Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:13 AM EDT

PDB ID	:	5WUX
Title	:	TNFalpha-certolizumab Fab
Authors	:	Heo, Y.S.; Lee, J.U.
Deposited on	:	2016-12-21
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

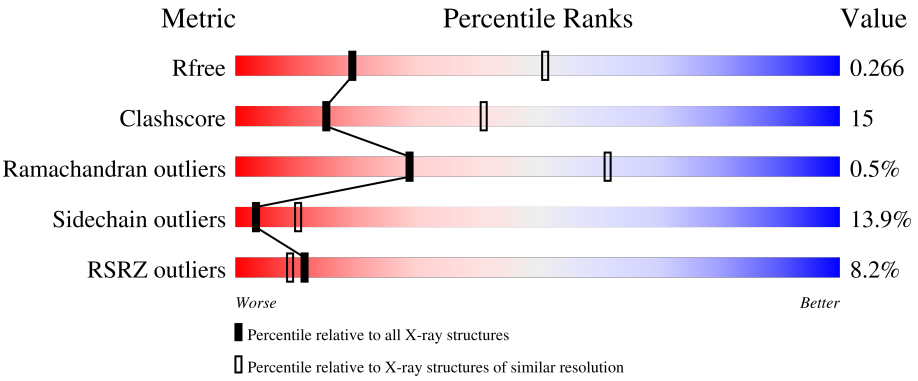
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	224	2% 63% 27% • 6%
1	C	224	10% 52% 36% • 10%
1	H	224	7% 58% 33% • 5%
2	B	214	8% 59% 32% 7% •
2	D	214	17% 54% 31% 8% • 6%

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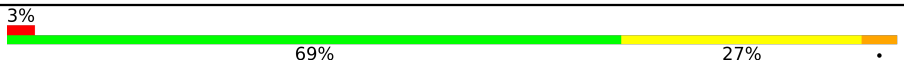
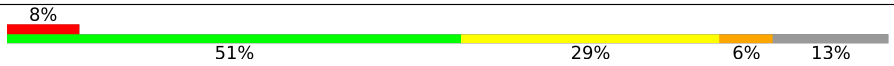
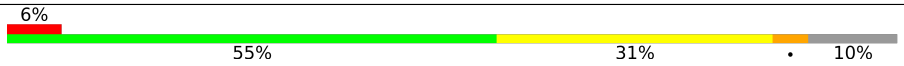
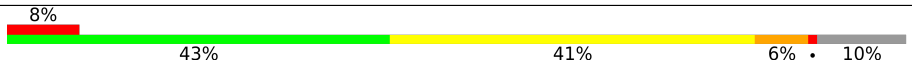
Mol	Chain	Length	Quality of chain
2	L	214	
3	E	157	
3	F	157	
3	G	157	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12793 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 heavy.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1586	1010	260	308	8			
1	C	202	Total	C	N	O	S	0	0	0
			1530	976	251	295	8			
1	H	212	Total	C	N	O	S	0	0	0
			1601	1019	263	311	8			

- Molecule 2 is a protein called light.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1632	1028	270	329	5			
2	D	201	Total	C	N	O	S	0	0	0
			1538	969	251	313	5			
2	L	213	Total	C	N	O	S	0	0	0
			1641	1033	271	332	5			

- Molecule 3 is a protein called Tumor necrosis factor alpha.

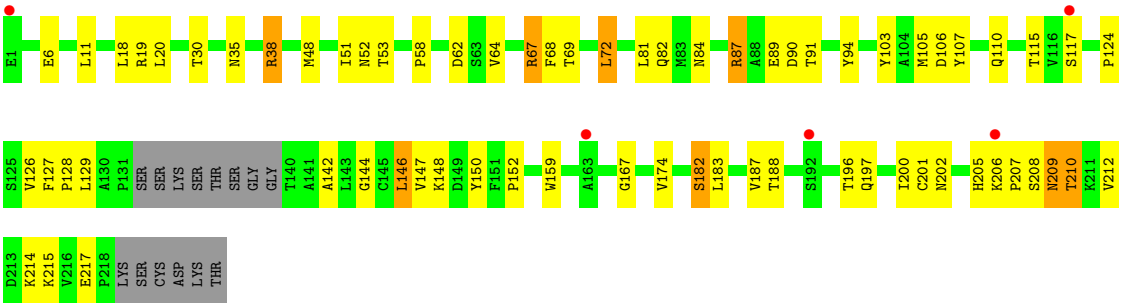
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	136	Total	C	N	O	S	0	0	0
			1057	681	177	197	2			
3	F	141	Total	C	N	O	S	0	0	0
			1104	708	190	204	2			
3	G	141	Total	C	N	O	S	0	0	0
			1104	708	190	204	2			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

