Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 07:22 PM EDT

PDB ID	:	5UOE
Title	:	Crystal Structure Analysis of Elbow-Engineered-Fab-Bound Human Insulin Degrading Enzyme (IDE)
Authors	:	Liang, W.G.; Bailey, L.; Kossiakoff, T.; Tang, W.J.
Deposited on	:	2017-01-31
Resolution	:	3.80 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 (1)) were used in the production of this report:

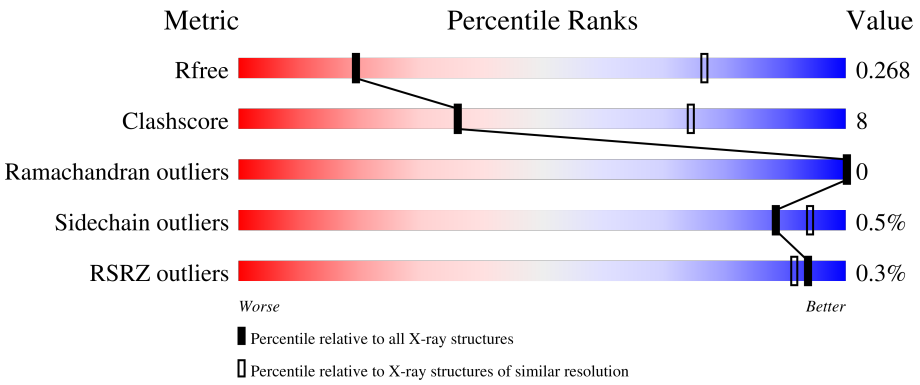
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	990	79% 17% ·
1	B	990	79% 17% ·
1	C	990	75% 21% ·
1	D	990	76% 20% ·
1	E	990	77% 19% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	229	44% 8% 48%
2	M	229	% 37% 14% 49%
2	P	229	32% 19% 48%
2	S	229	43% 8% 49%
2	V	229	39% 12% 49%
3	L	215	40% 10% • 50%
3	N	215	41% 9% 49%
3	Q	215	37% 13% 50%
3	T	215	34% 14% • 50%
3	W	215	34% 14% 51%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47331 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	953	7762	5003	1302	1435	22	0	0	0
1	B	952	7752	4997	1303	1430	22	0	0	0
1	C	953	7770	5009	1308	1431	22	0	0	0
1	D	953	7764	5006	1307	1429	22	0	0	0
1	E	953	7764	5006	1307	1429	22	0	0	0

There are 125 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
C	30	MET	-	expression tag	UNP P14735
C	31	HIS	-	expression tag	UNP P14735
C	32	HIS	-	expression tag	UNP P14735
C	33	HIS	-	expression tag	UNP P14735
C	34	HIS	-	expression tag	UNP P14735
C	35	HIS	-	expression tag	UNP P14735
C	36	HIS	-	expression tag	UNP P14735
C	37	ALA	-	expression tag	UNP P14735
C	38	ALA	-	expression tag	UNP P14735
C	39	GLY	-	expression tag	UNP P14735
C	40	ILE	-	expression tag	UNP P14735

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	PRO	-	expression tag	UNP P14735
C	110	LEU	CYS	engineered mutation	UNP P14735
C	171	SER	CYS	engineered mutation	UNP P14735
C	178	ALA	CYS	engineered mutation	UNP P14735
C	257	VAL	CYS	engineered mutation	UNP P14735
C	414	LEU	CYS	engineered mutation	UNP P14735
C	573	ASN	CYS	engineered mutation	UNP P14735
C	590	SER	CYS	engineered mutation	UNP P14735
C	789	SER	CYS	engineered mutation	UNP P14735
C	812	ALA	CYS	engineered mutation	UNP P14735
C	819	ALA	CYS	engineered mutation	UNP P14735
C	904	SER	CYS	engineered mutation	UNP P14735
C	966	ASN	CYS	engineered mutation	UNP P14735
C	974	ALA	CYS	engineered mutation	UNP P14735
D	30	MET	-	expression tag	UNP P14735
D	31	HIS	-	expression tag	UNP P14735
D	32	HIS	-	expression tag	UNP P14735
D	33	HIS	-	expression tag	UNP P14735
D	34	HIS	-	expression tag	UNP P14735
D	35	HIS	-	expression tag	UNP P14735
D	36	HIS	-	expression tag	UNP P14735
D	37	ALA	-	expression tag	UNP P14735
D	38	ALA	-	expression tag	UNP P14735
D	39	GLY	-	expression tag	UNP P14735
D	40	ILE	-	expression tag	UNP P14735
D	41	PRO	-	expression tag	UNP P14735
D	110	LEU	CYS	engineered mutation	UNP P14735
D	171	SER	CYS	engineered mutation	UNP P14735
D	178	ALA	CYS	engineered mutation	UNP P14735
D	257	VAL	CYS	engineered mutation	UNP P14735
D	414	LEU	CYS	engineered mutation	UNP P14735
D	573	ASN	CYS	engineered mutation	UNP P14735
D	590	SER	CYS	engineered mutation	UNP P14735
D	789	SER	CYS	engineered mutation	UNP P14735
D	812	ALA	CYS	engineered mutation	UNP P14735
D	819	ALA	CYS	engineered mutation	UNP P14735
D	904	SER	CYS	engineered mutation	UNP P14735
D	966	ASN	CYS	engineered mutation	UNP P14735
D	974	ALA	CYS	engineered mutation	UNP P14735
E	30	MET	-	expression tag	UNP P14735
E	31	HIS	-	expression tag	UNP P14735
E	32	HIS	-	expression tag	UNP P14735

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	HIS	-	expression tag	UNP P14735
E	34	HIS	-	expression tag	UNP P14735
E	35	HIS	-	expression tag	UNP P14735
E	36	HIS	-	expression tag	UNP P14735
E	37	ALA	-	expression tag	UNP P14735
E	38	ALA	-	expression tag	UNP P14735
E	39	GLY	-	expression tag	UNP P14735
E	40	ILE	-	expression tag	UNP P14735
E	41	PRO	-	expression tag	UNP P14735
E	110	LEU	CYS	engineered mutation	UNP P14735
E	171	SER	CYS	engineered mutation	UNP P14735
E	178	ALA	CYS	engineered mutation	UNP P14735
E	257	VAL	CYS	engineered mutation	UNP P14735
E	414	LEU	CYS	engineered mutation	UNP P14735
E	573	ASN	CYS	engineered mutation	UNP P14735
E	590	SER	CYS	engineered mutation	UNP P14735
E	789	SER	CYS	engineered mutation	UNP P14735
E	812	ALA	CYS	engineered mutation	UNP P14735
E	819	ALA	CYS	engineered mutation	UNP P14735
E	904	SER	CYS	engineered mutation	UNP P14735
E	966	ASN	CYS	engineered mutation	UNP P14735
E	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called FAB Heavy chain with engineered elbow.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	119	901	568	153	177	3	0	0	0
2	M	117	882	555	150	174	3	0	0	0
2	P	118	893	564	151	175	3	0	0	0
2	S	117	882	555	150	174	3	0	0	0
2	V	117	881	555	150	173	3	0	0	0

- Molecule 3 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	108	820	516	136	165	3	0	0	0

Continued on next page...

Continued from previous page...

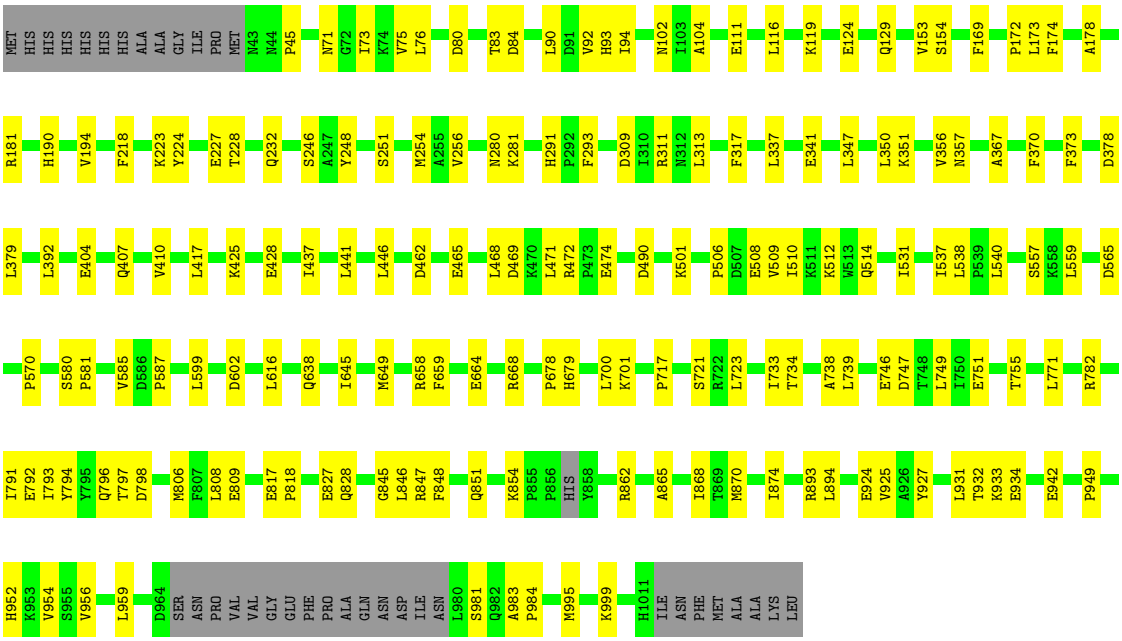
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	N	109	827	520	137	167	3	0	0	0
			Total	C	N	O	S			
3	Q	108	820	516	136	165	3	0	0	0
			Total	C	N	O	S			
3	T	107	815	513	135	164	3	0	0	0
			Total	C	N	O	S			
3	W	105	798	501	132	162	3	0	0	0

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.

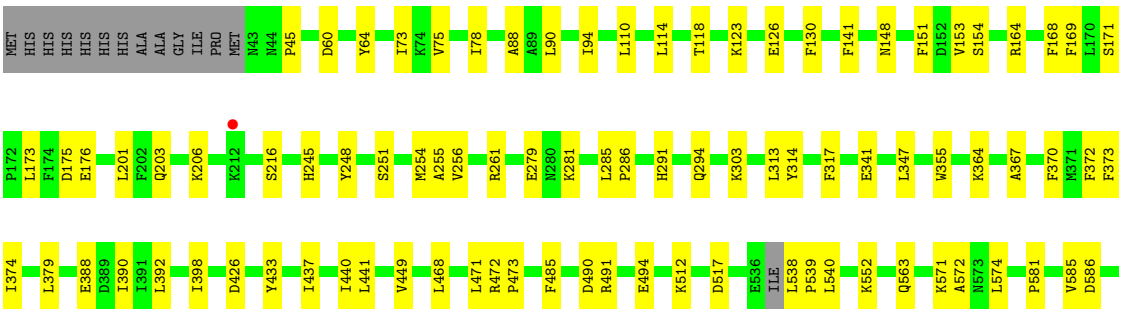
• Molecule 1: Insulin-degrading enzyme

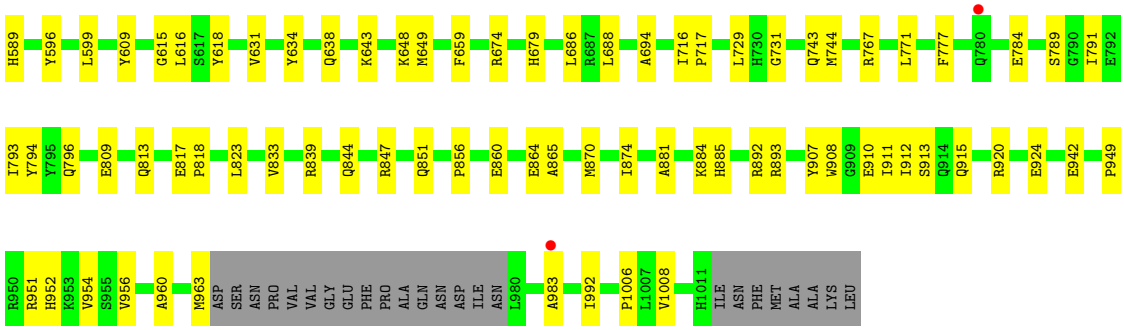
Chain A:



