



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:02 pm GMT

PDB ID : 3LTG
Title : Crystal structure of the Drosophila Epidermal Growth Factor Receptor ectodomain complexed with a low affinity Spitz mutant
Authors : Alvarado, D.; Klein, D.E.; Lemmon, M.A.
Deposited on : 2010-02-15
Resolution : 3.40 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

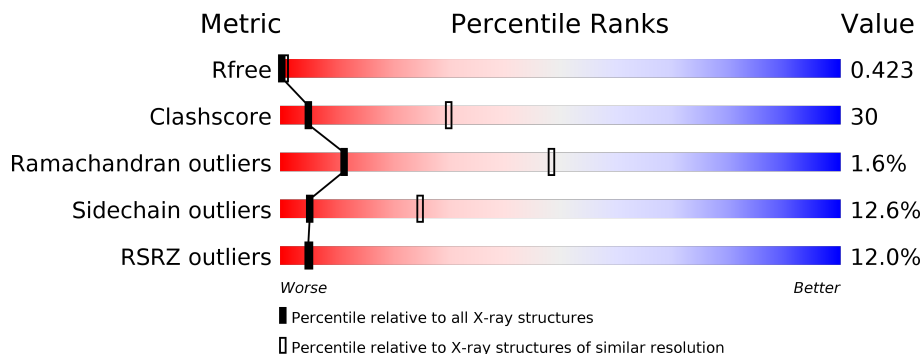
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	601	<div> <div>5%</div> <div>49%</div> <div>31%</div> <div>6% • 13%</div> </div>
1	C	601	<div> <div>15%</div> <div>45%</div> <div>34%</div> <div>8% • 12%</div> </div>
2	D	52	<div> <div>13%</div> <div>65%</div> <div>27%</div> <div>6% •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8529 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4013	2497	709	759	48			
1	C	531	Total	C	N	O	S	0	1	0
			4115	2565	732	768	50			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P04412
A	-4	HIS	-	EXPRESSION TAG	UNP P04412
A	-3	HIS	-	EXPRESSION TAG	UNP P04412
A	-2	HIS	-	EXPRESSION TAG	UNP P04412
A	-1	HIS	-	EXPRESSION TAG	UNP P04412
A	0	HIS	-	EXPRESSION TAG	UNP P04412
A	38	GLU	LYS	CONFLICT	UNP P04412
A	230	GLY	ALA	CONFLICT	UNP P04412
A	232	CYS	SER	CONFLICT	UNP P04412
A	359	LEU	ARG	CONFLICT	UNP P04412
A	493	ASN	THR	CONFLICT	UNP P04412
A	590	HIS	-	EXPRESSION TAG	UNP P04412
A	591	HIS	-	EXPRESSION TAG	UNP P04412
A	592	HIS	-	EXPRESSION TAG	UNP P04412
A	593	HIS	-	EXPRESSION TAG	UNP P04412
A	594	HIS	-	EXPRESSION TAG	UNP P04412
A	595	HIS	-	EXPRESSION TAG	UNP P04412
C	-5	HIS	-	EXPRESSION TAG	UNP P04412
C	-4	HIS	-	EXPRESSION TAG	UNP P04412
C	-3	HIS	-	EXPRESSION TAG	UNP P04412
C	-2	HIS	-	EXPRESSION TAG	UNP P04412
C	-1	HIS	-	EXPRESSION TAG	UNP P04412
C	0	HIS	-	EXPRESSION TAG	UNP P04412
C	38	GLU	LYS	CONFLICT	UNP P04412
C	230	GLY	ALA	CONFLICT	UNP P04412

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	232	CYS	SER	CONFLICT	UNP P04412
C	359	LEU	ARG	CONFLICT	UNP P04412
C	493	ASN	THR	CONFLICT	UNP P04412
C	590	HIS	-	EXPRESSION TAG	UNP P04412
C	591	HIS	-	EXPRESSION TAG	UNP P04412
C	592	HIS	-	EXPRESSION TAG	UNP P04412
C	593	HIS	-	EXPRESSION TAG	UNP P04412
C	594	HIS	-	EXPRESSION TAG	UNP P04412
C	595	HIS	-	EXPRESSION TAG	UNP P04412

- Molecule 2 is a protein called Protein spitz.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	51	Total	C	N	O	S	0	0	0
			401	259	62	73	7			

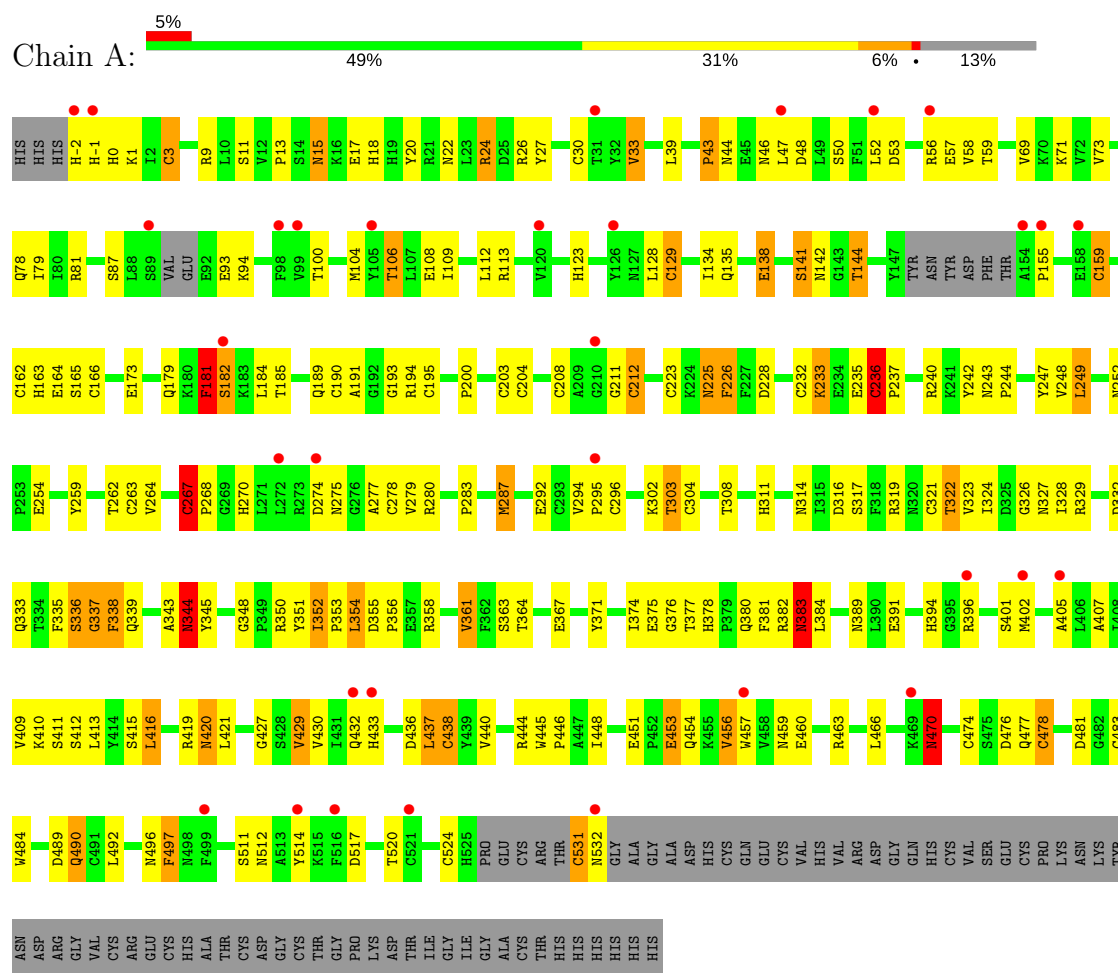
There is a discrepancy between the modelled and reference sequences:

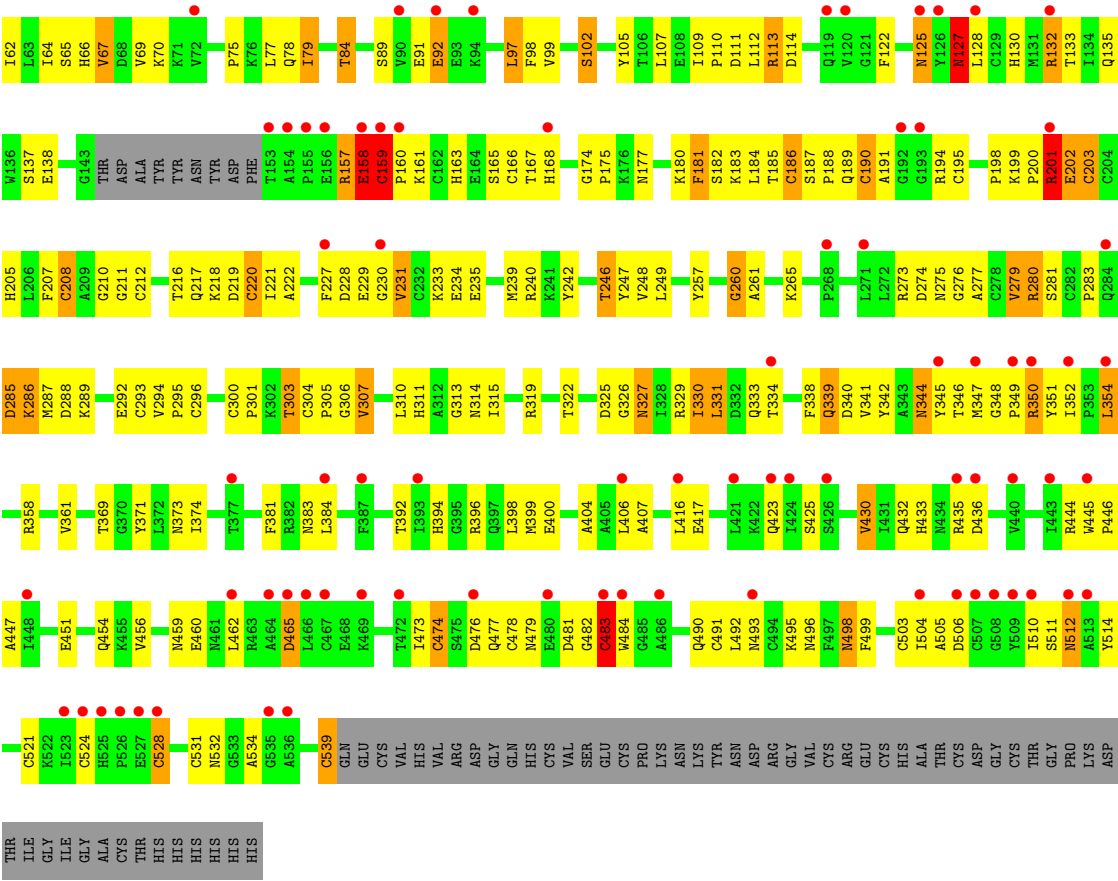
Chain	Residue	Modelled	Actual	Comment	Reference
D	52	ASP	-	EXPRESSION TAG	UNP Q01083

3 Residue-property plots [i](#)

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: Epidermal growth factor receptor





● Molecule 2: Protein spitz



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.75Å 120.15Å 274.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 46.58 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.7 (50.00-3.40) 82.7 (46.58-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.406 , 0.427 0.399 , 0.423	Depositor DCC
R_{free} test set	2886 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , -9.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	8529	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

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	0.78	9/4103 (0.2%)	0.85	11/5566 (0.2%)
1	C	0.72	3/4211 (0.1%)	0.87	7/5707 (0.1%)
2	D	0.68	0/413	0.77	1/560 (0.2%)
All	All	0.75	12/8727 (0.1%)	0.86	19/11833 (0.2%)

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	C	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	GLN	C-N	10.65	1.58	1.34
1	A	383	ASN	CG-ND2	-10.62	1.06	1.32
1	A	3	CYS	CB-SG	-10.10	1.65	1.82
1	A	470	ASN	CG-ND2	-10.00	1.07	1.32
1	C	436	ASP	CG-OD1	9.27	1.46	1.25
1	A	181	PHE	C-N	8.55	1.53	1.34
1	C	436	ASP	CB-CG	8.32	1.69	1.51
1	C	203	CYS	CB-SG	-6.47	1.71	1.82
1	A	470	ASN	CB-CG	6.28	1.65	1.51
1	A	267	CYS	CB-SG	-6.07	1.72	1.82
1	A	236	CYS	CB-SG	-5.74	1.72	1.81
1	A	438	CYS	CB-SG	-5.12	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ASP	CB-CG-OD2	-17.04	102.97	118.30
1	C	436	ASP	CB-CG-OD1	14.99	131.79	118.30
1	A	267	CYS	CA-CB-SG	-9.31	97.24	114.00
1	C	159	CYS	CA-CB-SG	-9.08	97.66	114.00
2	D	16	CYS	CA-CB-SG	-8.65	98.44	114.00
1	A	490	GLN	O-C-N	8.56	136.40	122.70
1	A	490	GLN	C-N-CA	-8.41	100.69	121.70
1	A	337	GLY	N-CA-C	-8.21	92.58	113.10
1	A	490	GLN	CA-C-N	-7.70	100.26	117.20
1	C	190	CYS	CA-CB-SG	-7.17	101.09	114.00
1	A	159	CYS	CA-CB-SG	-7.11	101.21	114.00
1	A	236	CYS	CA-CB-SG	-6.86	101.66	114.00
1	C	203	CYS	CA-CB-SG	-5.85	103.46	114.00
1	A	232	CYS	CA-CB-SG	-5.77	103.61	114.00
1	A	129	CYS	CA-CB-SG	-5.70	103.74	114.00
1	A	278	CYS	CA-CB-SG	-5.49	104.11	114.00
1	C	483	CYS	CA-CB-SG	-5.36	104.35	114.00
1	A	321	CYS	CA-CB-SG	-5.35	104.38	114.00
1	C	280	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	PHE	Mainchain
1	C	158	GLU	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	4013	0	3753	235	2
1	C	4115	0	3906	277	6
2	D	401	0	362	16	0
All	All	8529	0	8021	494	8

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 30.

