Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:53 PM GMT

PDB ID	:	1CZ8
Title	:	VASCULAR ENDOTHELIAL GROWTH FACTOR IN COMPLEX WITH AN AFFINITY MATURED ANTIBODY
Authors	:	Chen, Y.; Wiesmann, C.; Fuh, G.; Li, B.; Christinger, H.W.; McKay, P.; de Vos, A.M.; Lowman, H.B.
Deposited on	:	1999-09-01
Resolution	:	2.40 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 (i) symbol.

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

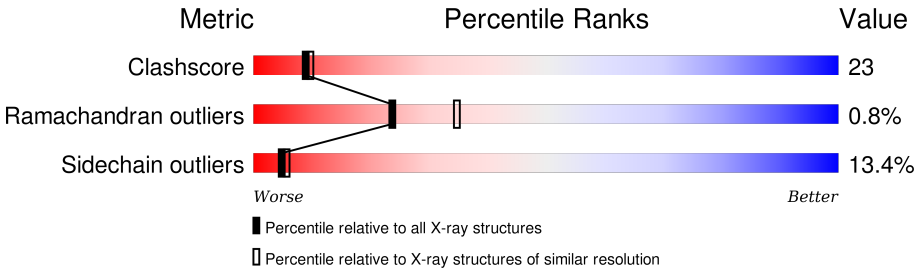
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	V	94	45% 44% 11%
1	W	94	40% 52% 6%
2	L	213	74% 23%
2	X	213	49% 37% 14%
3	H	218	72% 22% 5%
3	Y	218	61% 32% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8577 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 VASCULAR ENDOTHELIAL GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			
1	W	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			

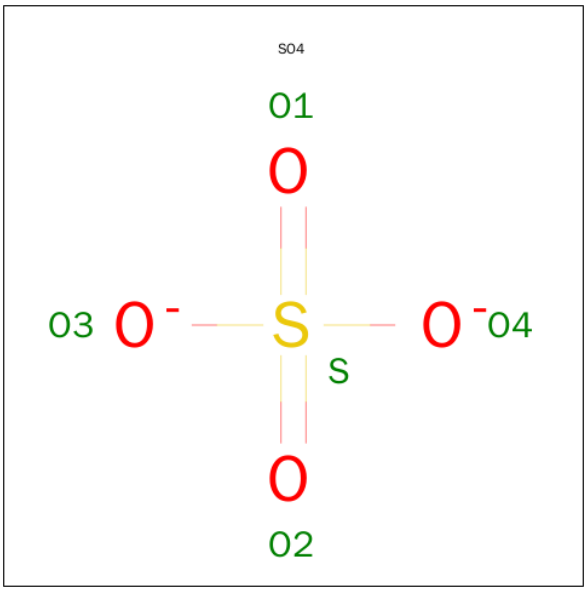
- Molecule 2 is a protein called LIGHT CHAIN OF NEUTRALIZING ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1644	1032	272	336	4			
2	X	213	Total	C	N	O	S	0	0	0
			1644	1032	272	336	4			

- Molecule 3 is a protein called HEAVY CHAIN OF NEUTRALIZING ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1669	1070	272	321	6			
3	Y	218	Total	C	N	O	S	0	0	0
			1669	1070	272	321	6			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	Y	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	149	Total O 149 149	0	0
5	L	148	Total O 148 148	0	0
5	V	18	Total O 18 18	0	0
5	W	15	Total O 15 15	0	0
5	X	39	Total O 39 39	0	0
5	Y	50	Total O 50 50	0	0

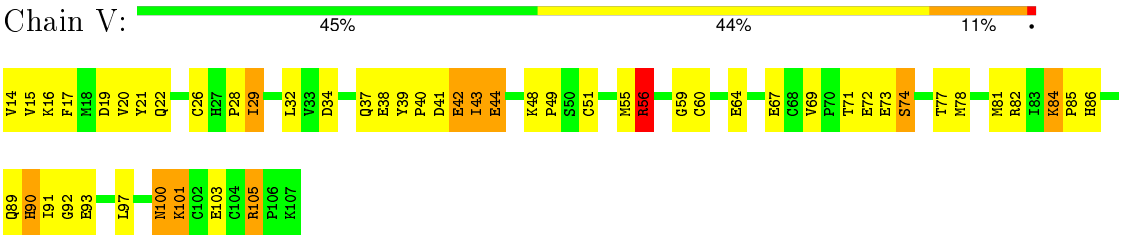
3 Residue-property plots (i)

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

Note EDS was not executed.

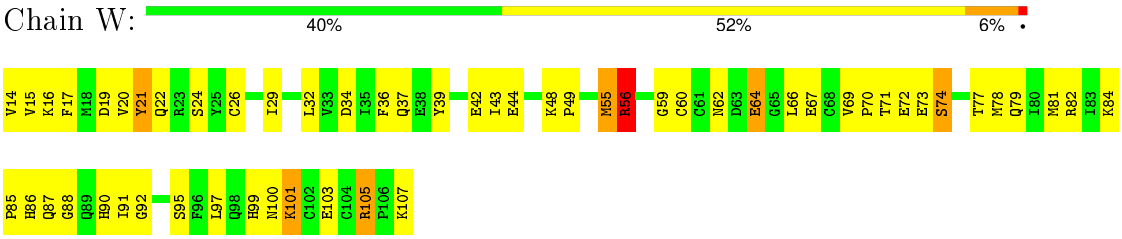
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

Chain V:



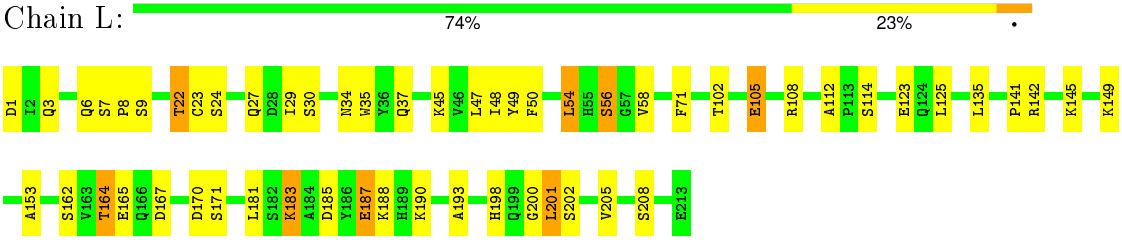
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

