



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:20 pm GMT

PDB ID : 1OB1
Title : Crystal structure of a Fab complex with Plasmodium falciparum MSP1-19
Authors : Pizarro, J.C.; Chitarra, V.; Verger, D.; Holm, I.; Petres, S.; Dartville, S.; Nato, F.; Longacre, S.; Bentley, G.A.
Deposited on : 2003-01-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

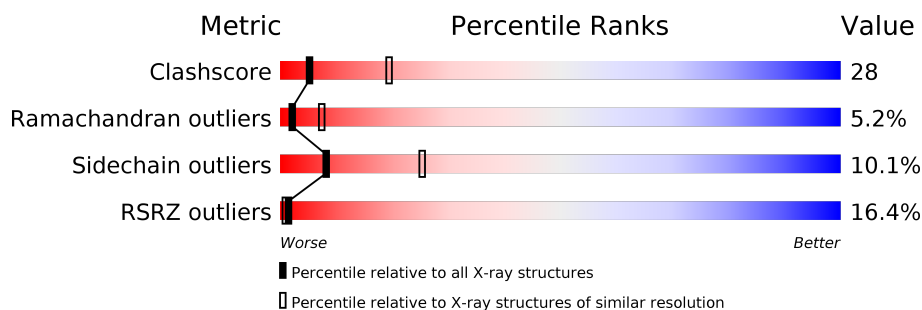
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>14%</div> <div>51% 39% 8%</div> </div>
1	D	215	<div> <div>24%</div> <div>52% 39% 9%</div> </div>
2	B	219	<div> <div>10%</div> <div>63% 27% 10%</div> </div>
2	E	219	<div> <div>26%</div> <div>64% 28% 7%</div> </div>
3	C	99	<div> <div>10%</div> <div>52% 34% 10%</div> </div>
3	F	99	<div> <div>4%</div> <div>48% 35% 13%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8149 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 ANTIBODY, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1660	1034	276	340	10			
1	D	215	Total	C	N	O	S	0	0	0
			1660	1034	276	340	10			

- Molecule 2 is a protein called ANTIBODY, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	1	0
			1674	1065	277	326	6			
2	E	219	Total	C	N	O	S	0	0	0
			1667	1061	274	326	6			

- Molecule 3 is a protein called MAJOR MEROZOITE SURFACE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	1
			734	436	133	153	12			
3	F	97	Total	C	N	O	S	0	0	1
			744	442	136	154	12			

There are 12 discrepancies between the modelled and reference sequences:

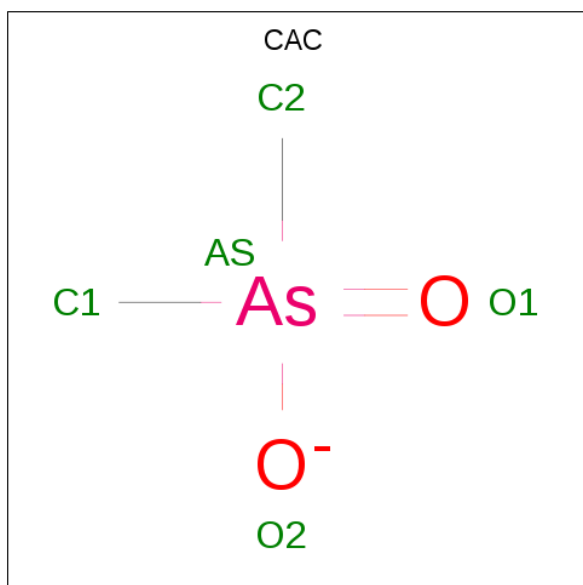
Chain	Residue	Modelled	Actual	Comment	Reference
C	94	HIS	-	expression tag	UNP Q25976
C	95	HIS	-	expression tag	UNP Q25976
C	96	HIS	-	expression tag	UNP Q25976
C	97	HIS	-	expression tag	UNP Q25976
C	98	HIS	-	expression tag	UNP Q25976
C	99	HIS	-	expression tag	UNP Q25976
F	94	HIS	-	expression tag	UNP Q25976
F	95	HIS	-	expression tag	UNP Q25976

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	96	HIS	-	expression tag	UNP Q25976
F	97	HIS	-	expression tag	UNP Q25976
F	98	HIS	-	expression tag	UNP Q25976
F	99	HIS	-	expression tag	UNP Q25976

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).

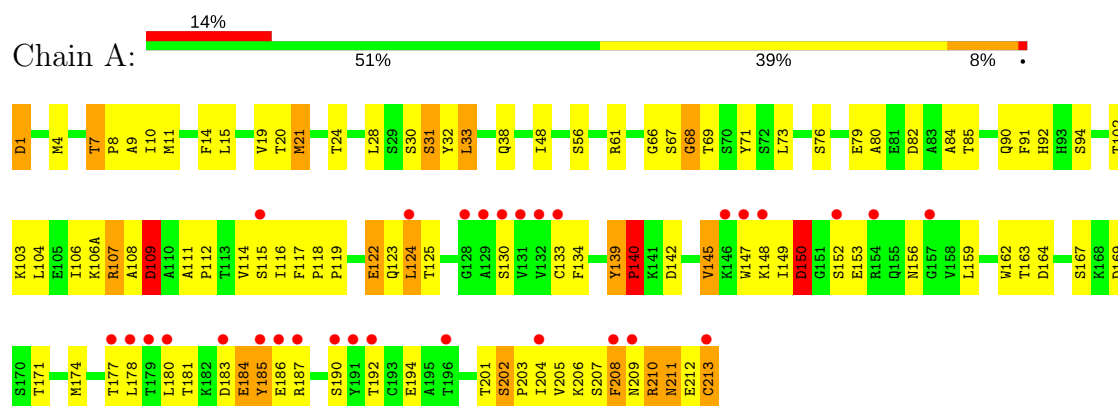


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	As	C	O	4	0
			5	1	2	2		
4	F	1	Total	As	C	O	4	0
			5	1	2	2		

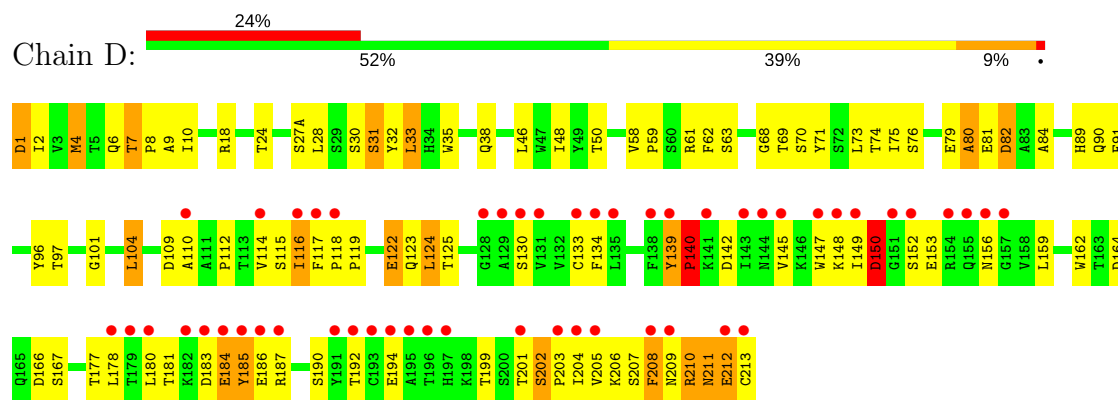
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

