	1.98	0.45
1:E:162:GLY:HA3	1:E:210:MSE:HE2	1.97	0.45
1:E:109:ALA:HB1	1:E:114:ILE:HB	1.98	0.45
1:F:66:LYS:HD2	1:F:66:LYS:HA	1.80	0.45
1:A:107:LEU:HD21	1:A:112:VAL:HG13	1.99	0.45
1:C:86:ASP:HB3	1:C:88:LEU:H	1.81	0.45
1:F:166:ARG:NH2	1:F:199:ASP:OD2	2.50	0.45
1:C:155:CYS:HB2	1:C:196:HIS:CE1	2.50	0.45
1:C:205:LEU:HD12	1:C:205:LEU:HA	1.84	0.45
1:J:205:LEU:HD12	1:J:205:LEU:HA	1.86	0.45
1:A:66:LYS:HD2	1:A:66:LYS:HA	1.79	0.45
1:D:148:LYS:HA	1:D:167:PRO:HA	1.99	0.45
1:A:152:ILE:HG13	1:A:163:LYS:HG2	1.99	0.44
1:A:210:MSE:HB3	1:A:215:LYS:HG2	1.99	0.44
1:H:222:LEU:HD23	1:I:152:ILE:HD13	1.98	0.44
1:F:64:GLU:C	1:F:66:LYS:H	2.21	0.44
1:E:75:LEU:HD22	1:E:75:LEU:HA	1.73	0.44
1:F:153:GLU:OE1	1:F:166:ARG:HD2	2.16	0.44
1:C:65:ILE:HG22	1:C:66:LYS:N	2.32	0.44
1:F:72:ASP:HA	1:F:73:PRO:HD3	1.84	0.44
1:B:166:ARG:NH2	1:B:199:ASP:OD2	2.50	0.44
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.51	0.44
1:G:143:GLU:HG3	1:I:142:VAL:HG11	1.99	0.44
1:I:76:ARG:CZ	1:I:205:LEU:HD22	2.48	0.44
1:C:189:ILE:HG12	1:C:193:ILE:HD12	2.00	0.44
1:F:105:ILE:HG21	1:F:105:ILE:HD13	1.62	0.44
1:H:79:SER:HB3	1:H:117:ARG:HG2	2.00	0.44
1:H:192:ARG:HH11	1:H:192:ARG:HD3	1.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:GLU:OE1	1:J:166:ARG:HD2	2.18	0.44
1:H:159:GLY:N	3:H:7303:HOH:O	2.50	0.44
1:G:64:GLU:HB3	1:G:66:LYS:HB2	1.99	0.43
1:H:234:SER:O	1:H:234:SER:OG	2.30	0.43
1:A:207:ILE:O	1:A:215:LYS:HE3	2.17	0.43
1:B:90:ARG:O	1:B:94:LYS:HG2	2.18	0.43
1:F:93:ARG:HD2	1:F:93:ARG:HA	1.69	0.43
1:F:119:ILE:HD11	1:F:198:PHE:HA	1.99	0.43
1:H:192:ARG:HD3	1:H:192:ARG:HA	1.78	0.43
1:I:230:LYS:HA	1:I:230:LYS:HD2	1.83	0.43
1:J:145:SER:HB3	1:J:169:ILE:H	1.83	0.43
1:J:158:PHE:C	1:J:160:ILE:N	2.71	0.43
1:J:175:TYR:OH	1:J:181:LYS:HD2	2.18	0.43
1:A:145:SER:HB2	1:A:169:ILE:HB	1.99	0.43
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.90	0.43
1:G:171:SER:HA	1:G:185:ILE:HD13	1.99	0.43
1:H:155:CYS:HB3	1:H:158:PHE:HD1	1.83	0.43
1:A:153:GLU:OE1	1:A:166:ARG:HD2	2.19	0.43
1:G:93:ARG:HD2	1:G:93:ARG:HA	1.82	0.43
1:G:98:ILE:HD13	1:G:98:ILE:N	2.34	0.43
1:B:158:PHE:C	1:B:160:ILE:H	2.21	0.43
1:B:234:SER:O	1:B:234:SER:OG	2.34	0.43
1:D:158:PHE:C	1:D:160:ILE:H	2.22	0.43