Chain W:



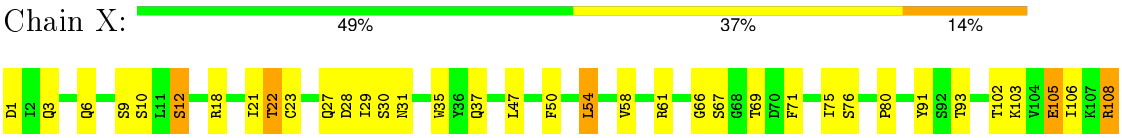
• Molecule 2: LIGHT CHAIN OF NEUTRALIZING ANTIBODY

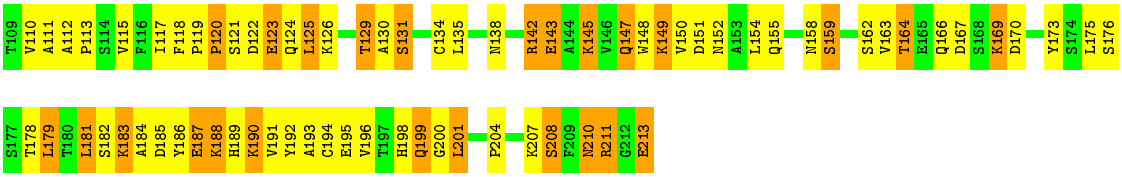
Chain L:



• Molecule 2: LIGHT CHAIN OF NEUTRALIZING ANTIBODY

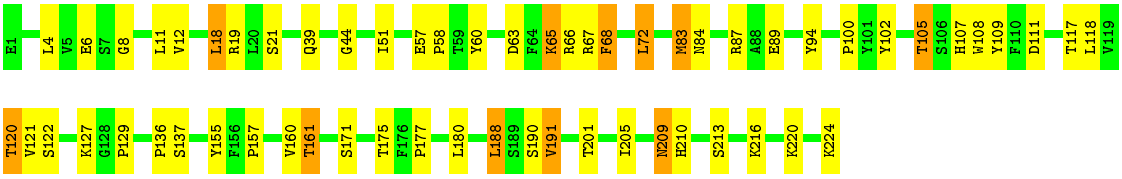
Chain X:





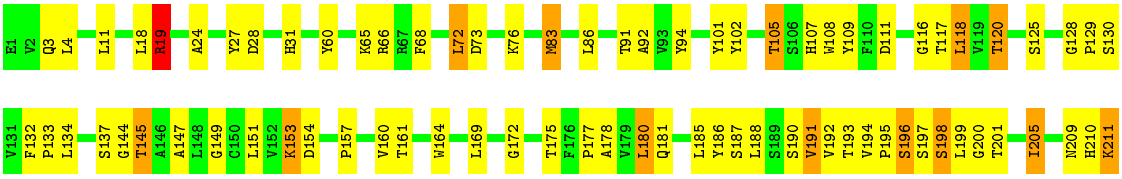
- Molecule 3: HEAVY CHAIN OF NEUTRALIZING ANTIBODY

Chain H:



- Molecule 3: HEAVY CHAIN OF NEUTRALIZING ANTIBODY

Chain Y:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.12Å 66.40Å 138.75Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.1 (20.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.208 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8577	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	V	0.49	0/779	0.78	3/1050 (0.3%)
1	W	0.49	0/779	0.73	1/1050 (0.1%)
2	L	0.65	0/1682	0.82	1/2288 (0.0%)
2	X	0.50	0/1682	0.71	1/2288 (0.0%)
3	H	0.66	0/1719	0.85	1/2348 (0.0%)
3	Y	0.55	0/1719	0.76	2/2348 (0.1%)
All	All	0.58	0/8360	0.78	9/11372 (0.1%)

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	W	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	56	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	V	56	ARG	NE-CZ-NH2	7.07	123.83	120.30
3	Y	19	ARG	NE-CZ-NH2	6.54	123.57	120.30
3	Y	19	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	W	56	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	V	56	ARG	CG-CD-NE	-5.48	100.30	111.80
3	H	19	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	X	75	ILE	N-CA-C	-5.21	96.94	111.00
2	L	170	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	21	TYR	Sidechain

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	V	761	0	726	53	0
1	W	761	0	726	52	0
2	L	1644	0	1587	34	0
2	X	1644	0	1587	151	0
3	H	1669	0	1603	44	0
3	Y	1669	0	1603	84	0
4	H	5	0	0	0	0
4	Y	5	0	0	1	0
5	H	149	0	0	9	0
5	L	148	0	0	10	0
5	V	18	0	0	4	0
5	W	15	0	0	0	0
5	X	39	0	0	6	0
5	Y	50	0	0	6	0
All	All	8577	0	7832	373	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 23.

