WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 PM GMT

PDB ID : 3W2D

Title : Crystal Structure of Staphylococcal Eenterotoxin B in complex with a novel neutralization monoclonal antibody Fab fragment

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Deposited on : 2012-11-28

Resolution : 3.10 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	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 3.10 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		50
Ramachandran outliers		8.4%
Sidechain outliers		19.7%
RSRZ outliers		1.7%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
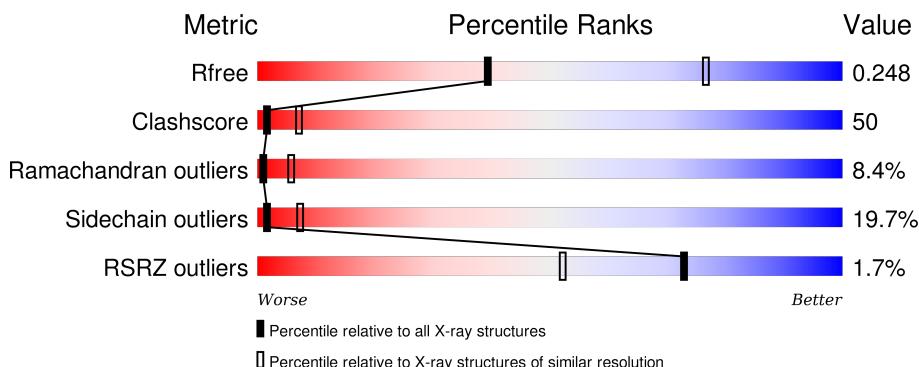
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	239	3% 27% / 51% / 13% / • / 6%
2	L	215	30% / 47% / 22% / •
3	H	223	2% 34% / 54% / 11% / •
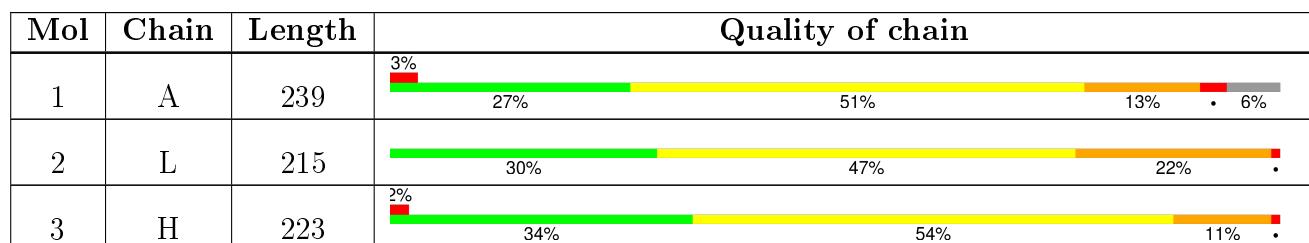
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5393 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 Enterotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1883	1208	305	360	10			

- Molecule 2 is a protein called Monoclonal Antibody 3E2 Fab figment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1647	1023	273	343	8			

- Molecule 3 is a protein called Monoclonal Antibody 3E2 Fab figment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	223	Total	C	N	O	S	0	0	0
			1723	1095	284	337	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
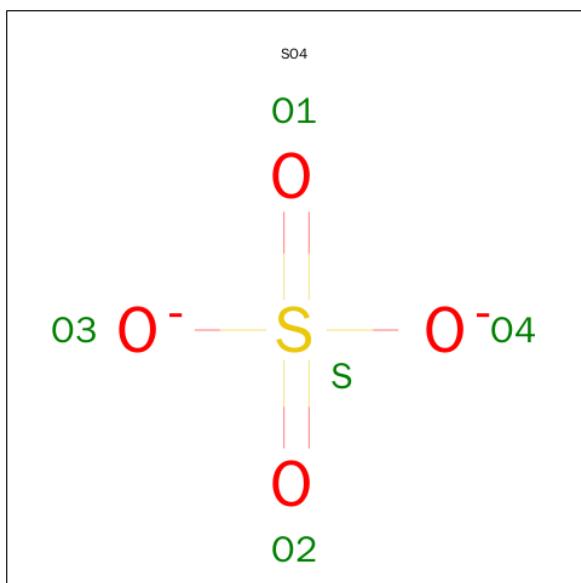
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total 40	O 40	0	0
5	L	47	Total 47	O 47	0	0
5	H	48	Total 48	O 48	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.

- Molecule 1: Enterotoxin type B
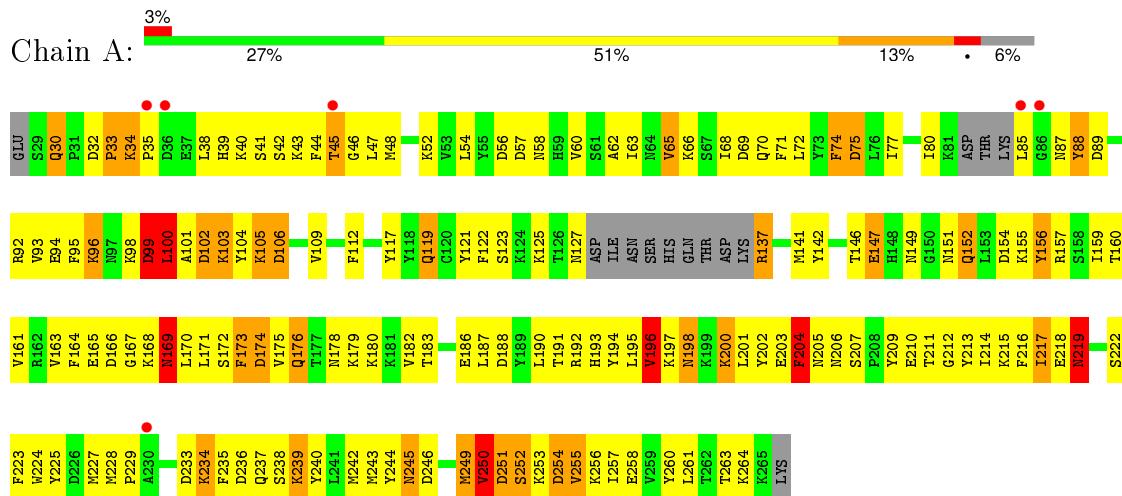
- Molecule 2: Monoclonal Antibody 3E2 Fab figment light chain
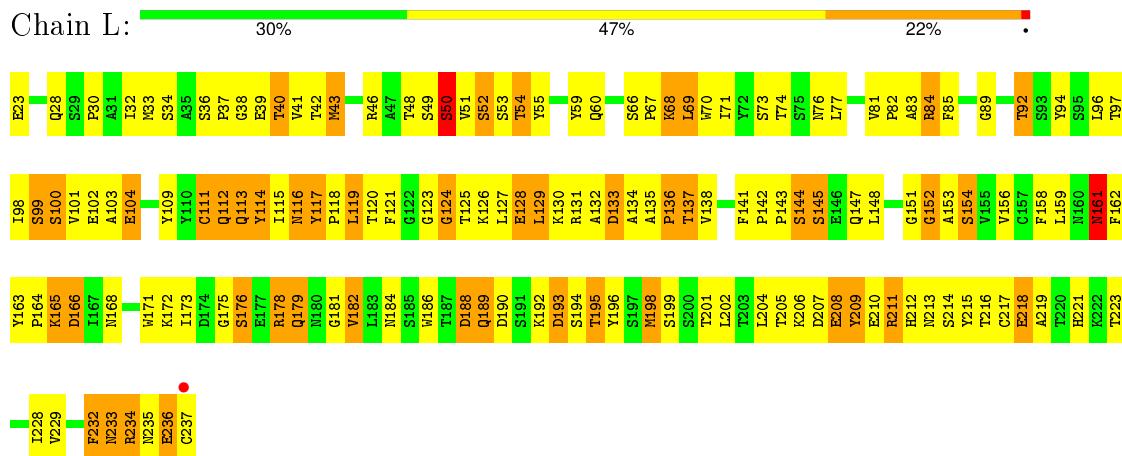
- Molecule 3: Monoclonal Antibody 3E2 Fab figment heavy chain