1:E:185:ILE:HD12	1:J:183:LEU:HB3	2.01	0.43
1:C:149:LEU:HD13	1:C:149:LEU:HA	1.80	0.43
1:J:217:LYS:HE3	1:J:217:LYS:HB3	1.69	0.43
1:B:221:LYS:H	1:B:221:LYS:HG2	1.59	0.42
1:C:218:VAL:HG22	1:C:221:LYS:HG3	2.01	0.42
1:A:70:TYR:HB2	1:A:158:PHE:CE2	2.54	0.42
1:F:70:TYR:HB2	1:F:158:PHE:CE2	2.53	0.42
1:I:111:GLN:HE21	1:I:111:GLN:HB3	1.62	0.42
1:I:75:LEU:HD12	1:I:75:LEU:HA	1.62	0.42
1:D:155:CYS:HB2	1:D:196:HIS:CE1	2.54	0.42
1:F:137:ILE:HD11	1:F:177:ILE:HD12	2.00	0.42
1:I:162:GLY:HA3	1:I:210:MSE:HE2	2.00	0.42
1:J:64:GLU:C	1:J:66:LYS:H	2.22	0.42
1:G:185:ILE:HG12	1:I:185:ILE:HG12	2.00	0.42
1:H:88:LEU:O	1:H:90:ARG:N	2.52	0.42
1:H:98:ILE:HG13	1:H:112:VAL:HG11	2.02	0.42
1:J:224:GLU:HA	1:J:227:ARG:HG3	2.02	0.42
1:C:94:LYS:HA	1:C:94:LYS:HD3	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:HG23	1:C:218:VAL:HG21	2.02	0.42
1:A:192:ARG:HD2	1:A:192:ARG:HA	1.81	0.42
1:B:98:ILE:H	1:B:98:ILE:HG12	1.58	0.42
1:E:95:MSE:HE2	1:E:95:MSE:HB3	1.93	0.42
1:D:202:ASN:HD22	1:D:202:ASN:HA	1.71	0.42
1:H:93:ARG:HD2	1:H:93:ARG:HA	1.84	0.42
1:H:99:MSE:HB2	1:H:107:LEU:HD22	2.01	0.42
1:J:76:ARG:HD3	1:J:205:LEU:HD22	2.01	0.42
1:G:146:LEU:HA	1:G:146:LEU:HD12	1.57	0.42
1:C:138:ASN:HB2	1:C:175:TYR:CD2	2.55	0.41
1:C:192:ARG:HD3	1:C:192:ARG:HA	1.82	0.41
1:D:96:PHE:CZ	1:D:120:VAL:HB	2.54	0.41
1:A:119:ILE:HG21	1:A:119:ILE:HD13	1.81	0.41
1:B:155:CYS:HB2	1:B:196:HIS:NE2	2.34	0.41
1:D:132:ASN:HD22	1:D:132:ASN:HA	1.70	0.41
1:I:187:LYS:HE2	1:I:187:LYS:HB3	1.35	0.41
1:J:82:THR:HB	1:J:138:ASN:HD21	1.85	0.41
1:J:130:GLU:H	1:J:130:GLU:HG3	1.54	0.41
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.94	0.41
1:E:199:ASP:OD2	1:E:209:LYS:NZ	2.45	0.41
1:H:109:ALA:HB1	1:H:114:ILE:HB	2.02	0.41
1:I:139:PRO:HB2	1:I:194:PHE:HZ	1.85	0.41
1:A:223:ASN:HA	1:A:226:ILE:HD12	2.03	0.41
1:C:160:ILE:CG2	1:C:161:GLU:N	2.83	0.41
1:D:192:ARG:HD2	1:D:192:ARG:HA	1.49	0.41
1:G:66:LYS:HB3	1:G:66:LYS:HE2	1.64	0.41
1:B:236:GLU:HA	1:B:237:PRO:HD3	1.78	0.41
1:G:119:ILE:HD13	1:G:119:ILE:HG21	1.89	0.41
1:G:221:LYS:H	1:G:221:LYS:HG2	1.40	0.41
1:G:149:LEU:HG	1:G:151:LEU:HD21	2.03	0.41
1:G:160:ILE:HD11	1:G:221:LYS:HB2	2.02	0.41
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.85	0.41