All (373) 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)
2:X:110:VAL:HG21	2:X:199:GLN:HE22	1.13	1.06
1:V:101:LYS:HA	5:V:120:HOH:O	1.61	1.00
2:X:188:LYS:HG2	2:X:188:LYS:O	1.64	0.96
2:X:190:LYS:HA	2:X:211:ARG:HG3	1.50	0.92
1:W:34:ASP:O	1:W:37:GLN:HB3	1.71	0.90
3:Y:224:LYS:HB3	3:Y:224:LYS:HZ2	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:72:GLU:HB3	1:W:101:LYS:HB2	1.54	0.88
1:V:72:GLU:HB2	1:V:101:LYS:HB2	1.55	0.88
3:Y:224:LYS:HB3	3:Y:224:LYS:NZ	1.89	0.87
1:W:74:SER:HB3	1:W:100:ASN:HD21	1.39	0.86
3:Y:28:ASP:OD2	3:Y:31:HIS:CD2	2.32	0.83
2:X:123:GLU:HB2	2:X:126:LYS:HE2	1.58	0.83
2:X:149:LYS:HB2	2:X:154:LEU:HD23	1.62	0.81
1:W:103:GLU:HB3	1:W:105:ARG:HD3	1.63	0.79
1:V:72:GLU:CB	1:V:101:LYS:HB2	2.13	0.79
1:V:15:VAL:CG2	1:W:78:MET:HG2	2.13	0.78
3:H:89:GLU:HG3	5:H:1140:HOH:O	1.84	0.77
2:X:50:PHE:HE1	5:X:233:HOH:O	1.67	0.77
3:Y:28:ASP:OD2	3:Y:31:HIS:HD2	1.67	0.76
2:X:18:ARG:HG3	2:X:76:SER:O	1.84	0.76
5:L:352:HOH:O	3:H:224:LYS:HE3	1.87	0.75
2:X:188:LYS:HD3	2:X:189:HIS:CD2	2.21	0.74
3:H:137:SER:HA	5:H:1098:HOH:O	1.86	0.74
2:X:110:VAL:HG21	2:X:199:GLN:NE2	1.96	0.73
3:Y:145:THR:HG22	3:Y:194:VAL:O	1.87	0.73
1:V:77:THR:HG22	1:W:14:VAL:HG13	1.69	0.73
1:V:74:SER:HB3	1:V:100:ASN:HD21	1.53	0.73
1:V:73:GLU:HB3	1:V:97:LEU:HD11	1.69	0.73
3:Y:211:LYS:HG3	5:Y:1018:HOH:O	1.87	0.73
2:X:188:LYS:HD3	2:X:189:HIS:HD2	1.53	0.72
2:X:110:VAL:CG2	2:X:199:GLN:HE22	1.99	0.72
1:W:71:THR:OG1	1:W:101:LYS:HB3	1.90	0.72
1:V:49:PRO:HG3	1:W:21:TYR:HA	1.72	0.71
2:X:113:PRO:HD3	2:X:198:HIS:CD2	2.26	0.71
3:Y:19:ARG:HH21	3:Y:19:ARG:HG2	1.55	0.71
2:X:150:VAL:HB	2:X:155:GLN:NE2	2.06	0.71
2:X:54:LEU:HD11	2:X:58:VAL:O	1.89	0.71
3:Y:73:ASP:CG	3:Y:76:LYS:HG3	2.11	0.71
1:W:42:GLU:OE1	1:W:82:ARG:NH2	2.24	0.70
2:X:124:GLN:HE22	2:X:131:SER:H	1.40	0.70
1:V:48:LYS:O	1:W:17:PHE:HE1	1.75	0.69
2:L:198:HIS:HD2	2:L:200:GLY:H	1.37	0.69
2:X:125:LEU:HD12	2:X:183:LYS:HB2	1.74	0.69
2:X:113:PRO:HD2	2:X:201:LEU:HD13	1.75	0.69
3:H:72:LEU:HD23	3:H:72:LEU:N	2.08	0.69
2:X:67:SER:HA	5:X:251:HOH:O	1.92	0.69
2:X:150:VAL:HG13	2:X:192:TYR:CE1	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:72:GLU:CB	1:W:101:LYS:HB2	2.23	0.68
2:L:198:HIS:CD2	2:L:200:GLY:H	2.11	0.68
2:X:179:LEU:HD21	2:X:181:LEU:HD21	1.76	0.67
3:Y:172:GLY:O	3:Y:192:VAL:HA	1.95	0.67
2:X:120:PRO:HG2	2:X:186:TYR:CE2	2.30	0.67
2:X:18:ARG:HG3	2:X:76:SER:HA	1.76	0.66
2:X:23:CYS:HB2	2:X:35:TRP:CH2	2.30	0.66
2:X:129:THR:HA	2:X:183:LYS:H	1.61	0.65
2:X:18:ARG:CG	2:X:76:SER:HA	2.26	0.65
2:L:164:THR:CG2	5:L:220:HOH:O	2.44	0.65
2:X:150:VAL:HG22	2:X:192:TYR:CD1	2.32	0.65
2:X:149:LYS:HE2	2:X:152:ASN:H	1.62	0.65
2:X:150:VAL:HG13	2:X:192:TYR:HE1	1.62	0.65
1:V:15:VAL:HG21	1:W:78:MET:HG2	1.78	0.65
1:V:103:GLU:HB3	1:V:105:ARG:HD3	1.78	0.65
2:X:162:SER:OG	3:Y:177:PRO:HD2	1.96	0.65
3:H:161:THR:HG22	5:H:1025:HOH:O	1.97	0.65
2:X:129:THR:HG22	2:X:182:SER:HA	1.78	0.64
3:H:216:LYS:NZ	5:H:1125:HOH:O	2.28	0.64
1:V:21:TYR:HA	1:W:49:PRO:HG3	1.79	0.64
2:X:149:LYS:NZ	2:X:191:VAL:HG12	2.13	0.64
1:V:56:ARG:NH2	1:V:97:LEU:O	2.31	0.64
2:X:113:PRO:HD2	2:X:201:LEU:CD1	2.29	0.63
3:Y:200:GLY:HA3	5:Y:1035:HOH:O	1.97	0.63
1:V:71:THR:OG1	1:V:101:LYS:HB3	1.97	0.63
2:X:190:LYS:HE3	2:X:211:ARG:N	2.13	0.63
2:X:142:ARG:HG3	2:X:173:TYR:CZ	2.33	0.63
2:X:145:LYS:O	2:X:145:LYS:HG3	1.96	0.63
2:X:142:ARG:HG3	2:X:173:TYR:CE1	2.34	0.63
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.79	0.63