Full wwPDB X-ray Structure Validation Report
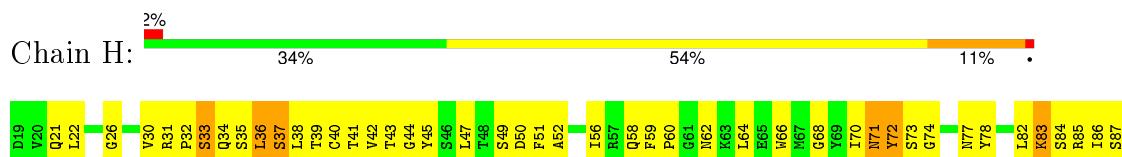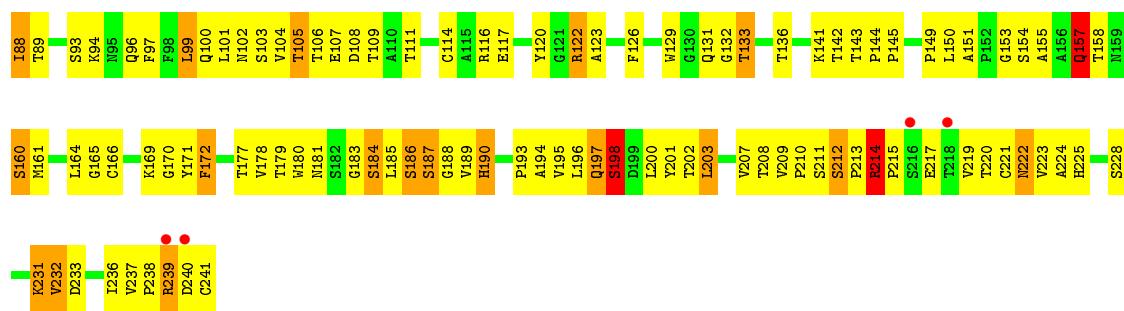
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	40.56Å 109.31Å 86.22Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	36.44 – 3.10 36.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.44-3.10) 92.4 (36.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.196 , 0.261 0.186 , 0.248	Depositor DCC
R_{free} test set	620 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 13506 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5393	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.57	0/1925	0.71	0/2586
2	L	0.56	0/1685	0.79	0/2292
3	H	0.57	0/1773	0.73	0/2430
All	All	0.57	0/5383	0.74	0/7308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1883	0	1831	179	0
2	L	1647	0	1564	215	0
3	H	1723	0	1662	141	0
4	H	5	0	0	0	0
5	A	40	0	0	1	0
5	H	48	0	0	2	0
5	L	47	0	0	4	0
All	All	5393	0	5057	518	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 50.