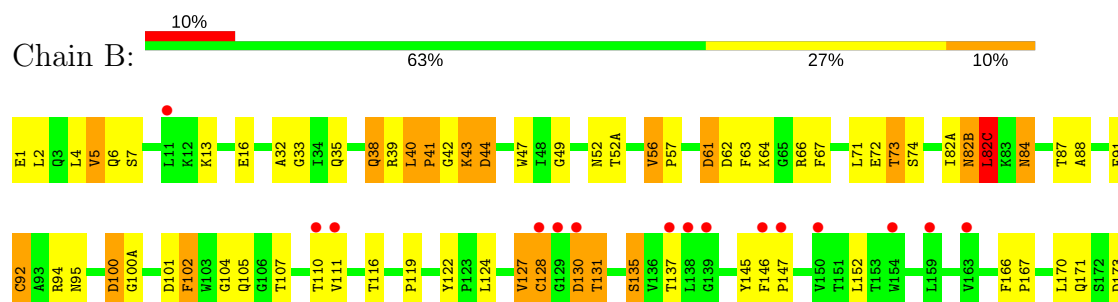
• Molecule 1: ANTIBODY, HEAVY CHAIN

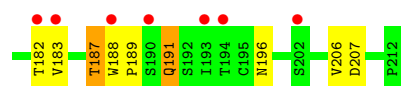


• Molecule 1: ANTIBODY, HEAVY CHAIN

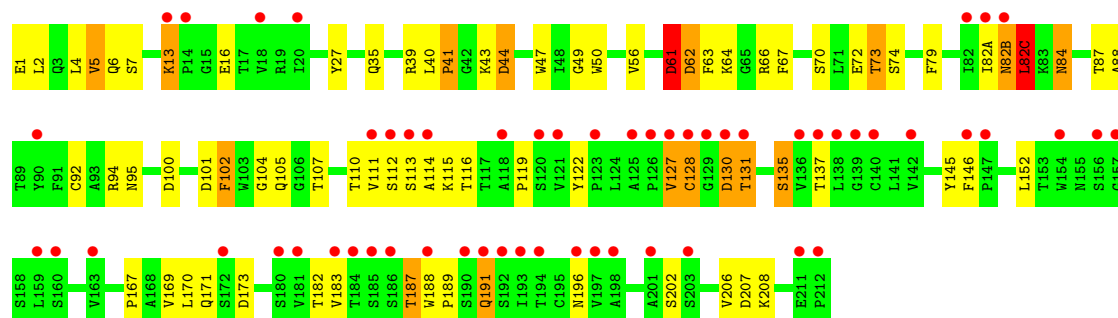


• Molecule 2: ANTIBODY, LIGHT CHAIN

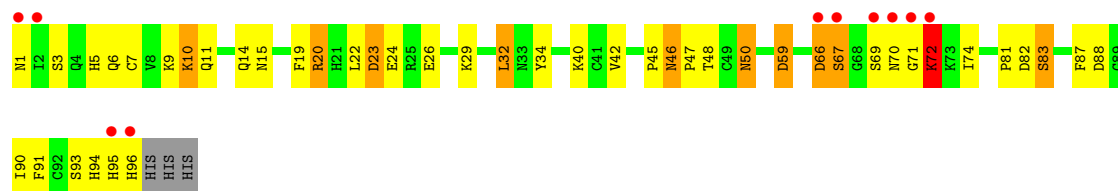




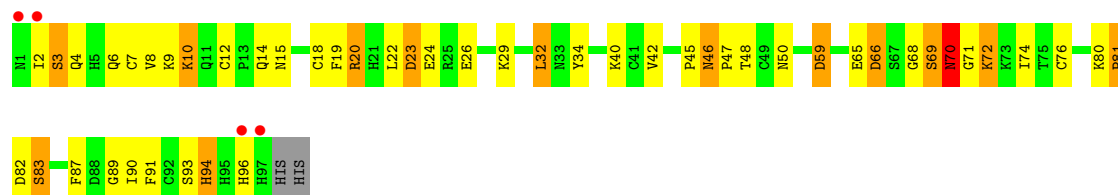
• Molecule 2: ANTIBODY, LIGHT CHAIN



• Molecule 3: MAJOR MEROZOITE SURFACE PROTEIN



• Molecule 3: MAJOR MEROZOITE SURFACE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.75Å 213.46Å 59.89Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	105.41 – 2.90 29.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (105.41-2.90) 96.7 (29.43-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.257 , 0.288 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8149	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/1702	0.84	7/2312 (0.3%)
1	D	0.36	0/1702	0.81	8/2312 (0.3%)
2	B	0.35	0/1723	0.74	7/2351 (0.3%)
2	E	0.33	0/1712	0.72	7/2337 (0.3%)
3	C	0.45	0/747	0.84	5/1004 (0.5%)
3	F	0.49	0/758	0.83	3/1019 (0.3%)
All	All	0.40	0/8344	0.79	37/11335 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	ASP	CB-CG-OD2	7.83	125.34	118.30
1	A	150	ASP	CB-CG-OD2	7.26	124.83	118.30
1	D	150	ASP	CB-CG-OD2	7.20	124.78	118.30
3	F	59	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	82	ASP	CB-CG-OD2	5.92	123.63	118.30
2	E	100	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	183	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	164	ASP	CB-CG-OD2	5.67	123.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	44	ASP	CB-CG-OD2	5.55	123.29	118.30
3	C	59	ASP	CB-CG-OD2	5.44	123.20	118.30
3	F	66	ASP	CB-CG-OD2	5.44	123.19	118.30
2	B	100	ASP	CA-C-N	5.43	127.05	116.20
2	B	207	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	183	ASP	CB-CG-OD2	5.40	123.16	118.30
2	E	207	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	109	ASP	CB-CG-OD2	5.33	123.09	118.30
3	C	88	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	44	ASP	CB-CG-OD2	5.30	123.07	118.30
2	E	130	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	1	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	130	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	1	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	169	ASP	CB-CG-OD2	5.21	122.99	118.30
2	E	173	ASP	CB-CG-OD2	5.21	122.99	118.30
2	E	62	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	166	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	142	ASP	CB-CG-OD2	5.18	122.96	118.30
3	F	23	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	109	ASP	CB-CG-OD2	5.14	122.92	118.30
2	B	173	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	100	ASP	O-C-N	-5.09	114.55	123.20
1	A	82	ASP	CB-CG-OD2	5.06	122.85	118.30
3	C	66	ASP	CB-CG-OD2	5.03	122.83	118.30
2	E	61	ASP	CB-CG-OD2	5.03	122.82	118.30
3	C	23	ASP	CB-CG-OD2	5.02	122.82	118.30
3	C	72	LYS	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Peptide
1	D	139	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1660	0	1570	114	0
1	D	1660	0	1570	123	0
2	B	1674	0	1634	74	0
2	E	1667	0	1625	72	0
3	C	734	0	661	46	0
3	F	744	0	668	55	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
All	All	8149	0	7728	449	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 28.