• Molecule 1: Insulin-degrading enzyme

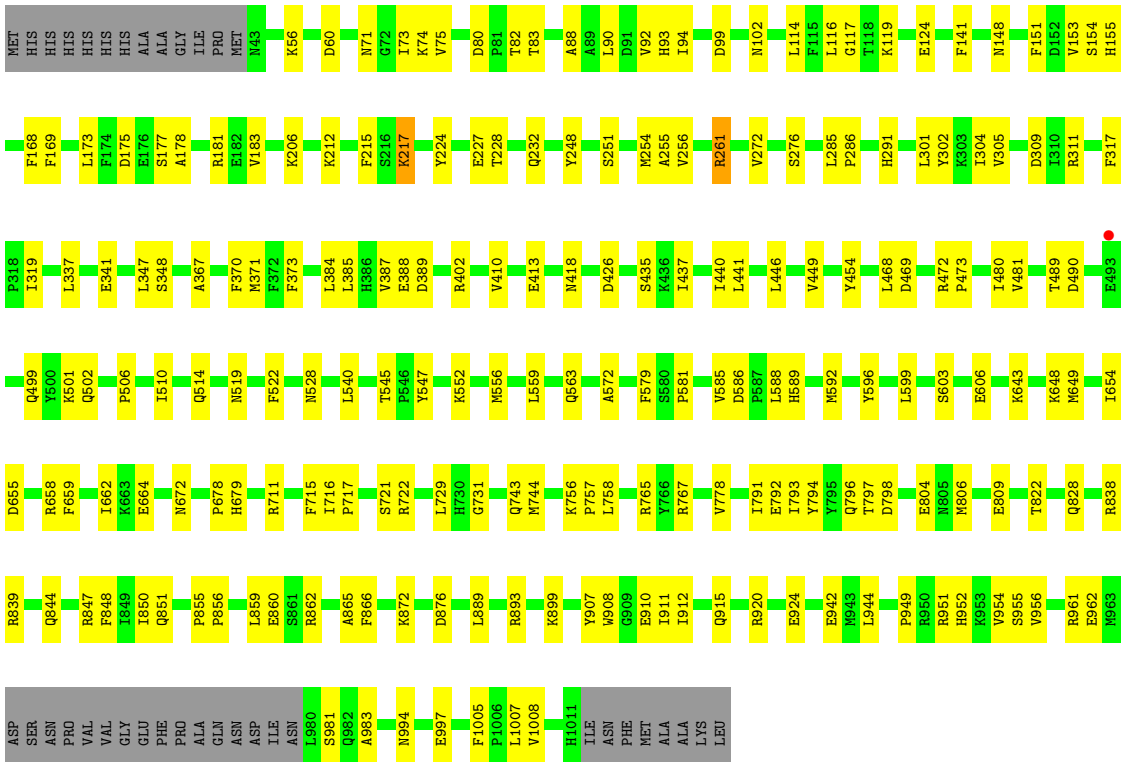
Chain B:





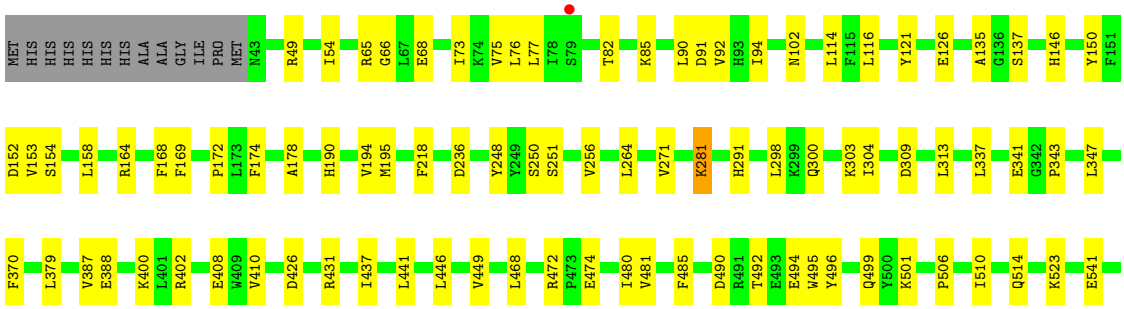
• Molecule 1: Insulin-degrading enzyme

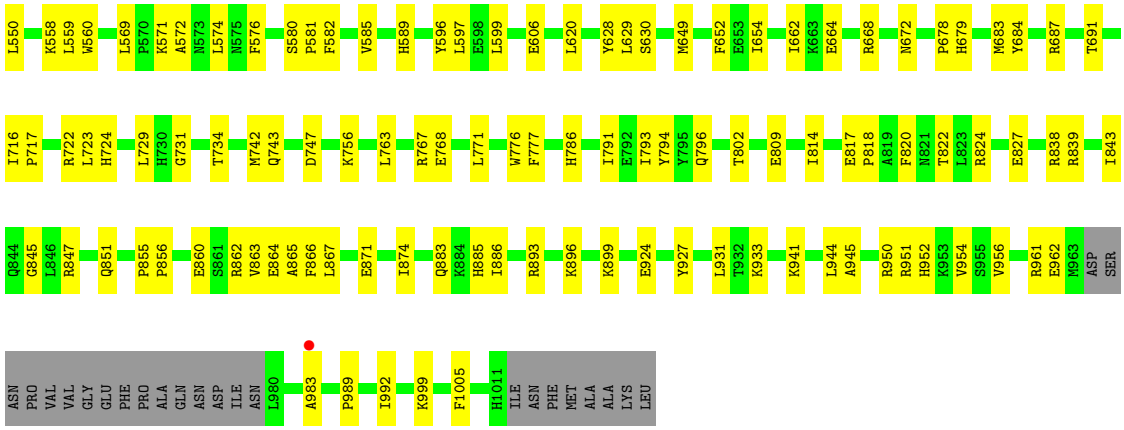
Chain C:



• Molecule 1: Insulin-degrading enzyme

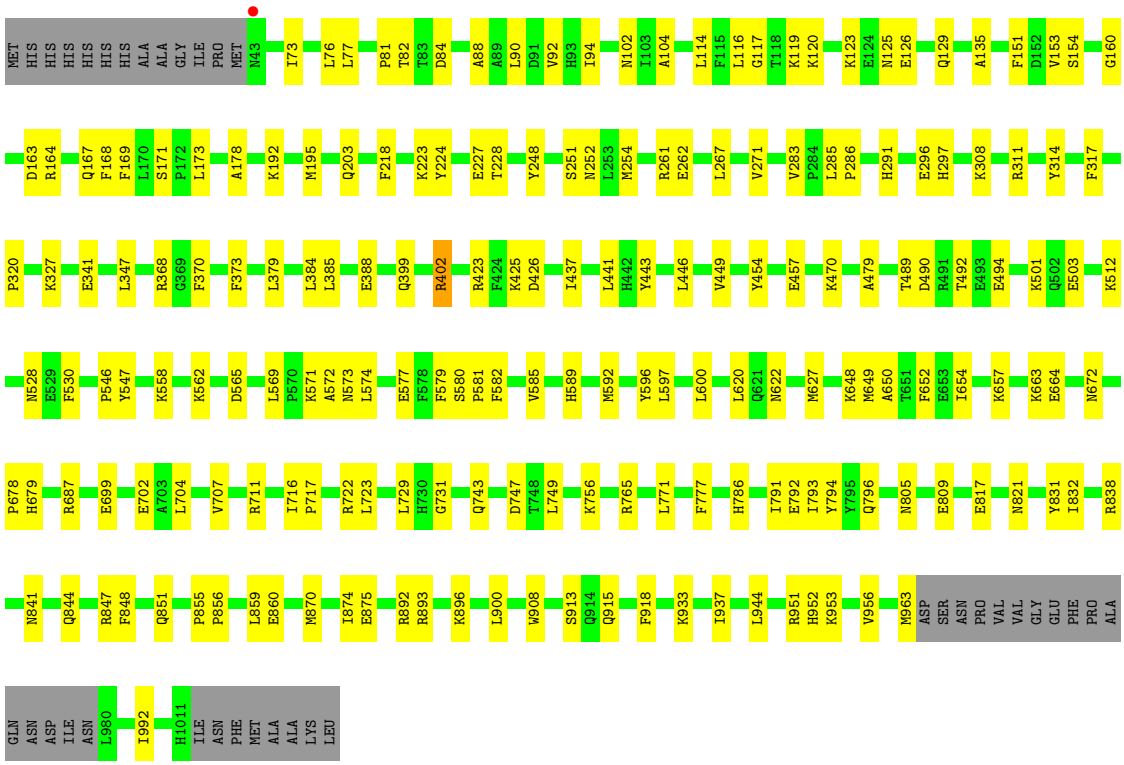
Chain D:





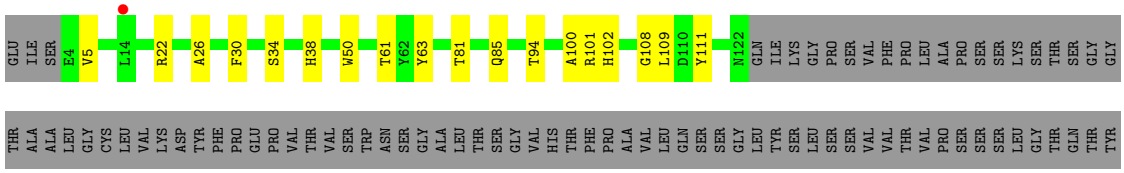
• Molecule 1: Insulin-degrading enzyme

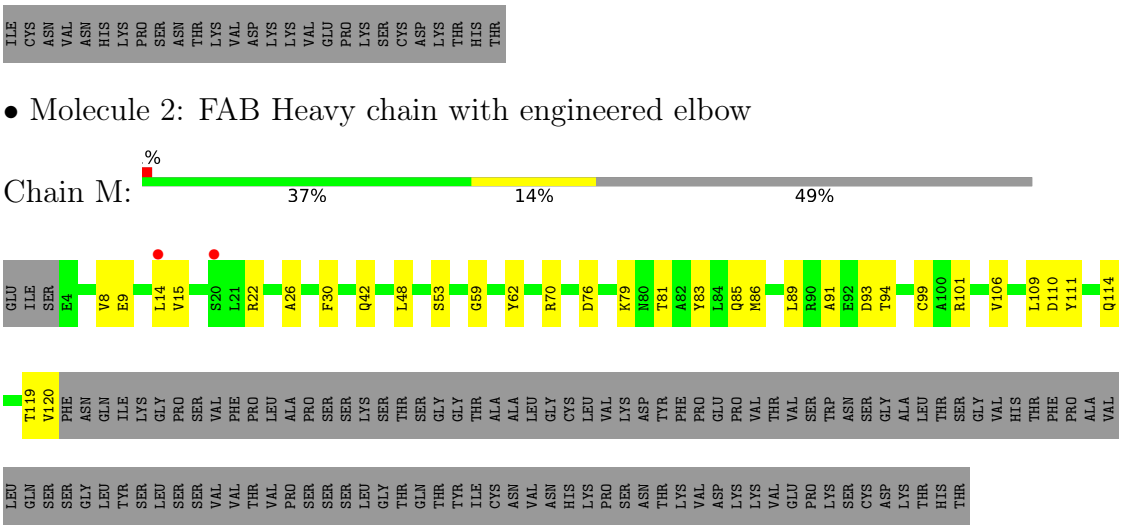
Chain E: 77% 19% •

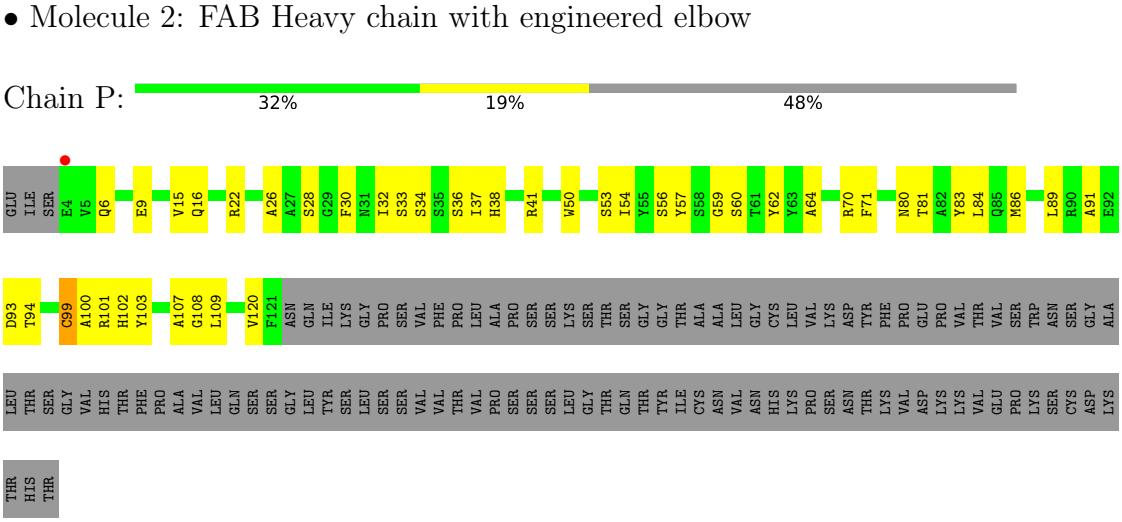


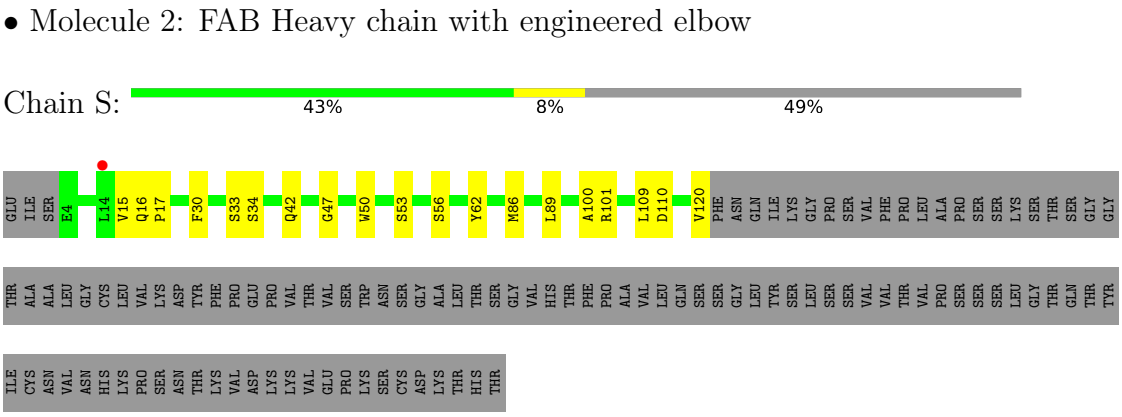
• Molecule 2: FAB Heavy chain with engineered elbow