All (518) 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:207:SER:O	1:A:264:LYS:NZ	1.85	1.10
2:L:172:LYS:HD2	2:L:216:THR:HG22	1.34	1.08
1:A:234:LYS:HD3	1:A:235:PHE:H	1.19	1.06
3:H:181:ASN:O	3:H:184:SER:OG	1.73	1.04
2:L:55:TYR:CD1	2:L:115:ILE:HD11	1.94	1.01
1:A:99:ASP:O	1:A:101:ALA:N	1.93	1.01
2:L:49:SER:O	2:L:50:SER:HB3	1.59	1.01
2:L:193:ASP:O	2:L:195:THR:N	1.98	0.96
3:H:100:GLN:NE2	3:H:102:ASN:OD1	2.01	0.94
3:H:78:TYR:HE1	3:H:88:ILE:HG13	1.31	0.94
1:A:234:LYS:CD	1:A:235:PHE:H	1.82	0.93
1:A:244:TYR:O	1:A:246:ASP:N	2.02	0.93
2:L:159:LEU:O	2:L:162:PHE:HE1	1.53	0.92
3:H:214:ARG:HD2	3:H:215:PRO:HA	1.51	0.91
2:L:113:GLN:NE2	2:L:114:TYR:O	2.03	0.90
1:A:234:LYS:HD3	1:A:235:PHE:N	1.85	0.90
2:L:113:GLN:HE21	2:L:113:GLN:C	1.74	0.90
2:L:23:GLU:HB2	2:L:118:PRO:HD2	1.51	0.90
1:A:88:TYR:HA	1:A:137:ARG:HB3	1.51	0.89
1:A:72:LEU:HD22	2:L:115:ILE:HG22	1.55	0.88
2:L:213:ASN:O	2:L:233:ASN:HA	1.72	0.88
2:L:211:ARG:HH11	2:L:211:ARG:HB2	1.38	0.87
1:A:156:TYR:HD2	1:A:156:TYR:N	1.74	0.86
1:A:168:LYS:O	1:A:170:LEU:N	2.06	0.86
3:H:160:SER:O	3:H:211:SER:N	2.07	0.86
3:H:213:PRO:O	3:H:214:ARG:HB2	1.74	0.86
2:L:178:ARG:CZ	2:L:178:ARG:HA	2.05	0.86
1:A:176:GLN:N	1:A:176:GLN:OE1	2.09	0.85
2:L:141:PHE:HB2	2:L:156:VAL:HG12	1.58	0.84
2:L:172:LYS:HE2	2:L:175:GLY:H	1.40	0.84
2:L:165:LYS:O	2:L:166:ASP:HB2	1.76	0.84
1:A:88:TYR:HB3	1:A:117:TYR:HE1	1.42	0.83
2:L:172:LYS:NZ	2:L:214:SER:OG	2.11	0.83
1:A:66:LYS:HD2	1:A:106:ASP:HA	1.60	0.83
2:L:136:PRO:O	2:L:137:THR:OG1	1.97	0.82
1:A:179:LYS:O	1:A:252:SER:OG	1.96	0.82
2:L:68:LYS:HB2	2:L:68:LYS:NZ	1.94	0.82
2:L:114:TYR:CZ	2:L:119:LEU:HD12	2.15	0.82
2:L:236:GLU:HB2	3:H:153:GLY:HA2	1.61	0.82
3:H:22:LEU:HD23	3:H:114:CYS:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:GLU:O	2:L:101:VAL:HG13	1.80	0.81
1:A:188:ASP:OD1	1:A:214:ILE:HD13	1.81	0.81
1:A:156:TYR:CD2	1:A:156:TYR:N	2.48	0.81
1:A:72:LEU:N	1:A:75:ASP:OD2	2.14	0.80
2:L:53:SER:HB2	2:L:74:THR:HG21	1.64	0.80
3:H:161:MET:HA	3:H:210:PRO:HA	1.62	0.80
2:L:70:TRP:HZ3	2:L:85:PHE:CE2	2.00	0.79
1:A:56:ASP:OD1	1:A:57:ASP:N	2.15	0.79
3:H:157:GLN:HE21	3:H:158:THR:HG23	1.49	0.78
2:L:172:LYS:HE2	2:L:175:GLY:N	1.98	0.77
1:A:70:GLN:HG3	1:A:75:ASP:O	1.84	0.77
2:L:41:VAL:HG12	2:L:42:THR:H	1.48	0.77
1:A:192:ARG:O	1:A:196:VAL:HG22	1.84	0.77
2:L:50:SER:HB2	2:L:92:THR:HG22	1.65	0.77
2:L:51:VAL:HG12	2:L:52:SER:O	1.86	0.76
2:L:33:MET:HG3	2:L:127:LEU:HD12	1.68	0.76
1:A:203:GLU:O	1:A:204:PHE:HB2	1.86	0.75
2:L:208:GLU:OE1	2:L:212:HIS:ND1	2.20	0.74
2:L:117:TYR:HE1	3:H:77:ASN:HD21	1.36	0.74
1:A:154:ASP:H	1:A:155:LYS:HB3	1.53	0.74
2:L:131:ARG:NH1	2:L:132:ALA:O	2.21	0.73
1:A:210:GLU:HG2	1:A:264:LYS:HG2	1.69	0.73
1:A:41:SER:OG	1:A:209:TYR:O	2.03	0.73
2:L:85:PHE:CE1	2:L:98:ILE:HG12	2.24	0.73
1:A:70:GLN:O	1:A:125:LYS:NZ	2.21	0.72
2:L:104:GLU:O	2:L:104:GLU:HG3	1.87	0.72
2:L:211:ARG:NH1	2:L:211:ARG:HB2	2.04	0.71
2:L:113:GLN:NE2	2:L:113:GLN:O	2.24	0.71
2:L:159:LEU:O	2:L:162:PHE:CE1	2.43	0.71
2:L:40:THR:HB	2:L:99:SER:HA	1.71	0.71
1:A:194:TYR:O	1:A:198:ASN:ND2	2.24	0.71
3:H:210:PRO:HB2	3:H:213:PRO:HD2	1.73	0.70
1:A:48:MET:HB3	1:A:204:PHE:H	1.56	0.70
3:H:78:TYR:CE1	3:H:88:ILE:HG13	2.22	0.70
1:A:200:LYS:N	1:A:200:LYS:HD2	2.07	0.70
2:L:55:TYR:HE1	3:H:122:ARG:HB2	1.55	0.69
2:L:46:ARG:HD3	5:L:308:HOH:O	1.92	0.69
3:H:66:TRP:CZ2	3:H:68:GLY:HA2	2.27	0.69
3:H:149:PRO:O	3:H:150:LEU:HD23	1.93	0.69
2:L:84:ARG:NH2	2:L:102:GLU:HB2	2.08	0.68
1:A:45:THR:O	1:A:45:THR:OG1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:GLU:CB	2:L:118:PRO:HD2	2.23	0.68
3:H:85:ARG:HB3	3:H:102:ASN:HB2	1.75	0.68
2:L:82:PRO:HB2	2:L:84:ARG:HD3	1.74	0.68
2:L:172:LYS:HD2	2:L:216:THR:CG2	2.18	0.68
3:H:196:LEU:HD13	3:H:201:TYR:CE1	2.29	0.68
1:A:210:GLU:HG2	1:A:264:LYS:HA	1.75	0.68
1:A:213:TYR:HA	1:A:227:MET:HG3	1.74	0.68
2:L:55:TYR:CE1	2:L:115:ILE:HD11	2.29	0.67
2:L:55:TYR:CG	2:L:115:ILE:HD11	2.29	0.67
1:A:154:ASP:N	1:A:155:LYS:HB3	2.09	0.67
2:L:193:ASP:OD2	2:L:195:THR:HG22	1.94	0.67
3:H:212:SER:HB2	3:H:213:PRO:HD3	1.76	0.67
1:A:75:ASP:HB3	1:A:92:ARG:HH21	1.59	0.67
2:L:213:ASN:HA	2:L:234:ARG:HH21	1.61	0.66
1:A:187:LEU:HD11	1:A:250:VAL:HG21	1.75	0.66
2:L:208:GLU:O	2:L:211:ARG:HD3	1.95	0.66
1:A:154:ASP:HB2	1:A:155:LYS:HB3	1.76	0.66
2:L:131:ARG:HG3	2:L:132:ALA:N	2.10	0.66
2:L:131:ARG:HG3	2:L:132:ALA:O	1.94	0.66
3:H:50:ASP:HB3	3:H:51:PHE:CE2	2.31	0.66
1:A:100:LEU:H	1:A:100:LEU:HD23	1.59	0.66
3:H:71:ASN:OD1	3:H:72:TYR:N	2.29	0.66
2:L:209:TYR:CD1	2:L:215:TYR:HE2	2.13	0.66
1:A:66:LYS:NZ	1:A:106:ASP:OD2	2.28	0.66
1:A:52:LYS:HB2	1:A:202:TYR:HB3	1.77	0.66
2:L:113:GLN:NE2	2:L:113:GLN:C	2.48	0.65
3:H:50:ASP:HB3	3:H:51:PHE:CD2	2.30	0.65
1:A:102:ASP:O	1:A:103:LYS:C	2.35	0.65
2:L:211:ARG:O	2:L:212:HIS:CD2	2.49	0.65
2:L:54:THR:O	2:L:73:SER:HA	1.96	0.65
1:A:47:LEU:H	1:A:234:LYS:HE2	1.62	0.64
2:L:145:SER:HA	2:L:148:LEU:HD12	1.78	0.64
2:L:206:LYS:C	2:L:208:GLU:H	2.00	0.64
1:A:34:LYS:H	1:A:35:PRO:CD	2.11	0.64
2:L:172:LYS:CD	2:L:216:THR:HG22	2.21	0.64
1:A:54:LEU:HD21	1:A:237:GLN:NE2	2.12	0.64
3:H:231:LYS:HE2	3:H:232:VAL:H	1.60	0.64
1:A:95:PHE:HB3	1:A:100:LEU:HD12	1.79	0.64
2:L:117:TYR:HE1	3:H:77:ASN:ND2	1.96	0.63
1:A:171:LEU:HD23	1:A:172:SER:N	2.13	0.63
3:H:186:SER:O	3:H:188:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:LEU:N	2:L:159:LEU:HD12	2.14	0.63
2:L:236:GLU:CB	3:H:153:GLY:HA2	2.29	0.63
2:L:70:TRP:CZ3	2:L:85:PHE:CE2	2.87	0.63
3:H:71:ASN:OD1	3:H:73:SER:N	2.29	0.63
3:H:109:THR:HG23	3:H:136:THR:HA	1.81	0.63
2:L:101:VAL:HG23	2:L:101:VAL:O	1.99	0.62
1:A:62:ALA:HB2	1:A:80:ILE:HD12	1.82	0.62
3:H:66:TRP:HH2	3:H:77:ASN:HD22	1.48	0.62
2:L:209:TYR:HA	2:L:215:TYR:OH	1.99	0.61
1:A:154:ASP:CA	1:A:155:LYS:HB3	2.30	0.61
1:A:101:ALA:O	1:A:105:LYS:HB2	2.01	0.61
1:A:161:VAL:N	1:A:173:PHE:O	2.30	0.61
1:A:39:HIS:O	1:A:211:THR:HG22	2.00	0.61
1:A:217:ILE:HG23	1:A:222:SER:HB3	1.83	0.61
2:L:153:ALA:N	2:L:204:LEU:O	2.30	0.61
1:A:172:SER:O	1:A:173:PHE:HB3	2.01	0.60
2:L:228:ILE:HD12	2:L:228:ILE:H	1.66	0.60
1:A:103:LYS:HD3	1:A:104:TYR:CE1	2.37	0.60
3:H:38:LEU:HD12	3:H:99:LEU:HD23	1.84	0.60
2:L:68:LYS:HZ3	2:L:68:LYS:HB2	1.67	0.60
2:L:119:LEU:HD11	3:H:126:PHE:HZ	1.67	0.60
1:A:99:ASP:O	1:A:100:LEU:C	2.37	0.60
1:A:33:PRO:HB3	1:A:224:TRP:CZ2	2.36	0.60
3:H:145:PRO:HD3	3:H:225:HIS:ND1	2.15	0.60
2:L:159:LEU:HD21	2:L:219:ALA:HB2	1.84	0.59
2:L:164:PRO:HD2	2:L:221:HIS:NE2	2.17	0.59
2:L:211:ARG:HD3	2:L:211:ARG:H	1.67	0.59
1:A:213:TYR:CE1	1:A:260:TYR:HB2	2.38	0.59
3:H:82:LEU:O	3:H:83:LYS:C	2.41	0.59
3:H:177:THR:HG22	3:H:224:ALA:HB3	1.84	0.59
3:H:59:PHE:HB3	3:H:60:PRO:HD2	1.84	0.59
3:H:179:THR:HB	3:H:183:GLY:HA2	1.85	0.59
1:A:165:GLU:HA	1:A:261:LEU:HB2	1.84	0.59
1:A:75:ASP:HB2	1:A:92:ARG:HE	1.67	0.59
2:L:46:ARG:HG2	2:L:46:ARG:HH11	1.67	0.59
1:A:154:ASP:CB	1:A:155:LYS:HB3	2.33	0.58
1:A:161:VAL:HG13	1:A:257:ILE:HG22	1.84	0.58
1:A:191:THR:HG21	1:A:257:ILE:HD13	1.85	0.58
2:L:228:ILE:N	2:L:228:ILE:HD12	2.18	0.58
1:A:157:ARG:HH11	1:A:252:SER:HB2	1.67	0.58
2:L:70:TRP:HZ3	2:L:85:PHE:CD2	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HD2	1:A:106:ASP:CA	2.32	0.58
1:A:56:ASP:CG	1:A:57:ASP:H	2.07	0.58
2:L:182:VAL:HA	2:L:201:THR:O	2.03	0.58
1:A:151:ASN:OD1	1:A:180:LYS:HB2	2.04	0.58
2:L:55:TYR:CD2	2:L:115:ILE:HG13	2.39	0.58
3:H:160:SER:HB3	5:H:413:HOH:O	2.03	0.58
1:A:48:MET:N	1:A:204:PHE:O	2.23	0.58
2:L:73:SER:O	2:L:74:THR:HG22	2.03	0.57
2:L:69:LEU:O	2:L:70:TRP:CD1	2.57	0.57
1:A:152:GLN:HE21	1:A:152:GLN:N	2.02	0.57