All (449) 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:D:118:PRO:HG3	1:D:208:PHE:CE2	1.32	1.62
1:A:118:PRO:HG3	1:A:208:PHE:CE2	1.33	1.59
1:D:118:PRO:CG	1:D:208:PHE:HE2	1.38	1.35
1:A:118:PRO:CG	1:A:208:PHE:HE2	1.38	1.34
1:D:209:ASN:O	1:D:213:CYS:O	1.54	1.21
1:D:210:ARG:O	1:D:212:GLU:N	1.73	1.20
1:A:118:PRO:CG	1:A:208:PHE:CE2	2.18	1.19
1:A:213:CYS:SG	2:B:127:VAL:HG22	1.83	1.18
1:D:30:SER:O	1:D:32:TYR:N	1.75	1.17
3:C:20:ARG:HH11	3:C:20:ARG:HG2	1.04	1.17
3:C:32:LEU:H	3:C:32:LEU:HD12	1.11	1.16
2:B:127:VAL:HG13	2:B:128:CYS:H	1.11	1.14
1:A:30:SER:O	1:A:32:TYR:N	1.78	1.14
1:D:118:PRO:CG	1:D:208:PHE:CE2	2.18	1.13
3:F:32:LEU:H	3:F:32:LEU:HD12	1.05	1.11
3:F:20:ARG:HH11	3:F:20:ARG:HG2	0.99	1.10
1:A:159:LEU:HD23	2:B:171:GLN:HE21	1.14	1.09
2:E:127:VAL:HG13	2:E:128:CYS:H	1.14	1.08
3:F:72:LYS:HZ2	3:F:72:LYS:HB3	1.23	1.02
3:F:93:SER:O	3:F:94:HIS:HB2	1.58	0.98
1:D:208:PHE:C	1:D:208:PHE:HD1	1.67	0.97
2:B:82(C):LEU:HD23	2:B:82(C):LEU:O	1.64	0.97
3:F:69:SER:O	3:F:71:GLY:N	1.97	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:HD1	1:A:208:PHE:C	1.67	0.95
2:E:82(C):LEU:O	2:E:82(C):LEU:HD23	1.66	0.95
1:D:139:TYR:CG	1:D:140:PRO:CD	2.51	0.94
1:A:139:TYR:CD1	1:A:140:PRO:CD	2.52	0.93
1:D:212:GLU:HG3	1:D:213:CYS:N	1.81	0.92
1:A:118:PRO:HG3	1:A:208:PHE:CZ	2.05	0.92
3:F:20:ARG:HG2	3:F:20:ARG:NH1	1.79	0.91
3:C:20:ARG:NH1	3:C:20:ARG:HG2	1.83	0.90
1:D:118:PRO:HG3	1:D:208:PHE:CZ	2.05	0.90
3:F:32:LEU:HD12	3:F:32:LEU:N	1.86	0.90
3:F:32:LEU:H	3:F:32:LEU:CD1	1.84	0.90
1:A:208:PHE:HD1	1:A:208:PHE:O	1.55	0.90
2:B:82(C):LEU:HD23	2:B:82(C):LEU:C	1.92	0.89
1:D:4:MET:HE1	1:D:97:THR:O	1.73	0.88
1:D:208:PHE:O	1:D:208:PHE:HD1	1.55	0.88
2:E:39:ARG:O	2:E:88:ALA:HB1	1.73	0.88
1:A:85:THR:OG1	1:A:103:LYS:HG2	1.73	0.88
2:B:127:VAL:HG13	2:B:128:CYS:N	1.87	0.87
2:B:40:LEU:HB3	2:B:41:PRO:HD2	1.56	0.87
2:E:82(C):LEU:C	2:E:82(C):LEU:HD23	1.94	0.87
3:C:32:LEU:N	3:C:32:LEU:HD12	1.89	0.87
2:B:40:LEU:HB3	2:B:41:PRO:CD	2.03	0.86
1:A:139:TYR:CD1	1:A:140:PRO:HD3	2.10	0.86
1:D:139:TYR:CD1	1:D:140:PRO:CD	2.59	0.86
1:A:139:TYR:CG	1:A:140:PRO:CD	2.58	0.86
1:A:208:PHE:CD1	1:A:208:PHE:C	2.44	0.86
1:A:201:THR:O	1:A:202:SER:HB3	1.76	0.84
3:C:32:LEU:H	3:C:32:LEU:CD1	1.90	0.84
2:E:127:VAL:HG13	2:E:128:CYS:N	1.92	0.84
3:F:45:PRO:C	3:F:46:ASN:HD22	1.81	0.84
1:D:208:PHE:C	1:D:208:PHE:CD1	2.44	0.83
3:C:45:PRO:C	3:C:46:ASN:HD22	1.82	0.83
1:D:201:THR:O	1:D:202:SER:HB3	1.78	0.83
1:A:107:ARG:O	1:A:139:TYR:CD1	2.31	0.82
1:D:2:ILE:HD12	1:D:2:ILE:H	1.46	0.81
1:D:119:PRO:HG3	1:D:130:SER:N	1.95	0.81
1:A:107:ARG:HE	1:A:171:THR:HG22	1.45	0.80
2:B:127:VAL:CG1	2:B:128:CYS:H	1.91	0.80
1:A:119:PRO:HG3	1:A:130:SER:N	1.97	0.80
1:A:139:TYR:CD1	1:A:140:PRO:HD2	2.15	0.80
3:C:22:LEU:HD13	3:C:96:HIS:N	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:ASP:O	2:E:131:THR:OG1	2.00	0.79
2:B:1:GLU:HG2	2:B:1:GLU:O	1.82	0.79
1:D:2:ILE:HD12	1:D:2:ILE:N	1.98	0.79
1:D:139:TYR:CD1	1:D:140:PRO:HD3	2.17	0.78
1:D:139:TYR:CD1	1:D:140:PRO:HD2	2.18	0.77
1:A:159:LEU:HD23	2:B:171:GLN:NE2	1.95	0.77
2:E:127:VAL:CG1	2:E:128:CYS:H	1.96	0.77
3:F:72:LYS:CB	3:F:72:LYS:HZ2	1.96	0.77
2:B:130:ASP:O	2:B:131:THR:OG1	2.03	0.76
1:D:119:PRO:HG3	1:D:130:SER:H	1.50	0.76
1:D:4:MET:CE	1:D:97:THR:O	2.34	0.75
1:A:117:PHE:CD2	2:B:124:LEU:HB3	2.22	0.75
1:D:89:HIS:HE1	1:D:96:TYR:O	1.70	0.75
3:F:20:ARG:HH11	3:F:20:ARG:CG	1.89	0.75
1:A:213:CYS:SG	2:B:127:VAL:CG2	2.71	0.74
2:E:1:GLU:O	2:E:1:GLU:HG2	1.88	0.74
1:A:119:PRO:HG3	1:A:130:SER:H	1.53	0.74
2:E:82(A):ILE:HG13	2:E:82(B):ASN:ND2	2.04	0.73
3:F:69:SER:C	3:F:71:GLY:H	1.92	0.73
1:D:159:LEU:HD23	2:E:171:GLN:HE21	1.54	0.73
1:A:118:PRO:CD	1:A:208:PHE:HE2	2.02	0.72
1:D:118:PRO:CD	1:D:208:PHE:HE2	2.02	0.72
3:F:46:ASN:HD22	3:F:46:ASN:N	1.83	0.72
1:A:61:ARG:NH2	3:F:59:ASP:OD2	2.22	0.72
1:D:73:LEU:HD23	1:D:74:THR:N	2.05	0.72
1:D:139:TYR:CG	1:D:140:PRO:HD2	2.23	0.72
2:B:39:ARG:O	2:B:88:ALA:HB1	1.90	0.72
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.55	0.71
2:B:82(A):ILE:HG13	2:B:82(B):ASN:ND2	2.06	0.71
2:E:113:SER:O	2:E:114:ALA:C	2.28	0.71
2:E:40:LEU:HB3	2:E:41:PRO:HD2	1.73	0.70
3:F:72:LYS:HB3	3:F:72:LYS:NZ	2.00	0.70
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.73	0.69
1:D:149:ILE:HD11	1:D:178:LEU:HD21	1.74	0.69
2:B:7:SER:O	2:B:107:THR:HG22	1.92	0.69
1:A:117:PHE:HD2	2:B:124:LEU:HB3	1.56	0.69
1:D:212:GLU:CG	1:D:213:CYS:N	2.55	0.69
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.73	0.69
3:C:22:LEU:CD1	3:C:96:HIS:N	2.56	0.69
1:A:139:TYR:CE1	1:A:140:PRO:HD3	2.28	0.68
1:A:162:TRP:O	2:B:167:PRO:HD2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:PHE:HB2	3:C:91:PHE:CD1	2.28	0.68
3:C:67:SER:HB2	3:C:71:GLY:HA2	1.76	0.67
3:C:6:GLN:HA	3:C:6:GLN:OE1	1.94	0.67
1:D:148:LYS:HB2	1:D:192:THR:HB	1.76	0.67
2:B:6:GLN:NE2	2:B:92:CYS:H	1.92	0.67
1:A:14:PHE:CE1	1:A:106(A):LYS:HD2	2.30	0.67
3:C:46:ASN:HD22	3:C:46:ASN:N	1.89	0.67
2:E:66:ARG:HH12	2:E:82(C):LEU:HA	1.60	0.67
2:E:113:SER:O	2:E:115:LYS:HG2	1.95	0.66
2:E:6:GLN:NE2	2:E:92:CYS:H	1.93	0.66
1:A:208:PHE:CD1	1:A:208:PHE:O	2.44	0.66
1:D:4:MET:HE2	1:D:90:GLN:HB3	1.78	0.66
1:A:149:ILE:HD11	1:A:178:LEU:HD21	1.76	0.66
1:A:210:ARG:O	1:A:212:GLU:N	2.24	0.66
1:D:139:TYR:CG	1:D:140:PRO:HD3	2.31	0.66
1:A:148:LYS:HB2	1:A:192:THR:HB	1.78	0.65
3:C:47:PRO:HD2	3:C:72:LYS:HG2	1.79	0.65
2:E:7:SER:O	2:E:107:THR:HG22	1.96	0.65
3:F:2:ILE:HG22	3:F:6:GLN:HG2	1.78	0.65
3:F:10:LYS:HD2	3:F:26:GLU:HB3	1.80	0.64
1:D:139:TYR:CE1	1:D:140:PRO:HD3	2.32	0.64
2:E:50:TRP:HZ2	3:F:8:VAL:O	1.80	0.64
1:D:208:PHE:O	1:D:208:PHE:CD1	2.45	0.64
1:A:211:ASN:C	1:A:213:CYS:H	2.00	0.63
3:F:69:SER:C	3:F:71:GLY:N	2.52	0.63
3:C:69:SER:O	3:C:70:ASN:HB2	1.98	0.62
3:F:72:LYS:CB	3:F:72:LYS:NZ	2.60	0.62
2:B:66:ARG:HH12	2:B:82(C):LEU:HA	1.63	0.62
3:C:29:LYS:HD3	3:C:91:PHE:CE2	2.34	0.62
2:E:87:THR:HG23	2:E:110:THR:HA	1.82	0.62
1:D:210:ARG:CZ	1:D:210:ARG:HB2	2.28	0.62
1:D:4:MET:HE1	1:D:90:GLN:H	1.65	0.62
1:A:139:TYR:CG	1:A:140:PRO:HD2	2.33	0.62
3:F:29:LYS:HB2	3:F:91:PHE:CZ	2.35	0.61
3:C:34:TYR:HA	3:C:42:VAL:O	2.00	0.61
3:C:10:LYS:HD2	3:C:26:GLU:HB3	1.83	0.61
3:F:34:TYR:HA	3:F:42:VAL:O	2.00	0.61
1:D:201:THR:O	1:D:202:SER:CB	2.47	0.61
2:E:35:GLN:HE21	2:E:47:TRP:HE1	1.48	0.60
2:B:35:GLN:HE21	2:B:47:TRP:HE1	1.47	0.60
1:D:152:SER:O	1:D:153:GLU:HB2	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:83:SER:OG	3:F:93:SER:O	2.20	0.60
1:A:201:THR:O	1:A:202:SER:CB	2.46	0.59
1:A:91:PHE:CG	2:B:100(A):GLY:HA3	2.38	0.59
1:D:159:LEU:HD21	2:E:169:VAL:CG1	2.31	0.59