3:Y:19:ARG:NH2	3:Y:19:ARG:HG2	2.13	0.62
3:H:205:ILE:HD13	3:H:220:LYS:HA	1.81	0.62
2:X:190:LYS:HA	2:X:211:ARG:CG	2.27	0.62
2:L:162:SER:OG	3:H:177:PRO:HD2	2.00	0.62
3:Y:205:ILE:HD13	3:Y:220:LYS:HA	1.82	0.62
2:X:118:PHE:CD1	3:Y:134:LEU:HB3	2.35	0.61
3:H:210:HIS:HD2	3:H:213:SER:OG	1.83	0.61
2:L:114:SER:HA	5:L:341:HOH:O	2.00	0.61
3:Y:195:PRO:O	3:Y:198:SER:HB2	2.00	0.61
2:X:134:CYS:HB2	2:X:148:TRP:CH2	2.36	0.61
2:X:115:VAL:HG22	2:X:196:VAL:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:169:LEU:HD21	3:Y:192:VAL:HG21	1.83	0.60
2:L:54:LEU:HD11	2:L:58:VAL:O	2.01	0.60
1:V:72:GLU:OE1	1:V:101:LYS:HD3	2.01	0.60
2:L:6:GLN:HA	2:L:22:THR:O	2.02	0.60
3:Y:194:VAL:HB	3:Y:195:PRO:HD2	1.83	0.60
2:X:193:ALA:HB2	2:X:208:SER:HB3	1.83	0.59
3:H:161:THR:CG2	5:H:1025:HOH:O	2.50	0.59
2:X:185:ASP:HB2	2:X:188:LYS:HD2	1.84	0.59
2:X:190:LYS:CA	2:X:211:ARG:HG3	2.29	0.59
2:X:159:SER:HA	2:X:178:THR:O	2.02	0.59
1:V:93:GLU:HG3	3:Y:101:TYR:OH	2.03	0.59
2:X:149:LYS:CD	2:X:193:ALA:HB3	2.33	0.59
1:V:32:LEU:HD13	1:W:59:GLY:HA2	1.85	0.59
2:X:124:GLN:HG3	3:Y:132:PHE:CE1	2.38	0.59
3:H:188:LEU:HD12	3:H:188:LEU:C	2.24	0.59
1:V:78:MET:HG2	1:W:15:VAL:HB	1.85	0.59
2:X:129:THR:HA	2:X:183:LYS:N	2.18	0.58
2:X:149:LYS:HZ2	2:X:191:VAL:HG12	1.67	0.58
3:Y:109:TYR:HE1	3:Y:111:ASP:HB3	1.68	0.58
2:X:147:GLN:CD	2:X:195:GLU:HB3	2.24	0.58
2:X:198:HIS:HB3	2:X:201:LEU:HD22	1.86	0.58
1:V:51:CYS:SG	1:W:24:SER:HB2	2.44	0.57
3:Y:205:ILE:HD13	3:Y:220:LYS:CA	2.34	0.57
3:Y:109:TYR:CE1	3:Y:111:ASP:HB3	2.40	0.57
2:L:56:SER:HB3	5:L:290:HOH:O	2.04	0.57
3:Y:129:PRO:HD2	3:Y:215:THR:HG21	1.86	0.57
2:X:189:HIS:O	2:X:211:ARG:HD3	2.05	0.57
1:V:28:PRO:O	5:V:125:HOH:O	2.17	0.57
3:Y:19:ARG:HH21	3:Y:19:ARG:CG	2.17	0.57
3:Y:118:LEU:HD13	3:Y:120:THR:HG22	1.85	0.57
3:Y:157:PRO:O	3:Y:210:HIS:HE1	1.87	0.57
1:V:43:ILE:HD12	1:V:44:GLU:HG3	1.87	0.57
2:L:30:SER:O	2:L:71:PHE:HZ	1.87	0.56
2:X:185:ASP:HA	2:X:188:LYS:HB3	1.87	0.56
2:X:210:ASN:CB	2:X:213:GLU:HB2	2.34	0.56
2:X:123:GLU:HG2	2:X:123:GLU:O	2.05	0.56
3:H:72:LEU:N	3:H:72:LEU:CD2	2.68	0.56
2:X:105:GLU:HG2	5:X:215:HOH:O	2.05	0.56
1:V:91:ILE:HD11	4:Y:992:SO4:O1	2.06	0.56
2:X:126:LYS:HG3	2:X:126:LYS:O	2.07	0.56
2:X:121:SER:CB	3:Y:133:PRO:HD2	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:190:LYS:HE3	2:X:211:ARG:H	1.72	0.55
1:W:74:SER:HB3	1:W:100:ASN:ND2	2.18	0.55
2:X:150:VAL:HB	2:X:155:GLN:HE21	1.71	0.55
3:H:72:LEU:HD23	3:H:72:LEU:H	1.72	0.55
2:X:129:THR:HG22	2:X:181:LEU:O	2.07	0.55
1:W:81:MET:HA	1:W:91:ILE:HA	1.88	0.55
2:X:110:VAL:HG11	2:X:199:GLN:NE2	2.22	0.55
2:X:183:LYS:O	2:X:183:LYS:HG2	2.06	0.55
2:L:164:THR:HG21	5:L:220:HOH:O	2.05	0.55
3:Y:196:SER:O	3:Y:199:LEU:HG	2.07	0.55
1:V:15:VAL:HG23	1:W:78:MET:HG2	1.89	0.55
2:X:121:SER:OG	3:Y:132:PHE:HB3	2.07	0.54
1:W:36:PHE:CZ	1:W:43:ILE:HA	2.42	0.54
2:X:125:LEU:CD1	2:X:130:ALA:HB2	2.38	0.54
3:H:68:PHE:HD1	3:H:68:PHE:N	2.05	0.54
3:Y:205:ILE:HD11	3:Y:220:LYS:HD2	1.90	0.54
1:V:34:ASP:O	1:V:37:GLN:HB3	2.08	0.54
3:H:157:PRO:O	3:H:210:HIS:HE1	1.90	0.53
1:V:38:GLU:O	1:V:40:PRO:HD3	2.07	0.53
1:V:92:GLY:HA3	3:Y:102:TYR:CE2	2.43	0.53
3:Y:188:LEU:HD12	3:Y:188:LEU:C	2.29	0.53
2:X:115:VAL:HB	2:X:207:LYS:HD3	1.89	0.53
2:X:192:TYR:O	2:X:208:SER:HA	2.09	0.53
2:X:125:LEU:HD21	2:X:186:TYR:CE1	2.44	0.53
3:H:68:PHE:CD1	3:H:68:PHE:N	2.76	0.53
3:H:60:TYR:CE1	3:H:65:LYS:HE2	2.45	0.52