1:I:92:VAL:HG13	1:I:120:VAL:HG11	2.03	0.41
1:G:111:GLN:HE21	1:G:111:GLN:HB3	1.72	0.41
1:I:63:ASP:HA	1:I:114:ILE:HD11	2.02	0.41
1:I:114:ILE:HG21	1:I:114:ILE:HD13	1.83	0.41
1:E:72:ASP:HA	1:E:73:PRO:HD3	1.85	0.40
1:H:150:LYS:HG2	1:H:165:GLU:HB2	2.01	0.40
1:C:227:ARG:HH11	1:C:227:ARG:HD3	1.72	0.40
1:G:76:ARG:HH11	1:G:76:ARG:HD3	1.75	0.40
1:H:119:ILE:HD13	1:H:119:ILE:HG21	1.72	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ASP:OD1	1:E:179:GLY:N	2.54	0.40
1:G:75:LEU:HA	1:G:75:LEU:HD12	1.74	0.40
1:H:96:PHE:CZ	1:H:120:VAL:HB	2.56	0.40
1:J:146:LEU:HD13	1:J:146:LEU:HA	1.91	0.40
1:A:158:PHE:HB3	1:A:160:ILE:HB	2.02	0.40
1:B:172:ILE:HD12	1:B:194:PHE:CE2	2.57	0.40
1:G:128:ARG:H	1:G:128:ARG:HG3	1.50	0.40
1:C:199:ASP:HB3	1:C:204:THR:HB	2.02	0.40
1:I:109:ALA:HB1	1:I:114:ILE:HB	2.03	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	177/183 (97%)	164 (93%)	12 (7%)	1 (1%)	25	56
1	B	177/183 (97%)	157 (89%)	20 (11%)	0	100	100
1	C	166/183 (91%)	154 (93%)	11 (7%)	1 (1%)	25	56
1	D	171/183 (93%)	153 (90%)	17 (10%)	1 (1%)	25	56
1	E	174/183 (95%)	160 (92%)	11 (6%)	3 (2%)	9	29
1	F	170/183 (93%)	157 (92%)	8 (5%)	5 (3%)	4	15
1	G	170/183 (93%)	149 (88%)	20 (12%)	1 (1%)	25	56
1	H	171/183 (93%)	154 (90%)	15 (9%)	2 (1%)	13	39
1	I	170/183 (93%)	160 (94%)	8 (5%)	2 (1%)	13	39
1	J	170/183 (93%)	157 (92%)	12 (7%)	1 (1%)	25	56
All	All	1716/1830 (94%)	1565 (91%)	134 (8%)	17 (1%)	15	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	89	LYS
1	J	159	GLY
1	A	117	ARG
1	C	65	ILE
1	I	70	TYR
1	D	70	TYR
1	E	217	LYS
1	F	86	ASP
1	E	159	GLY
1	F	128	ARG
1	E	70	TYR
1	F	65	ILE
1	F	230	LYS
1	G	88	LEU
1	F	70	TYR
1	H	65	ILE
1	I	159	GLY

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	168/169 (99%)	138 (82%)	30 (18%)	2 5
1	B	168/169 (99%)	140 (83%)	28 (17%)	2 6
1	C	157/169 (93%)	130 (83%)	27 (17%)	2 6
1	D	162/169 (96%)	133 (82%)	29 (18%)	2 5
1	E	165/169 (98%)	129 (78%)	36 (22%)	1 3
1	F	161/169 (95%)	132 (82%)	29 (18%)	1 5
1	G	161/169 (95%)	128 (80%)	33 (20%)	1 3
1	H	162/169 (96%)	133 (82%)	29 (18%)	2 5
1	I	161/169 (95%)	131 (81%)	30 (19%)	1 5
1	J	161/169 (95%)	126 (78%)	35 (22%)	1 3
All	All	1626/1690 (96%)	1320 (81%)	306 (19%)	1 5