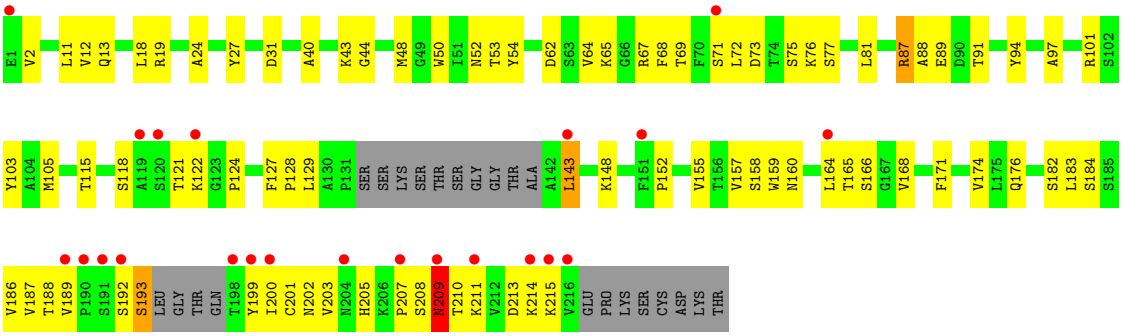
• Molecule 1: heavy

Chain A:



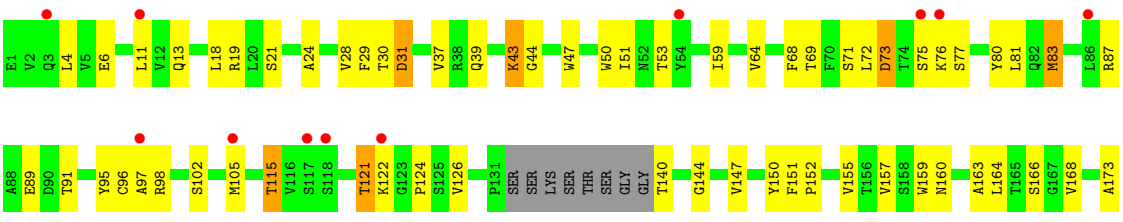
• Molecule 1: heavy

Chain C:



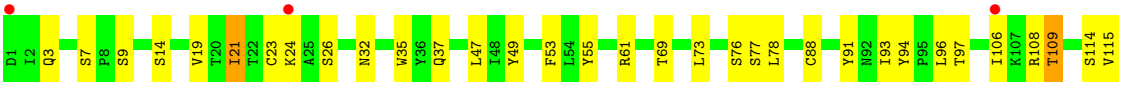
• Molecule 1: heavy

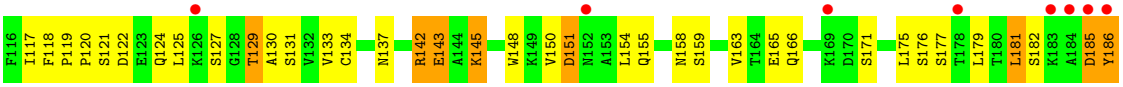
Chain H:

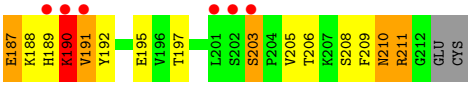


• Molecule 2: light

Chain B:

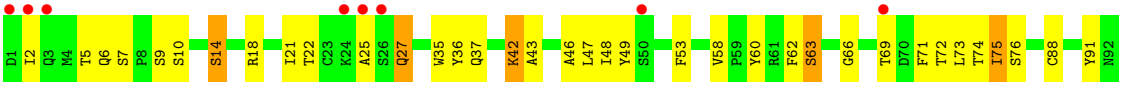


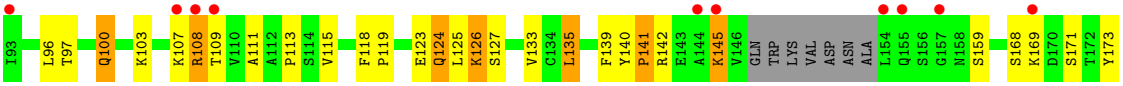


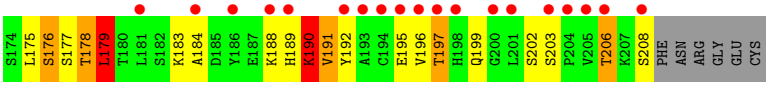


• Molecule 2: light

Chain D:

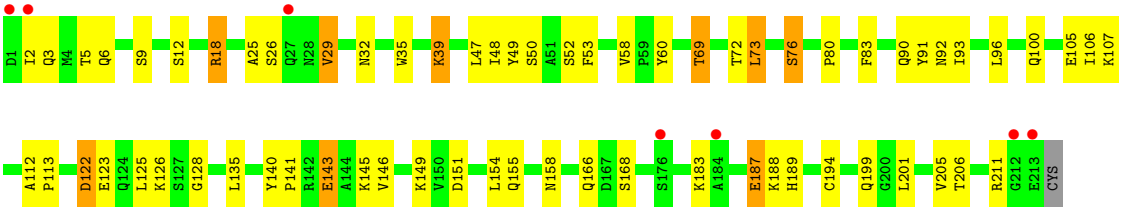






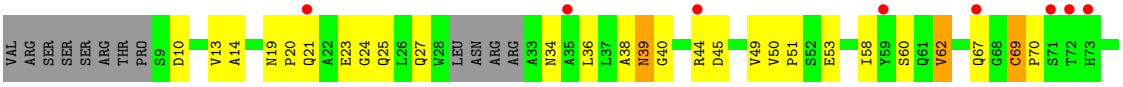
• Molecule 2: light

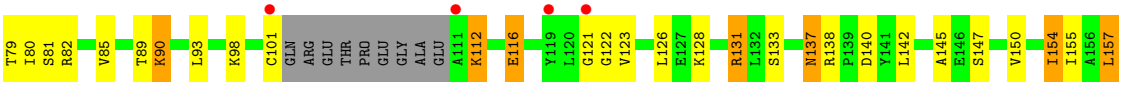
Chain L:



• Molecule 3: Tumor necrosis factor alpha

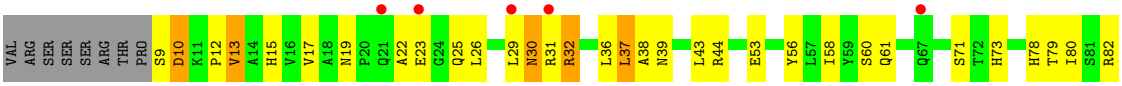
Chain E:

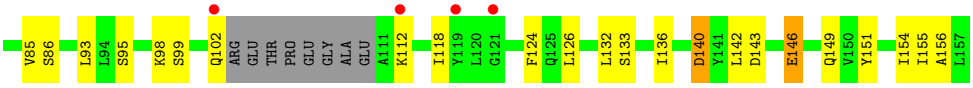




• Molecule 3: Tumor necrosis factor alpha

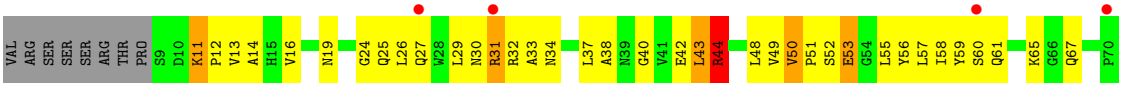
Chain F:

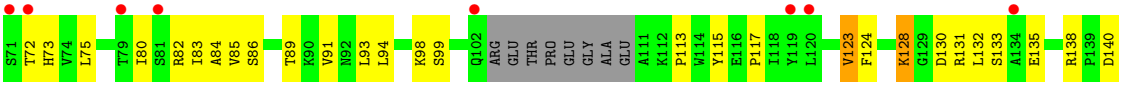


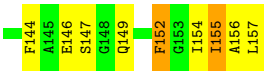


• Molecule 3: Tumor necrosis factor alpha

Chain G:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.59Å 207.22Å 112.63Å 90.00° 118.81° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 31.05 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.90) 95.2 (31.05-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.266 0.227 , 0.266	Depositor DCC
R_{free} test set	3217 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12793	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.37	0/1627	0.64	1/2219 (0.0%)
1	C	0.33	0/1569	0.63	0/2137
1	H	0.34	0/1642	0.57	0/2238
2	B	0.35	0/1669	0.60	0/2268
2	D	0.34	0/1571	0.66	1/2134 (0.0%)
2	L	0.34	0/1678	0.57	0/2280
3	E	0.38	0/1080	0.67	1/1468 (0.1%)
3	F	0.33	0/1128	0.61	0/1533
3	G	0.36	0/1128	0.63	0/1533
All	All	0.35	0/13092	0.62	3/17810 (0.0%)

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	3
1	C	0	2
2	D	0	1
3	E	0	1
3	G	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	179	LEU	CA-CB-CG	8.29	134.36	115.30
1	A	146	LEU	CA-CB-CG	8.04	133.78	115.30
3	E	157	LEU	CA-CB-CG	5.76	128.55	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ASN	Peptide
1	A	210	THR	Peptide
1	A	72	LEU	Peptide
1	C	209	ASN	Peptide
1	C	64	VAL	Peptide
2	D	141	PRO	Peptide
3	E	21	GLN	Peptide
3	G	43	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1586	0	1542	37	0
1	C	1530	0	1487	52	0
1	H	1601	0	1560	49	0
2	B	1632	0	1586	59	0
2	D	1538	0	1499	51	0
2	L	1641	0	1592	42	0
3	E	1057	0	1052	38	0
3	F	1104	0	1104	33	0
3	G	1104	0	1104	55	0
All	All	12793	0	12526	383	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 15.