3:H:83:MET:HE3	3:H:94:TYR:CE1	2.45	0.52
3:Y:144:GLY:O	3:Y:196:SER:HB2	2.09	0.52
3:H:209:ASN:HD22	3:H:210:HIS:N	2.08	0.52
3:Y:72:LEU:CD2	3:Y:72:LEU:N	2.72	0.52
3:Y:147:ALA:HB2	3:Y:193:THR:HG22	1.92	0.52
2:X:190:LYS:CE	2:X:210:ASN:HA	2.40	0.51
2:X:118:PHE:CB	3:Y:134:LEU:HD22	2.39	0.51
2:X:210:ASN:HB3	2:X:213:GLU:HB2	1.91	0.51
1:V:81:MET:HA	1:V:91:ILE:HA	1.93	0.51
2:X:121:SER:HB2	3:Y:133:PRO:HD2	1.91	0.51
2:X:66:GLY:O	2:X:67:SER:HB3	2.11	0.51
3:Y:175:THR:HA	3:Y:190:SER:HA	1.92	0.51
2:X:187:GLU:HA	2:X:211:ARG:NH1	2.25	0.51
2:X:198:HIS:CD2	2:X:200:GLY:H	2.29	0.51
3:Y:137:SER:OG	3:Y:223:PRO:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:79:GLN:HA	1:W:92:GLY:O	2.11	0.51
3:Y:149:GLY:HA2	3:Y:164:TRP:CH2	2.46	0.51
1:W:56:ARG:HD2	1:W:99:HIS:CE1	2.46	0.51
3:Y:73:ASP:OD1	3:Y:76:LYS:HG3	2.11	0.51
2:X:149:LYS:HA	2:X:154:LEU:HA	1.92	0.50
3:Y:145:THR:HG22	3:Y:194:VAL:C	2.32	0.50
1:V:77:THR:HG22	1:W:14:VAL:CG1	2.39	0.50
2:L:112:ALA:HB1	2:L:201:LEU:HD13	1.94	0.50
2:L:185:ASP:OD1	2:L:188:LYS:HE3	2.10	0.50
1:W:16:LYS:O	1:W:20:VAL:HG23	2.11	0.50
1:V:39:TYR:HB3	1:V:42:GLU:HG2	1.93	0.50
3:H:120:THR:CG2	5:H:1003:HOH:O	2.59	0.50
2:X:27:GLN:O	2:X:29:ILE:HG23	2.11	0.50
3:Y:68:PHE:CE2	3:Y:83:MET:CE	2.95	0.50
3:Y:83:MET:HB2	3:Y:86:LEU:HD21	1.93	0.50
1:W:73:GLU:HB3	1:W:97:LEU:HD11	1.94	0.50
2:X:135:LEU:CD2	3:Y:191:VAL:HG11	2.42	0.50
3:Y:205:ILE:HA	3:Y:219:LYS:O	2.11	0.50
1:V:32:LEU:HD13	1:W:59:GLY:CA	2.41	0.50
1:W:73:GLU:C	1:W:100:ASN:ND2	2.65	0.49
3:Y:102:TYR:HB2	3:Y:105:THR:O	2.12	0.49
2:X:186:TYR:CE2	2:X:192:TYR:CE2	3.00	0.49
2:X:115:VAL:CG2	2:X:196:VAL:HG21	2.42	0.49
2:X:123:GLU:OE2	3:Y:132:PHE:HD2	1.95	0.49
2:X:120:PRO:HG2	2:X:186:TYR:CZ	2.47	0.49
1:V:29:ILE:HA	5:V:125:HOH:O	2.11	0.49
3:H:129:PRO:HB3	3:H:155:TYR:HB3	1.95	0.49
2:X:149:LYS:O	2:X:149:LYS:HD3	2.13	0.49
3:Y:209:ASN:HD22	3:Y:216:LYS:HB3	1.78	0.49
2:X:66:GLY:HA3	2:X:71:PHE:HA	1.95	0.49
2:X:190:LYS:HA	2:X:211:ARG:HB2	1.95	0.48
2:L:201:LEU:HG	2:L:205:VAL:HG23	1.95	0.48
2:X:149:LYS:HD3	2:X:193:ALA:HB3	1.95	0.48
2:L:149:LYS:HA	2:L:153:ALA:O	2.13	0.48
2:L:1:ASP:HA	5:L:243:HOH:O	2.13	0.48
3:H:51:ILE:CD1	3:H:72:LEU:HD22	2.44	0.48
2:X:37:GLN:HB2	2:X:47:LEU:HD11	1.94	0.48
1:W:92:GLY:HA3	3:H:102:TYR:CE2	2.49	0.48
3:H:100:PRO:HD3	3:H:109:TYR:O	2.14	0.48
2:L:183:LYS:O	2:L:187:GLU:HG2	2.12	0.48
2:X:163:VAL:HG22	2:X:175:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:6:GLN:HA	2:X:22:THR:O	2.13	0.48
3:Y:92:ALA:HB2	5:Y:1022:HOH:O	2.12	0.48
2:X:210:ASN:HB2	2:X:213:GLU:HB2	1.95	0.48
2:X:129:THR:CG2	2:X:182:SER:HA	2.43	0.48
1:W:92:GLY:HA3	3:H:102:TYR:CD2	2.49	0.48
2:X:185:ASP:CB	2:X:188:LYS:HD2	2.44	0.47
2:X:124:GLN:NE2	2:X:131:SER:OG	2.47	0.47
3:H:136:PRO:O	3:H:137:SER:HB3	2.15	0.47
1:W:85:PRO:O	1:W:86:HIS:HB2	2.14	0.47
1:V:72:GLU:CD	1:V:101:LYS:HD3	2.35	0.47
2:X:190:LYS:HE2	2:X:210:ASN:HA	1.96	0.47
3:Y:197:SER:HB3	5:Y:1042:HOH:O	2.14	0.47
2:X:150:VAL:HG22	2:X:192:TYR:HD1	1.74	0.47
1:V:92:GLY:HA3	3:Y:102:TYR:CD2	2.49	0.47
3:Y:180:LEU:HG	3:Y:186:TYR:CE1	2.50	0.47
1:V:73:GLU:C	1:V:100:ASN:HD21	2.17	0.47
2:X:149:LYS:NZ	2:X:191:VAL:O	2.47	0.47
1:W:55:MET:O	1:W:56:ARG:HD3	2.15	0.47
1:W:70:PRO:HA	1:W:101:LYS:O	2.15	0.47
3:Y:28:ASP:HB3	3:Y:31:HIS:CD2	2.49	0.47
2:X:152:ASN:N	2:X:152:ASN:HD22	2.11	0.47
2:X:118:PHE:HB3	3:Y:134:LEU:HD22	1.97	0.47
2:X:149:LYS:HE2	2:X:152:ASN:HD22	1.80	0.47