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	64	GLU
1	A	66	LYS
1	A	67	ILE
1	A	72	ASP
1	A	78	ARG
1	A	79	SER
1	A	80	GLU
1	A	85	ASP
1	A	86	ASP
1	A	96	PHE
1	A	108	SER
1	A	116	LYS
1	A	124	LEU
1	A	134	ARG
1	A	144	GLN
1	A	146	LEU
1	A	156	LEU
1	A	160	ILE
1	A	170	VAL
1	A	173	SER
1	A	187	LYS
1	A	189	ILE
1	A	205	LEU
1	A	206	PHE
1	A	215	LYS
1	A	217	LYS
1	A	218	VAL
1	A	222	LEU
1	A	228	ASP
1	B	63	ASP
1	B	66	LYS
1	B	67	ILE
1	B	74	ILE
1	B	75	LEU
1	B	81	VAL
1	B	86	ASP
1	B	92	VAL
1	B	93	ARG
1	B	94	LYS
1	B	98	ILE
1	B	128	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	130	GLU
1	B	132	ASN
1	B	134	ARG
1	B	146	LEU
1	B	156	LEU
1	B	166	ARG
1	B	170	VAL
1	B	187	LYS
1	B	191	SER
1	B	206	PHE
1	B	208	ASP
1	B	211	THR
1	B	217	LYS
1	B	221	LYS
1	B	222	LEU
1	B	236	GLU
1	C	64	GLU
1	C	69	LYS
1	C	75	LEU
1	C	78	ARG
1	C	86	ASP
1	C	93	ARG
1	C	103	LYS
1	C	140	SER
1	C	144	GLN
1	C	145	SER
1	C	146	LEU
1	C	149	LEU
1	C	156	LEU
1	C	178	ASN
1	C	183	LEU
1	C	187	LYS
1	C	189	ILE
1	C	192	ARG
1	C	205	LEU
1	C	206	PHE
1	C	215	LYS
1	C	217	LYS
1	C	218	VAL
1	C	219	ARG
1	C	225	LEU
1	C	227	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	230	LYS
1	D	72	ASP
1	D	75	LEU
1	D	78	ARG
1	D	85	ASP
1	D	86	ASP
1	D	90	ARG
1	D	103	LYS
1	D	130	GLU
1	D	132	ASN
1	D	142	VAL
1	D	146	LEU
1	D	149	LEU
1	D	150	LYS
1	D	156	LEU
1	D	160	ILE
1	D	166	ARG
1	D	177	ILE
1	D	183	LEU
1	D	189	ILE
1	D	192	ARG
1	D	206	PHE
1	D	208	ASP
1	D	210	MSE
1	D	215	LYS
1	D	217	LYS
1	D	218	VAL
1	D	222	LEU
1	D	225	LEU
1	D	227	ARG
1	E	63	ASP
1	E	64	GLU
1	E	66	LYS
1	E	67	ILE
1	E	75	LEU
1	E	78	ARG
1	E	79	SER
1	E	84	PHE
1	E	85	ASP
1	E	86	ASP
1	E	94	LYS
1	E	98	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	128	ARG
1	E	129	LYS
1	E	130	GLU
1	E	144	GLN
1	E	146	LEU
1	E	150	LYS
1	E	156	LEU
1	E	160	ILE
1	E	161	GLU
1	E	170	VAL
1	E	183	LEU
1	E	187	LYS
1	E	191	SER
1	E	192	ARG
1	E	205	LEU
1	E	206	PHE
1	E	211	THR
1	E	215	LYS
1	E	217	LYS
1	E	218	VAL
1	E	221	LYS
1	E	222	LEU
1	E	225	LEU
1	E	236	GLU
1	F	65	ILE
1	F	66	LYS
1	F	69	LYS
1	F	70	TYR
1	F	75	LEU
1	F	79	SER
1	F	89	LYS
1	F	93	ARG
1	F	103	LYS
1	F	105	ILE
1	F	116	LYS
1	F	132	ASN
1	F	134	ARG
1	F	142	VAL
1	F	144	GLN
1	F	146	LEU
1	F	149	LEU
1	F	156	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	183	LEU