All (494) 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:A:354:LEU:HD12	1:A:355:ASP:N	1.12	1.44
1:A:354:LEU:CD1	1:A:355:ASP:O	1.76	1.34
1:C:311:HIS:CE1	1:C:351:TYR:CE1	2.21	1.28
1:A:354:LEU:HD12	1:A:355:ASP:CA	1.67	1.25
1:C:311:HIS:CE1	1:C:351:TYR:HE1	1.56	1.23
1:A:354:LEU:CD1	1:A:355:ASP:N	2.06	1.19
1:A:524:CYS:SG	1:A:531:CYS:SG	1.37	1.17
1:A:354:LEU:C	1:A:354:LEU:HD12	1.64	1.15
1:A:354:LEU:CD1	1:A:355:ASP:C	2.16	1.14
1:C:340:ASP:HB2	1:C:351:TYR:CE2	1.82	1.14
1:C:340:ASP:HB2	1:C:351:TYR:HE2	1.05	1.11
1:C:341:VAL:HG23	2:D:45:ARG:NH1	1.67	1.09
1:A:354:LEU:HD11	1:A:355:ASP:O	1.52	1.08
1:C:373:ASN:HB2	1:C:399:MET:HE3	1.34	1.08
1:A:352:ILE:HG13	1:A:352:ILE:O	1.41	1.07
1:C:36:ASN:OD1	1:C:61:TYR:CE1	2.09	1.05
1:A:524:CYS:SG	1:A:531:CYS:CB	2.43	1.05
1:C:15:ASN:HD22	1:C:18:HIS:HB2	1.22	1.04
1:C:531:CYS:SG	1:C:539:CYS:HB3	1.97	1.03
1:A:354:LEU:HD11	1:A:355:ASP:C	1.79	1.01
1:C:477:GLN:O	1:C:495:LYS:N	1.93	1.00
1:C:477:GLN:C	1:C:495:LYS:HB2	1.82	1.00
1:C:499:PHE:HB3	1:C:504:ILE:HD12	1.45	0.99
1:C:473:ILE:O	1:C:474:CYS:HB2	1.62	0.99
1:A:352:ILE:HD12	1:A:353:PRO:O	1.63	0.98
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.46	0.96
1:C:130:HIS:H	1:C:132:ARG:HH11	1.14	0.96
1:A:524:CYS:CB	1:A:531:CYS:SG	2.54	0.95
1:A:163:HIS:HD2	1:A:165:SER:H	1.12	0.94
1:A:194:ARG:O	1:A:204:CYS:HB2	1.68	0.94
1:C:227:PHE:CZ	1:C:230:GLY:HA2	2.02	0.94
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.33	0.94
1:C:12:VAL:HG11	1:C:41:TRP:CD1	2.04	0.93
1:A:287:MET:HB2	1:A:296:CYS:HB3	1.49	0.93
1:A:466:LEU:O	1:A:470:ASN:HB2	1.68	0.92
1:A:354:LEU:HD13	1:A:355:ASP:O	1.66	0.91
1:C:400:GLU:HG3	2:D:51:ILE:HD12	1.49	0.91
1:C:476:ASP:O	1:C:495:LYS:HD3	1.72	0.90
1:C:12:VAL:CG1	1:C:41:TRP:CD1	2.56	0.89
1:A:73:VAL:HG12	1:A:108:GLU:HB2	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PHE:CE2	1:C:230:GLY:HA2	2.10	0.86
1:C:130:HIS:H	1:C:132:ARG:NH1	1.73	0.86
1:C:307:VAL:HG11	1:C:314:ASN:HD22	1.43	0.84
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.43	0.82
1:C:287:MET:CE	1:C:301:PRO:HD2	2.09	0.82
1:C:311:HIS:HE1	1:C:351:TYR:HE1	1.22	0.81
1:A:193:GLY:HA3	1:C:201:ARG:HH12	1.43	0.81
1:A:354:LEU:HD12	1:A:355:ASP:C	1.91	0.81
1:A:163:HIS:CD2	1:A:165:SER:H	1.99	0.81
1:A:448:ILE:HD11	1:A:484:TRP:HZ2	1.45	0.81
1:C:287:MET:HE2	1:C:301:PRO:HD2	1.63	0.81
1:C:138:GLU:OE1	1:C:184:LEU:HG	1.81	0.80
1:A:100:THR:HG22	1:A:123:HIS:HB3	1.63	0.80
1:C:21:ARG:HG3	1:C:24:ARG:NH2	1.97	0.80
1:C:311:HIS:CE1	1:C:351:TYR:CD1	2.69	0.80
1:A:113:ARG:NH2	1:A:182:SER:OG	2.14	0.80
1:A:352:ILE:CD1	1:A:353:PRO:O	2.30	0.80
1:C:478:CYS:N	1:C:495:LYS:HB2	1.95	0.80
1:A:354:LEU:CD1	1:A:354:LEU:C	2.29	0.79
1:A:138:GLU:HB2	1:A:184:LEU:HG	1.65	0.79
1:C:373:ASN:CB	1:C:399:MET:HE3	2.12	0.79
1:A:354:LEU:CD1	1:A:355:ASP:CA	2.49	0.78
1:A:274:ASP:OD2	1:C:240:ARG:NH2	2.16	0.78
1:C:15:ASN:ND2	1:C:18:HIS:HB2	1.98	0.77
1:C:311:HIS:ND1	1:C:351:TYR:CD1	2.52	0.77
1:C:138:GLU:HB2	1:C:184:LEU:CD1	2.14	0.77
1:C:476:ASP:O	1:C:495:LYS:CD	2.34	0.76
1:A:225:ASN:HD22	1:A:225:ASN:H	1.30	0.75
1:A:248:VAL:HA	1:C:279:VAL:HG22	1.68	0.75
1:A:193:GLY:HA3	1:C:201:ARG:NH1	2.01	0.74
1:C:339:GLN:NE2	1:C:350[B]:ARG:NH2	2.36	0.74
1:C:340:ASP:OD2	1:C:351:TYR:OH	2.05	0.74
1:A:411:SER:OG	1:A:413:LEU:HD13	1.87	0.74
1:C:373:ASN:HB2	1:C:399:MET:CE	2.16	0.74
1:C:127:ASN:O	1:C:157:ARG:NH1	2.20	0.73
1:C:514:TYR:CZ	1:C:534:ALA:HB2	2.23	0.73
1:C:99:VAL:HG22	1:C:122:PHE:CD2	2.23	0.73
1:A:514:TYR:HB2	1:A:532:ASN:C	2.09	0.73
1:A:87:SER:HB2	1:A:93:GLU:O	1.89	0.73
1:C:15:ASN:HD22	1:C:18:HIS:CB	2.00	0.72
1:C:239:MET:CE	1:C:257:TYR:CE1	2.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:GLN:C	1:C:495:LYS:CB	2.57	0.72
1:C:477:GLN:HB3	1:C:503:CYS:HB3	1.72	0.72
1:C:132:ARG:HD3	1:C:132:ARG:H	1.55	0.72
1:C:287:MET:HE3	1:C:296:CYS:HB3	1.71	0.71
1:C:433:HIS:CE1	1:C:460:GLU:HG3	2.25	0.71
1:A:484:TRP:HB2	1:A:490:GLN:HG3	1.71	0.71
1:A:433:HIS:HB2	1:A:460:GLU:OE1	1.91	0.71
1:A:163:HIS:HD2	1:A:165:SER:N	1.88	0.71
1:C:113:ARG:HG3	1:C:113:ARG:NH1	2.05	0.70
1:C:189:GLN:OE1	1:C:200:PRO:HB3	1.92	0.70
1:C:36:ASN:HD21	1:C:84:THR:HB	1.56	0.70
1:A:138:GLU:HB2	1:A:184:LEU:CG	2.22	0.70
1:C:371:TYR:CE1	1:C:399:MET:HE2	2.27	0.70
1:A:411:SER:CB	1:A:413:LEU:HD13	2.22	0.70
1:C:102:SER:H	1:C:125:ASN:HB3	1.55	0.70
1:C:12:VAL:HG13	1:C:41:TRP:CD1	2.27	0.69
1:C:345:TYR:O	2:D:11:PHE:HZ	1.75	0.69