1:A:148:LYS:HG2	1:A:152:SER:O	2.02	0.59
3:F:6:GLN:OE1	3:F:6:GLN:HA	2.03	0.59
3:C:46:ASN:HA	3:C:72:LYS:HG2	1.84	0.59
1:A:152:SER:O	1:A:153:GLU:HB2	2.02	0.59
2:B:87:THR:HG23	2:B:110:THR:HA	1.83	0.59
1:A:147:TRP:O	1:A:153:GLU:HA	2.02	0.59
1:A:122:GLU:HB3	2:B:122:TYR:CD1	2.38	0.58
2:B:82(C):LEU:C	2:B:82(C):LEU:CD2	2.64	0.58
1:D:147:TRP:O	1:D:153:GLU:HA	2.03	0.58
1:D:123:GLN:O	1:D:125:THR:N	2.36	0.58
3:F:46:ASN:ND2	3:F:46:ASN:N	2.51	0.58
3:C:29:LYS:HB2	3:C:91:PHE:CZ	2.39	0.57
3:C:47:PRO:HD2	3:C:72:LYS:CG	2.34	0.57
3:F:19:PHE:HB2	3:F:91:PHE:CD1	2.39	0.57
3:F:47:PRO:HD2	3:F:72:LYS:HB2	1.85	0.57
1:D:162:TRP:O	2:E:167:PRO:HD2	2.05	0.57
2:E:82(C):LEU:C	2:E:82(C):LEU:CD2	2.66	0.57
3:C:6:GLN:O	3:C:20:ARG:HD3	2.04	0.57
1:D:123:GLN:C	1:D:125:THR:H	2.06	0.57
1:A:123:GLN:C	1:A:125:THR:H	2.08	0.56
1:D:4:MET:CE	1:D:90:GLN:HB3	2.34	0.56
2:B:82(C):LEU:O	2:B:82(C):LEU:CD2	2.44	0.56
3:F:82:ASP:OD1	3:F:82:ASP:O	2.24	0.56
3:F:93:SER:O	3:F:94:HIS:CB	2.37	0.56
1:D:213:CYS:SG	2:E:127:VAL:HG22	2.45	0.56
1:A:123:GLN:O	1:A:125:THR:N	2.39	0.56
2:B:130:ASP:C	2:B:131:THR:OG1	2.44	0.56
1:A:91:PHE:CD1	2:B:100(A):GLY:HA3	2.41	0.56
1:D:2:ILE:H	1:D:2:ILE:CD1	2.17	0.56
1:D:159:LEU:HD11	2:E:169:VAL:HB	1.88	0.55
1:D:30:SER:HB3	3:F:23:ASP:O	2.06	0.55
1:A:133:CYS:HB2	1:A:147:TRP:CH2	2.42	0.55
3:C:67:SER:CB	3:C:71:GLY:HA2	2.36	0.55
2:E:82(C):LEU:CD2	2:E:82(C):LEU:O	2.47	0.55
1:A:107:ARG:NH1	1:A:107:ARG:HG2	2.22	0.55
1:D:28:LEU:HB2	1:D:71:TYR:OH	2.07	0.55
1:A:209:ASN:O	1:A:213:CYS:C	2.45	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:SER:HB3	3:C:23:ASP:O	2.06	0.54
1:A:115:SER:HB3	1:A:117:PHE:HE1	1.73	0.54
1:D:145:VAL:HG23	1:D:145:VAL:O	2.07	0.54
1:A:11:MET:HE3	1:A:19:VAL:HG13	1.89	0.54
2:B:38:GLN:OE1	2:B:40:LEU:HD21	2.08	0.54
1:D:30:SER:O	1:D:31:SER:C	2.44	0.54
1:A:145:VAL:CG2	1:A:145:VAL:O	2.55	0.54
3:C:67:SER:HA	3:C:72:LYS:H	1.73	0.54
2:E:47:TRP:CH2	2:E:49:GLY:HA2	2.42	0.54
3:C:82:ASP:O	3:C:82:ASP:OD1	2.25	0.53
1:A:9:ALA:C	1:A:10:ILE:HD12	2.29	0.53
3:C:74:ILE:HG23	3:C:74:ILE:O	2.08	0.53
2:E:130:ASP:C	2:E:131:THR:OG1	2.46	0.53
1:D:212:GLU:HG3	1:D:213:CYS:H	1.67	0.53
2:E:130:ASP:N	2:E:130:ASP:OD1	2.41	0.53
1:D:211:ASN:C	1:D:212:GLU:HG2	2.29	0.52
1:D:116:ILE:C	1:D:117:PHE:HD1	2.13	0.52
1:D:30:SER:OG	1:D:30:SER:O	2.21	0.52
2:B:135:SER:HA	2:B:183:VAL:O	2.09	0.52
3:C:46:ASN:ND2	3:C:46:ASN:N	2.56	0.52
3:F:29:LYS:HD3	3:F:91:PHE:CE2	2.44	0.52
1:A:185:TYR:O	1:A:187:ARG:N	2.38	0.52
1:D:133:CYS:HB2	1:D:147:TRP:CH2	2.45	0.52
1:D:148:LYS:HG2	1:D:152:SER:O	2.09	0.52
1:A:210:ARG:HB2	1:A:210:ARG:CZ	2.40	0.52
3:C:74:ILE:CG2	3:C:74:ILE:O	2.57	0.52
2:E:16:GLU:O	2:E:82(C):LEU:HD13	2.10	0.52
1:D:184:GLU:O	1:D:185:TYR:C	2.48	0.52
3:F:20:ARG:NH2	3:F:24:GLU:OE1	2.43	0.52
2:B:72:GLU:O	2:B:74:SER:N	2.43	0.51
1:D:62:PHE:HD2	1:D:73:LEU:HD21	1.75	0.51
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.41	0.51
2:B:127:VAL:CG1	2:B:128:CYS:N	2.58	0.51
1:D:185:TYR:O	1:D:187:ARG:N	2.41	0.51
1:A:122:GLU:HB3	2:B:122:TYR:HD1	1.73	0.51
1:A:184:GLU:O	1:A:185:TYR:C	2.48	0.51
2:B:52:ASN:ND2	3:C:11:GLN:HG3	2.25	0.51
1:D:115:SER:HB3	1:D:117:PHE:HE1	1.76	0.51
2:B:130:ASP:N	2:B:130:ASP:OD1	2.44	0.51
1:A:159:LEU:CD2	2:B:171:GLN:HE21	2.03	0.51
2:E:135:SER:HA	2:E:183:VAL:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:O	1:A:212:GLU:HB3	2.10	0.51
3:C:20:ARG:NH1	3:C:20:ARG:CG	2.61	0.51
1:D:159:LEU:HD21	2:E:169:VAL:HG11	1.91	0.51
1:D:110:ALA:O	1:D:199:THR:HG21	2.10	0.51
3:F:6:GLN:O	3:F:20:ARG:HD3	2.11	0.51
1:D:46:LEU:HD23	2:E:101:ASP:HB3	1.92	0.51
1:D:61:ARG:HG3	1:D:75:ILE:HG23	1.93	0.50
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.75	0.50
2:B:187:THR:O	2:B:191:GLN:HG3	2.11	0.50
1:D:79:GLU:O	1:D:80:ALA:C	2.48	0.50
2:E:187:THR:O	2:E:191:GLN:HG3	2.12	0.50
1:A:192:THR:HA	1:A:207:SER:HB3	1.93	0.50
3:F:45:PRO:C	3:F:47:PRO:HD3	2.32	0.50
3:C:19:PHE:HB2	3:C:91:PHE:CE1	2.46	0.50
2:E:82(B):ASN:O	2:E:82(C):LEU:O	2.29	0.50
1:A:162:TRP:O	2:B:167:PRO:CD	2.60	0.50
2:B:4:LEU:O	2:B:104:GLY:HA2	2.12	0.50
1:A:149:ILE:O	1:A:150:ASP:OD1	2.30	0.50
3:C:20:ARG:NH2	3:C:24:GLU:OE1	2.45	0.50
3:C:83:SER:OG	3:C:93:SER:O	2.29	0.50
1:D:139:TYR:CD2	1:D:140:PRO:CD	2.95	0.50
1:A:107:ARG:NH1	1:A:108:ALA:O	2.45	0.49
1:A:116:ILE:C	1:A:117:PHE:HD1	2.14	0.49
1:D:202:SER:HB2	1:D:203:PRO:CD	2.42	0.49
1:D:59:PRO:HG2	1:D:62:PHE:HD1	1.76	0.49
2:B:6:GLN:HE22	2:B:92:CYS:H	1.58	0.49
3:F:87:PHE:O	3:F:90:ILE:HG12	2.13	0.49
2:B:152:LEU:HA	2:B:196:ASN:O	2.12	0.49
2:B:82(B):ASN:O	2:B:82(C):LEU:O	2.30	0.49
3:C:87:PHE:O	3:C:90:ILE:HG12	2.12	0.49
1:D:192:THR:HA	1:D:207:SER:HB3	1.94	0.49
1:D:211:ASN:HB3	1:D:212:GLU:HG2	1.94	0.49
1:D:208:PHE:HB2	1:D:213:CYS:OXT	2.13	0.49
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.47	0.48
3:C:59:ASP:OD2	1:D:61:ARG:NH2	2.46	0.48
1:A:116:ILE:C	1:A:117:PHE:CD1	2.87	0.48
1:D:162:TRP:O	2:E:167:PRO:CD	2.61	0.48
1:A:202:SER:HB2	1:A:203:PRO:CD	2.43	0.48
2:B:42:GLY:O	2:B:43:LYS:O	2.32	0.48
1:A:30:SER:OG	1:A:92:HIS:HD2	1.96	0.48
1:A:21:MET:CE	1:A:73:LEU:HD22	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:PRO:HB2	1:D:124:LEU:HG	1.95	0.48
1:D:81:GLU:CD	1:D:81:GLU:H	2.15	0.48
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.49	0.48
2:B:5:VAL:HG23	2:B:105:GLN:HE22	1.78	0.48
2:B:40:LEU:CB	2:B:41:PRO:CD	2.78	0.48
1:D:210:ARG:O	1:D:213:CYS:N	2.45	0.48
2:E:4:LEU:O	2:E:104:GLY:HA2	2.14	0.48
2:E:112:SER:OG	2:E:146:PHE:HZ	1.97	0.48
2:E:152:LEU:HA	2:E:196:ASN:O	2.13	0.48
1:D:122:GLU:HB3	2:E:122:TYR:HD1	1.79	0.48
1:A:163:THR:HG23	2:B:166:PHE:CD2	2.48	0.47
1:D:116:ILE:C	1:D:117:PHE:CD1	2.86	0.47
2:B:61:ASP:C	2:B:63:PHE:H	2.18	0.47
3:C:45:PRO:C	3:C:47:PRO:HD3	2.34	0.47
2:B:16:GLU:O	2:B:82(C):LEU:HD13	2.15	0.47
1:D:61:ARG:NH1	1:D:82:ASP:OD1	2.47	0.47
2:B:33:GLY:O	2:B:95:ASN:N	2.48	0.47
3:C:5:HIS:HA	3:C:20:ARG:HB3	1.97	0.47
2:E:6:GLN:HE21	2:E:104:GLY:HA3	1.80	0.47
1:A:133:CYS:HB2	1:A:147:TRP:HH2	1.79	0.47
1:A:30:SER:O	1:A:31:SER:C	2.44	0.47
1:D:79:GLU:O	1:D:81:GLU:N	2.47	0.47
1:A:112:PRO:HD2	1:A:204:ILE:CD1	2.45	0.47
2:B:127:VAL:C	2:B:128:CYS:SG	2.93	0.47
1:A:139:TYR:CG	1:A:140:PRO:N	2.82	0.46
1:A:38:GLN:O	1:A:84:ALA:HB1	2.16	0.46
1:A:211:ASN:C	1:A:213:CYS:N	2.64	0.46
1:D:212:GLU:CG	1:D:213:CYS:H	2.26	0.46
3:F:68:GLY:O	3:F:70:ASN:N	2.45	0.46
1:A:210:ARG:O	1:A:210:ARG:NH1	2.49	0.46
2:E:2:LEU:HD12	2:E:102:PHE:CE1	2.51	0.46
1:A:30:SER:C	1:A:32:TYR:N	2.64	0.46
2:E:72:GLU:O	2:E:74:SER:N	2.49	0.46
1:A:28:LEU:HB2	1:A:71:TYR:OH	2.15	0.46
2:B:32:ALA:O	2:B:52(A):THR:OG1	2.28	0.46
1:A:85:THR:HG1	1:A:103:LYS:HG2	1.80	0.46