1	F	187	LYS
1	F	189	ILE
1	F	191	SER
1	F	206	PHE
1	F	215	LYS
1	F	217	LYS
1	F	218	VAL
1	F	219	ARG
1	F	228	ASP
1	F	232	THR
1	G	63	ASP
1	G	64	GLU
1	G	66	LYS
1	G	75	LEU
1	G	79	SER
1	G	81	VAL
1	G	82	THR
1	G	84	PHE
1	G	86	ASP
1	G	93	ARG
1	G	94	LYS
1	G	113	ASN
1	G	116	LYS
1	G	127	LYS
1	G	130	GLU
1	G	132	ASN
1	G	134	ARG
1	G	142	VAL
1	G	146	LEU
1	G	149	LEU
1	G	156	LEU
1	G	178	ASN
1	G	183	LEU
1	G	187	LYS
1	G	192	ARG
1	G	205	LEU
1	G	206	PHE
1	G	211	THR
1	G	215	LYS
1	G	218	VAL
1	G	221	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	222	LEU
1	G	225	LEU
1	H	65	ILE
1	H	67	ILE
1	H	68	VAL
1	H	75	LEU
1	H	78	ARG
1	H	85	ASP
1	H	86	ASP
1	H	94	LYS
1	H	128	ARG
1	H	130	GLU
1	H	137	ILE
1	H	145	SER
1	H	146	LEU
1	H	156	LEU
1	H	160	ILE
1	H	170	VAL
1	H	172	ILE
1	H	183	LEU
1	H	187	LYS
1	H	189	ILE
1	H	192	ARG
1	H	205	LEU
1	H	206	PHE
1	H	210	MSE
1	H	215	LYS
1	H	216	LYS
1	H	218	VAL
1	H	222	LEU
1	H	236	GLU
1	I	66	LYS
1	I	69	LYS
1	I	75	LEU
1	I	81	VAL
1	I	85	ASP
1	I	86	ASP
1	I	93	ARG
1	I	98	ILE
1	I	103	LYS
1	I	116	LYS
1	I	128	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	145	SER
1	I	146	LEU
1	I	149	LEU
1	I	156	LEU
1	I	168	SER
1	I	170	VAL
1	I	173	SER
1	I	177	ILE
1	I	183	LEU
1	I	184	LYS
1	I	187	LYS
1	I	189	ILE
1	I	205	LEU
1	I	206	PHE
1	I	212	GLN
1	I	215	LYS
1	I	218	VAL
1	I	222	LEU
1	I	232	THR
1	J	63	ASP
1	J	64	GLU
1	J	65	ILE
1	J	66	LYS
1	J	67	ILE
1	J	69	LYS
1	J	70	TYR
1	J	75	LEU
1	J	79	SER
1	J	85	ASP
1	J	86	ASP
1	J	94	LYS
1	J	98	ILE
1	J	128	ARG
1	J	130	GLU
1	J	140	SER
1	J	142	VAL
1	J	145	SER
1	J	146	LEU
1	J	156	LEU
1	J	161	GLU
1	J	170	VAL
1	J	183	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	187	LYS
1	J	189	ILE
1	J	205	LEU
1	J	206	PHE
1	J	207	ILE
1	J	210	MSE
1	J	211	THR
1	J	215	LYS
1	J	217	LYS
1	J	222	LEU
1	J	225	LEU
1	J	228	ASP

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

Mol	Chain	Res	Type
1	A	113	ASN
1	A	144	GLN
1	B	113	ASN
1	B	144	GLN
1	B	182	HIS
1	B	202	ASN
1	C	111	GLN
1	C	113	ASN
1	C	202	ASN
1	D	111	GLN
1	D	132	ASN
1	D	144	GLN
1	D	202	ASN
1	E	144	GLN
1	E	202	ASN
1	F	111	GLN
1	F	113	ASN
1	F	132	ASN
1	F	144	GLN
1	F	202	ASN
1	G	113	ASN
1	G	132	ASN
1	G	144	GLN
1	G	202	ASN
1	G	223	ASN