1:A:448:ILE:HD11	1:A:484:TRP:CZ2	2.27	0.69
1:C:373:ASN:CG	1:C:399:MET:HE1	2.13	0.69
1:C:477:GLN:O	1:C:495:LYS:CB	2.40	0.69
1:C:180:LYS:C	1:C:181:PHE:HD1	1.96	0.69
1:C:330:ILE:HD11	1:C:381:PHE:CZ	2.28	0.69
1:C:347:MET:HE1	2:D:14:TRP:C	2.13	0.69
1:A:15:ASN:ND2	1:A:18:HIS:H	1.92	0.68
1:A:33:VAL:HG13	1:A:58:VAL:HG22	1.75	0.68
1:C:181:PHE:N	1:C:181:PHE:HD1	1.91	0.68
1:C:65:SER:OG	1:C:66:HIS:HD2	1.77	0.68
1:C:208:CYS:HB3	1:C:222:ALA:O	1.93	0.68
1:A:277:ALA:HB1	1:C:242:TYR:CD1	2.29	0.68
1:A:451:GLU:HB3	1:A:453:GLU:OE2	1.94	0.68
1:C:496:ASN:ND2	1:C:505:ALA:O	2.27	0.68
1:A:433:HIS:ND1	1:A:460:GLU:OE1	2.27	0.67
1:C:181:PHE:N	1:C:181:PHE:CD1	2.60	0.67
1:C:341:VAL:CG2	2:D:45:ARG:NH1	2.54	0.67
1:C:417:GLU:OE1	1:C:490:GLN:NE2	2.27	0.67
1:A:351:TYR:O	1:A:352:ILE:C	2.31	0.67
1:A:33:VAL:CG1	1:A:58:VAL:HG22	2.25	0.67
1:A:324:ILE:CD1	1:A:328:ILE:HD11	2.23	0.66
1:C:44:ASN:O	1:C:47:LEU:HD23	1.94	0.66
1:C:183:LYS:HG2	1:C:184:LEU:HD23	1.76	0.66
1:A:336:SER:O	1:A:353:PRO:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:TRP:NE1	1:A:492:LEU:CD2	2.59	0.66
1:A:191:ALA:O	1:C:201:ARG:HD2	1.96	0.66
1:C:373:ASN:ND2	1:C:399:MET:HE1	2.10	0.66
1:C:228:ASP:OD2	1:C:233:LYS:HE3	1.96	0.65
1:A:327:ASN:OD1	1:A:371:TYR:CE2	2.50	0.65
1:A:270:HIS:HA	1:A:396:ARG:HG2	1.79	0.65
1:C:287:MET:HE3	1:C:296:CYS:CB	2.27	0.65
1:C:239:MET:CE	1:C:257:TYR:CZ	2.80	0.65
1:C:114:ASP:OD2	1:C:194:ARG:NH1	2.30	0.64
1:C:344:ASN:N	1:C:344:ASN:OD1	2.30	0.64
1:C:12:VAL:HG11	1:C:41:TRP:CG	2.32	0.64
1:A:405:ALA:HB2	1:A:427:GLY:HA3	1.80	0.64
1:C:180:LYS:C	1:C:181:PHE:CD1	2.71	0.64
1:C:400:GLU:HG3	2:D:51:ILE:CD1	2.24	0.64
1:C:319:ARG:HA	1:C:361:VAL:HG13	1.79	0.63
1:A:383:ASN:HA	1:A:415:SER:O	1.97	0.63
1:A:57:GLU:HG3	1:A:79:ILE:HB	1.81	0.63
1:C:138:GLU:HB2	1:C:184:LEU:HD11	1.79	0.63
1:C:44:ASN:OD1	1:C:47:LEU:HD22	1.98	0.63
1:C:77:LEU:HD23	1:C:78:GLN:N	2.14	0.63
1:A:477:GLN:O	1:A:478:CYS:SG	2.56	0.63
1:C:477:GLN:O	1:C:495:LYS:HB2	1.97	0.63
1:A:411:SER:HB2	1:A:413:LEU:CD1	2.28	0.63
1:C:327:ASN:HB3	1:C:371:TYR:H	1.62	0.63
1:A:374:ILE:HD13	1:A:384:LEU:HD21	1.80	0.62
1:C:373:ASN:CG	1:C:399:MET:CE	2.67	0.62
1:A:411:SER:HB2	1:A:413:LEU:HD13	1.81	0.62
1:A:267:CYS:SG	1:A:268:PRO:HD2	2.39	0.62
1:A:391:GLU:HA	1:A:420:ASN:O	1.99	0.62
1:C:114:ASP:CG	1:C:194:ARG:NH1	2.53	0.62
1:C:306:GLY:N	1:C:325:ASP:O	2.32	0.62
1:A:138:GLU:HB2	1:A:184:LEU:CD1	2.30	0.62
1:C:514:TYR:OH	1:C:534:ALA:HB2	1.99	0.62
1:A:354:LEU:O	1:A:354:LEU:HG	1.99	0.62
1:C:383:ASN:HB2	1:C:417:GLU:HG3	1.82	0.62
1:C:483:CYS:HB3	1:C:491:CYS:HA	1.82	0.61
1:A:81:ARG:NH2	1:A:223:CYS:O	2.18	0.61
1:C:36:ASN:OD1	1:C:61:TYR:CZ	2.52	0.61
1:A:437:LEU:HD11	1:A:440:VAL:HG13	1.82	0.61
1:C:130:HIS:N	1:C:132:ARG:HH11	1.93	0.61
1:C:49:LEU:HD22	1:C:69:VAL:HG11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:SER:OG	2:D:36:GLU:OE2	2.15	0.61
1:A:226:PHE:HB2	1:A:233:LYS:O	2.00	0.61
1:C:294:VAL:HG13	1:C:295:PRO:HD2	1.83	0.61
1:C:45:GLU:O	1:C:46:ASN:HB2	2.01	0.61
1:A:413:LEU:HB2	1:A:437:LEU:HD23	1.82	0.61
2:D:27:ILE:HG13	2:D:27:ILE:O	1.98	0.61
1:A:279:VAL:HA	1:C:247:TYR:O	2.01	0.60
1:C:373:ASN:CB	1:C:399:MET:CE	2.78	0.60
1:A:378:HIS:HD2	1:A:380:GLN:H	1.50	0.60
1:C:36:ASN:OD1	1:C:61:TYR:CD1	2.52	0.60
1:C:275:ASN:OD1	1:C:276:GLY:N	2.35	0.60
1:A:410:LYS:HG3	1:A:433:HIS:HD2	1.66	0.60
1:A:437:LEU:HD12	1:A:440:VAL:HG22	1.84	0.60
1:C:77:LEU:HD23	1:C:77:LEU:C	2.22	0.60
1:C:287:MET:HE1	1:C:301:PRO:HD2	1.82	0.60
1:C:311:HIS:ND1	1:C:351:TYR:HD1	1.97	0.60
1:C:114:ASP:CG	1:C:194:ARG:HH12	2.05	0.59
1:C:228:ASP:O	1:C:231:VAL:HG13	2.02	0.59
1:C:183:LYS:HG2	1:C:184:LEU:N	2.18	0.59
1:A:378:HIS:CD2	1:A:380:GLN:H	2.19	0.59
1:C:473:ILE:O	1:C:474:CYS:CB	2.39	0.59
1:C:186:CYS:HB3	1:C:198:PRO:HA	1.85	0.59
1:C:374:ILE:HD13	1:C:384:LEU:HD21	1.84	0.59
1:C:163:HIS:ND1	1:C:165:SER:HB3	2.17	0.58
1:C:200:PRO:O	1:C:201:ARG:CB	2.51	0.58
1:C:211:GLY:O	1:C:220:CYS:HB3	2.04	0.58
1:A:484:TRP:NE1	1:A:492:LEU:HD23	2.19	0.57
2:D:16:CYS:HB3	2:D:20:ALA:HB3	1.86	0.57
1:A:437:LEU:HD13	1:A:438:CYS:H	1.68	0.57
1:A:524:CYS:SG	1:A:531:CYS:HB2	2.40	0.57
1:C:109:ILE:HG22	1:C:112:LEU:HB2	1.87	0.57
1:C:36:ASN:HD22	1:C:36:ASN:N	2.02	0.57
1:C:51:PHE:CD2	1:C:52:LEU:HD13	2.39	0.57
1:C:504:ILE:HG22	1:C:506:ASP:H	1.70	0.57
1:C:199:LYS:HB2	1:C:202:GLU:OE2	2.04	0.57
1:C:341:VAL:HG23	2:D:45:ARG:CZ	2.33	0.57
1:A:402:MET:HE1	1:A:430:VAL:CG1	2.35	0.57