3:H:160:SER:O	3:H:210:PRO:HA	2.04	0.57
1:A:119:GLN:NE2	1:A:236:ASP:OD1	2.23	0.57
1:A:88:TYR:HB3	1:A:117:TYR:CE1	2.33	0.57
3:H:166:CYS:HB2	3:H:180:TRP:CH2	2.40	0.57
2:L:208:GLU:O	2:L:209:TYR:C	2.43	0.57
3:H:82:LEU:O	3:H:84:SER:N	2.38	0.57
3:H:239:ARG:HD3	3:H:239:ARG:N	2.20	0.57
1:A:183:THR:O	1:A:186:GLU:HB3	2.05	0.57
2:L:119:LEU:HD11	3:H:126:PHE:CZ	2.40	0.56
3:H:171:TYR:O	3:H:172:PHE:HB2	2.05	0.56
1:A:74:PHE:CD2	1:A:74:PHE:N	2.74	0.56
2:L:179:GLN:HA	2:L:179:GLN:OE1	2.05	0.56
3:H:59:PHE:HB3	3:H:60:PRO:CD	2.35	0.56
1:A:98:LYS:NZ	3:H:117:GLU:OE2	2.39	0.56
3:H:186:SER:O	3:H:187:SER:C	2.45	0.55
3:H:42:VAL:HG21	3:H:47:LEU:HD21	1.86	0.55
3:H:52:ALA:HB3	3:H:117:GLU:CD	2.27	0.55
1:A:154:ASP:HB2	1:A:155:LYS:CB	2.36	0.55
2:L:235:ASN:HA	5:L:343:HOH:O	2.06	0.55
3:H:66:TRP:HH2	3:H:77:ASN:ND2	2.05	0.55
3:H:213:PRO:HA	3:H:217:GLU:OE1	2.06	0.55
1:A:171:LEU:HD23	1:A:172:SER:O	2.06	0.55
3:H:26:GLY:HA3	3:H:38:LEU:HD23	1.87	0.55
3:H:106:THR:C	3:H:108:ASP:H	2.09	0.55
3:H:70:ILE:HD11	3:H:74:GLY:HA2	1.88	0.55
2:L:172:LYS:HZ1	2:L:214:SER:HG	1.54	0.55
1:A:168:LYS:HB2	1:A:170:LEU:HG	1.88	0.55
2:L:172:LYS:HE2	2:L:175:GLY:CA	2.37	0.55
1:A:253:LYS:O	1:A:255:VAL:N	2.37	0.55
2:L:23:GLU:HB2	2:L:118:PRO:CD	2.32	0.55
3:H:240:ASP:O	3:H:241:CYS:HB2	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:HB3	1:A:77:ILE:HD12	1.87	0.54
2:L:172:LYS:C	2:L:172:LYS:HD3	2.28	0.54
3:H:194:ALA:HB2	3:H:203:LEU:HB2	1.89	0.54
2:L:84:ARG:HH22	2:L:102:GLU:HB2	1.71	0.54
1:A:182:VAL:HG13	1:A:250:VAL:HG23	1.90	0.54
2:L:41:VAL:HG12	2:L:42:THR:N	2.21	0.54
2:L:30:PRO:O	2:L:125:THR:HG23	2.07	0.54
2:L:128:GLU:HB3	2:L:189:GLN:NE2	2.22	0.54
3:H:169:LYS:HA	3:H:202:THR:HG23	1.89	0.54
3:H:71:ASN:CG	3:H:72:TYR:N	2.61	0.54
3:H:164:LEU:HD11	3:H:219:VAL:HG11	1.90	0.54
3:H:171:TYR:CZ	3:H:201:TYR:HB2	2.43	0.54
2:L:236:GLU:HG3	3:H:153:GLY:HA2	1.89	0.54
2:L:70:TRP:CZ2	2:L:81:VAL:HG12	2.42	0.54
2:L:151:GLY:O	2:L:152:GLY:O	2.25	0.54
3:H:129:TRP:N	3:H:129:TRP:CD1	2.76	0.54
2:L:208:GLU:O	2:L:210:GLU:N	2.41	0.53
2:L:135:ALA:HA	2:L:223:THR:OG1	2.08	0.53
2:L:50:SER:CB	2:L:92:THR:HG22	2.37	0.53
3:H:71:ASN:C	3:H:71:ASN:OD1	2.47	0.53
2:L:193:ASP:OD2	2:L:195:THR:CG2	2.57	0.53
3:H:141:LYS:HE2	3:H:142:THR:O	2.08	0.53
2:L:161:ASN:HD22	2:L:195:THR:HG21	1.73	0.53
2:L:158:PHE:C	2:L:159:LEU:HD12	2.29	0.53
2:L:53:SER:HB2	2:L:74:THR:CG2	2.36	0.53
1:A:244:TYR:C	1:A:246:ASP:H	2.12	0.53
2:L:129:LEU:CD2	2:L:129:LEU:N	2.71	0.53
1:A:60:VAL:O	1:A:112:PHE:HA	2.09	0.53
1:A:63:ILE:HD12	1:A:63:ILE:N	2.23	0.53
2:L:69:LEU:O	2:L:70:TRP:HD1	1.91	0.52
2:L:190:ASP:HB2	2:L:193:ASP:OD1	2.08	0.52
1:A:165:GLU:C	1:A:167:GLY:H	2.13	0.52
2:L:84:ARG:HH22	2:L:102:GLU:CB	2.21	0.52
2:L:43:MET:HE2	2:L:125:THR:CG2	2.40	0.52
2:L:37:PRO:HA	2:L:101:VAL:O	2.10	0.52
3:H:212:SER:CB	3:H:213:PRO:HD3	2.38	0.52
1:A:202:TYR:OH	1:A:227:MET:O	2.26	0.52
3:H:197:GLN:O	3:H:198:SER:C	2.48	0.52
2:L:103:ALA:HA	2:L:129:LEU:HD11	1.90	0.52
2:L:141:PHE:HB3	2:L:142:PRO:HD2	1.91	0.52
2:L:186:TRP:CD1	2:L:198:MET:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:161:ASN:HB3	2:L:195:THR:HG21	1.91	0.52
1:A:236:ASP:OD2	1:A:239:LYS:HB2	2.10	0.52
2:L:171:TRP:CD1	2:L:182:VAL:HG11	2.45	0.51
3:H:222:ASN:HB3	3:H:233:ASP:OD1	2.10	0.51
2:L:123:GLY:O	2:L:124:GLY:O	2.27	0.51
3:H:58:GLN:HG3	3:H:62:ASN:O	2.10	0.51
1:A:44:PHE:CZ	1:A:46:GLY:HA3	2.45	0.51
1:A:194:TYR:C	1:A:198:ASN:HD21	2.13	0.51
3:H:179:THR:OG1	3:H:183:GLY:N	2.44	0.51
1:A:42:SER:HB3	1:A:264:LYS:CD	2.40	0.51
1:A:182:VAL:HG13	1:A:250:VAL:CG2	2.41	0.51
3:H:161:MET:HA	3:H:210:PRO:CA	2.36	0.51
3:H:120:TYR:O	3:H:123:ALA:HB3	2.10	0.51
2:L:213:ASN:HA	2:L:234:ARG:NH2	2.26	0.51
1:A:195:LEU:O	1:A:196:VAL:C	2.50	0.51
1:A:203:GLU:O	1:A:204:PHE:CB	2.56	0.51
2:L:173:ILE:O	2:L:214:SER:O	2.29	0.51
1:A:100:LEU:N	1:A:100:LEU:HD23	2.25	0.51
2:L:73:SER:HB2	2:L:76:ASN:OD1	2.11	0.51
1:A:201:LEU:HD21	1:A:227:MET:HE2	1.92	0.51
1:A:39:HIS:HB2	1:A:228:MET:HB2	1.93	0.51
3:H:178:VAL:HG22	3:H:179:THR:N	2.26	0.51
3:H:169:LYS:HG3	3:H:202:THR:HG23	1.92	0.51
2:L:123:GLY:O	5:L:341:HOH:O	2.19	0.51
1:A:65:VAL:CG1	5:A:309:HOH:O	2.59	0.51
1:A:34:LYS:N	1:A:35:PRO:CD	2.73	0.50
3:H:231:LYS:NZ	3:H:233:ASP:OD1	2.44	0.50
1:A:40:LYS:HD2	1:A:43:LYS:HD2	1.93	0.50
2:L:51:VAL:HG12	2:L:52:SER:N	2.26	0.50
3:H:133:THR:O	3:H:133:THR:HG23	2.12	0.50
1:A:71:PHE:N	1:A:75:ASP:OD2	2.43	0.50
1:A:182:VAL:CG1	1:A:250:VAL:HG23	2.42	0.50
1:A:242:MET:HG2	1:A:242:MET:O	2.11	0.50
2:L:181:GLY:O	2:L:202:LEU:HD12	2.12	0.50
2:L:195:THR:HG23	2:L:196:TYR:N	2.27	0.50
1:A:154:ASP:N	1:A:155:LYS:O	2.45	0.50
2:L:159:LEU:N	2:L:159:LEU:CD1	2.74	0.50
2:L:142:PRO:HG3	2:L:236:GLU:CD	2.33	0.50
1:A:52:LYS:HB2	1:A:202:TYR:CB	2.42	0.50
2:L:28:GLN:HE22	2:L:124:GLY:CA	2.24	0.50
2:L:209:TYR:CD1	2:L:215:TYR:CE2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD1	1:A:70:GLN:N	2.43	0.50
2:L:193:ASP:CG	2:L:195:THR:HG22	2.33	0.50
2:L:114:TYR:CZ	2:L:119:LEU:CD1	2.90	0.49
1:A:57:ASP:HA	1:A:193:HIS:NE2	2.27	0.49
1:A:263:THR:HG22	1:A:264:LYS:N	2.28	0.49
3:H:217:GLU:CD	3:H:217:GLU:H	2.15	0.49
3:H:161:MET:HG2	3:H:210:PRO:N	2.27	0.49
2:L:142:PRO:HG3	2:L:236:GLU:OE2	2.12	0.49
1:A:161:VAL:O	1:A:172:SER:HA	2.13	0.49
2:L:236:GLU:CG	3:H:153:GLY:HA2	2.42	0.49
2:L:166:ASP:OD1	5:L:304:HOH:O	2.18	0.49
2:L:209:TYR:CE1	2:L:215:TYR:HE2	2.30	0.49
1:A:234:LYS:CD	1:A:235:PHE:N	2.59	0.49
1:A:187:LEU:CD1	1:A:250:VAL:HG21	2.41	0.49
2:L:186:TRP:HE1	2:L:198:MET:CE	2.25	0.49
3:H:111:THR:HG23	3:H:133:THR:H	1.77	0.49
1:A:88:TYR:CB	1:A:117:TYR:HE1	2.22	0.49
3:H:200:LEU:HD12	3:H:200:LEU:N	2.27	0.49
2:L:172:LYS:HB3	2:L:216:THR:HG22	1.95	0.49
2:L:163:TYR:CD2	2:L:164:PRO:HA	2.47	0.49
2:L:178:ARG:NE	2:L:178:ARG:HA	2.27	0.49
1:A:88:TYR:N	1:A:88:TYR:CD2	2.81	0.49
2:L:143:PRO:O	2:L:144:SER:OG	2.24	0.49
3:H:105:THR:O	3:H:108:ASP:HB2	2.13	0.49
1:A:96:LYS:HD2	1:A:245:ASN:ND2	2.27	0.48
3:H:144:PRO:HG3	3:H:228:SER:HB2	1.94	0.48
3:H:58:GLN:HB2	3:H:64:LEU:CD2	2.43	0.48
2:L:70:TRP:CD2	2:L:81:VAL:HG11	2.48	0.48
2:L:206:LYS:C	2:L:208:GLU:N	2.66	0.48
3:H:21:GLN:O	3:H:22:LEU:HD12	2.13	0.48
3:H:195:VAL:HG12	3:H:196:LEU:H	1.77	0.48
1:A:161:VAL:HG21	1:A:191:THR:HG22	1.95	0.48
2:L:43:MET:HE2	2:L:125:THR:HG21	1.95	0.48
2:L:172:LYS:HE2	2:L:175:GLY:HA2	1.96	0.48
1:A:155:LYS:C	1:A:156:TYR:HD2	2.16	0.48
1:A:188:ASP:OD1	1:A:214:ILE:HG21	2.13	0.48
1:A:121:TYR:CG	1:A:122:PHE:N	2.81	0.48
3:H:169:LYS:HG3	3:H:202:THR:CG2	2.43	0.48
3:H:66:TRP:CE2	3:H:68:GLY:HA2	2.48	0.48
3:H:161:MET:HB3	3:H:208:THR:HG22	1.95	0.48
1:A:39:HIS:HB2	1:A:228:MET:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HD3	1:A:104:TYR:CZ	2.49	0.48
2:L:131:ARG:HG2	2:L:163:TYR:CG	2.49	0.48
3:H:42:VAL:HG21	3:H:47:LEU:CD2	2.43	0.48
2:L:193:ASP:O	2:L:193:ASP:CG	2.51	0.48
2:L:215:TYR:HB2	2:L:232:PHE:CD2	2.49	0.47
2:L:113:GLN:HG3	2:L:120:THR:HB	1.95	0.47
3:H:161:MET:HG2	3:H:210:PRO:CD	2.43	0.47
1:A:87:ASN:O	1:A:137:ARG:HG2	2.14	0.47
2:L:133:ASP:HB3	2:L:223:THR:HG22	1.96	0.47
1:A:240:TYR:O	1:A:243:MET:HG2	2.14	0.47
1:A:217:ILE:HD12	1:A:217:ILE:N	2.29	0.47
2:L:101:VAL:CG2	2:L:101:VAL:O	2.62	0.47
2:L:41:VAL:O	2:L:97:THR:HG23	2.14	0.47
2:L:145:SER:O	2:L:148:LEU:HB2	2.14	0.47
1:A:195:LEU:N	1:A:195:LEU:HD23	2.29	0.47
2:L:126:LYS:HB2	2:L:126:LYS:HE3	1.70	0.47
1:A:41:SER:CB	1:A:207:SER:HB3	2.45	0.47
3:H:145:PRO:HB3	3:H:171:TYR:HB3	1.97	0.47
1:A:39:HIS:ND1	1:A:228:MET:O	2.33	0.47
1:A:244:TYR:C	1:A:246:ASP:N	2.68	0.47
1:A:165:GLU:O	1:A:166:ASP:HB3	2.14	0.47