All (383) 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:B:151:ASP:H	2:B:191:VAL:HG12	1.25	1.01
3:E:131:ARG:HH11	3:E:131:ARG:HB2	1.25	1.01
1:C:128:PRO:HD3	1:C:214:LYS:HZ3	1.24	0.99
1:C:128:PRO:HD3	1:C:214:LYS:NZ	1.86	0.89
2:D:125:LEU:O	2:D:183:LYS:NZ	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:LYS:HE3	2:D:43:ALA:H	1.41	0.84
3:G:50:VAL:HB	3:G:128:LYS:NZ	1.94	0.82
1:H:11:LEU:HD23	1:H:121:THR:HG22	1.59	0.81
2:B:186:TYR:O	2:B:192:TYR:OH	1.99	0.80
3:E:98:LYS:HE2	3:G:98:LYS:HZ3	1.47	0.79
2:L:106:ILE:O	2:L:166:GLN:NE2	2.16	0.79
1:C:121:THR:HG22	1:C:152:PRO:HD3	1.65	0.79
2:D:159:SER:HB2	2:D:179:LEU:HD13	1.65	0.79
1:A:148:LYS:HA	1:A:182:SER:HB2	1.65	0.78
3:E:137:ASN:HB3	3:E:138:ARG:HG2	1.64	0.78
1:A:48:MET:HG2	1:A:64:VAL:HG11	1.65	0.78
1:H:215:LYS:NZ	1:H:217:GLU:HG3	1.99	0.76
1:C:40:ALA:HB3	1:C:43:LYS:HB3	1.67	0.76
3:G:53:GLU:HA	3:G:128:LYS:HE3	1.65	0.76
2:B:129:THR:HA	2:B:182:SER:HA	1.69	0.75
2:B:189:HIS:O	2:B:211:ARG:NH2	2.19	0.75
2:B:3:GLN:HB2	2:B:26:SER:HB3	1.66	0.75
1:A:144:GLY:HA2	1:A:159:TRP:HH2	1.54	0.73
2:D:18:ARG:HG3	2:D:76:SER:HA	1.69	0.73
3:E:98:LYS:HD2	3:E:116:GLU:HG3	1.69	0.72
3:F:79:THR:HG23	3:F:95:SER:HB3	1.72	0.71
1:A:53:THR:HA	1:A:72:LEU:HD11	1.70	0.71
3:G:30:ASN:O	3:G:32:ARG:N	2.24	0.71
1:H:124:PRO:HB3	1:H:150:TYR:HB3	1.71	0.71
3:G:50:VAL:HB	3:G:128:LYS:HZ3	1.55	0.71
2:L:6:GLN:H	2:L:100:GLN:HE22	1.37	0.70
1:C:205:HIS:HB3	1:C:210:THR:HB	1.73	0.69
3:E:50:VAL:HG21	3:E:126:LEU:HD12	1.74	0.69
2:D:191:VAL:HG12	2:D:192:TYR:H	1.56	0.69
3:G:11:LYS:HG3	3:G:12:PRO:HD2	1.75	0.69
2:B:187:GLU:HA	2:B:211:ARG:HH12	1.58	0.69
3:F:13:VAL:HG23	3:F:155:ILE:HB	1.75	0.68
1:H:11:LEU:HB2	1:H:152:PRO:HG3	1.74	0.68
3:E:10:ASP:O	3:E:39:ASN:ND2	2.27	0.68
1:A:126:VAL:HG21	1:A:212:VAL:HG11	1.77	0.67
3:E:112:LYS:HD2	3:F:73:HIS:HB3	1.77	0.67
2:L:39:LYS:NZ	2:L:83:PHE:O	2.26	0.67
2:L:151:ASP:OD2	2:L:189:HIS:HB3	1.95	0.67
1:A:208:SER:OG	1:A:209:ASN:O	2.14	0.66
1:A:64:VAL:HB	1:A:68:PHE:HD2	1.60	0.66
2:B:114:SER:HB2	2:B:137:ASN:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG3	1:A:82:GLN:HG2	1.78	0.66
2:B:155:GLN:HB3	2:B:158:ASN:HD21	1.60	0.66
3:E:25:GLN:HG2	3:E:27:GLN:HB2	1.78	0.66
1:C:43:LYS:HG3	1:C:44:GLY:H	1.62	0.65
1:C:13:GLN:HE22	1:C:118:SER:HA	1.60	0.65
3:F:13:VAL:HG12	3:F:38:ALA:HB3	1.79	0.64
1:C:11:LEU:HB2	1:C:152:PRO:HG3	1.78	0.64
2:D:115:VAL:HG21	2:D:196:VAL:HG21	1.80	0.64
3:E:60:SER:HB3	3:E:80:ILE:HD11	1.78	0.64
3:F:38:ALA:HB1	3:F:39:ASN:HD22	1.63	0.63