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.50	0.47
1:W:17:PHE:CD2	3:Y:31:HIS:HE1	2.33	0.46
2:X:61:ARG:HG2	2:X:61:ARG:HH11	1.80	0.46
1:V:14:VAL:HG13	1:W:77:THR:HG22	1.96	0.46
3:Y:200:GLY:CA	5:Y:1035:HOH:O	2.60	0.46
2:X:123:GLU:OE2	3:Y:132:PHE:CD2	2.69	0.46
2:X:158:ASN:O	2:X:179:LEU:HA	2.16	0.46
2:X:163:VAL:HG12	2:X:164:THR:N	2.30	0.46
2:X:175:LEU:HD23	2:X:176:SER:N	2.31	0.46
2:X:149:LYS:HD2	2:X:193:ALA:HB3	1.97	0.46
3:H:39:GLN:HG3	3:H:44:GLY:O	2.15	0.46
1:V:42:GLU:OE1	1:V:82:ARG:NH2	2.38	0.46
1:V:77:THR:CG2	1:W:14:VAL:HG22	2.46	0.46
3:H:6:GLU:HA	3:H:21:SER:O	2.16	0.46
2:X:150:VAL:CG1	2:X:192:TYR:HE1	2.27	0.46
3:Y:178:ALA:HA	3:Y:188:LEU:HB3	1.98	0.46
1:V:67:GLU:HG3	1:V:69:VAL:HG13	1.98	0.45
1:V:72:GLU:HB3	1:V:101:LYS:HB2	1.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:149:LYS:HB2	2:X:154:LEU:CD2	2.39	0.45
3:Y:169:LEU:CD2	3:Y:192:VAL:HG21	2.46	0.45
3:Y:210:HIS:HD2	3:Y:213:SER:OG	2.00	0.45
2:X:18:ARG:HG3	2:X:76:SER:CA	2.43	0.45
1:V:41:ASP:C	1:V:43:ILE:H	2.19	0.45
2:X:1:ASP:HA	5:X:235:HOH:O	2.16	0.45
2:X:182:SER:C	2:X:184:ALA:N	2.70	0.45
3:Y:195:PRO:HG2	3:Y:198:SER:OG	2.16	0.45
1:W:39:TYR:HB3	1:W:42:GLU:HG2	1.97	0.45
3:Y:94:TYR:O	3:Y:116:GLY:HA2	2.17	0.45
2:X:167:ASP:OD1	2:X:170:ASP:N	2.47	0.45
2:X:21:ILE:HG12	2:X:102:THR:HG21	1.99	0.45
2:L:141:PRO:O	2:L:198:HIS:HE1	1.99	0.45
3:H:72:LEU:HD23	5:H:1101:HOH:O	2.16	0.45
1:V:17:PHE:HE1	1:W:48:LYS:O	1.99	0.45
2:X:119:PRO:HA	2:X:120:PRO:HD3	1.85	0.45
1:W:84:LYS:HD3	1:W:87:GLN:OE1	2.17	0.45
2:X:181:LEU:HD12	2:X:186:TYR:HB2	1.99	0.44
2:X:210:ASN:O	2:X:211:ARG:C	2.55	0.44
3:H:51:ILE:HD11	3:H:72:LEU:HD22	1.99	0.44
1:W:19:ASP:O	1:W:20:VAL:C	2.56	0.44
1:W:64:GLU:HA	1:W:64:GLU:OE2	2.15	0.44
3:Y:128:GLY:HA2	3:Y:210:HIS:HD2	1.82	0.44
3:H:63:ASP:C	5:H:1117:HOH:O	2.56	0.44
3:Y:181:GLN:HG3	3:Y:185:LEU:O	2.18	0.44
1:V:73:GLU:C	1:V:100:ASN:ND2	2.71	0.44
1:W:67:GLU:HG3	1:W:69:VAL:HG13	2.00	0.44
2:X:50:PHE:CG	3:Y:107:HIS:CE1	3.05	0.44
3:Y:68:PHE:CE2	3:Y:83:MET:HE2	2.52	0.44
3:Y:24:ALA:HB1	3:Y:27:TYR:CE2	2.53	0.44
3:Y:72:LEU:H	3:Y:72:LEU:HD23	1.82	0.44
2:X:135:LEU:HD22	3:Y:191:VAL:HG11	2.00	0.44
2:X:163:VAL:HG12	2:X:164:THR:O	2.18	0.44
2:X:80:PRO:HA	2:X:106:ILE:HG12	2.00	0.44
1:V:16:LYS:O	1:V:20:VAL:HG23	2.17	0.44
2:L:34:ASN:OD1	2:L:49:TYR:HA	2.17	0.44
2:L:9:SER:O	2:L:102:THR:HA	2.18	0.44
2:X:188:LYS:CG	2:X:188:LYS:O	2.50	0.43
2:X:143:GLU:H	2:X:143:GLU:CD	2.20	0.43
2:L:105:GLU:OE1	2:L:142:ARG:NH2	2.51	0.43
3:Y:72:LEU:HD23	3:Y:72:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:169:LYS:HE2	2:X:169:LYS:HB2	1.72	0.43
1:W:73:GLU:HB3	1:W:97:LEU:CD1	2.49	0.43
3:H:87:ARG:HD2	3:H:89:GLU:OE2	2.18	0.43
1:V:77:THR:O	1:W:14:VAL:HG13	2.17	0.43
1:V:85:PRO:O	1:V:86:HIS:HB2	2.17	0.43
2:X:142:ARG:HG3	2:X:173:TYR:CD1	2.53	0.43
2:X:142:ARG:HG3	2:X:173:TYR:CE2	2.53	0.43
2:X:190:LYS:HG2	2:X:211:ARG:HB2	1.99	0.43
2:X:117:ILE:HB	2:X:207:LYS:HB3	2.00	0.43
2:X:147:GLN:OE1	2:X:195:GLU:HB3	2.18	0.43
2:L:164:THR:HG23	5:L:220:HOH:O	2.14	0.43
2:L:47:LEU:C	2:L:48:ILE:HG13	2.39	0.43
2:X:10:SER:HA	2:X:103:LYS:O	2.19	0.43
3:H:84:ASN:ND2	5:H:1108:HOH:O	2.51	0.43
2:L:123:GLU:HB2	5:L:301:HOH:O	2.19	0.43
1:V:59:GLY:HA2	1:W:32:LEU:HD13	2.00	0.43
3:Y:211:LYS:HG3	3:Y:211:LYS:H	1.55	0.43
2:X:67:SER:HB2	5:X:251:HOH:O	2.19	0.43
2:L:7:SER:HA	2:L:8:PRO:C	2.40	0.43
3:H:8:GLY:O	3:H:18:LEU:HD21	2.19	0.43
1:W:56:ARG:HA	1:W:56:ARG:HD3	1.77	0.42