3:H:35:SER:HA	3:H:101:LEU:O	2.14	0.47
3:H:171:TYR:CE2	3:H:201:TYR:HB2	2.50	0.47
2:L:43:MET:HG2	2:L:96:LEU:HB3	1.96	0.47
2:L:60:GLN:HG3	2:L:109:TYR:CE1	2.49	0.47
1:A:215:LYS:HE2	1:A:222:SER:HB2	1.96	0.47
2:L:141:PHE:CD2	2:L:156:VAL:HG13	2.49	0.47
2:L:46:ARG:HG2	2:L:46:ARG:NH1	2.29	0.47
3:H:215:PRO:HB3	3:H:238:PRO:HG3	1.97	0.47
2:L:130:LYS:HA	2:L:163:TYR:OH	2.15	0.47
2:L:186:TRP:HE1	2:L:198:MET:HE2	1.80	0.47
1:A:204:PHE:C	1:A:204:PHE:HD2	2.19	0.46
2:L:116:ASN:HD22	2:L:116:ASN:HA	1.52	0.46
2:L:163:TYR:CG	2:L:164:PRO:HA	2.51	0.46
2:L:112:GLN:HA	2:L:120:THR:O	2.15	0.46
2:L:68:LYS:HZ2	2:L:68:LYS:HB2	1.78	0.46
1:A:193:HIS:O	1:A:197:LYS:HG2	2.15	0.46
1:A:251:ASP:O	1:A:255:VAL:HG12	2.16	0.46
3:H:71:ASN:CG	3:H:72:TYR:H	2.17	0.46
3:H:26:GLY:HA3	3:H:38:LEU:CD2	2.44	0.46
3:H:209:VAL:CG2	3:H:213:PRO:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:C	1:A:168:LYS:HD3	2.36	0.46
1:A:204:PHE:CD2	1:A:204:PHE:C	2.89	0.46
2:L:152:GLY:HA2	2:L:205:THR:HA	1.98	0.46
2:L:172:LYS:NZ	2:L:173:ILE:O	2.41	0.46
2:L:138:VAL:HA	2:L:158:PHE:O	2.16	0.46
1:A:66:LYS:HE3	1:A:66:LYS:HB3	1.80	0.46
3:H:101:LEU:HG	3:H:104:VAL:HG12	1.97	0.46
2:L:175:GLY:O	2:L:176:SER:C	2.54	0.46
1:A:236:ASP:HB3	1:A:239:LYS:HB2	1.98	0.46
2:L:193:ASP:C	2:L:195:THR:N	2.64	0.46
2:L:208:GLU:O	2:L:211:ARG:N	2.42	0.45
1:A:75:ASP:CB	1:A:92:ARG:HE	2.29	0.45
1:A:52:LYS:HG2	1:A:52:LYS:O	2.15	0.45
1:A:71:PHE:O	2:L:116:ASN:O	2.33	0.45
2:L:67:PRO:O	2:L:68:LYS:HG3	2.16	0.45
2:L:55:TYR:CE1	3:H:122:ARG:HB2	2.44	0.45
2:L:37:PRO:HG3	2:L:129:LEU:HD12	1.97	0.45
2:L:154:SER:HA	2:L:202:LEU:O	2.16	0.45
2:L:119:LEU:HD22	3:H:66:TRP:HB2	1.99	0.45
2:L:115:ILE:HD12	2:L:115:ILE:HG23	1.70	0.45
2:L:84:ARG:NH2	2:L:102:GLU:CB	2.79	0.45
3:H:157:GLN:HG2	3:H:158:THR:N	2.32	0.45
1:A:253:LYS:HG3	1:A:254:ASP:OD1	2.17	0.45
3:H:30:VAL:HG11	3:H:104:VAL:HG21	1.98	0.45
2:L:215:TYR:HB2	2:L:232:PHE:HD2	1.82	0.45
2:L:114:TYR:O	2:L:116:ASN:N	2.46	0.45
2:L:115:ILE:HD13	2:L:115:ILE:N	2.32	0.45
2:L:82:PRO:HB2	2:L:84:ARG:CD	2.44	0.45
2:L:34:SER:HA	2:L:128:GLU:O	2.17	0.45
3:H:32:PRO:O	3:H:33:SER:CB	2.65	0.45
1:A:216:PHE:O	1:A:222:SER:HA	2.17	0.45
1:A:44:PHE:CE1	1:A:235:PHE:HB2	2.52	0.44
3:H:97:PHE:CZ	3:H:114:CYS:HB2	2.52	0.44
2:L:102:GLU:HG2	2:L:103:ALA:H	1.81	0.44
2:L:70:TRP:HZ3	2:L:85:PHE:CZ	2.35	0.44
2:L:32:ILE:HG21	2:L:128:GLU:OE2	2.16	0.44
2:L:28:GLN:NE2	2:L:124:GLY:CA	2.80	0.44
2:L:173:ILE:HG23	2:L:215:TYR:CE1	2.52	0.44
2:L:188:ASP:O	2:L:189:GLN:C	2.56	0.44
3:H:237:VAL:HG23	3:H:238:PRO:HD2	1.98	0.44
3:H:132:GLY:O	3:H:133:THR:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB2	1:A:92:ARG:NE	2.31	0.44
1:A:137:ARG:NH1	1:A:137:ARG:HA	2.33	0.44
2:L:237:CYS:SG	3:H:241:CYS:HA	2.58	0.44
3:H:145:PRO:HA	3:H:170:GLY:O	2.18	0.44
1:A:228:MET:HA	1:A:229:PRO:HD3	1.63	0.44
1:A:74:PHE:H	1:A:74:PHE:HD2	1.66	0.44
3:H:43:THR:C	3:H:45:TYR:H	2.21	0.44
2:L:173:ILE:HD11	2:L:179:GLN:CG	2.46	0.44
3:H:217:GLU:CD	3:H:217:GLU:N	2.71	0.44
1:A:38:LEU:HD13	1:A:211:THR:HB	1.99	0.44
2:L:134:ALA:C	2:L:223:THR:HG21	2.38	0.44
2:L:136:PRO:HA	2:L:162:PHE:HB3	2.00	0.44
1:A:88:TYR:N	1:A:88:TYR:HD2	2.16	0.44
1:A:165:GLU:HB3	1:A:170:LEU:HD12	2.00	0.43
3:H:155:ALA:HA	3:H:157:GLN:CD	2.38	0.43
1:A:62:ALA:C	1:A:63:ILE:HD12	2.37	0.43
3:H:197:GLN:HE21	3:H:197:GLN:HB3	1.62	0.43
1:A:146:THR:HG22	1:A:249:MET:SD	2.58	0.43
3:H:188:GLY:O	3:H:207:VAL:HA	2.17	0.43
1:A:152:GLN:HE21	1:A:152:GLN:CA	2.30	0.43
2:L:43:MET:SD	2:L:96:LEU:HD12	2.59	0.43
1:A:165:GLU:O	1:A:167:GLY:N	2.46	0.43
3:H:171:TYR:HB2	3:H:225:HIS:CE1	2.54	0.43
1:A:253:LYS:C	1:A:255:VAL:H	2.19	0.43
3:H:83:LYS:O	3:H:86:ILE:HG22	2.19	0.43
1:A:236:ASP:OD2	1:A:239:LYS:HD3	2.18	0.43
2:L:48:THR:O	2:L:49:SER:C	2.56	0.43
1:A:219:ASN:H	1:A:219:ASN:ND2	2.16	0.43
1:A:72:LEU:CD2	2:L:116:ASN:ND2	2.81	0.43
3:H:212:SER:CB	3:H:213:PRO:CD	2.96	0.43
2:L:28:GLN:OE1	2:L:111:CYS:SG	2.76	0.43
1:A:75:ASP:CB	1:A:92:ARG:HH21	2.29	0.43
2:L:114:TYR:CE2	2:L:119:LEU:HD12	2.53	0.43
1:A:210:GLU:HG2	1:A:264:LYS:CA	2.44	0.43
1:A:96:LYS:HD2	1:A:245:ASN:CG	2.39	0.43
2:L:59:TYR:CD1	2:L:69:LEU:HA	2.53	0.43
3:H:151:ALA:HB3	3:H:239:ARG:NE	2.34	0.43
3:H:41:THR:HA	3:H:96:GLN:HB3	2.01	0.43
3:H:189:VAL:HG12	3:H:190:HIS:N	2.34	0.43
2:L:119:LEU:HD23	2:L:119:LEU:C	2.39	0.42
1:A:154:ASP:H	1:A:155:LYS:CB	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:HA2	1:A:260:TYR:O	2.19	0.42
1:A:159:ILE:O	1:A:174:ASP:HA	2.19	0.42
2:L:147:GLN:O	2:L:151:GLY:O	2.37	0.42
2:L:141:PHE:HD2	2:L:156:VAL:HG13	1.84	0.42
2:L:142:PRO:HA	2:L:143:PRO:HD3	1.93	0.42
3:H:143:THR:HA	3:H:144:PRO:HD3	1.88	0.42
1:A:186:GLU:O	1:A:190:LEU:HG	2.20	0.42
2:L:161:ASN:N	2:L:196:TYR:O	2.53	0.42
2:L:77:LEU:HB3	2:L:81:VAL:HG23	2.02	0.42
3:H:36:LEU:HD11	3:H:38:LEU:HD11	2.01	0.42
2:L:171:TRP:CH2	2:L:217:CYS:HB3	2.55	0.42
3:H:169:LYS:CG	3:H:202:THR:HG23	2.49	0.42
2:L:114:TYR:CE2	2:L:119:LEU:CD1	3.02	0.42
1:A:200:LYS:O	1:A:201:LEU:C	2.57	0.42
1:A:250:VAL:HG23	1:A:251:ASP:H	1.85	0.42
3:H:177:THR:CG2	3:H:224:ALA:HB3	2.50	0.42
3:H:165:GLY:C	3:H:180:TRP:HH2	2.23	0.42
1:A:42:SER:HB3	1:A:264:LYS:HE3	2.01	0.42
3:H:50:ASP:C	3:H:51:PHE:CD2	2.93	0.42
1:A:251:ASP:O	1:A:253:LYS:N	2.53	0.42
3:H:169:LYS:CB	3:H:202:THR:HG23	2.50	0.42
2:L:55:TYR:CG	2:L:115:ILE:CG1	3.03	0.41
3:H:161:MET:CA	3:H:210:PRO:HA	2.42	0.41
1:A:213:TYR:HB2	1:A:225:TYR:O	2.19	0.41
3:H:179:THR:HB	3:H:183:GLY:CA	2.49	0.41
2:L:112:GLN:HG3	2:L:121:PHE:CE1	2.55	0.41
3:H:36:LEU:HD22	3:H:36:LEU:C	2.40	0.41
2:L:89:GLY:HA3	2:L:94:TYR:HA	2.02	0.41
2:L:128:GLU:HB3	2:L:189:GLN:HE21	1.85	0.41
3:H:106:THR:C	3:H:108:ASP:N	2.74	0.41
1:A:93:VAL:HG22	1:A:141:MET:HG3	2.01	0.41
1:A:165:GLU:O	1:A:166:ASP:CB	2.69	0.41
1:A:99:ASP:HA	1:A:102:ASP:OD2	2.20	0.41
2:L:36:SER:HA	2:L:37:PRO:HD3	1.84	0.41
2:L:82:PRO:O	2:L:84:ARG:N	2.54	0.41
2:L:52:SER:OG	2:L:54:THR:HG23	2.21	0.41
3:H:197:GLN:HG3	3:H:202:THR:OG1	2.21	0.41
1:A:30:GLN:HG2	1:A:223:PHE:HA	2.03	0.41
2:L:190:ASP:CB	2:L:193:ASP:OD1	2.68	0.41
1:A:204:PHE:O	1:A:204:PHE:HD2	2.03	0.41
1:A:34:LYS:H	1:A:35:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB2	1:A:207:SER:CB	2.51	0.41
1:A:142:TYR:HB3	1:A:245:ASN:HA	2.02	0.41
3:H:100:GLN:HB2	5:H:405:HOH:O	2.21	0.41
2:L:168:ASN:O	2:L:219:ALA:HA	2.20	0.41
2:L:163:TYR:CD2	2:L:164:PRO:CA	3.04	0.41
3:H:171:TYR:O	3:H:200:LEU:HA	2.21	0.41
3:H:37:SER:HA	3:H:99:LEU:O	2.20	0.41
3:H:223:VAL:CG1	3:H:224:ALA:N	2.84	0.41
1:A:164:PHE:CE2	1:A:169:ASN:HA	2.55	0.41
2:L:184:ASN:HA	2:L:199:SER:O	2.21	0.41
1:A:56:ASP:HA	1:A:197:LYS:NZ	2.36	0.41
3:H:143:THR:HG22	3:H:171:TYR:HA	2.03	0.41
2:L:117:TYR:HA	2:L:118:PRO:HA	1.66	0.40
3:H:97:PHE:HZ	3:H:114:CYS:HB2	1.86	0.40
2:L:82:PRO:CB	2:L:84:ARG:CD	2.99	0.40
1:A:217:ILE:HG22	1:A:218:GLU:O	2.20	0.40
2:L:38:GLY:HA2	2:L:100:SER:OG	2.21	0.40
1:A:109:VAL:HG12	1:A:147:GLU:HA	2.02	0.40
1:A:99:ASP:HB2	1:A:100:LEU:H	1.62	0.40
3:H:43:THR:O	3:H:45:TYR:N	2.54	0.40
2:L:218:GLU:HB2	2:L:229:VAL:HG12	2.03	0.40
1:A:69:ASP:HB3	1:A:77:ILE:HB	2.04	0.40
1:A:96:LYS:HA	3:H:122:ARG:NH2	2.36	0.40
3:H:196:LEU:HD13	3:H:201:TYR:CZ	2.56	0.40
3:H:40:CYS:O	3:H:96:GLN:HB2	2.21	0.40
2:L:204:LEU:HD23	2:L:208:GLU:CG	2.52	0.40
3:H:42:VAL:CG2	3:H:47:LEU:HD21	2.51	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	219/239 (92%)	158 (72%)	41 (19%)	20 (9%)	1	5
2	L	213/215 (99%)	161 (76%)	30 (14%)	22 (10%)	1	4
3	H	221/223 (99%)	177 (80%)	31 (14%)	13 (6%)	2	12
All	All	653/677 (96%)	496 (76%)	102 (16%)	55 (8%)	1	6