1:A:139:TYR:CG	1:A:140:PRO:HD3	2.41	0.46
1:A:145:VAL:HG23	1:A:145:VAL:O	2.16	0.46
1:A:67:SER:O	1:A:68:GLY:C	2.54	0.46
1:D:123:GLN:C	1:D:125:THR:N	2.69	0.46
1:A:119:PRO:HB2	1:A:124:LEU:HG	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82(A):ILE:HG13	2:E:82(B):ASN:CG	2.37	0.45
2:E:6:GLN:HE22	2:E:92:CYS:H	1.60	0.45
2:E:119:PRO:HB3	2:E:145:TYR:CB	2.44	0.45
3:F:23:ASP:O	3:F:24:GLU:HB2	2.17	0.45
3:F:72:LYS:HZ3	3:F:72:LYS:HA	1.81	0.45
3:F:74:ILE:O	3:F:74:ILE:CG2	2.65	0.45
2:B:101:ASP:O	2:B:102:PHE:O	2.34	0.45
3:C:67:SER:HB2	3:C:71:GLY:CA	2.46	0.45
1:A:150:ASP:HB3	1:A:190:SER:H	1.81	0.45
3:F:12:CYS:SG	3:F:18:CYS:HB2	2.57	0.45
2:B:119:PRO:HB3	2:B:145:TYR:CB	2.43	0.45
2:E:119:PRO:CB	2:E:145:TYR:HB3	2.44	0.45
2:B:116:THR:HA	2:B:146:PHE:O	2.17	0.45
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.44	0.45
3:C:22:LEU:C	3:C:24:GLU:H	2.19	0.45
2:E:188:TRP:CG	2:E:189:PRO:HA	2.52	0.45
2:B:188:TRP:CG	2:B:189:PRO:HA	2.51	0.45
1:D:181:THR:OG1	1:D:184:GLU:HB3	2.16	0.45
2:E:116:THR:HG22	2:E:202:SER:HB3	1.98	0.45
3:F:14:GLN:O	3:F:15:ASN:HB2	2.17	0.45
1:D:89:HIS:CE1	1:D:96:TYR:O	2.60	0.45
3:F:74:ILE:O	3:F:74:ILE:HG23	2.17	0.45
2:B:35:GLN:NE2	2:B:47:TRP:HE1	2.14	0.44
1:D:139:TYR:CG	1:D:140:PRO:N	2.85	0.44
1:A:150:ASP:OD1	1:A:150:ASP:C	2.55	0.44
2:B:63:PHE:HD1	2:B:67:PHE:CE2	2.34	0.44
1:D:59:PRO:HG2	1:D:62:PHE:CD1	2.52	0.44
1:A:7:THR:HA	1:A:8:PRO:HA	1.73	0.44
2:B:35:GLN:HG3	2:B:95:ASN:HB2	2.00	0.44
1:D:185:TYR:HE2	1:D:210:ARG:HH21	1.64	0.44
1:D:18:ARG:HA	1:D:76:SER:O	2.18	0.44
3:C:6:GLN:CA	3:C:6:GLN:OE1	2.64	0.44
1:D:112:PRO:HD2	1:D:204:ILE:CD1	2.47	0.44
1:D:90:GLN:O	1:D:96:TYR:HB3	2.18	0.44
1:A:33:LEU:HD22	1:A:71:TYR:CG	2.53	0.44
2:B:71:LEU:N	2:B:71:LEU:HD23	2.31	0.44
3:F:72:LYS:HA	3:F:72:LYS:NZ	2.33	0.44
1:A:145:VAL:HG11	1:A:174:MET:SD	2.58	0.44
3:C:34:TYR:CA	3:C:42:VAL:O	2.64	0.44
1:D:211:ASN:CB	1:D:212:GLU:HG2	2.48	0.44
1:D:206:LYS:HB2	1:D:206:LYS:HE2	1.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:PHE:HB2	3:F:91:PHE:CE1	2.53	0.44
1:A:111:ALA:HA	1:A:112:PRO:HD3	1.89	0.43
1:A:181:THR:OG1	1:A:184:GLU:HB3	2.18	0.43
1:D:212:GLU:HG3	1:D:213:CYS:CB	2.48	0.43
3:F:34:TYR:CA	3:F:42:VAL:O	2.65	0.43
1:A:123:GLN:C	1:A:125:THR:N	2.71	0.43
1:D:123:GLN:OE1	2:E:122:TYR:CE2	2.71	0.43
1:D:139:TYR:CD2	1:D:140:PRO:HD3	2.52	0.43
1:D:7:THR:HA	1:D:8:PRO:HA	1.71	0.43
1:A:21:MET:HE3	1:A:73:LEU:HD22	2.00	0.43
2:B:56:VAL:HA	2:B:57:PRO:HD3	1.77	0.43
1:D:122:GLU:HB3	2:E:122:TYR:CD1	2.53	0.43
1:A:123:GLN:OE1	2:B:122:TYR:CE2	2.71	0.43
3:F:2:ILE:HG22	3:F:6:GLN:CG	2.46	0.43
1:A:114:VAL:HA	1:A:134:PHE:O	2.18	0.43
1:A:79:GLU:O	1:A:80:ALA:C	2.57	0.43
1:D:91:PHE:HE1	2:E:35:GLN:HE22	1.65	0.43
3:F:76:CYS:HB2	3:F:89:GLY:HA3	2.01	0.43
2:B:137:THR:HG22	2:B:182:THR:HG23	2.01	0.43
1:D:116:ILE:O	1:D:117:PHE:CD1	2.72	0.43
2:E:84:ASN:HA	2:E:111:VAL:CG1	2.48	0.43
3:F:65:GLU:O	3:F:72:LYS:NZ	2.52	0.43
3:F:72:LYS:CA	3:F:72:LYS:NZ	2.82	0.43
1:A:206:LYS:HB2	1:A:206:LYS:HE2	1.90	0.43
1:D:181:THR:OG1	1:D:184:GLU:CB	2.67	0.43
2:E:61:ASP:C	2:E:63:PHE:H	2.22	0.43
2:E:64:LYS:HE3	2:E:64:LYS:HB2	1.76	0.43
2:E:70:SER:OG	2:E:79:PHE:HB2	2.19	0.43
1:A:211:ASN:O	1:A:212:GLU:CB	2.66	0.43
1:A:85:THR:HA	1:A:102:THR:O	2.19	0.43
1:D:150:ASP:HB3	1:D:190:SER:H	1.82	0.43
1:D:159:LEU:CD2	2:E:169:VAL:HG11	2.49	0.43
1:D:58:VAL:HA	1:D:59:PRO:HD2	1.89	0.43
1:A:30:SER:OG	1:A:92:HIS:CD2	2.71	0.43
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.54	0.43
2:E:112:SER:HG	2:E:146:PHE:HZ	1.59	0.42
1:D:210:ARG:HG3	1:D:211:ASN:N	2.34	0.42
3:F:20:ARG:CG	3:F:20:ARG:NH1	2.57	0.42
1:D:159:LEU:HB3	1:D:177:THR:HB	2.01	0.42
1:D:33:LEU:HD22	1:D:71:TYR:CB	2.50	0.42
1:A:11:MET:CE	1:A:19:VAL:HG13	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:O	1:A:213:CYS:HB2	2.18	0.42
1:D:211:ASN:O	1:D:212:GLU:HB3	2.19	0.42
1:D:35:TRP:HB2	1:D:48:ILE:HB	2.01	0.42
1:A:181:THR:OG1	1:A:184:GLU:CB	2.67	0.42
1:D:33:LEU:HD22	1:D:71:TYR:CG	2.54	0.42
3:C:14:GLN:O	3:C:15:ASN:HB2	2.19	0.42
3:C:67:SER:CA	3:C:71:GLY:HA2	2.49	0.42
1:D:9:ALA:C	1:D:10:ILE:HD12	2.40	0.42
2:E:5:VAL:HG23	2:E:105:GLN:HE22	1.85	0.42
2:B:6:GLN:HE22	2:B:91:PHE:HA	1.85	0.42
2:E:137:THR:HG22	2:E:182:THR:HG23	2.02	0.42
1:D:38:GLN:O	1:D:84:ALA:HB1	2.20	0.42
2:E:50:TRP:CZ2	3:F:8:VAL:O	2.68	0.42
1:A:15:LEU:HD21	1:A:106:ILE:HD13	2.02	0.42
2:B:146:PHE:HA	2:B:147:PRO:HA	1.74	0.42
1:D:114:VAL:HA	1:D:134:PHE:O	2.20	0.42
2:B:64:LYS:HE3	2:B:64:LYS:HB2	1.80	0.41
2:B:82(A):ILE:HG13	2:B:82(B):ASN:CG	2.39	0.41
2:B:84:ASN:HA	2:B:111:VAL:CG1	2.50	0.41
3:F:22:LEU:C	3:F:24:GLU:H	2.23	0.41
1:D:139:TYR:CZ	1:D:140:PRO:HD3	2.55	0.41
1:A:194:GLU:HG2	1:A:205:VAL:HG22	2.02	0.41
3:C:22:LEU:HD11	3:C:96:HIS:N	2.34	0.41
1:D:133:CYS:HB2	1:D:147:TRP:HH2	1.84	0.41
1:A:159:LEU:HB3	1:A:177:THR:HB	2.03	0.41
1:A:24:THR:HA	1:A:69:THR:O	2.21	0.41
3:C:7:CYS:SG	3:C:26:GLU:CG	3.08	0.41
1:D:6:GLN:CD	1:D:101:GLY:H	2.24	0.41
1:D:104:LEU:HA	1:D:104:LEU:HD23	1.81	0.41
2:E:63:PHE:HD1	2:E:67:PHE:CE2	2.39	0.41
3:F:7:CYS:SG	3:F:26:GLU:CG	3.09	0.41
1:A:109:ASP:HA	1:A:139:TYR:HB3	2.03	0.41
1:A:10:ILE:HG13	1:A:103:LYS:HB2	2.03	0.41
1:A:48:ILE:HD12	1:A:73:LEU:HD12	2.03	0.41
3:C:50:ASN:HD22	3:C:50:ASN:HA	1.53	0.41
1:A:118:PRO:HG3	1:A:208:PHE:HE2	0.65	0.41
1:A:30:SER:C	1:A:32:TYR:H	2.12	0.41
1:D:204:ILE:HG22	1:D:204:ILE:O	2.21	0.41
2:E:116:THR:HA	2:E:146:PHE:O	2.21	0.41
2:E:2:LEU:HD22	2:E:27:TYR:CD1	2.55	0.41
2:E:35:GLN:HG3	2:E:95:ASN:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:TYR:CD2	1:D:140:PRO:N	2.89	0.40
1:D:50:THR:O	1:D:50:THR:HG22	2.21	0.40
1:D:4:MET:HE3	1:D:97:THR:O	2.19	0.40
2:E:116:THR:CG2	2:E:202:SER:HB3	2.51	0.40
3:F:3:SER:H	3:F:6:GLN:HB2	1.86	0.40
2:B:61:ASP:O	2:B:63:PHE:N	2.54	0.40
2:E:35:GLN:NE2	2:E:47:TRP:HE1	2.17	0.40
1:D:24:THR:HA	1:D:69:THR:O	2.21	0.40
2:E:208:LYS:HD3	2:E:208:LYS:HA	1.95	0.40
3:F:80:LYS:O	3:F:81:PRO:C	2.59	0.40
2:B:2:LEU:HD12	2:B:102:PHE:CE1	2.56	0.40
1:D:194:GLU:HG2	1:D:205:VAL:HG22	2.03	0.40
2:E:113:SER:C	2:E:114:ALA:O	2.58	0.40
1:A:116:ILE:O	1:A:117:PHE:CD1	2.75	0.40
2:E:13:LYS:NZ	2:E:13:LYS:H	2.20	0.40
2:E:40:LEU:HB3	2:E:41:PRO:CD	2.46	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	213/215 (99%)	174 (82%)	26 (12%)	13 (6%)	1	5
1	D	213/215 (99%)	178 (84%)	22 (10%)	13 (6%)	1	5
2	B	218/219 (100%)	192 (88%)	16 (7%)	10 (5%)	2	10
2	E	217/219 (99%)	191 (88%)	18 (8%)	8 (4%)	4	15
3	C	94/99 (95%)	79 (84%)	10 (11%)	5 (5%)	2	7
3	F	95/99 (96%)	80 (84%)	9 (10%)	6 (6%)	1	4
All	All	1050/1066 (98%)	894 (85%)	101 (10%)	55 (5%)	2	7