1:C:451:GLU:O	1:C:454:GLN:HG3	2.05	0.57
1:A:191:ALA:O	1:C:201:ARG:CD	2.53	0.57
1:A:295:PRO:HG3	1:C:295:PRO:HG3	1.86	0.56
1:A:335:PHE:HE1	1:A:376:GLY:HA3	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:O	1:A:352:ILE:O	2.23	0.56
1:A:416:LEU:HD21	1:A:440:VAL:HG12	1.88	0.56
1:C:340:ASP:HB3	1:C:349:PRO:HD2	1.86	0.56
1:A:302:LYS:O	1:A:322:THR:HG22	2.04	0.56
1:A:87:SER:HB3	1:A:94:LYS:HA	1.87	0.56
1:C:200:PRO:O	1:C:201:ARG:HB2	2.04	0.56
1:A:319:ARG:HA	1:A:361:VAL:HG12	1.87	0.56
1:C:342:TYR:HD1	1:C:346:THR:HG23	1.70	0.56
1:C:42:LEU:HD23	1:C:49:LEU:HD11	1.87	0.56
1:C:482:GLY:C	1:C:483:CYS:SG	2.83	0.56
1:A:182:SER:HB2	1:A:194:ARG:HD3	1.88	0.56
1:C:195:CYS:HB3	1:C:203:CYS:SG	2.46	0.56
1:A:433:HIS:CG	1:A:460:GLU:OE1	2.58	0.55
1:A:303:THR:CG2	1:A:304:CYS:N	2.68	0.55
1:A:189:GLN:OE1	1:A:200:PRO:HB2	2.07	0.55
1:C:53:ASP:HA	1:C:75:PRO:HD2	1.87	0.55
1:A:323:VAL:HG22	1:A:367:GLU:HB2	1.89	0.55
1:C:307:VAL:HG11	1:C:314:ASN:ND2	2.17	0.55
1:A:437:LEU:HD13	1:A:438:CYS:N	2.22	0.55
1:C:330:ILE:HD11	1:C:381:PHE:CE1	2.40	0.55
1:A:433:HIS:CB	1:A:460:GLU:OE1	2.54	0.55
1:A:259:TYR:O	1:A:262:THR:HB	2.07	0.55
1:A:242:TYR:CE2	1:C:277:ALA:HB1	2.41	0.55
1:A:247:TYR:O	1:C:279:VAL:HA	2.06	0.55
1:C:478:CYS:CA	1:C:495:LYS:HB2	2.37	0.55
1:A:262:THR:HG22	1:A:264:VAL:HG13	1.89	0.54
1:A:228:ASP:HB3	1:A:233:LYS:HD3	1.88	0.54
1:A:327:ASN:HD22	1:A:327:ASN:N	2.06	0.54
1:A:233:LYS:HG3	1:A:235:GLU:O	2.08	0.54
1:A:283:PRO:HG3	1:C:240:ARG:NH2	2.23	0.54
1:C:287:MET:HE1	1:C:301:PRO:CD	2.36	0.54
1:C:163:HIS:ND1	1:C:175:PRO:HG3	2.23	0.54
1:A:15:ASN:C	1:A:15:ASN:HD22	2.11	0.54
1:A:274:ASP:O	1:C:249:LEU:HD11	2.08	0.54
1:C:369:THR:HA	1:C:394:HIS:HB2	1.89	0.54
1:A:275:ASN:HD21	1:C:275:ASN:ND2	2.05	0.53
1:A:225:ASN:N	1:A:225:ASN:HD22	2.01	0.53
1:C:239:MET:HE3	1:C:257:TYR:CZ	2.44	0.53
1:C:478:CYS:HA	1:C:495:LYS:N	2.24	0.53
1:A:100:THR:HA	1:A:123:HIS:O	2.07	0.53
1:A:402:MET:HE2	1:A:430:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:HIS:ND1	1:C:165:SER:CB	2.71	0.53
1:A:477:GLN:O	1:A:478:CYS:CB	2.55	0.53
1:C:21:ARG:CG	1:C:24:ARG:NH2	2.71	0.53
1:A:242:TYR:CD2	1:C:277:ALA:HB1	2.44	0.53
1:A:402:MET:HE1	1:A:430:VAL:HG13	1.90	0.53
1:C:341:VAL:CG2	2:D:45:ARG:CZ	2.87	0.53
1:A:437:LEU:HD12	1:A:440:VAL:CG2	2.39	0.53
1:A:451:GLU:H	1:A:454:GLN:NE2	2.07	0.53
1:A:22:ASN:OD1	1:A:401:SER:HB3	2.09	0.53
1:A:109:ILE:HG22	1:A:112:LEU:HB2	1.90	0.53
1:C:163:HIS:CE1	1:C:175:PRO:HG3	2.44	0.53
1:A:134:ILE:O	1:A:135:GLN:HB3	2.09	0.53
1:C:319:ARG:HH11	1:C:319:ARG:HG3	1.74	0.52
2:D:26:LYS:HA	2:D:30:LEU:O	2.09	0.52
1:A:134:ILE:O	1:A:179:GLN:OE1	2.27	0.52
1:A:484:TRP:HE1	1:A:492:LEU:CD2	2.22	0.52
1:C:33:VAL:CG1	1:C:58:VAL:HG22	2.39	0.52
1:A:280:ARG:N	1:C:247:TYR:O	2.40	0.52
1:A:409:VAL:HG12	1:A:410:LYS:HD3	1.91	0.52
1:A:225:ASN:OD1	1:A:233:LYS:C	2.48	0.52
1:C:37:LEU:HD12	1:C:37:LEU:C	2.30	0.52
1:A:338:PHE:O	1:A:338:PHE:CD1	2.63	0.52
1:A:444:ARG:HG2	1:A:481:ASP:HA	1.92	0.52
1:A:335:PHE:O	1:A:353:PRO:HB3	2.10	0.52
1:C:218:LYS:HE2	1:C:230:GLY:O	2.10	0.52
1:C:339:GLN:NE2	1:C:350[B]:ARG:HH22	2.08	0.52
1:A:193:GLY:CA	1:C:201:ARG:NH1	2.71	0.52
1:A:453:GLU:H	1:A:453:GLU:CD	2.12	0.52
1:A:496:ASN:O	1:A:497:PHE:CB	2.57	0.52
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.21	0.51
1:C:239:MET:HE1	1:C:257:TYR:CE1	2.44	0.51
1:A:326:GLY:C	1:A:327:ASN:HD22	2.13	0.51
1:C:138:GLU:O	1:C:183:LYS:HD3	2.10	0.51
1:A:437:LEU:CD1	1:A:440:VAL:HG13	2.40	0.51
1:C:333:GLN:HE22	2:D:47:GLU:HB2	1.75	0.51
1:A:377:THR:HA	1:A:412:SER:OG	2.10	0.51
1:A:193:GLY:CA	1:C:201:ARG:HH12	2.17	0.51
1:C:239:MET:HE2	1:C:257:TYR:CE1	2.46	0.51
1:A:333:GLN:HG3	1:A:338:PHE:HB2	1.92	0.51
1:A:20:TYR:CD1	1:A:47:LEU:HD22	2.46	0.51
1:C:33:VAL:HG13	1:C:58:VAL:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASP:CG	1:C:351:TYR:HH	2.14	0.51
1:A:474:CYS:SG	1:A:483:CYS:N	2.84	0.51
1:C:217:GLN:HB2	1:C:231:VAL:HG23	1.93	0.51
1:A:181:PHE:CE2	1:A:184:LEU:HD12	2.46	0.50
1:A:344:ASN:N	1:A:344:ASN:OD1	2.35	0.50
1:A:314:ASN:O	1:A:317:SER:OG	2.22	0.50
1:C:499:PHE:HB3	1:C:504:ILE:CD1	2.29	0.50
1:A:208:CYS:SG	1:A:212:CYS:HB3	2.51	0.50
1:C:444:ARG:NH1	1:C:447:ALA:HB2	2.26	0.50
1:A:343:ALA:C	1:A:345:TYR:H	2.14	0.50
1:C:340:ASP:HB2	1:C:351:TYR:CZ	2.41	0.50
1:C:492:LEU:O	1:C:493:ASN:ND2	2.37	0.50
1:A:421:LEU:HD23	1:A:484:TRP:CH2	2.47	0.50
1:C:207:PHE:CE1	1:C:234:GLU:HB2	2.47	0.49
1:A:351:TYR:C	1:A:352:ILE:O	2.49	0.49