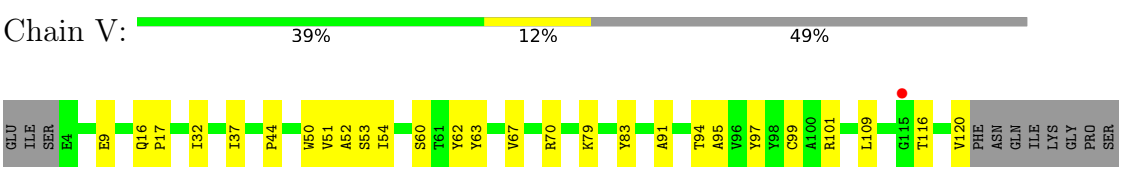
Chain H: 44% 8% 48%

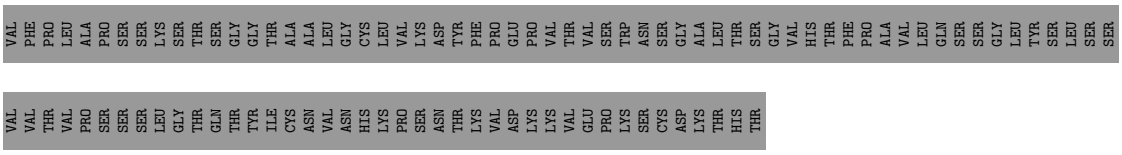



ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR
• Molecule 2: FAB Heavy chain with engineered elbow
Chain M:
%
37%
14%
49%
GLU ILE SER E4 V8 E9 L14 V15 S20 L21 R22 A26 F30 Q42 L48 S53 G59 Y62 R70 D76 K79 N80 T81 A82 Y83 L84 Q85 M86 L89 R90 A91 E92 D93 T94 C99 A100 R101 V106 L109 D110 Y111 Q114
T119 V120 PHE ASN GLN ILE LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL
LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR


• Molecule 2: FAB Heavy chain with engineered elbow
Chain P:
32%
19%
48%
GLU ILE SER E4 V5 Q6 E9 V15 Q16 R22 A26 A27 S28 G29 F30 N31 I32 S33 S34 S35 S36 I37 H38 R41 W50 S53 I54 Y55 S56 Y57 S58 G59 S60 T61 Y62 Y63 A64 R70 F71 N80 T81 A82 Y83 L84 Q85 M86 L89 R90 A91 E92
D93 T94 C99 A100 R101 H102 Y103 A107 G108 L109 V120 F121 ASN GLN ILE LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA
LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS
THR HIS THR

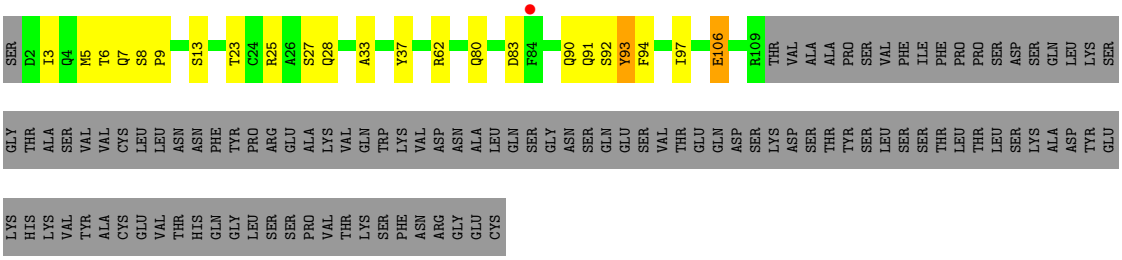

• Molecule 2: FAB Heavy chain with engineered elbow
Chain S:
43%
8%
49%
GLU ILE SER E4 L14 V15 Q16 P17 F30 S33 S34 Q42 G47 W50 S53 S56 Y62 M86 L89 A100 R101 L109 D110 V120 PHE ASN GLN ILE LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY
THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR
ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR


• Molecule 2: FAB Heavy chain with engineered elbow
Chain V:
39%
12%
49%
GLU ILE SER E4 E9 Q16 P17 I32 I37 P44 W50 V51 A52 S53 I54 S60 T61 Y62 Y63 V67 R70 K79 Y83 A91 T94 A95 Y96 Y97 Y98 C99 A100 R101 L109 G115 T116 V120 PHE ASN GLN ILE LYS GLY PRO SER



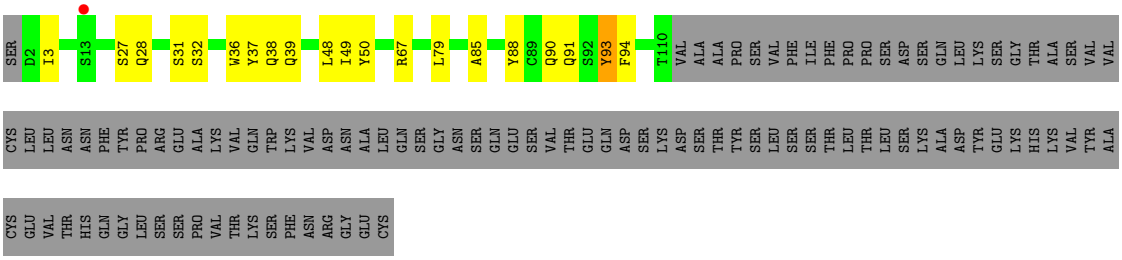
• Molecule 3: FAB light chain

Chain L:



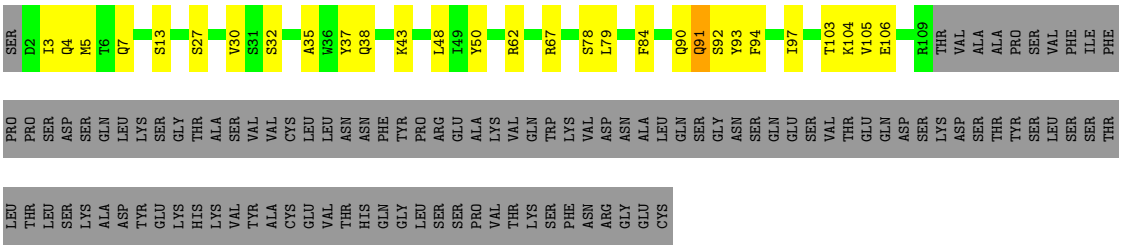
• Molecule 3: FAB light chain

Chain N:



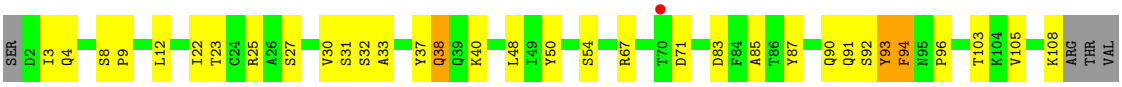
• Molecule 3: FAB light chain

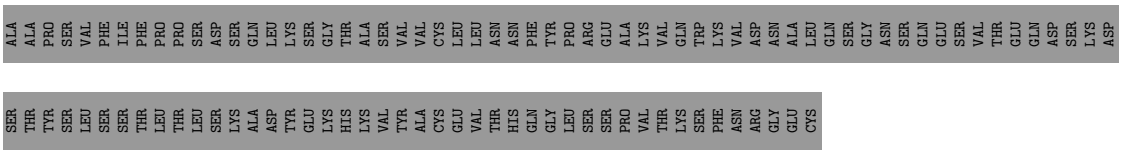
Chain Q:



• Molecule 3: FAB light chain

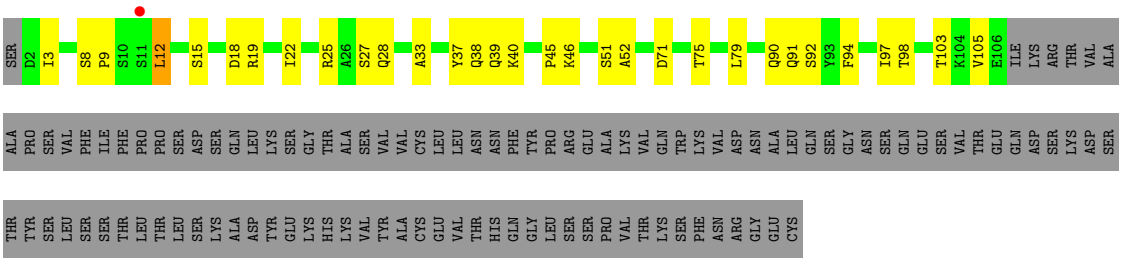
Chain T:





• Molecule 3: FAB light chain

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.32Å 242.05Å 310.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.80 49.24 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-3.80) 91.4 (49.24-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.220 , 0.270 0.220 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	47331	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% 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)

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	0.26	0/7955	0.42	0/10764
1	B	0.26	0/7946	0.42	0/10752
1	C	0.27	0/7965	0.43	0/10777
1	D	0.26	0/7959	0.42	0/10771
1	E	0.26	0/7959	0.42	0/10771
2	H	0.28	0/922	0.50	0/1253
2	M	0.26	0/902	0.50	0/1226
2	P	0.26	0/914	0.48	0/1242
2	S	0.26	0/902	0.47	0/1226
2	V	0.29	0/901	0.51	0/1224
3	L	0.35	0/838	0.55	1/1137 (0.1%)
3	N	0.28	0/845	0.50	0/1147
3	Q	0.35	0/838	0.53	0/1137
3	T	0.27	0/833	0.49	0/1130
3	W	0.29	0/816	0.54	0/1108
All	All	0.27	0/48495	0.44	1/65665 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	93	TYR	C-N-CA	-5.01	109.18	121.70

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	7762	0	7681	98	0
1	B	7752	0	7669	100	0
1	C	7770	0	7703	132	0
1	D	7764	0	7695	120	0
1	E	7764	0	7695	114	0
2	H	901	0	856	16	0
2	M	882	0	841	28	0
2	P	893	0	850	38	0
2	S	882	0	841	14	0
2	V	881	0	840	21	0
3	L	820	0	797	19	0
3	N	827	0	804	16	0
3	Q	820	0	797	26	0
3	T	815	0	795	29	0
3	W	798	0	771	23	0
All	All	47331	0	46635	755	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 8.