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	99	ASP
1	A	100	LEU
1	A	169	ASN
1	A	245	ASN
1	A	251	ASP
1	A	254	ASP
2	L	50	SER
2	L	99	SER
2	L	124	GLY
2	L	136	PRO
2	L	137	THR
2	L	152	GLY
2	L	166	ASP
2	L	193	ASP
2	L	194	SER
3	H	34	GLN
3	H	107	GLU
3	H	154	SER
3	H	172	PHE
3	H	187	SER
1	A	89	ASP
1	A	102	ASP
1	A	103	LYS
1	A	173	PHE
1	A	204	PHE
1	A	252	SER
2	L	83	ALA
2	L	144	SER
2	L	176	SER
2	L	178	ARG
2	L	207	ASP
2	L	208	GLU
2	L	209	TYR

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Mol	Chain	Res	Type
2	L	232	PHE
3	H	33	SER
3	H	133	THR
3	H	198	SER
3	H	214	ARG
1	A	200	LYS
1	A	219	ASN
2	L	119	LEU
2	L	192	LYS
3	H	83	LYS
1	A	33	PRO
2	L	133	ASP
2	L	161	ASN
3	H	157	GLN
1	A	205	ASN
1	A	34	LYS
1	A	196	VAL
2	L	117	TYR
1	A	250	VAL
3	H	44	GLY
3	H	232	VAL