1	H	144	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	178	ASN
1	H	202	ASN
1	I	113	ASN
1	I	144	GLN
1	I	202	ASN
1	J	132	ASN
1	J	202	ASN
1	J	233	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	176/183 (96%)	0.14	4 (2%)	60	51	32, 54, 96, 104	0
1	B	176/183 (96%)	0.20	6 (3%)	45	35	22, 46, 96, 106	0
1	C	165/183 (90%)	0.05	4 (2%)	59	49	13, 38, 81, 92	0
1	D	170/183 (92%)	0.08	3 (1%)	68	61	21, 47, 92, 102	0
1	E	173/183 (94%)	0.15	7 (4%)	38	28	23, 47, 99, 106	0
1	F	169/183 (92%)	-0.12	2 (1%)	79	73	15, 32, 80, 104	0
1	G	169/183 (92%)	0.12	6 (3%)	42	32	18, 43, 88, 104	0
1	H	170/183 (92%)	-0.06	4 (2%)	59	49	17, 39, 82, 106	0
1	I	169/183 (92%)	0.13	7 (4%)	37	27	18, 42, 90, 105	0
1	J	169/183 (92%)	0.05	6 (3%)	42	32	20, 42, 89, 105	0
All	All	1706/1830 (93%)	0.08	49 (2%)	51	41	13, 43, 92, 106	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	ASP	14.2
1	E	63	ASP	11.9
1	J	63	ASP	10.8
1	I	63	ASP	10.4
1	G	63	ASP	9.8
1	C	65	ILE	9.3
1	C	231	ALA	8.3
1	A	63	ASP	7.0
1	I	65	ILE	5.0
1	B	241	HIS	4.8
1	I	64	GLU	4.4
1	B	240	HIS	4.3
1	B	239	GLU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	64	GLU	3.7
1	E	237	PRO	3.6
1	F	65	ILE	3.6
1	A	235	GLU	3.6
1	F	233	HIS	3.4
1	H	65	ILE	3.4
1	A	123	ALA	3.3
1	B	238	LEU	3.2
1	E	238	LEU	3.2
1	H	233	HIS	3.1
1	J	126	GLU	3.1
1	G	66	LYS	3.0
1	J	64	GLU	3.0
1	J	66	LYS	2.9
1	D	94	LYS	2.9
1	B	237	PRO	2.9
1	A	107	LEU	2.8
1	H	235	GLU	2.8
1	E	126	GLU	2.7
1	G	65	ILE	2.6
1	G	229	TYR	2.6
1	I	66	LYS	2.5
1	H	236	GLU	2.5
1	D	131	GLU	2.3
1	E	235	GLU	2.3
1	E	123	ALA	2.3
1	J	119	ILE	2.3
1	C	64	GLU	2.2
1	C	230	LYS	2.2
1	G	64	GLU	2.2
1	I	128	ARG	2.1
1	G	160	ILE	2.1
1	J	123	ALA	2.0
1	I	130	GLU	2.0
1	I	90	ARG	2.0
1	E	130	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO	C	2300	1/1	0.98	0.13	35,35,35,35	0
2	CO	D	3300	1/1	0.98	0.11	34,34,34,34	0
2	CO	H	7300	1/1	0.98	0.11	34,34,34,34	0
2	CO	B	1300	1/1	0.99	0.11	39,39,39,39	0
2	CO	G	6300	1/1	0.99	0.11	30,30,30,30	0
2	CO	A	300	1/1	0.99	0.10	46,46,46,46	0
2	CO	I	8300	1/1	0.99	0.09	45,45,45,45	0
2	CO	J	9300	1/1	0.99	0.10	44,44,44,44	0
2	CO	E	4300	1/1	1.00	0.11	39,39,39,39	0
2	CO	F	5300	1/1	1.00	0.14	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.