All (755) 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:402:ARG:HG3	1:C:468:LEU:HD21	1.46	0.97
1:E:716:ILE:HB	1:E:717:PRO:HD3	1.58	0.86
3:W:3:ILE:HG13	3:W:27:SER:HB3	1.60	0.84
1:C:599:LEU:HD23	1:C:662:ILE:HD12	1.61	0.83
1:C:893:ARG:HG3	1:C:893:ARG:HH11	1.42	0.82
1:E:838:ARG:HB2	1:E:847:ARG:HD3	1.66	0.78
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.65	0.77
1:C:94:ILE:HG13	1:C:248:TYR:HB3	1.66	0.77
2:M:86:MET:HB3	2:M:89:LEU:HD21	1.69	0.74
3:L:8:SER:HB3	3:L:9:PRO:HD3	1.71	0.73
1:C:596:TYR:OH	1:C:649:MET:O	2.08	0.72
1:E:574:LEU:HG	1:E:729:LEU:HD22	1.72	0.71
1:E:489:THR:HA	1:E:501:LYS:HB2	1.74	0.70
2:H:109:LEU:HB2	3:L:37:TYR:OH	1.93	0.69
3:L:8:SER:HB2	3:L:23:THR:HB	1.74	0.68
2:S:101:ARG:O	2:S:109:LEU:HA	1.94	0.67
1:B:809:GLU:HG3	1:B:839:ARG:HH22	1.60	0.67
2:S:86:MET:HB3	2:S:89:LEU:HD21	1.75	0.67
1:B:538:LEU:N	1:B:539:PRO:CD	2.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:9:PRO:O	3:W:103:THR:HG22	1.95	0.66
1:E:203:GLN:HB3	1:E:494:GLU:OE2	1.95	0.66
3:T:8:SER:HB3	3:T:9:PRO:HD3	1.78	0.66
1:C:596:TYR:CD1	1:C:716:ILE:HG12	2.30	0.66
1:A:508:GLU:O	1:A:512:LYS:HG3	1.96	0.65
1:B:123:LYS:HB2	1:B:126:GLU:HB2	1.77	0.65
1:C:893:ARG:HG3	1:C:893:ARG:NH1	2.10	0.65
1:A:124:GLU:OE2	1:A:181:ARG:NH2	2.30	0.65
2:V:50:TRP:HZ2	2:V:53:SER:HB3	1.61	0.65
2:V:51:VAL:HG12	2:V:52:ALA:H	1.59	0.65
1:D:822:THR:O	1:D:827:GLU:HG2	1.96	0.65
3:W:8:SER:HB3	3:W:9:PRO:HD3	1.78	0.65
1:A:678:PRO:HD2	1:A:851:GLN:NE2	2.13	0.64
1:A:73:ILE:HG12	1:A:254:MET:HB2	1.78	0.64
1:D:796:GLN:HB3	1:D:952:HIS:HB2	1.81	0.63
1:E:262:GLU:HB2	1:E:267:LEU:HG	1.80	0.63
1:E:129:GLN:HA	1:E:817:GLU:HG3	1.80	0.63
1:E:114:LEU:HD13	1:E:168:PHE:HB3	1.81	0.63
2:P:70:ARG:NH1	2:P:93:ASP:OD2	2.31	0.62
2:P:86:MET:HB3	2:P:89:LEU:HD21	1.79	0.62
1:B:789:SER:HB3	1:B:856:PRO:HG3	1.81	0.62
1:A:45:PRO:HG3	1:B:176:GLU:HB3	1.82	0.62
1:E:512:LYS:HE2	3:W:94:PHE:CE2	2.35	0.62
2:M:101:ARG:O	2:M:109:LEU:HA	1.99	0.62
3:T:90:GLN:HG2	3:T:91:GLN:H	1.65	0.61
1:C:337:LEU:HD21	1:C:410:VAL:HG11	1.82	0.61
1:E:94:ILE:HG13	1:E:248:TYR:HB3	1.81	0.61
1:C:92:VAL:HG22	1:C:254:MET:HG2	1.83	0.60
2:V:9:GLU:OE2	2:V:99:CYS:HB3	2.01	0.60
2:M:110:ASP:OD1	2:M:111:TYR:N	2.33	0.60
1:C:942:GLU:HA	1:C:949:PRO:HD2	1.82	0.59
1:D:771:LEU:HB2	1:D:952:HIS:HB3	1.85	0.59
3:N:90:GLN:HG2	3:N:91:GLN:N	2.17	0.59
1:A:392:LEU:HD22	3:L:94:PHE:HD2	1.67	0.59
1:B:839:ARG:HG2	1:B:844:GLN:HB3	1.85	0.59
2:V:32:ILE:HB	2:V:37:ILE:HD11	1.85	0.59
1:D:809:GLU:OE1	1:D:893:ARG:NH1	2.36	0.58
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.85	0.58
1:E:944:LEU:O	1:E:951:ARG:NH1	2.36	0.58
1:A:679:HIS:ND1	1:A:851:GLN:OE1	2.37	0.57
3:Q:3:ILE:HB	3:Q:91:GLN:OE1	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LEU:N	1:B:539:PRO:HD3	2.19	0.57
1:D:574:LEU:HD22	1:D:729:LEU:HD22	1.86	0.57
2:S:109:LEU:HB2	3:T:37:TYR:OH	2.05	0.57
1:A:350:LEU:HD13	1:A:356:VAL:HG21	1.86	0.57
3:T:30:VAL:HG12	3:T:32:SER:O	2.05	0.57
1:E:224:TYR:HA	1:E:228:THR:HB	1.85	0.57
1:E:490:ASP:OD2	1:E:501:LYS:HG3	2.04	0.57
1:D:77:LEU:HD21	1:D:271:VAL:HG21	1.87	0.57
2:P:50:TRP:CD2	3:Q:97:ILE:HB	2.38	0.57
3:Q:30:VAL:HG23	3:Q:93:TYR:CE2	2.40	0.57
1:B:809:GLU:OE1	1:B:893:ARG:NH1	2.37	0.57
1:C:413:GLU:OE2	1:C:528:ASN:HB2	2.05	0.57
1:C:581:PRO:HD3	1:C:758:LEU:HD21	1.85	0.56
1:E:76:LEU:HD23	1:E:437:ILE:HG21	1.85	0.56
1:D:73:ILE:HG13	1:D:251:SER:HB2	1.87	0.56
1:D:678:PRO:HD2	1:D:851:GLN:HE21	1.69	0.56
1:B:341:GLU:HB2	1:B:609:TYR:CD1	2.41	0.56
1:D:400:LYS:HZ3	1:D:523:LYS:HA	1.69	0.56
1:A:942:GLU:HA	1:A:949:PRO:HD2	1.87	0.56
1:C:441:LEU:HD11	1:C:446:LEU:HD23	1.86	0.56
1:C:572:ALA:HA	1:C:731:GLY:HA3	1.87	0.56
1:D:400:LYS:NZ	1:D:523:LYS:HA	2.21	0.56
1:B:616:LEU:HD11	1:B:638:GLN:HG3	1.88	0.56
1:D:767:ARG:HD3	1:D:1005:PHE:O	2.05	0.56
1:C:75:VAL:HG22	1:C:256:VAL:HB	1.88	0.56
1:C:599:LEU:HD13	1:C:654:ILE:HG23	1.86	0.56
1:D:92:VAL:HG12	1:D:94:ILE:H	1.71	0.56
3:L:33:ALA:HB1	3:L:92:SER:O	2.05	0.56
1:B:572:ALA:HA	1:B:731:GLY:HA3	1.87	0.55
1:C:116:LEU:HD22	1:C:124:GLU:HG2	1.88	0.55
1:C:116:LEU:HD13	1:C:178:ALA:HB1	1.88	0.55
1:B:45:PRO:HB3	1:E:120:LYS:HB2	1.88	0.55
1:E:135:ALA:HA	1:E:892:ARG:HH11	1.72	0.55
1:B:596:TYR:OH	1:B:649:MET:O	2.23	0.55
1:C:73:ILE:HG13	1:C:251:SER:HB2	1.87	0.55
2:H:108:GLY:O	3:L:37:TYR:OH	2.25	0.55
1:C:556:MET:HA	1:C:757:PRO:HB3	1.88	0.55
1:E:123:LYS:HB2	1:E:126:GLU:HB2	1.87	0.55
1:E:832:ILE:HB	1:E:851:GLN:HB3	1.88	0.55
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.87	0.55
2:P:50:TRP:HD1	2:P:64:ALA:HB2	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ARG:HD2	1:A:959:LEU:HB2	1.89	0.55
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.89	0.55
1:D:65:ARG:HB2	1:D:264:LEU:HD13	1.88	0.55
3:W:3:ILE:HD12	3:W:28:GLN:HB2	1.88	0.55
1:C:679:HIS:HB3	1:C:851:GLN:HB2	1.89	0.54
3:Q:3:ILE:HG23	3:Q:27:SER:HB2	1.89	0.54
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.89	0.54
2:H:61:THR:HB	2:H:63:TYR:CE2	2.42	0.54
1:C:678:PRO:HD2	1:C:851:GLN:NE2	2.22	0.54
1:E:793:ILE:O	1:E:847:ARG:HA	2.07	0.54
2:H:5:VAL:HG13	2:H:30:PHE:CE2	2.41	0.54
2:V:101:ARG:O	2:V:109:LEU:HA	2.07	0.54
1:E:441:LEU:HD11	1:E:446:LEU:HD23	1.90	0.54
1:E:501:LYS:HE2	1:E:503:GLU:OE2	2.08	0.54
2:H:102:HIS:HA	2:H:109:LEU:H	1.71	0.54
1:D:809:GLU:OE2	1:D:839:ARG:NH2	2.38	0.54
1:A:75:VAL:HG22	1:A:256:VAL:HB	1.90	0.54
1:B:813:GLN:OE1	1:B:892:ARG:NH2	2.40	0.54
1:E:123:LYS:CB	1:E:126:GLU:HB2	2.38	0.54
2:M:70:ARG:NH1	2:M:93:ASP:OD2	2.40	0.54
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.23	0.54
2:S:100:ALA:HB3	2:S:109:LEU:HD22	1.89	0.53
1:D:794:TYR:HB3	1:D:954:VAL:HG13	1.90	0.53
1:D:304:ILE:HB	1:D:481:VAL:HG22	1.90	0.53
1:D:402:ARG:NH1	1:D:468:LEU:O	2.40	0.53
1:D:716:ILE:HB	1:D:717:PRO:HD3	1.90	0.53
1:E:546:PRO:C	1:E:562:LYS:HE3	2.28	0.53
3:T:32:SER:H	3:T:67:ARG:NH1	2.07	0.53
2:V:52:ALA:HB2	2:V:63:TYR:HD1	1.72	0.53
1:A:865:ALA:HB2	1:A:983:ALA:HA	1.90	0.53
1:C:402:ARG:HG3	1:C:468:LEU:CD2	2.28	0.53
1:E:771:LEU:HB2	1:E:952:HIS:HB3	1.91	0.53
1:E:913:SER:O	1:E:915:GLN:HG3	2.08	0.53
3:Q:32:SER:HB3	3:Q:67:ARG:NH1	2.23	0.53
1:C:552:LYS:NZ	1:C:743:GLN:HG3	2.23	0.53
1:D:309:ASP:N	1:D:672:ASN:OD1	2.38	0.53
1:D:945:ALA:O	1:D:951:ARG:NH1	2.41	0.53
2:P:101:ARG:O	2:P:109:LEU:HA	2.09	0.53
1:A:441:LEU:HD11	1:A:446:LEU:HD23	1.89	0.53
1:B:512:LYS:HD3	2:M:106:VAL:HG13	1.90	0.53
1:E:92:VAL:HG12	1:E:94:ILE:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:HG13	1:D:248:TYR:HB3	1.91	0.53
3:N:90:GLN:HG2	3:N:91:GLN:H	1.73	0.53
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.44	0.52
1:B:618:TYR:HB2	1:B:631:VAL:HG22	1.89	0.52
1:C:559:LEU:HD11	1:C:729:LEU:HG	1.92	0.52
1:C:850:ILE:HG21	1:C:859:LEU:HD22	1.91	0.52
1:E:119:LYS:HD2	1:E:171:SER:HB2	1.91	0.52
1:E:722:ARG:HG2	1:E:756:LYS:HB2	1.90	0.52
2:M:9:GLU:OE2	2:M:9:GLU:N	2.42	0.52
1:B:552:LYS:NZ	1:B:743:GLN:HG2	2.25	0.52
1:E:341:GLU:HG2	1:E:347:LEU:HD23	1.91	0.52
1:E:679:HIS:HB3	1:E:851:GLN:HB2	1.90	0.52
2:M:30:PHE:CE2	2:M:101:ARG:HD2	2.44	0.52
3:L:13:SER:HA	3:L:106:GLU:O	2.09	0.52
2:P:107:ALA:HB1	3:Q:35:ALA:HB2	1.91	0.52
3:Q:5:MET:HE3	3:Q:91:GLN:HB2	1.92	0.52
2:V:50:TRP:CG	3:W:97:ILE:HB	2.45	0.52
1:C:586:ASP:OD1	1:C:589:HIS:ND1	2.42	0.52
1:D:150:TYR:HE1	1:D:431:ARG:HE	1.58	0.52
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.92	0.52
1:C:679:HIS:ND1	1:C:851:GLN:OE1	2.37	0.52
1:D:441:LEU:HD11	1:D:446:LEU:HD23	1.90	0.52
1:B:291:HIS:O	1:B:294:GLN:NE2	2.42	0.52
1:C:793:ILE:O	1:C:847:ARG:HA	2.10	0.52
1:D:580:SER:HB2	1:D:723:LEU:HD23	1.92	0.52
3:Q:38:GLN:HB2	3:Q:48:LEU:HD11	1.92	0.52
1:A:827:GLU:OE2	1:A:862:ARG:HD2	2.10	0.52
1:D:114:LEU:HD13	1:D:168:PHE:HB3	1.90	0.52
1:D:678:PRO:HD2	1:D:851:GLN:NE2	2.24	0.52
2:M:22:ARG:HA	2:M:85:GLN:HA	1.91	0.52
1:B:279:GLU:HG2	1:B:281:LYS:HE3	1.92	0.51
1:C:490:ASP:HB2	1:C:501:LYS:HD3	1.92	0.51
1:C:655:ASP:HB3	1:C:658:ARG:HB2	1.91	0.51
1:A:679:HIS:HB3	1:A:851:GLN:HB2	1.90	0.51
1:C:56:LYS:NZ	1:C:60:ASP:O	2.26	0.51
2:H:22:ARG:HA	2:H:85:GLN:HA	1.92	0.51
2:M:91:ALA:HA	2:M:120:VAL:HG21	1.90	0.51
3:Q:32:SER:N	3:Q:67:ARG:HH11	2.08	0.51
3:T:12:LEU:HD11	3:T:105:VAL:HG13	1.92	0.51
1:A:510:ILE:O	1:A:514:GLN:HG2	2.10	0.51
1:B:392:LEU:HD22	3:N:94:PHE:HD2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:GLU:HA	1:B:949:PRO:HD2	1.92	0.51
1:D:121:TYR:CD2	1:D:164:ARG:HG3	2.45	0.51
2:V:94:THR:OG1	2:V:120:VAL:HG22	2.11	0.51
1:C:865:ALA:HB2	1:C:983:ALA:HA	1.91	0.51
1:D:864:GLU:OE2	1:D:951:ARG:NH2	2.44	0.51
1:E:875:GLU:HG2	1:E:937:ILE:HD13	1.93	0.51
2:M:109:LEU:HB2	3:N:37:TYR:OH	2.10	0.51
1:C:92:VAL:HG12	1:C:94:ILE:H	1.75	0.51
1:D:343:PRO:HA	1:D:606:GLU:OE2	2.10	0.51
2:H:101:ARG:O	2:H:109:LEU:HA	2.10	0.51
2:M:86:MET:CB	2:M:89:LEU:HD21	2.40	0.51
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.93	0.51