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	211/225 (94%)	166 (79%)	45 (21%)	1	6
2	L	188/188 (100%)	153 (81%)	35 (19%)	2	9
3	H	195/195 (100%)	158 (81%)	37 (19%)	2	8
All	All	594/608 (98%)	477 (80%)	117 (20%)	1	7

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	45	THR
1	A	58	ASN
1	A	65	VAL
1	A	68	ILE
1	A	74	PHE
1	A	75	ASP
1	A	85	LEU
1	A	88	TYR
1	A	94	GLU
1	A	96	LYS
1	A	99	ASP
1	A	100	LEU
1	A	105	LYS
1	A	106	ASP
1	A	119	GLN
1	A	123	SER
1	A	127	ASN
1	A	137	ARG
1	A	147	GLU
1	A	149	ASN
1	A	152	GLN
1	A	156	TYR
1	A	160	THR
1	A	163	VAL
1	A	169	ASN
1	A	174	ASP
1	A	175	VAL
1	A	176	GLN
1	A	178	ASN
1	A	196	VAL
1	A	198	ASN
1	A	204	PHE
1	A	206	ASN
1	A	217	ILE
1	A	219	ASN
1	A	233	ASP
1	A	234	LYS
1	A	238	SER
1	A	239	LYS
1	A	249	MET
1	A	250	VAL
1	A	255	VAL