2:L:52:SER:CB	3:E:137:ASN:HD21	2.10	0.63
2:B:145:LYS:HE2	2:B:145:LYS:HA	1.80	0.63
1:C:43:LYS:HG3	1:C:44:GLY:N	2.14	0.62
2:D:18:ARG:NH2	3:G:72:THR:OG1	2.18	0.62
1:H:173:ALA:HA	1:H:183:LEU:HB3	1.81	0.62
1:C:87:ARG:HD3	1:C:88:ALA:H	1.63	0.62
1:A:87:ARG:HB2	1:A:89:GLU:HG2	1.80	0.62
1:A:215:LYS:HG2	1:A:217:GLU:OE2	2.00	0.62
1:C:157:VAL:HG22	1:C:203:VAL:HG22	1.80	0.62
1:H:164:LEU:HD21	1:H:187:VAL:HG21	1.81	0.61
1:H:31:ASP:OD2	3:E:44:ARG:NH2	2.25	0.61
1:A:142:ALA:HB2	1:A:188:THR:HG22	1.82	0.61
3:G:94:LEU:HD21	3:G:124:PHE:HZ	1.66	0.61
2:D:184:ALA:O	2:D:188:LYS:HB2	2.01	0.60
1:H:140:THR:N	1:H:191:SER:HG	1.98	0.60
1:C:87:ARG:HD3	1:C:88:ALA:N	2.16	0.60
2:B:187:GLU:HA	2:B:211:ARG:NH1	2.16	0.60
2:B:49:TYR:O	2:B:53:PHE:HB2	2.02	0.60
1:A:20:LEU:HB2	1:A:81:LEU:HB3	1.83	0.60
1:H:31:ASP:OD1	3:E:131:ARG:NE	2.34	0.60
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.32	0.59
3:G:60:SER:HB3	3:G:80:ILE:HD11	1.85	0.59
1:C:97:ALA:HB1	1:C:105:MET:HB3	1.84	0.59
1:C:208:SER:O	1:C:210:THR:N	2.34	0.59
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.84	0.59
3:F:82:ARG:HB2	3:F:93:LEU:HD11	1.85	0.58
2:L:60:TYR:OH	3:E:24:GLY:HA2	2.03	0.58
1:H:215:LYS:HZ2	1:H:217:GLU:HG3	1.65	0.58
2:B:142:ARG:HD3	2:B:143:GLU:OE2	2.04	0.58
2:D:10:SER:HB2	2:D:103:LYS:HB3	1.85	0.58
3:E:131:ARG:HH11	3:E:131:ARG:CB	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:140:ASP:OD1	3:F:140:ASP:N	2.29	0.58
3:F:12:PRO:HA	3:F:39:ASN:HB2	1.84	0.58
3:F:12:PRO:HD2	3:F:156:ALA:HB3	1.84	0.58
1:A:124:PRO:HB3	1:A:147:VAL:CG1	2.34	0.58
2:B:187:GLU:C	2:B:211:ARG:HH22	2.08	0.58
1:H:6:GLU:OE2	1:H:95:TYR:HA	2.04	0.57
1:H:47:TRP:CG	2:L:96:LEU:HB2	2.39	0.57
2:D:140:TYR:CD1	2:D:141:PRO:HA	2.39	0.57
1:C:205:HIS:CE1	1:C:207:PRO:HB2	2.39	0.57
2:D:113:PRO:O	2:D:115:VAL:HG23	2.05	0.57
1:A:144:GLY:HA2	1:A:159:TRP:CH2	2.39	0.57
2:L:122:ASP:HA	2:L:125:LEU:HD12	1.87	0.57
2:D:49:TYR:O	2:D:53:PHE:HB2	2.05	0.56
1:H:215:LYS:HZ3	1:H:217:GLU:HG3	1.68	0.56
2:B:191:VAL:HA	2:B:210:ASN:HD21	1.71	0.56
2:B:186:TYR:CG	2:B:187:GLU:N	2.72	0.56
2:D:2:ILE:HG23	2:D:27:GLN:HG3	1.88	0.56
1:H:97:ALA:HB1	1:H:105:MET:HB3	1.87	0.56
1:C:186:VAL:HG11	2:D:135:LEU:HD22	1.87	0.56
2:B:148:TRP:HE1	2:B:177:SER:HG	1.54	0.56
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.88	0.56
3:G:67:GLN:HA	3:G:113:PRO:HA	1.88	0.56
2:B:120:PRO:HG2	2:B:125:LEU:HD11	1.86	0.55
1:H:102:SER:OG	2:L:91:TYR:O	2.24	0.55
1:A:106:ASP:OD2	1:A:107:TYR:N	2.38	0.55
1:C:13:GLN:NE2	1:C:118:SER:HA	2.22	0.55