1:A:116:LEU:HD13	1:A:178:ALA:HB1	1.93	0.51
1:B:437:ILE:HA	1:B:440:ILE:HG12	1.93	0.51
1:C:806:MET:SD	1:C:924:GLU:HB3	2.51	0.51
1:D:76:LEU:HD23	1:D:437:ILE:HG21	1.93	0.51
3:N:38:GLN:HB3	3:N:48:LEU:HD21	1.93	0.51
1:D:490:ASP:HB2	1:D:501:LYS:HD3	1.92	0.50
1:B:881:ALA:O	1:B:885:HIS:ND1	2.40	0.50
1:C:469:ASP:OD1	1:C:472:ARG:NH2	2.39	0.50
2:V:50:TRP:CD2	3:W:97:ILE:HB	2.47	0.50
1:A:797:THR:HG23	1:A:845:GLY:HA2	1.92	0.50
1:D:121:TYR:HB3	1:D:126:GLU:HG2	1.93	0.50
2:M:8:VAL:HG23	2:M:26:ALA:HB3	1.92	0.50
1:B:920:ARG:O	1:B:924:GLU:HG3	2.11	0.50
1:C:224:TYR:HA	1:C:228:THR:OG1	2.11	0.50
1:E:84:ASP:OD2	1:E:896:LYS:NZ	2.43	0.50
2:H:5:VAL:HG13	2:H:30:PHE:CD2	2.47	0.50
1:C:603:SER:CB	1:C:648:LYS:HZ1	2.23	0.50
1:D:54:ILE:HD11	1:D:66:GLY:H	1.77	0.50
1:E:308:LYS:HD3	1:E:672:ASN:HB3	1.94	0.50
2:M:26:ALA:HA	2:M:81:THR:HG22	1.93	0.50
1:A:224:TYR:HA	1:A:228:THR:HB	1.93	0.50
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.93	0.50
1:C:228:THR:O	1:C:232:GLN:HG3	2.12	0.50
1:C:545:THR:OG1	1:C:547:TYR:O	2.28	0.50
1:D:722:ARG:HE	1:D:756:LYS:HB2	1.76	0.50
3:W:19:ARG:HH11	3:W:75:THR:HG21	1.76	0.50
1:A:472:ARG:HD2	1:A:474:GLU:OE2	2.12	0.50
1:B:674:ARG:HD2	1:B:784:GLU:OE1	2.11	0.50
2:S:50:TRP:HZ2	2:S:53:SER:HB3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HE2	1:A:357:ASN:HA	1.92	0.49
1:B:203:GLN:HG3	1:B:494:GLU:OE2	2.11	0.49
1:B:206:LYS:HB3	1:B:216:SER:HA	1.94	0.49
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.94	0.49
1:E:716:ILE:HB	1:E:717:PRO:CD	2.38	0.49
3:L:90:GLN:HG2	3:L:91:GLN:N	2.26	0.49
3:L:90:GLN:HE21	3:L:97:ILE:HD13	1.77	0.49
3:W:38:GLN:OE1	3:W:40:LYS:NZ	2.40	0.49
1:A:80:ASP:O	1:A:83:THR:HG22	2.12	0.49
1:C:255:ALA:HB1	1:C:441:LEU:HD23	1.93	0.49
1:D:684:TYR:O	1:D:687:ARG:HG2	2.11	0.49
3:L:3:ILE:HG12	3:L:28:GLN:HG2	1.94	0.49
1:A:508:GLU:HG3	1:A:509:VAL:N	2.27	0.49
1:A:717:PRO:O	1:A:721:SER:OG	2.26	0.49
1:E:73:ILE:HG13	1:E:251:SER:HB2	1.94	0.49
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.94	0.49
1:B:341:GLU:HG2	1:B:347:LEU:HD23	1.92	0.49
1:B:686:LEU:HB2	1:B:956:VAL:HG21	1.94	0.49
1:C:519:ASN:HB3	1:C:522:PHE:HD2	1.76	0.49
1:C:809:GLU:HB3	1:C:889:LEU:HD21	1.95	0.49
1:D:337:LEU:HD21	1:D:410:VAL:HG11	1.93	0.49
1:A:874:ILE:O	1:A:933:LYS:HD3	2.13	0.49
1:C:155:HIS:NE2	1:C:261:ARG:HG2	2.27	0.49
1:B:679:HIS:HB3	1:B:851:GLN:HB2	1.95	0.49
1:C:175:ASP:OD2	1:C:177:SER:HB3	2.12	0.49
1:C:291:HIS:CD2	1:C:370:PHE:HB2	2.48	0.49
1:C:908:TRP:NE1	1:C:912:ILE:HD11	2.27	0.49
1:E:317:PHE:HB2	1:E:373:PHE:HB3	1.94	0.49
1:B:865:ALA:HB2	1:B:983:ALA:HA	1.94	0.49
1:D:874:ILE:O	1:D:933:LYS:HD3	2.13	0.49
2:P:32:ILE:HG22	2:P:37:ILE:HD11	1.95	0.49
2:P:50:TRP:CD1	2:P:64:ALA:HB2	2.48	0.49
1:B:110:LEU:HD11	1:B:245:HIS:HB2	1.94	0.49
1:E:492:THR:O	1:E:492:THR:HG22	2.13	0.49
2:M:76:ASP:HB2	2:M:83:TYR:HE2	1.78	0.49
3:T:38:GLN:HB3	3:T:48:LEU:HD11	1.94	0.49
1:C:93:HIS:O	1:C:93:HIS:ND1	2.44	0.49
2:P:6:GLN:HB2	2:P:28:SER:HB2	1.95	0.49
1:C:581:PRO:O	1:C:585:VAL:HG23	2.13	0.48
1:C:792:GLU:HA	1:C:848:PHE:O	2.12	0.48
2:V:50:TRP:NE1	3:W:97:ILE:HD12	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.48	0.48
1:E:860:GLU:OE1	1:E:953:LYS:NZ	2.40	0.48
2:H:30:PHE:CE1	2:H:101:ARG:HD2	2.48	0.48
3:T:3:ILE:HG23	3:T:27:SER:HB2	1.95	0.48
1:A:747:ASP:O	1:A:751:GLU:HG2	2.13	0.48
1:C:387:VAL:HG11	1:C:480:ILE:HD11	1.96	0.48
1:C:716:ILE:HB	1:C:717:PRO:HD3	1.94	0.48
1:C:721:SER:O	1:C:722:ARG:NH1	2.40	0.48
2:S:110:ASP:OD1	2:S:110:ASP:N	2.42	0.48
2:V:37:ILE:HB	2:V:54:ILE:HG23	1.96	0.48
1:A:602:ASP:OD1	1:A:658:ARG:NH2	2.45	0.48
1:D:85:LYS:NZ	1:D:135:ALA:O	2.46	0.48
1:D:691:THR:O	1:D:999:LYS:NZ	2.35	0.48
1:D:827:GLU:CD	1:D:862:ARG:HH22	2.16	0.48
1:E:125:ASN:HB3	1:E:821:ASN:ND2	2.29	0.48
1:E:320:PRO:HD3	1:E:470:LYS:HD2	1.94	0.48
2:P:91:ALA:HA	2:P:120:VAL:HG21	1.94	0.48
2:P:109:LEU:HB2	3:Q:37:TYR:OH	2.13	0.48
2:V:67:VAL:HG12	2:V:70:ARG:NH2	2.29	0.48
3:W:12:LEU:HD11	3:W:105:VAL:HG22	1.95	0.48
3:W:90:GLN:HG2	3:W:91:GLN:N	2.28	0.48
1:D:313:LEU:HB2	1:D:379:LEU:HD11	1.95	0.48
1:B:388:GLU:HB2	2:M:62:TYR:OH	2.14	0.48
1:B:908:TRP:NE1	1:B:912:ILE:HD11	2.28	0.48
1:C:794:TYR:HB3	1:C:954:VAL:HG13	1.95	0.48
1:E:125:ASN:HD22	1:E:821:ASN:HD22	1.61	0.48
2:P:38:HIS:HB3	2:P:50:TRP:CH2	2.49	0.48
1:C:305:VAL:HB	1:C:499:GLN:HB2	1.95	0.48
1:C:915:GLN:HG2	1:C:1008:VAL:HG11	1.94	0.48
1:D:76:LEU:HD22	1:D:449:VAL:HG21	1.96	0.48
2:H:38:HIS:HD1	2:H:50:TRP:HE1	1.60	0.48
3:T:22:ILE:HG21	3:T:103:THR:HG21	1.95	0.48
1:A:291:HIS:HD2	1:A:293:PHE:O	1.97	0.48
1:A:357:ASN:HB2	1:A:378:ASP:OD2	2.13	0.48
1:A:392:LEU:HD22	3:L:94:PHE:CD2	2.48	0.48
1:B:517:ASP:OD2	3:N:93:TYR:OH	2.26	0.48
1:B:793:ILE:O	1:B:847:ARG:HA	2.13	0.48
1:D:172:PRO:HG2	1:D:174:PHE:CE2	2.49	0.48
3:Q:90:GLN:HG2	3:Q:91:GLN:N	2.29	0.48
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.96	0.48
1:E:580:SER:HB2	1:E:723:LEU:HD23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:ILE:HD11	1:B:860:GLU:OE2	2.13	0.48
1:D:90:LEU:HD13	1:D:169:PHE:CE2	2.48	0.48
1:D:506:PRO:HB3	2:S:34:SER:O	2.14	0.48
1:E:870:MET:O	1:E:874:ILE:HG13	2.14	0.48
2:M:15:VAL:HG11	2:M:89:LEU:HD13	1.96	0.48
1:B:255:ALA:HB1	1:B:441:LEU:HD23	1.96	0.47
1:D:559:LEU:HD13	1:D:742:MET:HE3	1.96	0.47
1:D:950:ARG:HG2	1:D:952:HIS:CE1	2.50	0.47
2:P:26:ALA:HA	2:P:81:THR:HG23	1.96	0.47
3:T:90:GLN:HG2	3:T:91:GLN:N	2.29	0.47
1:A:472:ARG:HB3	1:A:474:GLU:HG2	1.95	0.47
1:B:864:GLU:CD	1:B:951:ARG:HH12	2.15	0.47
1:D:426:ASP:HB3	1:D:899:LYS:HB3	1.96	0.47
2:H:50:TRP:CD1	3:L:97:ILE:HB	2.50	0.47
3:Q:4:GLN:O	3:Q:27:SER:OG	2.28	0.47
1:C:309:ASP:N	1:C:672:ASN:OD1	2.42	0.47
1:D:137:SER:N	1:D:152:ASP:OD1	2.43	0.47
1:D:190:HIS:O	1:D:194:VAL:HG23	2.14	0.47
1:D:944:LEU:O	1:D:951:ARG:NH1	2.47	0.47
3:N:39:GLN:O	3:N:85:ALA:HB1	2.14	0.47
1:A:794:TYR:HB3	1:A:954:VAL:HG13	1.95	0.47
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.96	0.47
1:C:304:ILE:HB	1:C:481:VAL:HG22	1.95	0.47
1:C:579:PHE:HZ	1:C:765:ARG:CZ	2.28	0.47
1:C:862:ARG:NH1	1:C:981:SER:O	2.47	0.47
1:D:250:SER:HB2	1:D:281:LYS:HB3	1.97	0.47
1:E:678:PRO:HD2	1:E:851:GLN:NE2	2.29	0.47
2:M:42:GLN:HB2	2:M:48:LEU:HD23	1.96	0.47
1:A:246:SER:C	1:A:281:LYS:HZ3	2.17	0.47
1:B:468:LEU:HD12	1:B:471:LEU:HD12	1.96	0.47
1:C:119:LYS:HD3	1:D:236:ASP:HB2	1.95	0.47
2:P:30:PHE:CE2	2:P:101:ARG:HD2	2.50	0.47
1:A:417:LEU:HD21	1:A:531:ILE:HG22	1.97	0.47
2:P:54:ILE:HA	2:P:60:SER:O	2.14	0.47
2:P:102:HIS:HA	2:P:109:LEU:H	1.78	0.47
1:A:119:LYS:HA	1:A:173:LEU:HD21	1.96	0.47
1:A:425:LYS:HD2	1:A:428:GLU:OE2	2.15	0.47
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.95	0.47
1:B:586:ASP:OD1	1:B:589:HIS:ND1	2.48	0.47
1:B:870:MET:O	1:B:874:ILE:HG13	2.15	0.47
1:C:348:SER:HB2	1:C:606:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ALA:HB3	1:C:370:PHE:CE1	2.49	0.47
1:E:581:PRO:O	1:E:585:VAL:HG23	2.15	0.47
3:L:62:ARG:NE	3:L:83:ASP:OD2	2.46	0.47
1:B:388:GLU:OE1	2:M:62:TYR:OH	2.26	0.47
1:C:778:VAL:HG22	1:C:955:SER:HB2	1.97	0.47
1:D:441:LEU:HD13	1:D:449:VAL:HG11	1.96	0.47
1:E:569:LEU:O	1:E:571:LYS:N	2.44	0.47
1:E:663:LYS:HG3	1:E:704:LEU:HD21	1.96	0.47
3:T:50:TYR:O	3:T:54:SER:OG	2.30	0.47
1:D:572:ALA:HA	1:D:731:GLY:HA3	1.97	0.47
1:E:163:ASP:O	1:E:167:GLN:HG2	2.15	0.47
1:E:809:GLU:OE1	1:E:893:ARG:NH1	2.48	0.47
2:M:9:GLU:OE1	2:M:99:CYS:HB3	2.14	0.47
2:V:44:PRO:HD3	2:V:95:ALA:HA	1.97	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.50	0.46
1:B:864:GLU:OE2	1:B:951:ARG:NH1	2.32	0.46
1:E:657:LYS:HA	1:E:657:LYS:HD2	1.70	0.46
1:E:777:PHE:HB3	1:E:992:ILE:HD11	1.97	0.46
2:P:91:ALA:O	2:P:94:THR:HG22	2.15	0.46
3:T:32:SER:OG	3:T:33:ALA:N	2.48	0.46
1:B:881:ALA:HA	1:B:884:LYS:HE2	1.97	0.46
1:C:90:LEU:HD13	1:C:169:PHE:CE2	2.50	0.46
1:C:301:LEU:HD13	2:P:57:TYR:HE1	1.80	0.46
2:H:100:ALA:HB3	2:H:109:LEU:HD22	1.96	0.46
2:P:53:SER:OG	2:P:62:TYR:HB2	2.15	0.46
3:T:8:SER:N	3:T:23:THR:O	2.38	0.46
1:C:341:GLU:HG2	1:C:347:LEU:HD23	1.98	0.46
1:C:791:ILE:HA	1:C:956:VAL:O	2.16	0.46
1:C:804:GLU:C	1:C:844:GLN:HE22	2.19	0.46
1:A:809:GLU:OE1	1:A:893:ARG:NH1	2.48	0.46
1:B:643:LYS:HD2	1:B:744:MET:HG2	1.97	0.46
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.97	0.46
1:C:722:ARG:NE	1:C:756:LYS:HB2	2.30	0.46
1:C:856:PRO:HA	1:C:859:LEU:HD12	1.98	0.46
1:D:794:TYR:CE1	1:D:845:GLY:HA3	2.50	0.46
2:P:15:VAL:HG22	2:P:16:GLN:H	1.81	0.46
3:T:83:ASP:O	3:T:87:TYR:OH	2.27	0.46
1:A:749:LEU:HB3	1:A:755:THR:OG1	2.16	0.46
1:B:75:VAL:HA	1:B:256:VAL:O	2.15	0.46
1:C:994:ASN:HB3	1:C:997:GLU:HB3	1.97	0.46
1:D:153:VAL:HG22	1:D:154:SER:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:TYR:OH	1:D:649:MET:O	2.32	0.46
3:T:9:PRO:HG2	3:T:22:ILE:HA	1.98	0.46
1:B:540:LEU:HA	1:B:563:GLN:HE22	1.81	0.46
1:D:218:PHE:HB2	1:D:495:TRP:NE1	2.31	0.46