2:L:27:GLN:O	2:L:29:ILE:HG23	2.19	0.42
2:X:190:LYS:HE2	2:X:210:ASN:CG	2.39	0.42
3:Y:129:PRO:HD2	3:Y:215:THR:CG2	2.48	0.42
3:H:109:TYR:CE1	3:H:111:ASP:HB3	2.55	0.42
3:Y:153:LYS:HE3	3:Y:154:ASP:OD2	2.19	0.42
2:X:213:GLU:O	2:X:213:GLU:HG3	2.19	0.42
2:X:54:LEU:HD21	2:X:58:VAL:HG12	2.02	0.42
2:L:164:THR:HG23	2:L:165:GLU:O	2.19	0.42
3:H:12:VAL:O	3:H:121:VAL:HA	2.19	0.42
2:X:190:LYS:HA	2:X:211:ARG:CB	2.49	0.42
1:V:91:ILE:HG21	3:Y:31:HIS:ND1	2.34	0.42
3:H:175:THR:HA	3:H:190:SER:HA	2.00	0.42
2:L:135:LEU:CD2	3:H:191:VAL:HG11	2.50	0.42
2:X:18:ARG:HG3	2:X:76:SER:C	2.39	0.42
3:Y:91:THR:O	3:Y:92:ALA:HB2	2.20	0.42
3:Y:210:HIS:CD2	3:Y:213:SER:OG	2.73	0.42
2:X:12:SER:HA	2:X:105:GLU:O	2.20	0.42
2:X:30:SER:O	2:X:71:PHE:HZ	2.03	0.42
3:Y:60:TYR:CE1	3:Y:65:LYS:HE2	2.55	0.42
2:X:148:TRP:CZ3	2:X:194:CYS:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:61:ARG:NH1	2:X:61:ARG:HG2	2.36	0.41
3:H:57:GLU:HA	3:H:58:PRO:HD3	1.94	0.41
2:L:193:ALA:HB2	2:L:208:SER:HB3	2.02	0.41
1:V:90:HIS:HA	3:Y:31:HIS:O	2.20	0.41
2:X:193:ALA:HA	2:X:207:LYS:O	2.20	0.41
2:X:31:ASN:HB2	5:X:233:HOH:O	2.20	0.41
1:V:100:ASN:O	1:V:101:LYS:HD2	2.20	0.41
2:X:175:LEU:HD23	2:X:175:LEU:C	2.40	0.41
2:X:112:ALA:HB1	2:X:201:LEU:CD1	2.50	0.41
1:W:73:GLU:C	1:W:100:ASN:HD21	2.24	0.41
3:Y:72:LEU:HD23	5:Y:998:HOH:O	2.20	0.41
2:L:50:PHE:CG	3:H:107:HIS:CE1	3.08	0.41
1:V:90:HIS:N	1:V:90:HIS:CD2	2.88	0.41
2:X:182:SER:C	2:X:184:ALA:H	2.23	0.41
1:V:84:LYS:NZ	5:V:121:HOH:O	2.54	0.41
2:X:151:ASP:OD2	2:X:189:HIS:ND1	2.53	0.41
2:X:124:GLN:HE22	2:X:131:SER:N	2.12	0.41
2:X:28:ASP:HA	2:X:69:THR:HG22	2.02	0.41
2:L:167:ASP:O	2:L:171:SER:HA	2.21	0.41
1:W:66:LEU:O	1:W:107:LYS:HE3	2.20	0.41
3:Y:205:ILE:HD13	3:Y:220:LYS:CB	2.49	0.41
2:X:189:HIS:O	2:X:211:ARG:HG3	2.21	0.40
1:V:48:LYS:O	1:W:17:PHE:CE1	2.65	0.40
2:X:125:LEU:HD13	2:X:130:ALA:HB2	2.03	0.40
3:H:67:ARG:C	3:H:68:PHE:HD1	2.24	0.40
1:V:19:ASP:O	1:V:20:VAL:C	2.58	0.40
2:L:108:ARG:HB2	5:L:304:HOH:O	2.21	0.40
2:X:91:TYR:HB2	3:Y:108:TRP:HB2	2.03	0.40
1:W:88:GLY:HA3	3:H:108:TRP:CZ3	2.56	0.40
2:X:118:PHE:CE1	3:Y:134:LEU:O	2.73	0.40
3:Y:209:ASN:ND2	3:Y:216:LYS:HB3	2.36	0.40
3:H:136:PRO:O	3:H:137:SER:CB	2.69	0.40
1:W:21:TYR:CE1	1:W:62:ASN:ND2	2.90	0.40
1:W:39:TYR:HB3	1:W:42:GLU:CG	2.51	0.40
1:W:69:VAL:HB	1:W:70:PRO:HD2	2.04	0.40
2:X:18:ARG:HG2	2:X:76:SER:HA	2.03	0.40
2:L:145:LYS:HE2	5:L:239:HOH:O	2.21	0.40
3:H:102:TYR:HB2	3:H:105:THR:O	2.21	0.40
2:X:108:ARG:NH1	2:X:111:ALA:HB2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	V	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	8 9
1	W	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	17 25
2	L	211/213 (99%)	201 (95%)	10 (5%)	0	100 100
2	X	211/213 (99%)	188 (89%)	19 (9%)	4 (2%)	10 12
3	H	214/218 (98%)	209 (98%)	5 (2%)	0	100 100
3	Y	214/218 (98%)	198 (92%)	15 (7%)	1 (0%)	34 48
All	All	1034/1050 (98%)	961 (93%)	65 (6%)	8 (1%)	24 35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	138	ASN
1	V	26	CYS
1	V	42	GLU
1	W	26	CYS
2	X	204	PRO
3	Y	201	THR
2	X	122	ASP
2	X	120	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	V	89/89 (100%)	74 (83%)	15 (17%)	2 3
1	W	89/89 (100%)	77 (86%)	12 (14%)	5 5
2	L	190/190 (100%)	175 (92%)	15 (8%)	15 23
2	X	190/190 (100%)	157 (83%)	33 (17%)	2 2
3	H	182/182 (100%)	160 (88%)	22 (12%)	6 8
3	Y	182/182 (100%)	155 (85%)	27 (15%)	4 4
All	All	922/922 (100%)	798 (87%)	124 (13%)	5 6