2:L:143:GLU:CD	2:L:143:GLU:H	2.10	0.55
1:C:31:ASP:OD1	3:G:131:ARG:NH1	2.40	0.55
2:D:25:ALA:HB3	2:D:69:THR:HA	1.89	0.55
3:F:58:ILE:HD11	3:F:126:LEU:HD11	1.89	0.55
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.88	0.55
1:C:87:ARG:HD2	1:C:89:GLU:OE2	2.07	0.55
1:H:68:PHE:HB3	1:H:81:LEU:HD11	1.89	0.55
1:H:160:ASN:HB2	1:H:164:LEU:H	1.72	0.55
1:C:208:SER:O	1:C:210:THR:OG1	2.20	0.55
1:C:171:PHE:CE2	2:D:176:SER:HB3	2.42	0.54
1:H:53:THR:HA	1:H:72:LEU:HD11	1.89	0.54
1:H:168:VAL:HG22	1:H:187:VAL:HB	1.89	0.54
1:A:6:GLU:H	1:A:110:GLN:HE22	1.56	0.54
1:A:200:ILE:HG13	1:A:215:LYS:HA	1.90	0.53
1:H:201:CYS:O	1:H:213:ASP:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:HB3	2:B:121:SER:OG	2.08	0.53
3:G:50:VAL:HB	3:G:128:LYS:HZ1	1.74	0.53
2:B:185:ASP:O	2:B:188:LYS:HB2	2.09	0.53
1:C:24:ALA:HB3	1:C:77:SER:HB3	1.91	0.53
1:C:129:LEU:HB3	2:D:118:PHE:CD2	2.44	0.53
3:G:57:LEU:HB2	3:G:157:LEU:HD11	1.90	0.53
3:G:31:ARG:O	3:G:32:ARG:NH1	2.40	0.53
2:B:208:SER:OG	2:B:209:PHE:N	2.40	0.53
1:C:168:VAL:HG22	1:C:187:VAL:HB	1.91	0.53
3:F:31:ARG:O	3:F:32:ARG:HG2	2.09	0.52
3:G:52:SER:N	3:G:128:LYS:HD2	2.24	0.52
2:B:118:PHE:HB2	2:B:133:VAL:HB	1.92	0.52
1:H:6:GLU:OE2	1:H:96:CYS:N	2.43	0.52
2:L:189:HIS:O	2:L:211:ARG:NH1	2.43	0.52
3:E:98:LYS:CE	3:G:98:LYS:HZ3	2.20	0.52
3:G:61:GLN:NE2	3:G:149:GLN:O	2.42	0.52
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.90	0.52
2:D:190:LYS:CG	2:D:191:VAL:H	2.23	0.52
1:C:53:THR:HA	1:C:72:LEU:HD11	1.90	0.52
1:H:151:PHE:HB2	1:H:180:LEU:HD22	1.92	0.52
2:B:211:ARG:H	2:B:211:ARG:HD2	1.75	0.52
2:B:150:VAL:HG13	2:B:191:VAL:O	2.09	0.52
1:H:91:THR:HG23	1:H:115:THR:HA	1.92	0.52
2:L:3:GLN:HB3	2:L:26:SER:HB3	1.93	0.51
3:E:98:LYS:HE2	3:G:117:PRO:HD2	1.92	0.51
3:F:60:SER:HB3	3:F:80:ILE:HD11	1.92	0.51
2:B:159:SER:HB3	2:B:179:LEU:HD13	1.93	0.51
2:D:107:LYS:HB2	2:D:107:LYS:NZ	2.25	0.51
2:B:166:GLN:HE21	2:B:171:SER:HB3	1.75	0.51
1:A:110:GLN:OE1	1:A:110:GLN:N	2.44	0.51
1:A:52:ASN:ND2	3:F:86:SER:O	2.40	0.51
2:L:47:LEU:HA	2:L:58:VAL:HG21	1.92	0.50
3:G:57:LEU:O	3:G:154:ILE:HA	2.10	0.50
3:E:98:LYS:HD2	3:E:116:GLU:CG	2.39	0.50
2:B:187:GLU:CA	2:B:211:ARG:HH12	2.24	0.50
3:E:140:ASP:OD1	3:E:140:ASP:N	2.45	0.50
3:G:53:GLU:CA	3:G:128:LYS:HE3	2.38	0.50
2:D:108:ARG:HH21	2:D:111:ALA:HB2	1.76	0.50
1:H:4:LEU:HD11	1:H:98:ARG:HB2	1.94	0.49
1:A:91:THR:HG23	1:A:115:THR:HA	1.93	0.49
1:A:124:PRO:HB3	1:A:147:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:GLU:HA	2:B:206:THR:HA	1.93	0.49