1:D:628:TYR:CZ	1:D:630:SER:HB2	2.50	0.46
1:D:776:TRP:CD2	1:D:989:PRO:HB3	2.51	0.46
1:D:927:TYR:CE2	1:D:931:LEU:HD21	2.51	0.46
3:W:25:ARG:NE	3:W:71:ASP:OD1	2.44	0.46
1:C:797:THR:OG1	1:C:798:ASP:N	2.49	0.46
2:M:53:SER:OG	2:M:62:TYR:HB2	2.16	0.46
1:A:223:LYS:HE3	1:A:227:GLU:OE2	2.16	0.46
1:E:796:GLN:HB3	1:E:952:HIS:HB2	1.98	0.46
2:M:101:ARG:NH1	2:M:110:ASP:OD2	2.49	0.46
3:Q:7:GLN:NE2	3:Q:103:THR:OG1	2.49	0.46
1:B:688:LEU:HD22	1:B:694:ALA:HB1	1.97	0.46
1:C:387:VAL:HG21	1:C:480:ILE:HD13	1.97	0.46
1:D:102:ASN:OD1	1:D:102:ASN:N	2.47	0.46
1:D:664:GLU:OE2	1:D:668:ARG:NE	2.46	0.46
1:D:856:PRO:O	1:D:860:GLU:N	2.40	0.46
1:D:871:GLU:OE2	1:D:941:LYS:NZ	2.47	0.46
1:E:192:LYS:HD3	1:E:831:TYR:HD2	1.80	0.46
1:E:791:ILE:HA	1:E:956:VAL:O	2.15	0.46
2:V:16:GLN:HB3	2:V:17:PRO:CD	2.46	0.46
1:C:75:VAL:HA	1:C:256:VAL:O	2.15	0.45
1:E:547:TYR:CD1	1:E:918:PHE:HB3	2.50	0.45
2:P:30:PHE:CZ	2:P:101:ARG:HD2	2.51	0.45
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.98	0.45
1:B:201:LEU:HD13	1:B:314:TYR:HE2	1.81	0.45
1:C:88:ALA:HB3	1:C:151:PHE:CE1	2.51	0.45
1:C:272:VAL:O	1:C:276:SER:OG	2.22	0.45
1:D:91:ASP:OD1	1:D:146:HIS:ND1	2.43	0.45
1:D:777:PHE:HB3	1:D:992:ILE:HD11	1.98	0.45
1:E:223:LYS:HE3	1:E:227:GLU:OE2	2.15	0.45
1:E:838:ARG:HB2	1:E:847:ARG:CD	2.42	0.45
1:A:868:ILE:HD11	1:A:984:PRO:HB3	1.98	0.45
1:B:64:TYR:CD2	1:B:78:ILE:HG12	2.51	0.45
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.51	0.45
1:B:317:PHE:HB2	1:B:373:PHE:HB3	1.97	0.45
1:C:944:LEU:O	1:C:951:ARG:NH2	2.47	0.45
1:E:441:LEU:HD13	1:E:449:VAL:HG11	1.97	0.45
1:B:141:PHE:CE1	1:B:148:ASN:HB3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:HIS:CD2	1:C:261:ARG:HG2	2.51	0.45
1:D:768:GLU:HB3	1:D:843:ILE:HG13	1.98	0.45
1:E:291:HIS:CD2	1:E:370:PHE:HB2	2.51	0.45
1:E:596:TYR:OH	1:E:649:MET:O	2.31	0.45
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.99	0.45
1:B:913:SER:O	1:B:915:GLN:HG3	2.17	0.45
1:C:99:ASP:O	1:C:217:LYS:HE3	2.17	0.45
1:C:441:LEU:HD13	1:C:449:VAL:HG11	1.98	0.45
1:D:388:GLU:HB3	3:T:94:PHE:CE2	2.51	0.45
2:P:71:PHE:HB3	2:P:84:LEU:HD11	1.99	0.45
1:D:569:LEU:O	1:D:571:LYS:N	2.48	0.45
1:E:704:LEU:HA	1:E:707:VAL:HG12	1.99	0.45
3:W:33:ALA:HB1	3:W:92:SER:O	2.16	0.45
1:A:104:ALA:HB1	1:A:218:PHE:HB3	1.98	0.45
1:B:910:GLU:OE1	1:B:920:ARG:NH2	2.33	0.45
1:C:579:PHE:HZ	1:C:765:ARG:NH1	2.14	0.45
1:D:116:LEU:HD13	1:D:178:ALA:HB1	1.98	0.45
3:L:80:GLN:H	3:L:83:ASP:HB2	1.80	0.45
2:P:107:ALA:HA	3:Q:92:SER:OG	2.15	0.45
1:A:791:ILE:HA	1:A:956:VAL:O	2.15	0.45
1:B:303:LYS:HB3	1:B:485:PHE:CD2	2.52	0.45
1:C:643:LYS:HD2	1:C:744:MET:HG2	1.98	0.45
1:C:822:THR:HG21	1:C:866:PHE:CD1	2.52	0.45
1:E:573:ASN:ND2	1:E:900:LEU:HG	2.32	0.45
1:E:597:LEU:HD11	1:E:627:MET:HG2	1.98	0.45
3:Q:5:MET:CE	3:Q:91:GLN:HB2	2.47	0.45
1:A:792:GLU:HA	1:A:848:PHE:O	2.17	0.45
1:A:797:THR:OG1	1:A:798:ASP:N	2.49	0.45
1:C:489:THR:HA	1:C:501:LYS:HB2	1.99	0.45
1:E:597:LEU:HD12	1:E:622:ASN:HB3	1.99	0.45
1:A:645:ILE:O	1:A:649:MET:HB2	2.17	0.45
1:C:117:GLY:O	1:C:173:LEU:HB2	2.17	0.45
1:D:582:PHE:O	1:D:589:HIS:HB3	2.17	0.45
1:E:102:ASN:OD1	1:E:102:ASN:N	2.50	0.45
2:M:30:PHE:CZ	2:M:101:ARG:HD2	2.52	0.45
3:T:25:ARG:HG3	3:T:71:ASP:OD2	2.17	0.45
1:A:71:ASN:O	1:A:280:ASN:ND2	2.50	0.44
1:C:722:ARG:CD	1:C:756:LYS:HB2	2.47	0.44
1:D:863:VAL:O	1:D:867:LEU:HG	2.17	0.44
1:E:192:LYS:HB3	1:E:192:LYS:HE2	1.71	0.44
1:E:699:GLU:O	1:E:702:GLU:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:41:ARG:NH1	2:P:93:ASP:HA	2.32	0.44
3:W:79:LEU:HD23	3:W:79:LEU:HA	1.84	0.44
1:A:559:LEU:HD23	1:A:739:LEU:HD23	1.98	0.44
3:T:4:GLN:HG3	3:T:27:SER:OG	2.16	0.44
2:V:79:LYS:HE3	2:V:83:TYR:OH	2.18	0.44
2:V:91:ALA:HA	2:V:120:VAL:HG21	1.98	0.44
1:D:961:ARG:HD2	1:D:962:GLU:OE2	2.17	0.44
2:P:32:ILE:HG23	2:P:80:ASN:OD1	2.17	0.44
3:Q:13:SER:HA	3:Q:106:GLU:O	2.17	0.44
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.53	0.44
1:B:313:LEU:HB2	1:B:379:LEU:HD11	1.99	0.44
1:C:90:LEU:HD13	1:C:169:PHE:CZ	2.52	0.44
1:E:252:ASN:ND2	1:E:283:VAL:O	2.50	0.44
1:E:699:GLU:HA	1:E:702:GLU:OE2	2.18	0.44
1:E:856:PRO:HA	1:E:859:LEU:HD12	1.99	0.44
2:M:79:LYS:O	2:M:81:THR:HG23	2.16	0.44
1:A:190:HIS:O	1:A:194:VAL:HG23	2.18	0.44
1:B:615:GLY:HA3	1:B:634:TYR:HE1	1.82	0.44
1:A:93:HIS:O	1:A:93:HIS:ND1	2.49	0.44
1:D:387:VAL:HG11	1:D:480:ILE:HD11	2.00	0.44
1:D:883:GLN:HA	1:D:886:ILE:HB	1.98	0.44
3:N:31:SER:HA	3:N:67:ARG:CZ	2.47	0.44
2:P:38:HIS:ND1	2:P:50:TRP:HH2	2.16	0.44
3:Q:43:LYS:HA	3:Q:43:LYS:HD2	1.64	0.44
1:A:854:LYS:HD2	1:A:854:LYS:HA	1.66	0.44
1:B:173:LEU:HD22	1:B:175:ASP:HB2	1.98	0.44
1:B:441:LEU:HD13	1:B:449:VAL:HG11	2.00	0.44
1:C:388:GLU:OE1	2:P:59:GLY:HA3	2.18	0.44
1:E:650:ALA:HB2	1:E:749:LEU:HD23	2.00	0.44
2:P:36:SER:OG	2:P:38:HIS:NE2	2.41	0.44
1:D:303:LYS:HB3	1:D:485:PHE:CD2	2.53	0.44
1:D:388:GLU:HB2	2:S:62:TYR:OH	2.18	0.44
1:D:652:PHE:CE2	1:D:654:ILE:HD13	2.53	0.44
1:E:314:TYR:HB2	1:E:479:ALA:HB3	1.99	0.44
2:P:9:GLU:OE2	2:P:99:CYS:HB3	2.17	0.44
3:Q:84:PHE:HD1	3:Q:105:VAL:O	1.99	0.44
2:S:16:GLN:HB3	2:S:17:PRO:HD2	1.99	0.44
2:V:97:TYR:O	2:V:116:THR:HG22	2.18	0.44
1:B:648:LYS:HE3	1:B:648:LYS:HB3	1.80	0.44
1:B:823:LEU:HB2	1:B:833:VAL:HG11	1.99	0.44
1:C:102:ASN:OD1	1:C:102:ASN:N	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:HD13	1:C:168:PHE:HB3	1.99	0.44
1:C:385:LEU:HD22	2:P:60:SER:HB3	2.00	0.44
1:D:541:GLU:OE2	1:D:734:THR:HB	2.17	0.44
1:D:814:ILE:HG12	1:D:885:HIS:ND1	2.32	0.44
1:A:129:GLN:HA	1:A:817:GLU:HG3	2.00	0.43
1:A:557:SER:OG	1:A:746:GLU:OE1	2.30	0.43
1:C:599:LEU:HD21	1:C:659:PHE:HA	2.00	0.43
1:D:492:THR:OG1	1:D:499:GLN:HG3	2.18	0.43
1:D:581:PRO:O	1:D:585:VAL:HG23	2.17	0.43
3:Q:90:GLN:HG2	3:Q:91:GLN:H	1.83	0.43
1:A:71:ASN:HB2	1:A:251:SER:OG	2.18	0.43
1:D:722:ARG:HA	1:D:756:LYS:O	2.17	0.43
1:A:537:ILE:HD11	1:A:570:PRO:HD3	2.00	0.43
1:B:355:TRP:HB3	1:B:390:ILE:HD11	2.01	0.43
1:D:791:ILE:HD11	1:D:860:GLU:OE2	2.19	0.43
1:E:379:LEU:HD13	1:E:384:LEU:HA	2.01	0.43
2:P:33:SER:HA	2:P:56:SER:HB2	1.99	0.43
2:S:42:GLN:HG3	2:S:47:GLY:O	2.18	0.43
1:A:153:VAL:HG22	1:A:154:SER:H	1.82	0.43
1:E:368:ARG:HH12	1:E:443:TYR:HD1	1.67	0.43
2:H:94:THR:HG23	2:H:94:THR:O	2.17	0.43
3:T:38:GLN:HE22	3:T:40:LYS:NZ	2.16	0.43
1:E:160:GLY:O	1:E:164:ARG:NH1	2.52	0.43
1:E:577:GLU:HB2	1:E:908:TRP:CZ2	2.54	0.43
1:C:860:GLU:OE2	1:C:955:SER:HB3	2.18	0.43
1:D:597:LEU:HD22	1:D:620:LEU:HD21	1.99	0.43
1:B:367:ALA:HB3	1:B:370:PHE:CE1	2.53	0.43
1:C:181:ARG:HB3	1:C:828:GLN:HG3	2.01	0.43
1:D:153:VAL:HG11	1:D:158:LEU:HA	1.99	0.43
1:D:550:LEU:HD11	1:D:558:LYS:CG	2.49	0.43
3:N:3:ILE:HD12	3:N:28:GLN:HB2	2.01	0.43
1:A:462:ASP:OD1	1:A:462:ASP:N	2.52	0.43
1:A:771:LEU:HB2	1:A:952:HIS:HB3	2.01	0.43
1:B:88:ALA:HB3	1:B:151:PHE:CE1	2.54	0.43
1:D:494:GLU:HB3	1:D:496:TYR:H	1.83	0.43
3:T:31:SER:HA	3:T:67:ARG:CZ	2.48	0.43
3:T:91:GLN:HE21	3:T:93:TYR:HB2	1.84	0.43
1:C:183:VAL:HG11	1:C:227:GLU:OE2	2.18	0.43
2:M:94:THR:OG1	2:M:120:VAL:HG22	2.19	0.43
3:N:3:ILE:HG13	3:N:27:SER:HB2	2.01	0.43
3:Q:104:LYS:HB2	3:Q:104:LYS:HE3	1.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:15:VAL:O	2:S:120:VAL:HA	2.19	0.43
3:W:15:SER:N	3:W:18:ASP:OD2	2.48	0.43
3:W:91:GLN:HB3	3:W:98:THR:H	1.83	0.43
1:A:581:PRO:O	1:A:585:VAL:HG23	2.19	0.43
1:A:793:ILE:O	1:A:847:ARG:HA	2.18	0.43
1:B:552:LYS:HZ1	1:B:743:GLN:HG2	1.83	0.43
1:C:153:VAL:HG22	1:C:154:SER:H	1.84	0.43
1:C:540:LEU:HA	1:C:563:GLN:OE1	2.19	0.43
1:D:82:THR:O	1:D:896:LYS:NZ	2.40	0.43
1:E:426:ASP:OD1	1:E:571:LYS:HE3	2.19	0.43
1:E:600:LEU:HD23	1:E:620:LEU:HD21	2.00	0.43
1:E:805:ASN:HA	1:E:844:GLN:HE22	1.84	0.43
3:N:39:GLN:HE21	3:N:88:TYR:HE2	1.65	0.43
3:W:90:GLN:HE21	3:W:97:ILE:HD13	1.84	0.43
1:A:806:MET:SD	1:A:924:GLU:HB3	2.59	0.42
1:D:865:ALA:HB2	1:D:983:ALA:HA	2.00	0.42
1:B:398:ILE:HD13	1:B:471:LEU:HB3	2.01	0.42
1:B:433:TYR:CZ	1:B:437:ILE:HD11	2.54	0.42
1:B:716:ILE:HB	1:B:717:PRO:HD3	2.01	0.42
1:C:437:ILE:HA	1:C:440:ILE:HG12	2.01	0.42
1:D:794:TYR:CE1	1:D:838:ARG:HD3	2.54	0.42
1:E:582:PHE:O	1:E:589:HIS:HB3	2.19	0.42
1:B:73:ILE:HG12	1:B:254:MET:HB2	2.00	0.42
1:B:777:PHE:HB3	1:B:992:ILE:HD11	2.01	0.42
1:C:472:ARG:HG2	1:C:473:PRO:HD2	2.01	0.42
1:D:599:LEU:HD13	1:D:654:ILE:HD12	2.01	0.42
1:E:81:PRO:HA	1:E:261:ARG:HG2	2.01	0.42
1:E:116:LEU:HD13	1:E:178:ALA:HB1	2.01	0.42
2:M:109:LEU:CD1	3:N:90:GLN:HE22	2.33	0.42
1:B:75:VAL:HG22	1:B:256:VAL:HB	2.02	0.42
1:D:291:HIS:CD2	1:D:370:PHE:HB2	2.54	0.42
1:E:528:ASN:OD1	1:E:530:PHE:HB2	2.19	0.42
1:E:579:PHE:CE2	1:E:765:ARG:NH1	2.88	0.42
3:L:3:ILE:HG23	3:L:27:SER:HB2	2.01	0.42
2:V:109:LEU:HB2	3:W:37:TYR:OH	2.19	0.42
1:B:915:GLN:HG2	1:B:1008:VAL:HG11	2.01	0.42
1:C:767:ARG:HG2	1:C:1007:LEU:HD21	2.01	0.42
1:D:743:GLN:HG3	1:D:747:ASP:OD2	2.20	0.42
1:E:90:LEU:HD13	1:E:169:PHE:CE2	2.54	0.42