1:C:300:CYS:O	1:C:301:PRO:C	2.51	0.49
1:A:247:TYR:HB2	1:C:280:ARG:HG3	1.95	0.49
1:C:37:LEU:HD12	1:C:38:GLU:N	2.28	0.49
1:C:504:ILE:HD13	1:C:510:ILE:HD12	1.94	0.49
1:A:240:ARG:NH1	1:A:249:LEU:HD13	2.28	0.49
1:C:315:ILE:HD12	1:C:354:LEU:HD11	1.95	0.49
1:C:20:TYR:CD1	1:C:47:LEU:HD12	2.46	0.49
1:A:477:GLN:C	1:A:478:CYS:SG	2.92	0.48
1:C:350[A]:ARG:HG2	1:C:350[A]:ARG:HH11	1.78	0.48
1:A:374:ILE:CD1	1:A:384:LEU:HD21	2.42	0.48
1:C:130:HIS:N	1:C:132:ARG:NH1	2.54	0.48
1:C:274:ASP:O	1:C:275:ASN:C	2.51	0.48
1:A:142:ASN:HB2	1:A:144:THR:HG22	1.95	0.48
1:A:355:ASP:HB2	1:A:356:PRO:HD2	1.96	0.48
1:C:484:TRP:CE2	1:C:492:LEU:HD11	2.47	0.48
1:A:416:LEU:HD21	1:A:440:VAL:CG1	2.42	0.48
1:A:489:ASP:N	1:A:489:ASP:OD1	2.30	0.48
1:A:211:GLY:C	1:A:212:CYS:SG	2.92	0.48
1:A:356:PRO:HG3	1:A:381:PHE:HB2	1.95	0.48
1:C:465:ASP:N	1:C:465:ASP:OD1	2.47	0.48
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.13	0.48
1:C:130:HIS:HA	1:C:133:THR:HG23	1.94	0.48
1:A:228:ASP:HA	1:A:263:CYS:HB2	1.95	0.48
1:A:283:PRO:HG3	1:C:240:ARG:HH21	1.77	0.48
1:A:287:MET:SD	1:A:296:CYS:HB2	2.54	0.48
1:C:157:ARG:O	1:C:158:GLU:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ASN:ND2	1:C:18:HIS:CB	2.69	0.48
1:C:310:LEU:HA	1:C:314:ASN:HD21	1.79	0.48
1:A:134:ILE:O	1:A:135:GLN:CB	2.61	0.47
1:A:329:ARG:HD3	1:A:371:TYR:HE1	1.79	0.47
1:A:484:TRP:NE1	1:A:492:LEU:HD21	2.28	0.47
1:C:44:ASN:O	1:C:47:LEU:CD2	2.62	0.47
1:A:43:PRO:HD2	1:A:44:ASN:H	1.79	0.47
1:C:477:GLN:O	1:C:495:LYS:CA	2.62	0.47
1:A:26:ARG:HG2	1:A:27:TYR:CD1	2.48	0.47
1:C:99:VAL:CG2	1:C:122:PHE:CD2	2.97	0.47
1:C:183:LYS:HE2	1:C:184:LEU:CD2	2.44	0.47
1:C:445:TRP:N	1:C:446:PRO:HD2	2.29	0.47
1:C:64:ILE:HG23	1:C:67:VAL:HG11	1.96	0.47
1:A:270:HIS:CD2	1:A:270:HIS:H	2.32	0.47
1:A:484:TRP:HE1	1:A:492:LEU:HD23	1.80	0.47
1:C:187:SER:HB3	1:C:188:PRO:HD2	1.96	0.47
1:A:274:ASP:CG	1:C:240:ARG:HH22	2.13	0.47
1:A:514:TYR:CB	1:A:532:ASN:C	2.83	0.47
1:C:70:LYS:HG2	1:C:105:TYR:CD1	2.51	0.46
1:C:479:ASN:OD1	1:C:481:ASP:HB2	2.14	0.46
1:C:97:LEU:HD23	1:C:98:PHE:N	2.31	0.46
2:D:8:PRO:HD2	2:D:33:TYR:CE2	2.50	0.46
1:A:228:ASP:CB	1:A:233:LYS:HD3	2.45	0.46
1:A:240:ARG:NH2	1:C:283:PRO:HG3	2.30	0.46
1:A:407:ALA:HA	1:A:430:VAL:O	2.16	0.46
1:A:413:LEU:CB	1:A:437:LEU:HD23	2.44	0.46
1:C:260:GLY:O	1:C:261:ALA:HB3	2.15	0.46
1:A:338:PHE:HD1	1:A:338:PHE:H	1.63	0.46
1:A:432:GLN:HA	1:A:459:ASN:O	2.15	0.46
1:A:283:PRO:CG	1:C:240:ARG:NH2	2.78	0.46
1:C:499:PHE:HB2	1:C:521:CYS:HB2	1.97	0.46
1:C:57:GLU:HG3	1:C:79:ILE:HG12	1.98	0.46
1:C:342:TYR:CE1	1:C:348:GLY:HA2	2.51	0.46
1:C:371:TYR:CE1	1:C:399:MET:CE	2.96	0.46
1:C:78:GLN:HA	1:C:112:LEU:HA	1.96	0.46
1:A:195:CYS:HA	1:A:203:CYS:HA	1.97	0.46
1:A:410:LYS:HD2	1:A:433:HIS:HB3	1.98	0.46
1:A:517:ASP:HB3	1:A:520:THR:H	1.80	0.46
1:C:183:LYS:HE2	1:C:184:LEU:HD21	1.98	0.46
1:C:99:VAL:HG22	1:C:122:PHE:HD2	1.76	0.46
1:A:484:TRP:CE2	1:A:492:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:SER:O	1:A:389:ASN:ND2	2.48	0.45
1:C:392:THR:HG22	1:C:423:GLN:HB3	1.99	0.45
1:A:240:ARG:HB3	1:A:249:LEU:HD22	1.98	0.45
1:C:174:GLY:H	1:C:177:ASN:HD22	1.63	0.45
1:A:444:ARG:HD3	1:A:481:ASP:OD1	2.17	0.45
1:C:512:ASN:O	1:C:524:CYS:N	2.50	0.45
1:C:205:HIS:HD2	1:C:207:PHE:H	1.63	0.45
1:C:303:THR:HG23	1:C:304:CYS:N	2.32	0.45
1:C:77:LEU:CD2	1:C:77:LEU:C	2.84	0.45
1:A:333:GLN:HB3	1:A:338:PHE:HB3	1.97	0.45
1:C:483:CYS:HA	1:C:492:LEU:HD12	1.99	0.45
1:C:138:GLU:CB	1:C:184:LEU:HD11	2.46	0.45
1:C:216:THR:O	1:C:219:ASP:HB2	2.17	0.45
1:C:476:ASP:O	1:C:495:LYS:HD2	2.16	0.45
1:A:381:PHE:O	1:A:412:SER:O	2.35	0.45
1:C:350[A]:ARG:CG	1:C:350[A]:ARG:HH11	2.30	0.45
1:C:7:LYS:O	1:C:7:LYS:HG3	2.17	0.45
1:C:99:VAL:CG2	1:C:122:PHE:HD2	2.30	0.44
1:C:286:LYS:HA	1:C:295:PRO:HA	1.97	0.44
1:C:40:THR:HA	1:C:65:SER:O	2.17	0.44
1:A:514:TYR:HB3	1:A:532:ASN:H	1.82	0.44
1:C:138:GLU:HB2	1:C:184:LEU:HD12	1.98	0.44
1:C:246:THR:OG1	1:C:248:VAL:HG12	2.17	0.44
1:C:327:ASN:HB3	1:C:371:TYR:N	2.28	0.44
1:C:36:ASN:HD21	1:C:84:THR:CB	2.28	0.44
1:C:512:ASN:OD1	1:C:512:ASN:N	2.50	0.44
1:A:3:CYS:HB2	1:A:33:VAL:HA	2.00	0.44
1:C:407:ALA:HA	1:C:430:VAL:O	2.17	0.44
1:C:374:ILE:CD1	1:C:384:LEU:HD21	2.48	0.44
1:C:492:LEU:C	1:C:493:ASN:HD22	2.20	0.44
1:A:109:ILE:CG2	1:A:112:LEU:HB2	2.46	0.44
1:A:316:ASP:OD1	1:A:358:ARG:NH2	2.51	0.44
1:C:404:ALA:HB2	1:C:430:VAL:CG1	2.48	0.44
1:A:138:GLU:HB2	1:A:184:LEU:HD11	2.00	0.44