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	22	GLN
1	V	29	ILE
1	V	43	ILE
1	V	44	GLU
1	V	55	MET
1	V	56	ARG
1	V	60	CYS
1	V	64	GLU
1	V	74	SER
1	V	84	LYS
1	V	89	GLN
1	V	90	HIS
1	V	100	ASN
1	V	101	LYS
1	V	105	ARG
1	W	22	GLN
1	W	29	ILE
1	W	44	GLU
1	W	55	MET
1	W	56	ARG
1	W	60	CYS
1	W	64	GLU
1	W	74	SER
1	W	90	HIS
1	W	95	SER
1	W	101	LYS
1	W	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	3	GLN
2	L	22	THR
2	L	24	SER
2	L	45	LYS
2	L	54	LEU
2	L	56	SER
2	L	105	GLU
2	L	125	LEU
2	L	164	THR
2	L	181	LEU
2	L	183	LYS
2	L	187	GLU
2	L	190	LYS
2	L	201	LEU
2	L	202	SER
3	H	4	LEU
3	H	11	LEU
3	H	18	LEU
3	H	65	LYS
3	H	66	ARG
3	H	68	PHE
3	H	72	LEU
3	H	83	MET
3	H	105	THR
3	H	117	THR
3	H	118	LEU
3	H	120	THR
3	H	122	SER
3	H	127	LYS
3	H	160	VAL
3	H	161	THR
3	H	171	SER
3	H	180	LEU
3	H	188	LEU
3	H	191	VAL
3	H	201	THR
3	H	209	ASN
2	X	3	GLN
2	X	9	SER
2	X	12	SER
2	X	22	THR
2	X	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	93	THR
2	X	105	GLU
2	X	108	ARG
2	X	123	GLU
2	X	125	LEU
2	X	129	THR
2	X	131	SER
2	X	142	ARG
2	X	143	GLU
2	X	145	LYS
2	X	147	GLN
2	X	149	LYS
2	X	159	SER
2	X	164	THR
2	X	166	GLN
2	X	169	LYS
2	X	179	LEU
2	X	181	LEU
2	X	183	LYS
2	X	187	GLU
2	X	188	LYS
2	X	190	LYS
2	X	199	GLN
2	X	201	LEU
2	X	208	SER
2	X	210	ASN
2	X	211	ARG
2	X	213	GLU
3	Y	3	GLN
3	Y	4	LEU
3	Y	11	LEU
3	Y	18	LEU
3	Y	19	ARG
3	Y	66	ARG
3	Y	72	LEU
3	Y	83	MET
3	Y	105	THR
3	Y	117	THR
3	Y	118	LEU
3	Y	120	THR
3	Y	125	SER
3	Y	130	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Y	145	THR
3	Y	151	LEU
3	Y	153	LYS
3	Y	160	VAL
3	Y	161	THR
3	Y	180	LEU
3	Y	187	SER
3	Y	191	VAL
3	Y	196	SER
3	Y	198	SER
3	Y	205	ILE
3	Y	211	LYS
3	Y	224	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	75	ASN
1	V	89	GLN
1	V	100	ASN
1	W	75	ASN
1	W	100	ASN
2	L	152	ASN
2	L	198	HIS
3	H	209	ASN
3	H	210	HIS
2	X	31	ASN
2	X	124	GLN
2	X	152	ASN
2	X	155	GLN
2	X	160	GLN
2	X	198	HIS
2	X	199	GLN
3	Y	31	HIS
3	Y	209	ASN
3	Y	210	HIS
3	Y	214	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	H	991	-	4,4,4	0.99	0	6,6,6	0.65	0
4	SO4	Y	992	-	4,4,4	1.17	0	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	H	991	-	-	0/0/0/0	0/0/0/0
4	SO4	Y	992	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	992	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.