1:E:652:PHE:CE2	1:E:654:ILE:HD13	2.54	0.42
2:P:15:VAL:HG11	2:P:89:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:92:SER:HA	3:Q:97:ILE:CD1	2.50	0.42
3:W:22:ILE:CG2	3:W:103:THR:HG21	2.50	0.42
1:A:341:GLU:HG2	1:A:347:LEU:HD22	2.01	0.42
1:A:927:TYR:CE2	1:A:931:LEU:HD21	2.54	0.42
1:C:285:LEU:HD12	1:C:286:PRO:HD2	2.00	0.42
1:D:794:TYR:CD1	1:D:838:ARG:HD3	2.55	0.42
2:V:50:TRP:CZ2	2:V:53:SER:HB3	2.48	0.42
3:W:51:SER:O	3:W:52:ALA:HB3	2.19	0.42
1:B:794:TYR:HB3	1:B:954:VAL:HG13	2.02	0.42
1:E:77:LEU:HD21	1:E:271:VAL:HG21	2.01	0.42
1:E:368:ARG:NH1	1:E:443:TYR:CD1	2.88	0.42
3:L:6:THR:HG22	3:L:25:ARG:O	2.20	0.42
2:M:76:ASP:HB2	2:M:83:TYR:CE2	2.54	0.42
1:A:317:PHE:HB2	1:A:373:PHE:HB3	2.02	0.42
1:A:580:SER:HB2	1:A:723:LEU:HD23	2.02	0.42
1:B:581:PRO:O	1:B:585:VAL:HG23	2.20	0.42
1:C:855:PRO:HA	1:C:856:PRO:HD3	1.95	0.42
1:D:802:THR:HG23	1:D:924:GLU:HG2	2.02	0.42
1:D:855:PRO:HA	1:D:856:PRO:HD3	1.92	0.42
1:E:855:PRO:HA	1:E:963:MET:CE	2.50	0.42
3:T:108:LYS:HB3	3:T:108:LYS:HE2	1.82	0.42
1:C:80:ASP:OD1	1:C:82:THR:HG22	2.19	0.42
1:C:586:ASP:OD2	1:C:588:LEU:HB3	2.20	0.42
1:D:791:ILE:HA	1:D:956:VAL:O	2.20	0.42
1:E:88:ALA:HB3	1:E:151:PHE:CE1	2.55	0.42
1:E:558:LYS:HE3	1:E:558:LYS:HB2	1.88	0.42
3:N:79:LEU:HD23	3:N:79:LEU:HA	1.88	0.42
1:A:75:VAL:HA	1:A:256:VAL:O	2.19	0.42
1:A:178:ALA:HA	1:A:181:ARG:HH21	1.84	0.42
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.24	0.42
1:A:404:GLU:HG2	1:A:407:GLN:NE2	2.35	0.42
1:A:733:ILE:HD13	1:A:738:ALA:HB2	2.02	0.42
1:B:130:PHE:CE1	1:B:164:ARG:NH1	2.88	0.42
1:B:426:ASP:OD1	1:B:571:LYS:NZ	2.44	0.42
1:C:592:MET:HE3	1:C:715:PHE:CD1	2.55	0.42
1:D:599:LEU:HD23	1:D:662:ILE:HD12	2.02	0.42
1:D:793:ILE:O	1:D:847:ARG:HA	2.20	0.42
1:E:153:VAL:HG22	1:E:154:SER:H	1.85	0.42
2:M:14:LEU:HA	2:M:119:THR:O	2.20	0.42
2:P:103:TYR:H	2:P:108:GLY:HA3	1.84	0.42
3:T:40:LYS:HG2	3:T:85:ALA:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD21	1:A:410:VAL:HG11	2.01	0.41
1:C:141:PHE:CE1	1:C:148:ASN:HB3	2.55	0.41
1:C:510:ILE:O	1:C:514:GLN:HG3	2.19	0.41
1:D:550:LEU:HB2	1:D:560:TRP:CH2	2.55	0.41
1:D:820:PHE:CZ	1:D:824:ARG:HD3	2.54	0.41
1:E:565:ASP:OD1	1:E:565:ASP:N	2.53	0.41
3:N:36:TRP:HD1	3:N:49:ILE:HB	1.85	0.41
1:A:181:ARG:HB3	1:A:828:GLN:HG3	2.02	0.41
1:C:426:ASP:HB3	1:C:899:LYS:HB3	2.01	0.41
1:D:90:LEU:HD22	1:D:169:PHE:CE1	2.55	0.41
1:D:679:HIS:O	1:D:683:MET:HG3	2.20	0.41
1:D:724:HIS:CD2	1:D:763:LEU:HD21	2.55	0.41
2:H:101:ARG:NH1	2:H:111:TYR:HD2	2.19	0.41
2:P:100:ALA:HB3	2:P:109:LEU:HD22	2.02	0.41
2:S:30:PHE:CE2	2:S:101:ARG:HD2	2.54	0.41
1:A:862:ARG:NH2	1:A:981:SER:O	2.49	0.41
1:C:389:ASP:HA	3:Q:94:PHE:CD2	2.56	0.41
1:C:872:LYS:HE2	1:C:876:ASP:OD2	2.21	0.41
1:D:472:ARG:HD2	1:D:474:GLU:OE2	2.20	0.41
1:E:104:ALA:HB1	1:E:218:PHE:HB3	2.03	0.41
1:B:60:ASP:OD2	1:B:64:TYR:OH	2.30	0.41
1:B:153:VAL:HG22	1:B:154:SER:H	1.86	0.41
1:D:576:PHE:HB2	1:D:629:LEU:HB3	2.02	0.41
1:E:385:LEU:HD22	2:V:60:SER:HB3	2.02	0.41
1:E:388:GLU:OE1	2:V:62:TYR:OH	2.26	0.41
3:L:6:THR:OG1	3:L:7:GLN:N	2.54	0.41
1:A:228:THR:O	1:A:232:GLN:HB2	2.21	0.41
1:B:388:GLU:OE1	2:M:59:GLY:HA3	2.21	0.41
1:C:796:GLN:O	1:C:952:HIS:HB2	2.20	0.41
1:E:856:PRO:HD3	1:E:963:MET:HE2	2.02	0.41
1:B:118:THR:HB	1:B:171:SER:O	2.20	0.41
1:B:643:LYS:NZ	1:B:744:MET:HG2	2.36	0.41
1:B:907:TYR:O	1:B:911:ILE:HG13	2.20	0.41
1:C:80:ASP:O	1:C:83:THR:HG22	2.20	0.41
1:C:212:LYS:HA	1:C:212:LYS:HD2	1.81	0.41
1:C:506:PRO:HB3	2:P:34:SER:O	2.21	0.41
1:D:195:MET:HB2	1:D:786:HIS:CE1	2.55	0.41
3:Q:92:SER:HA	3:Q:97:ILE:HD12	2.03	0.41
2:S:33:SER:HA	2:S:56:SER:HB2	2.01	0.41
1:A:76:LEU:HD23	1:A:437:ILE:HG21	2.01	0.41
1:A:313:LEU:HB2	1:A:379:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASN:HB2	1:C:251:SER:OG	2.20	0.41
1:C:206:LYS:HG2	1:C:215:PHE:CE2	2.56	0.41
1:C:910:GLU:OE2	1:C:920:ARG:NE	2.39	0.41
1:D:550:LEU:HD12	1:D:559:LEU:O	2.20	0.41
1:D:817:GLU:HB3	1:D:818:PRO:HD3	2.02	0.41
1:D:822:THR:HG21	1:D:866:PHE:CD1	2.56	0.41
1:E:285:LEU:HD12	1:E:286:PRO:HD2	2.03	0.41
1:E:425:LYS:HD3	1:E:454:TYR:CE2	2.55	0.41
3:W:39:GLN:HB2	3:W:45:PRO:HG3	2.02	0.41
1:C:317:PHE:HB2	1:C:373:PHE:HB3	2.03	0.41
1:C:893:ARG:NH1	1:C:893:ARG:CG	2.80	0.41
1:E:399:GLN:O	1:E:402:ARG:HG2	2.20	0.41
3:L:90:GLN:NE2	3:L:97:ILE:HD13	2.35	0.41
3:T:38:GLN:HE22	3:T:40:LYS:HG3	1.86	0.41
1:A:92:VAL:HG12	1:A:94:ILE:H	1.86	0.41
1:A:94:ILE:HG13	1:A:248:TYR:HB3	2.02	0.41
1:A:808:LEU:HD11	1:A:846:LEU:HD13	2.03	0.41
1:B:472:ARG:HG3	1:B:473:PRO:HD2	2.03	0.41
1:C:148:ASN:OD1	1:C:435:SER:OG	2.26	0.41
1:C:907:TYR:O	1:C:911:ILE:HG13	2.20	0.41
1:D:190:HIS:CE1	1:D:218:PHE:HZ	2.38	0.41
1:E:195:MET:HB2	1:E:786:HIS:CE1	2.56	0.41
1:E:317:PHE:O	1:E:373:PHE:N	2.53	0.41
1:E:572:ALA:HA	1:E:731:GLY:HA3	2.03	0.41
1:A:870:MET:O	1:A:874:ILE:HG13	2.21	0.41
1:E:311:ARG:HH22	1:E:664:GLU:CD	2.22	0.41
1:E:327:LYS:HD2	1:E:457:GLU:OE2	2.21	0.41
3:L:8:SER:N	3:L:23:THR:O	2.54	0.41
3:N:31:SER:HA	3:N:67:ARG:NH2	2.36	0.41
2:S:50:TRP:CZ3	3:T:96:PRO:HA	2.56	0.41
3:W:46:LYS:HD3	3:W:46:LYS:HA	1.89	0.41
1:A:468:LEU:HD12	1:A:471:LEU:HD12	2.03	0.40
1:A:506:PRO:HB3	2:H:34:SER:O	2.21	0.40
1:A:540:LEU:HD11	1:A:565:ASP:HB3	2.03	0.40
1:A:932:THR:HG22	1:A:934:GLU:H	1.85	0.40
1:A:995:MET:O	1:A:999:LYS:HG3	2.20	0.40
1:C:961:ARG:HD2	1:C:962:GLU:OE2	2.20	0.40
1:D:49:ARG:NH1	1:D:68:GLU:OE1	2.54	0.40
1:D:298:LEU:O	1:D:300:GLN:HG2	2.21	0.40
1:E:592:MET:SD	1:E:711:ARG:HG3	2.61	0.40
2:H:26:ALA:HA	2:H:81:THR:HG23	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:79:LEU:HD23	3:Q:79:LEU:HA	1.82	0.40
1:A:309:ASP:O	1:A:668:ARG:NH1	2.48	0.40
1:A:490:ASP:OD1	1:A:501:LYS:HG3	2.22	0.40
1:B:364:LYS:HD2	1:B:374:ILE:CG2	2.52	0.40
1:E:117:GLY:O	1:E:173:LEU:HB2	2.21	0.40
1:E:874:ILE:O	1:E:933:LYS:HD3	2.21	0.40
2:P:50:TRP:CE3	2:P:50:TRP:HA	2.56	0.40
2:P:107:ALA:O	3:Q:50:TYR:HB2	2.21	0.40
3:Q:62:ARG:HD2	3:Q:78:SER:O	2.20	0.40
3:T:31:SER:HA	3:T:67:ARG:NH1	2.36	0.40
1:A:465:GLU:O	1:A:469:ASP:HB2	2.21	0.40
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.03	0.40
1:C:319:ILE:HG13	1:C:371:MET:HB2	2.03	0.40
1:C:711:ARG:HA	1:C:711:ARG:HD2	1.88	0.40
1:D:75:VAL:HA	1:D:256:VAL:O	2.21	0.40
1:D:341:GLU:HG2	1:D:347:LEU:HD23	2.03	0.40
1:E:82:THR:HA	1:E:261:ARG:HH21	1.85	0.40
3:T:33:ALA:HB1	3:T:92:SER:O	2.21	0.40
1:A:102:ASN:OD1	1:A:102:ASN:N	2.53	0.40
1:A:587:PRO:HB3	1:A:700:LEU:HD23	2.02	0.40
1:B:490:ASP:OD1	1:B:491:ARG:N	2.50	0.40
1:C:74:LYS:HD2	1:C:74:LYS:H	1.87	0.40
1:C:302:TYR:CD2	1:C:502:GLN:HB3	2.57	0.40
1:C:311:ARG:HD2	1:C:384:LEU:HD22	2.03	0.40
1:C:838:ARG:HB2	1:C:847:ARG:HD3	2.04	0.40
1:E:73:ILE:HG12	1:E:254:MET:HB2	2.02	0.40
3:N:32:SER:N	3:N:67:ARG:NH1	2.69	0.40
2:P:22:ARG:NH1	2:P:83:TYR:CG	2.89	0.40
1:C:311:ARG:HH22	1:C:664:GLU:CD	2.25	0.40
1:C:418:ASN:HB3	1:C:454:TYR:O	2.21	0.40
1:C:579:PHE:HZ	1:C:765:ARG:NH2	2.19	0.40
1:D:510:ILE:O	1:D:514:GLN:HG3	2.21	0.40
1:D:827:GLU:CG	1:D:862:ARG:HH22	2.35	0.40
1:E:296:GLU:HG3	1:E:297:HIS:CE1	2.57	0.40
1:E:743:GLN:HG3	1:E:747:ASP:OD2	2.21	0.40
1:E:792:GLU:HA	1:E:848:PHE:O	2.21	0.40
1:E:794:TYR:CD1	1:E:838:ARG:HD3	2.56	0.40
3:T:8:SER:HB3	3:T:23:THR:HB	2.04	0.40
3:T:32:SER:N	3:T:67:ARG:NH1	2.70	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	947/990 (96%)	924 (98%)	23 (2%)	0	100	100
1	B	946/990 (96%)	922 (98%)	24 (2%)	0	100	100
1	C	949/990 (96%)	923 (97%)	26 (3%)	0	100	100
1	D	949/990 (96%)	926 (98%)	23 (2%)	0	100	100
1	E	949/990 (96%)	919 (97%)	30 (3%)	0	100	100
2	H	117/229 (51%)	110 (94%)	7 (6%)	0	100	100
2	M	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	P	116/229 (51%)	110 (95%)	6 (5%)	0	100	100
2	S	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	V	115/229 (50%)	108 (94%)	7 (6%)	0	100	100
3	L	106/215 (49%)	97 (92%)	9 (8%)	0	100	100
3	N	107/215 (50%)	103 (96%)	4 (4%)	0	100	100
3	Q	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
3	T	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
3	W	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
All	All	5845/7170 (82%)	5654 (97%)	191 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	840/879 (96%)	837 (100%)	3 (0%)	91	95
1	B	838/879 (95%)	837 (100%)	1 (0%)	93	97
1	C	841/879 (96%)	837 (100%)	4 (0%)	88	94
1	D	840/879 (96%)	838 (100%)	2 (0%)	93	97
1	E	840/879 (96%)	835 (99%)	5 (1%)	86	92
2	H	94/191 (49%)	94 (100%)	0	100	100
2	M	92/191 (48%)	91 (99%)	1 (1%)	73	85
2	P	93/191 (49%)	92 (99%)	1 (1%)	73	85
2	S	92/191 (48%)	92 (100%)	0	100	100
2	V	92/191 (48%)	92 (100%)	0	100	100
3	L	93/190 (49%)	90 (97%)	3 (3%)	39	65
3	N	94/190 (50%)	92 (98%)	2 (2%)	53	74
3	Q	93/190 (49%)	92 (99%)	1 (1%)	73	85
3	T	93/190 (49%)	90 (97%)	3 (3%)	39	65
3	W	91/190 (48%)	90 (99%)	1 (1%)	73	85
All	All	5126/6300 (81%)	5099 (100%)	27 (0%)	88	94