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Mol	Chain	Res	Type
1	A	256	LYS
1	A	258	GLU
2	L	40	THR
2	L	43	MET
2	L	50	SER
2	L	52	SER
2	L	54	THR
2	L	66	SER
2	L	68	LYS
2	L	69	LEU
2	L	71	ILE
2	L	84	ARG
2	L	92	THR
2	L	100	SER
2	L	104	GLU
2	L	111	CYS
2	L	112	GLN
2	L	113	GLN
2	L	114	TYR
2	L	116	ASN
2	L	128	GLU
2	L	129	LEU
2	L	145	SER
2	L	154	SER
2	L	161	ASN
2	L	165	LYS
2	L	179	GLN
2	L	182	VAL
2	L	188	ASP
2	L	189	GLN
2	L	195	THR
2	L	198	MET
2	L	211	ARG
2	L	218	GLU
2	L	233	ASN
2	L	234	ARG
2	L	236	GLU
3	H	31	ARG
3	H	36	LEU
3	H	37	SER
3	H	39	THR
3	H	49	SER

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Mol	Chain	Res	Type
3	H	56	ILE
3	H	71	ASN
3	H	72	TYR
3	H	87	SER
3	H	88	ILE
3	H	89	THR
3	H	93	SER
3	H	94	LYS
3	H	99	LEU
3	H	103	SER
3	H	105	THR
3	H	116	ARG
3	H	122	ARG
3	H	131	GLN
3	H	157	GLN
3	H	160	SER
3	H	184	SER
3	H	185	LEU
3	H	186	SER
3	H	190	HIS
3	H	193	PRO
3	H	197	GLN
3	H	198	SER
3	H	203	LEU
3	H	212	SER
3	H	214	ARG
3	H	220	THR
3	H	221	CYS
3	H	222	ASN
3	H	231	LYS
3	H	236	ILE
3	H	239	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	152	GLN
1	A	198	ASN
1	A	219	ASN
1	A	237	GLN
1	A	245	ASN

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Mol	Chain	Res	Type
2	L	24	ASN
2	L	113	GLN
2	L	116	ASN
2	L	161	ASN
2	L	189	GLN
2	L	233	ASN
3	H	157	GLN
3	H	197	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	301	-	4,4,4	0.27	0	6,6,6	0.20	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	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	225/239 (94%)	-0.13	6 (2%)	58	34	18, 45, 69, 85	0
2	L	215/215 (100%)	-0.14	1 (0%)	91	83	13, 40, 80, 103	0
3	H	223/223 (100%)	-0.24	4 (1%)	71	50	13, 32, 96, 117	0
All	All	663/677 (97%)	-0.17	11 (1%)	73	52	13, 40, 84, 117	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	4.2
1	A	86	GLY	2.9
1	A	45	THR	2.7
1	A	36	ASP	2.5
2	L	237	CYS	2.5
1	A	230	ALA	2.4
3	H	239	ARG	2.4
3	H	216	SER	2.3
3	H	240	ASP	2.2
1	A	85	LEU	2.1
3	H	218	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	H	301	5/5	0.98	0.13	-1.63	30,31,38,44	0

6.5 Other polymers (i)

There are no such residues in this entry.