1:A:433:HIS:HA	1:A:460:GLU:HB3	1.99	0.44
1:A:56:ARG:HD2	1:A:78:GLN:HE21	1.83	0.44
1:A:39:LEU:HD11	1:A:52:LEU:HD11	2.00	0.44
1:C:67:VAL:HG13	1:C:102:SER:OG	2.18	0.44
1:C:325:ASP:C	1:C:325:ASP:OD1	2.55	0.44
1:A:367:GLU:OE1	1:A:394:HIS:HE1	2.01	0.43
1:A:445:TRP:HB2	1:A:456:VAL:HG11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:CYS:HB2	1:C:539:CYS:HB2	1.88	0.43
1:A:163:HIS:CD2	1:A:164:GLU:N	2.86	0.43
1:C:338:PHE:O	1:C:351:TYR:HD2	2.01	0.43
1:A:181:PHE:HB2	1:A:185:THR:OG1	2.18	0.43
1:A:50:SER:O	1:A:53:ASP:HB2	2.18	0.43
1:A:335:PHE:CZ	1:A:381:PHE:CD1	3.07	0.43
1:C:329:ARG:HG2	1:C:373:ASN:HB3	2.01	0.43
1:A:252:ASN:OD1	1:A:254:GLU:N	2.51	0.43
1:C:53:ASP:HA	1:C:75:PRO:CD	2.47	0.43
1:C:212:CYS:HA	1:C:220:CYS:HA	2.00	0.43
1:C:339:GLN:HE22	1:C:350[B]:ARG:HH22	1.67	0.43
1:A:138:GLU:CB	1:A:184:LEU:HD11	2.48	0.43
1:A:336:SER:C	1:A:337:GLY:O	2.55	0.43
1:A:512:ASN:HB2	1:A:524:CYS:SG	2.58	0.43
1:C:279:VAL:HG13	1:C:281:SER:H	1.84	0.43
1:C:350[B]:ARG:NH1	1:C:350[B]:ARG:HB2	2.33	0.43
1:C:514:TYR:OH	1:C:534:ALA:CB	2.66	0.43
1:A:15:ASN:ND2	1:A:17:GLU:N	2.66	0.43
1:A:332:ASP:O	1:A:336:SER:HB3	2.18	0.43
1:C:110:PRO:O	1:C:111:ASP:CB	2.67	0.43
1:C:138:GLU:OE2	1:C:183:LYS:HB3	2.18	0.43
1:A:279:VAL:CA	1:C:247:TYR:O	2.66	0.43
1:C:325:ASP:OD1	1:C:326:GLY:N	2.52	0.43
1:C:451:GLU:H	1:C:454:GLN:NE2	2.17	0.43
1:A:46:ASN:OD1	1:A:47:LEU:N	2.51	0.42
1:C:273:ARG:HD3	1:C:292:GLU:OE2	2.19	0.42
1:C:374:ILE:HD13	1:C:384:LEU:HD11	2.00	0.42
1:C:62:ILE:HD11	1:C:77:LEU:HD11	2.01	0.42
1:A:343:ALA:C	1:A:345:TYR:N	2.72	0.42
1:A:236:CYS:SG	1:A:237:PRO:HD2	2.59	0.42
1:A:59:THR:O	1:A:81:ARG:HB2	2.19	0.42
1:C:344:ASN:HB2	1:C:346:THR:HG22	2.01	0.42
1:A:292:GLU:HG2	1:A:294:VAL:HG23	2.01	0.42
1:A:444:ARG:O	1:A:444:ARG:HG3	2.18	0.42
1:A:445:TRP:N	1:A:446:PRO:CD	2.82	0.42
1:A:1:LYS:HG2	1:A:30:CYS:HA	2.02	0.42
1:C:416:LEU:O	1:C:417:GLU:HB2	2.20	0.42
1:A:336:SER:OG	1:A:337:GLY:O	2.30	0.42
1:A:338:PHE:N	1:A:338:PHE:CD1	2.87	0.42
1:C:331:LEU:O	1:C:334:THR:HB	2.19	0.42
1:C:325:ASP:HA	1:C:369:THR:OG1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:HIS:HB3	1:A:-1:HIS:H	1.58	0.42
1:A:402:MET:HE2	1:A:457:TRP:CE3	2.55	0.42
1:C:531:CYS:CB	1:C:539:CYS:HB3	2.50	0.42
1:C:159:CYS:SG	1:C:160:PRO:HD2	2.60	0.41
1:C:2:ILE:CG2	1:C:3:CYS:N	2.82	0.41
1:C:498:ASN:HD22	1:C:499:PHE:N	2.18	0.41
1:A:311:HIS:CD2	1:A:338:PHE:CE1	3.09	0.41
1:C:285:ASP:N	1:C:285:ASP:OD1	2.54	0.41
2:D:42:MET:HG2	2:D:50:GLU:HG2	2.01	0.41
1:C:45:GLU:O	1:C:46:ASN:CB	2.68	0.41
1:A:134:ILE:HD13	1:A:134:ILE:HA	1.87	0.41
1:A:15:ASN:ND2	1:A:17:GLU:H	2.19	0.41
1:A:308:THR:O	1:A:329:ARG:HG3	2.20	0.41
1:C:432:GLN:HA	1:C:459:ASN:O	2.20	0.41
1:C:53:ASP:HA	1:C:75:PRO:HG2	2.03	0.41
1:C:15:ASN:ND2	1:C:18:HIS:H	2.18	0.41
1:A:71:LYS:HG2	1:A:106:THR:HG23	2.03	0.41
1:A:15:ASN:HB3	1:A:18:HIS:CD2	2.55	0.41
1:A:243:ASN:HA	1:A:244:PRO:HD2	1.93	0.41
1:C:288:ASP:OD2	1:C:289:LYS:O	2.39	0.41
1:C:304:CYS:HA	1:C:305:PRO:HD2	1.90	0.41
1:A:339:GLN:OE1	1:A:348:GLY:O	2.39	0.41
1:C:369:THR:O	1:C:396:ARG:HB2	2.21	0.41
1:A:429:VAL:HG13	1:A:456:VAL:HB	2.02	0.41
1:A:335:PHE:CE1	1:A:376:GLY:HA3	2.54	0.41
1:A:419:ARG:C	1:A:421:LEU:H	2.25	0.41
1:A:87:SER:CB	1:A:93:GLU:O	2.65	0.41
1:C:157:ARG:O	1:C:158:GLU:C	2.59	0.41
1:C:45:GLU:HA	1:C:69:VAL:HA	2.03	0.41
1:C:477:GLN:NE2	1:C:505:ALA:HA	2.36	0.41
1:A:329:ARG:HD3	1:A:371:TYR:CE1	2.56	0.41
1:A:141:SER:O	1:A:142:ASN:CB	2.69	0.40
1:A:514:TYR:CB	1:A:532:ASN:O	2.70	0.40
1:C:183:LYS:CG	1:C:184:LEU:N	2.81	0.40
1:C:89:SER:O	1:C:91:GLU:O	2.38	0.40
1:A:327:ASN:OD1	1:A:371:TYR:CZ	2.75	0.40
1:A:382:ARG:O	1:A:383:ASN:O	2.40	0.40
1:A:477:GLN:O	1:A:478:CYS:HB2	2.21	0.40
1:C:190:CYS:O	1:C:191:ALA:C	2.58	0.40
1:C:394:HIS:O	1:C:425:SER:HB2	2.21	0.40
1:A:163:HIS:O	1:A:166:CYS:HB2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLY:O	1:C:221:ILE:HD12	2.22	0.40
1:C:228:ASP:O	1:C:229:GLU:HB2	2.22	0.40
2:D:47:GLU:N	2:D:47:GLU:OE1	2.51	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:THR:O	1:C:313:GLY:CA[3_554]	1.18	1.02
1:A:48:ASP:CB	1:A:350:ARG:O[4_545]	1.91	0.29
1:C:181:PHE:CD2	1:C:352:ILE:CG2[3_554]	1.99	0.21
1:C:167:THR:O	1:C:313:GLY:C[3_554]	2.02	0.18
1:C:168:HIS:CE1	1:C:352:ILE:N[3_554]	2.03	0.17
1:C:168:HIS:NE2	1:C:352:ILE:N[3_554]	2.04	0.16
1:A:46:ASN:CG	1:A:351:TYR:CE2[4_545]	2.12	0.08
1:C:135:GLN:NE2	1:C:358:ARG:CD[3_554]	2.14	0.06