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	124	LEU
1	A	140	PRO
1	A	150	ASP
1	A	185	TYR
1	A	202	SER
1	A	211	ASN
2	B	41	PRO
2	B	43	LYS
2	B	73	THR
2	B	82(C)	LEU
2	B	102	PHE
3	C	48	THR
3	C	66	ASP
1	D	31	SER
1	D	80	ALA
1	D	124	LEU
1	D	140	PRO
1	D	150	ASP
1	D	185	TYR
1	D	202	SER
1	D	211	ASN
1	D	212	GLU
2	E	82(C)	LEU
3	F	48	THR
3	F	70	ASN
1	A	68	GLY
1	A	186	GLU
1	D	186	GLU
2	E	43	LYS
2	E	73	THR
2	E	102	PHE
3	F	69	SER
2	B	62	ASP
3	C	67	SER
1	A	109	ASP
3	C	72	LYS
1	D	68	GLY
3	F	94	HIS
1	A	76	SER
1	A	156	ASN
1	A	184	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	135	SER
1	D	156	ASN
1	D	184	GLU
2	E	41	PRO
2	E	62	ASP
3	F	96	HIS
2	B	40	LEU
2	B	100	ASP
2	E	135	SER
3	C	81	PRO
2	B	127	VAL
2	E	127	VAL
3	F	81	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/190 (100%)	170 (90%)	20 (10%)	7	23
1	D	190/190 (100%)	175 (92%)	15 (8%)	13	37
2	B	188/187 (100%)	170 (90%)	18 (10%)	9	28
2	E	187/187 (100%)	171 (91%)	16 (9%)	11	33
3	C	86/90 (96%)	74 (86%)	12 (14%)	4	11
3	F	87/90 (97%)	74 (85%)	13 (15%)	3	10
All	All	928/934 (99%)	834 (90%)	94 (10%)	8	25