2:D:188:LYS:HE3	2:D:189:HIS:CE1	2.47	0.49
1:C:103:TYR:HA	2:D:91:TYR:CD2	2.47	0.49
3:F:112:LYS:HD2	3:G:73:HIS:HB3	1.94	0.49
3:F:56:TYR:CE2	3:F:156:ALA:HB2	2.47	0.49
1:C:68:PHE:HD2	1:C:81:LEU:HD11	1.78	0.49
1:H:37:VAL:O	1:H:95:TYR:N	2.27	0.48
1:H:43:LYS:HD2	1:H:44:GLY:H	1.77	0.48
2:L:128:GLY:HA2	2:L:183:LYS:HB2	1.95	0.48
2:B:190:LYS:O	2:B:210:ASN:ND2	2.47	0.48
2:D:175:LEU:HD23	2:D:176:SER:N	2.29	0.48
2:D:66:GLY:HA3	2:D:71:PHE:HA	1.94	0.48
2:L:29:VAL:HG12	2:L:92:ASN:HB3	1.95	0.48
3:E:49:VAL:HG22	3:E:131:ARG:HG2	1.95	0.48
3:F:25:GLN:HG2	3:F:26:LEU:N	2.29	0.48
2:L:91:TYR:HA	2:L:96:LEU:HD22	1.95	0.48
2:L:50:SER:HB3	2:L:53:PHE:CD1	2.49	0.48
2:L:80:PRO:HB2	2:L:168:SER:O	2.14	0.48
3:E:58:ILE:O	3:E:121:GLY:HA2	2.14	0.48
3:E:123:VAL:HG21	3:G:155:ILE:HG21	1.95	0.47
1:H:50:TRP:HE3	1:H:59:ILE:HD13	1.79	0.47
1:C:91:THR:HG23	1:C:115:THR:HA	1.95	0.47
1:H:68:PHE:HD1	1:H:83:MET:HB3	1.79	0.47
3:F:37:LEU:HD21	3:F:43:LEU:HB2	1.95	0.47
1:C:54:TYR:CD2	3:G:86:SER:HA	2.49	0.47
1:C:124:PRO:HD2	1:C:210:THR:HG21	1.97	0.47
3:G:11:LYS:HG2	3:G:156:ALA:O	2.14	0.47
3:G:80:ILE:HA	3:G:133:SER:O	2.14	0.47
1:C:73:ASP:OD1	1:C:75:SER:OG	2.29	0.47
3:G:14:ALA:HB3	3:G:154:ILE:HG13	1.97	0.47
2:B:191:VAL:HA	2:B:210:ASN:ND2	2.29	0.47
1:H:73:ASP:HB3	1:H:80:TYR:HE2	1.80	0.47
1:H:140:THR:N	1:H:191:SER:OG	2.47	0.47
1:A:103:TYR:HA	2:B:91:TYR:CD1	2.50	0.46
2:L:48:ILE:HD12	2:L:73:LEU:HD12	1.97	0.46
1:A:35:ASN:HD22	1:A:105:MET:HG3	1.80	0.46
2:B:23:CYS:HB2	2:B:35:TRP:CH2	2.50	0.46
2:D:133:VAL:HG22	2:D:178:THR:HG22	1.98	0.46
2:D:169:LYS:HD3	2:D:169:LYS:HA	1.69	0.46
1:H:164:LEU:HD22	1:H:199:TYR:HD1	1.80	0.46
2:B:130:ALA:N	2:B:181:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:55:LEU:HD23	3:G:55:LEU:HA	1.67	0.46
2:B:188:LYS:HG2	2:B:189:HIS:ND1	2.30	0.46
1:H:64:VAL:HB	1:H:68:PHE:HD2	1.79	0.46
2:L:18:ARG:HG3	2:L:76:SER:O	2.15	0.46
3:E:51:PRO:O	3:E:128:LYS:HG3	2.15	0.46
3:G:128:LYS:HA	3:G:128:LYS:HD3	1.61	0.46
1:C:19:ARG:O	1:C:19:ARG:HG3	2.16	0.46
1:H:28:VAL:HG12	1:H:31:ASP:H	1.80	0.46
3:F:17:VAL:O	3:F:29:LEU:N	2.48	0.46
3:G:75:LEU:HD23	3:G:99:SER:HB3	1.98	0.46
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.51	0.46
2:B:151:ASP:OD1	2:B:190:LYS:N	2.49	0.46
1:C:101:ARG:HB3	3:G:89:THR:HG22	1.98	0.46
2:D:14:SER:HA	2:D:107:LYS:O	2.16	0.46
2:L:183:LYS:HG2	2:L:187:GLU:OE1	2.16	0.46
3:E:62:VAL:HG12	3:E:150:VAL:HG13	1.97	0.46
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.51	0.46
2:D:140:TYR:CG	2:D:141:PRO:HA	2.50	0.46