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	514/601 (86%)	466 (91%)	38 (7%)	10 (2%)	9	45
1	C	528/601 (88%)	494 (94%)	27 (5%)	7 (1%)	14	53
2	D	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
All	All	1091/1254 (87%)	1006 (92%)	68 (6%)	17 (2%)	11	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	ASN
1	A	478	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	158	GLU
1	A	212	CYS
1	A	344	ASN
1	A	420	ASN
1	A	497	PHE
1	A	511	SER
1	C	92	GLU
1	C	201	ARG
1	C	260	GLY
1	C	127	ASN
1	C	474	CYS
1	A	155	PRO
1	C	159	CYS
1	A	43	PRO
1	A	13	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	440/531 (83%)	394 (90%)	46 (10%)	8	34
1	C	454/531 (86%)	385 (85%)	69 (15%)	3	18
2	D	42/45 (93%)	38 (90%)	4 (10%)	10	38
All	All	936/1107 (85%)	817 (87%)	119 (13%)	5	25

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	9	ARG
1	A	11	SER
1	A	15	ASN
1	A	24	ARG
1	A	33	VAL
1	A	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	MET
1	A	106	THR
1	A	128	LEU
1	A	129	CYS
1	A	138	GLU
1	A	141	SER
1	A	144	THR
1	A	159	CYS
1	A	162	CYS
1	A	173	GLU
1	A	182	SER
1	A	190	CYS
1	A	225	ASN
1	A	226	PHE
1	A	233	LYS
1	A	236	CYS
1	A	249	LEU
1	A	267	CYS
1	A	287	MET
1	A	303	THR
1	A	322	THR
1	A	336	SER
1	A	338	PHE
1	A	344	ASN
1	A	352	ILE
1	A	354	LEU
1	A	361	VAL
1	A	364	THR
1	A	375	GLU
1	A	416	LEU
1	A	429	VAL
1	A	436	ASP
1	A	437	LEU
1	A	453	GLU
1	A	456	VAL
1	A	463	ARG
1	A	470	ASN
1	A	476	ASP
1	A	531	CYS
1	C	7	LYS
1	C	8	SER
1	C	12	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	14	SER
1	C	31	THR
1	C	33	VAL
1	C	36	ASN
1	C	37	LEU
1	C	42	LEU
1	C	44	ASN
1	C	52	LEU
1	C	67	VAL
1	C	79	ILE
1	C	84	THR
1	C	92	GLU
1	C	97	LEU
1	C	102	SER
1	C	107	LEU
1	C	113	ARG
1	C	125	ASN
1	C	127	ASN
1	C	128	LEU
1	C	132	ARG
1	C	137	SER
1	C	157	ARG
1	C	159	CYS
1	C	161	LYS
1	C	166	CYS
1	C	181	PHE
1	C	182	SER
1	C	185	THR
1	C	186	CYS
1	C	201	ARG
1	C	202	GLU
1	C	208	CYS
1	C	220	CYS
1	C	231	VAL
1	C	235	GLU
1	C	246	THR
1	C	265	LYS
1	C	279	VAL
1	C	285	ASP
1	C	286	LYS
1	C	293	CYS
1	C	303	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	307	VAL
1	C	322	THR
1	C	327	ASN
1	C	330	ILE
1	C	331	LEU
1	C	339	GLN
1	C	344	ASN
1	C	350[A]	ARG
1	C	350[B]	ARG
1	C	354	LEU
1	C	398	LEU
1	C	406	LEU
1	C	430	VAL
1	C	435	ARG
1	C	456	VAL
1	C	462	LEU
1	C	465	ASP
1	C	483	CYS
1	C	498	ASN
1	C	511	SER
1	C	512	ASN
1	C	528	CYS
1	C	532	ASN
1	C	539	CYS
2	D	4	THR
2	D	6	LYS
2	D	27	ILE
2	D	42	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	HIS
1	A	163	HIS
1	A	168	HIS
1	A	179	GLN
1	A	225	ASN
1	A	270	HIS
1	A	275	ASN
1	A	311	HIS
1	A	327	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	HIS
1	A	394	HIS
1	A	420	ASN
1	A	433	HIS
1	A	449	GLN
1	A	454	GLN
1	A	490	GLN
1	C	15	ASN
1	C	36	ASN
1	C	66	HIS
1	C	177	ASN
1	C	205	HIS
1	C	333	GLN
1	C	339	GLN
1	C	373	ASN
1	C	394	HIS
1	C	420	ASN
1	C	432	GLN
1	C	454	GLN
1	C	477	GLN
1	C	493	ASN
1	C	498	ASN
2	D	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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	522/601 (86%)	0.60	32 (6%) 22 21	35, 60, 83, 106	0
1	C	531/601 (88%)	0.99	93 (17%) 2 2	35, 56, 80, 97	0
2	D	51/52 (98%)	1.04	7 (13%) 3 4	41, 50, 58, 61	0
All	All	1104/1254 (88%)	0.80	132 (11%) 5 5	35, 58, 81, 106	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	THR	12.0
1	A	-2	HIS	8.0
1	C	154	ALA	7.2
1	C	506	ASP	5.9
1	C	51	PHE	5.5
1	C	192	GLY	5.4
1	C	507	CYS	5.3
2	D	15	TYR	5.1
1	C	523	ILE	5.0
1	C	421	LEU	5.0
1	C	12	VAL	4.8
1	C	10	LEU	4.7
1	C	524	CYS	4.6
1	C	443	ILE	4.5
2	D	19	ASP	4.5
1	C	525	HIS	4.5
1	C	3	CYS	4.4
1	C	155	PRO	4.3
1	C	126	TYR	4.3
1	C	424	ILE	4.3
1	A	89	SER	4.3
1	C	349	PRO	4.3
1	C	448	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	484	TRP	4.2
1	C	230	GLY	4.2
2	D	11	PHE	4.0
1	C	423	GLN	3.9
2	D	28	ALA	3.9
1	C	416	LEU	3.8
1	A	155	PRO	3.8
1	C	510	ILE	3.7
1	C	55	ILE	3.7
1	C	526	PRO	3.7
1	A	433	HIS	3.7
1	C	486	ALA	3.7
1	C	159	CYS	3.6
1	C	435	ARG	3.6
1	C	27	TYR	3.6
1	C	536	ALA	3.5
1	C	23	LEU	3.4
1	C	535	GLY	3.4
1	C	90	VAL	3.3
1	C	30	CYS	3.3
1	C	350[A]	ARG	3.3
1	A	-1	HIS	3.2
1	A	105	TYR	3.2
1	C	483	CYS	3.1
1	A	98	PHE	3.1
1	C	465	ASP	3.1
1	C	436	ASP	3.0
1	C	387	PHE	3.0
1	C	393	ILE	2.9
1	A	402	MET	2.9
1	C	513	ALA	2.9
1	C	347	MET	2.9
1	C	469	LYS	2.8
1	C	464	ALA	2.8
1	A	521	CYS	2.8
1	A	295	PRO	2.8
1	C	512	ASN	2.8
1	C	94	LYS	2.8
1	C	160	PRO	2.7
1	A	56	ARG	2.7
1	C	284	GLN	2.7
1	C	168	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	432	GLN	2.6
1	C	440	VAL	2.6
1	C	20	TYR	2.6
1	C	120	VAL	2.6
1	C	352	ILE	2.6
1	C	41	TRP	2.5
1	C	193	GLY	2.5
1	C	92	GLU	2.5
1	C	128	LEU	2.4
1	A	516	PHE	2.4
1	A	154	ALA	2.4
1	C	504	ILE	2.4
2	D	14	TRP	2.4
1	A	31	THR	2.4
1	C	466	LEU	2.4
1	A	126	TYR	2.4
1	C	227	PHE	2.4
1	C	377	THR	2.4
1	C	53	ASP	2.4
1	C	445	TRP	2.4
1	C	345	TYR	2.4
1	C	527	GLU	2.3
1	C	462	LEU	2.3
1	C	476	ASP	2.3
1	C	132	ARG	2.3
1	A	532	ASN	2.3
1	C	72	VAL	2.3
1	C	125	ASN	2.3
1	A	99	VAL	2.3
1	C	49	LEU	2.3
1	C	528	CYS	2.3
1	C	38	GLU	2.3
1	A	457	TRP	2.2
1	C	480	GLU	2.2
1	A	274	ASP	2.2
1	A	499	PHE	2.2
1	C	268	PRO	2.2
1	A	47	LEU	2.2
1	C	271	LEU	2.2
1	C	0	HIS	2.2
1	C	509	TYR	2.2
1	C	158	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	514	TYR	2.2
1	A	272	LEU	2.2
1	C	472	THR	2.2
2	D	18	ASN	2.2
1	A	396	ARG	2.2
1	C	201	ARG	2.2
1	C	467	CYS	2.2
2	D	20	ALA	2.2
1	C	334	THR	2.2
1	A	210	GLY	2.1
1	A	158	GLU	2.1
1	C	426	SER	2.1
1	C	156	GLU	2.1
1	C	493	ASN	2.1
1	C	508	GLY	2.1
1	A	120	VAL	2.1
1	C	52	LEU	2.1
1	A	405	ALA	2.1
1	C	384	LEU	2.1
1	A	52	LEU	2.1
1	A	182	SER	2.1
1	A	469	LYS	2.0
1	C	354	LEU	2.0
1	C	119	GLN	2.0
1	C	406	LEU	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.