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	4	MET
1	A	7	THR
1	A	20	THR
1	A	21	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	33	LEU
1	A	56	SER
1	A	90	GLN
1	A	94	SER
1	A	104	LEU
1	A	107	ARG
1	A	122	GLU
1	A	140	PRO
1	A	142	ASP
1	A	145	VAL
1	A	167	SER
1	A	180	LEU
1	A	208	PHE
1	A	210	ARG
1	A	213	CYS
2	B	5	VAL
2	B	13	LYS
2	B	38	GLN
2	B	44	ASP
2	B	56	VAL
2	B	61	ASP
2	B	73	THR
2	B	82(B)	ASN
2	B	82(C)	LEU
2	B	84	ASN
2	B	92	CYS
2	B	94	ARG
2	B	128	CYS
2	B	131	THR
2	B	170	LEU
2	B	187	THR
2	B	191	GLN
2	B	206	VAL
3	C	1	ASN
3	C	3	SER
3	C	9	LYS
3	C	10	LYS
3	C	20	ARG
3	C	32	LEU
3	C	40	LYS
3	C	46	ASN
3	C	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	83	SER
3	C	94	HIS
3	C	95	HIS
1	D	1	ASP
1	D	4	MET
1	D	7	THR
1	D	27(A)	SER
1	D	33	LEU
1	D	63	SER
1	D	70	SER
1	D	104	LEU
1	D	116	ILE
1	D	122	GLU
1	D	140	PRO
1	D	167	SER
1	D	180	LEU
1	D	208	PHE
1	D	210	ARG
2	E	5	VAL
2	E	13	LYS
2	E	44	ASP
2	E	56	VAL
2	E	61	ASP
2	E	73	THR
2	E	82(B)	ASN
2	E	82(C)	LEU
2	E	84	ASN
2	E	94	ARG
2	E	128	CYS
2	E	131	THR
2	E	170	LEU
2	E	187	THR
2	E	191	GLN
2	E	206	VAL
3	F	3	SER
3	F	4	GLN
3	F	9	LYS
3	F	10	LYS
3	F	20	ARG
3	F	32	LEU
3	F	40	LYS
3	F	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	50	ASN
3	F	66	ASP
3	F	70	ASN
3	F	72	LYS
3	F	83	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	92	HIS
1	A	197	HIS
2	B	6	GLN
2	B	35	GLN
2	B	164	HIS
2	B	171	GLN
3	C	4	GLN
3	C	44	ASN
3	C	46	ASN
3	C	50	ASN
3	C	52	ASN
3	C	95	HIS
1	D	89	HIS
1	D	92	HIS
1	D	197	HIS
1	D	211	ASN
2	E	6	GLN
2	E	35	GLN
2	E	171	GLN
3	F	36	GLN
3	F	44	ASN
3	F	46	ASN
3	F	50	ASN
3	F	52	ASN
3	F	96	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CAC	C	1096	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	F	1097	-	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAC	C	1096	-	-	0/0/0/0	0/0/0/0
4	CAC	F	1097	-	-	0/0/0/0	0/0/0/0