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	111	GLU
1	A	701	LYS
1	B	261	ARG
1	C	217	LYS
1	C	261	ARG
1	C	839	ARG
1	C	1005	PHE
1	D	281	LYS
1	D	408	GLU
1	E	402	ARG
1	E	423	ARG
1	E	648	LYS
1	E	687	ARG
1	E	841	ASN
3	L	5	MET
3	L	93	TYR
3	L	106	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	114	GLN
3	N	50	TYR
3	N	93	TYR
2	P	99	CYS
3	Q	91	GLN
3	T	38	GLN
3	T	93	TYR
3	T	94	PHE
3	W	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	ASN
1	D	190	HIS
2	H	42	GLN

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)

There are no ligands in this entry.

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	953/990 (96%)	-0.28	0	100	100	55, 72, 89, 121	0
1	B	952/990 (96%)	-0.18	3 (0%)	94	91	56, 76, 92, 128	0
1	C	953/990 (96%)	-0.28	1 (0%)	95	95	55, 72, 90, 117	0
1	D	953/990 (96%)	-0.20	2 (0%)	95	94	54, 77, 93, 121	0
1	E	953/990 (96%)	-0.25	1 (0%)	95	95	51, 73, 90, 120	0
2	H	119/229 (51%)	0.02	1 (0%)	86	81	64, 78, 98, 106	0
2	M	117/229 (51%)	0.24	2 (1%)	70	62	73, 92, 106, 125	0
2	P	118/229 (51%)	0.14	1 (0%)	86	81	71, 88, 105, 112	0
2	S	117/229 (51%)	0.17	1 (0%)	84	79	71, 89, 105, 116	0
2	V	117/229 (51%)	0.03	1 (0%)	84	79	70, 89, 110, 119	0
3	L	108/215 (50%)	0.08	1 (0%)	84	79	64, 77, 96, 113	0
3	N	109/215 (50%)	0.28	1 (0%)	84	79	71, 89, 103, 109	0
3	Q	108/215 (50%)	0.15	0	100	100	63, 81, 96, 100	0
3	T	107/215 (49%)	0.25	1 (0%)	84	79	64, 82, 95, 104	0
3	W	105/215 (48%)	0.20	1 (0%)	82	76	70, 85, 99, 108	0
All	All	5889/7170 (82%)	-0.16	17 (0%)	94	91	51, 76, 96, 128	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	14	LEU	3.5
2	M	20	SER	2.8
1	C	493	GLU	2.8
1	E	43	ASN	2.6
2	S	14	LEU	2.6
1	B	983	ALA	2.5
3	L	84	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	212	LYS	2.3
1	B	780	GLN	2.3
1	D	983	ALA	2.3
3	N	13	SER	2.3
3	T	70	THR	2.2
2	V	115	GLY	2.2
3	W	11	SER	2.2
1	D	79	SER	2.1
2	P	4	GLU	2.1
2	H	14	LEU	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.