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, 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	215/215 (100%)	0.35	30 (13%) 2 2	8, 11, 13, 16	0
1	D	215/215 (100%)	1.27	51 (23%) 0 0	9, 11, 13, 16	0
2	B	219/219 (100%)	0.65	22 (10%) 7 5	10, 11, 12, 15	0
2	E	219/219 (100%)	1.43	57 (26%) 0 0	10, 11, 12, 13	0
3	C	96/99 (96%)	0.32	10 (10%) 6 4	9, 11, 17, 23	0
3	F	97/99 (97%)	-0.01	4 (4%) 37 32	9, 11, 16, 21	0
All	All	1061/1066 (99%)	0.78	174 (16%) 1 1	8, 11, 13, 23	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	96	HIS	18.9
2	E	128	CYS	13.6
2	E	131	THR	12.7
2	E	127	VAL	12.2
1	A	213	CYS	12.0
1	D	204	ILE	11.5
2	B	129	GLY	11.4
1	A	180	LEU	11.0
1	D	185	TYR	10.9
1	A	129	ALA	10.8
1	D	147	TRP	9.9
3	F	1	ASN	9.6
2	E	129	GLY	9.2
2	E	112	SER	8.9
2	E	147	PRO	8.7
1	D	196	THR	8.3
1	D	145	VAL	8.3
3	F	2	ILE	8.0
2	B	130	ASP	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	149	ILE	7.1
1	D	213	CYS	7.1
1	D	195	ALA	7.0
1	D	143	ILE	6.9
2	E	137	THR	6.7
1	D	203	PRO	6.7
1	D	129	ALA	6.7
1	D	180	LEU	6.5
1	D	187	ARG	6.3
2	B	128	CYS	6.2
2	E	192	SER	6.1
2	E	183	VAL	5.8
1	D	154	ARG	5.7
2	E	130	ASP	5.7
3	C	1	ASN	5.7
2	E	125	ALA	5.6
1	D	192	THR	5.5
1	D	197	HIS	5.5
2	E	138	LEU	5.4
2	E	136	VAL	5.4
1	D	152	SER	5.3
2	E	190	SER	5.3
1	D	186	GLU	5.2
2	E	188	TRP	5.2
1	D	205	VAL	5.1
1	A	196	THR	5.1
2	E	113	SER	5.1
2	B	182	THR	5.1
1	D	133	CYS	5.0
1	D	148	LYS	5.0
1	A	178	LEU	4.9
3	C	95	HIS	4.8
1	D	131	VAL	4.8
2	E	191	GLN	4.6
2	B	11	LEU	4.6
1	D	183	ASP	4.5
3	F	97	HIS	4.4
2	B	190	SER	4.4
1	A	179	THR	4.4
2	E	126	PRO	4.3
1	D	178	LEU	4.3
3	C	71	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	157	GLY	4.2
2	E	184	THR	4.1
1	D	191	TYR	4.1
2	E	186	SER	4.1
1	A	128	GLY	4.1
1	D	110	ALA	4.0
1	D	117	PHE	4.0
1	A	186	GLU	4.0
1	D	141	LYS	3.9
3	C	66	ASP	3.9
1	A	124	LEU	3.9
1	D	151	GLY	3.9
2	E	82(B)	ASN	3.8
2	E	163	VAL	3.7
1	D	128	GLY	3.7
2	E	211	GLU	3.7
1	D	157	GLY	3.7
2	E	142	VAL	3.7
2	B	183	VAL	3.6
1	D	118	PRO	3.6
2	B	110	THR	3.6
2	E	146	PHE	3.6
2	E	181	VAL	3.6
2	E	197	VAL	3.5
1	A	191	TYR	3.4
1	D	193	CYS	3.4
2	E	120	SER	3.3
2	E	139	GLY	3.3
2	E	82(A)	ILE	3.3
2	E	159	LEU	3.2
1	D	208	PHE	3.2
2	E	194	THR	3.2
2	B	111	VAL	3.1
2	B	193	ILE	3.1
1	A	208	PHE	3.1
2	B	159	LEU	3.1
2	B	202	SER	3.1
2	E	193	ILE	3.0
2	E	13	LYS	3.0
2	B	154	TRP	3.0
1	D	156	ASN	3.0
2	E	196	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	160	SER	3.0
1	A	187	ARG	3.0
2	E	201	ALA	2.9
1	A	146	LYS	2.9
2	E	156	SER	2.9
2	E	140	CYS	2.9
2	B	147	PRO	2.9
1	A	204	ILE	2.9
2	B	138	LEU	2.9
2	E	198	ALA	2.9
3	C	72	LYS	2.9
1	A	148	LYS	2.9
1	A	147	TRP	2.9
2	E	20	ILE	2.8
1	A	132	VAL	2.8
2	E	123	PRO	2.8
2	B	137	THR	2.8
2	B	194	THR	2.8
1	A	183	ASP	2.8
2	E	111	VAL	2.8
2	E	203	SER	2.7
2	B	146	PHE	2.7
1	A	185	TYR	2.6
1	D	179	THR	2.6
1	A	130	SER	2.6
2	B	188	TRP	2.6
3	C	67	SER	2.6
1	D	155	GLN	2.6
2	E	121	VAL	2.6
1	A	209	ASN	2.5
1	D	139	TYR	2.5
1	D	114	VAL	2.5
1	D	134	PHE	2.5
1	D	184	GLU	2.5
1	D	135	LEU	2.5
1	A	190	SER	2.4
2	E	185	SER	2.4
1	D	194	GLU	2.4
1	A	152	SER	2.4
1	D	116	ILE	2.4
1	D	182	LYS	2.4
2	E	154	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	70	ASN	2.4
2	E	118	ALA	2.4
1	A	133	CYS	2.4
1	A	154	ARG	2.3
1	D	130	SER	2.3
3	C	2	ILE	2.3
1	A	157	GLY	2.3
1	D	209	ASN	2.3
1	A	192	THR	2.2
3	C	69	SER	2.2
2	E	18	VAL	2.2
2	E	172	SER	2.2
2	E	180	SER	2.2
1	A	131	VAL	2.2
2	B	139	GLY	2.2
3	F	96	HIS	2.2
1	D	138	PHE	2.1
1	A	115	SER	2.1
2	E	14	PRO	2.1
1	D	201	THR	2.1
2	E	212	PRO	2.1
1	D	144	ASN	2.1
1	D	212	GLU	2.1
2	B	163	VAL	2.1
2	E	90	TYR	2.0
2	B	150	VAL	2.0
2	E	114	ALA	2.0
2	E	82	ILE	2.0
1	A	177	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CAC	C	1096	5/5	0.92	0.08	20,20,20,79	4
4	CAC	F	1097	5/5	0.95	0.10	20,20,20,76	4

6.5 Other polymers [i](#)

There are no such residues in this entry.