2:L:155:GLN:HB3	2:L:158:ASN:HD21	1.80	0.46
3:E:40:GLY:C	3:E:51:PRO:HB3	2.36	0.46
2:B:32:ASN:HB3	2:B:91:TYR:CD1	2.51	0.46
2:B:192:TYR:HD2	2:B:209:PHE:CZ	2.34	0.45
1:C:143:LEU:HD11	1:C:159:TRP:CZ3	2.51	0.45
2:D:108:ARG:HD3	2:D:171:SER:HB2	1.98	0.45
3:F:15:HIS:H	3:F:36:LEU:HB2	1.82	0.45
2:B:91:TYR:HA	2:B:96:LEU:HD22	1.99	0.45
3:G:65:LYS:HD2	3:G:115:TYR:CE1	2.51	0.45
2:B:211:ARG:H	2:B:211:ARG:CD	2.29	0.45
2:D:35:TRP:CH2	2:D:88:CYS:HB3	2.51	0.45
1:H:175:LEU:HD12	1:H:180:LEU:O	2.16	0.45
3:G:33:ALA:O	3:G:34:ASN:HB2	2.16	0.45
3:G:84:ALA:HA	3:G:130:ASP:OD1	2.15	0.45
1:A:11:LEU:HB2	1:A:152:PRO:HG3	1.98	0.45
1:A:30:THR:HA	1:A:53:THR:OG1	2.17	0.45
1:A:196:THR:OG1	1:A:197:GLN:N	2.49	0.45
2:B:151:ASP:HB3	2:B:190:LYS:HB3	1.98	0.45
1:H:186:VAL:HG11	2:L:135:LEU:HD22	1.97	0.45
1:A:206:LYS:HB3	1:A:207:PRO:HD3	1.99	0.45
2:D:197:THR:O	2:D:197:THR:OG1	2.34	0.45
3:G:82:ARG:HB2	3:G:93:LEU:HD11	1.99	0.45
3:G:83:ILE:HA	3:G:89:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:SER:OG	3:F:10:ASP:N	2.49	0.45
2:L:2:ILE:HD12	2:L:90:GLN:CD	2.37	0.45
2:L:194:CYS:O	2:L:206:THR:HA	2.16	0.45
3:G:83:ILE:HB	3:G:131:ARG:HB2	1.98	0.45
2:D:188:LYS:HB3	2:D:188:LYS:HE2	1.58	0.45
3:G:44:ARG:CZ	3:G:44:ARG:HB3	2.47	0.44
1:A:128:PRO:HD3	1:A:214:LYS:HE2	1.99	0.44
2:D:123:GLU:O	2:D:126:LYS:HB3	2.18	0.44
1:H:144:GLY:HA2	1:H:159:TRP:CH2	2.52	0.44
1:C:158:SER:O	1:C:202:ASN:N	2.31	0.44
3:F:19:ASN:ND2	3:F:22:ALA:HB2	2.32	0.44
1:C:192:SER:O	1:C:193:SER:OG	2.30	0.44
1:H:124:PRO:HD3	1:H:205:HIS:ND1	2.32	0.44
2:B:106:ILE:H	2:B:166:GLN:HE22	1.66	0.44
1:A:142:ALA:HA	1:A:188:THR:HA	2.00	0.44
2:B:21:ILE:HD11	2:B:35:TRP:HZ3	1.82	0.44
1:H:73:ASP:OD1	1:H:75:SER:HB2	2.17	0.44
2:B:188:LYS:HE2	2:B:189:HIS:CE1	2.52	0.44
1:H:126:VAL:HG22	1:H:147:VAL:HG22	1.99	0.44
3:G:16:VAL:HG23	3:G:152:PHE:HB3	2.00	0.44
1:C:160:ASN:HD21	1:C:199:TYR:HD1	1.65	0.44
1:A:51:ILE:HA	1:A:58:PRO:HA	2.00	0.44
1:C:62:ASP:O	1:C:65:LYS:HB3	2.18	0.44
1:H:155:VAL:HG23	1:H:205:HIS:HB2	1.99	0.44
2:L:145:LYS:HD2	2:L:146:VAL:H	1.82	0.44
3:E:82:ARG:HB2	3:E:93:LEU:HD11	1.99	0.44
2:B:35:TRP:CH2	2:B:88:CYS:HB3	2.53	0.43
1:C:205:HIS:O	1:C:210:THR:N	2.50	0.43
2:L:149:LYS:HG3	2:L:154:LEU:HD12	1.99	0.43
2:B:49:TYR:HB3	2:B:55:TYR:CE2	2.54	0.43
1:C:157:VAL:HA	1:C:202:ASN:O	2.18	0.43
2:L:52:SER:HB2	3:E:137:ASN:HD21	1.80	0.43
1:A:124:PRO:HA	1:A:150:TYR:HB3	1.99	0.43
1:C:202:ASN:ND2	1:C:213:ASP:OD1	2.31	0.43
2:D:6:GLN:H	2:D:100:GLN:NE2	2.16	0.43
2:D:91:TYR:HA	2:D:96:LEU:HD22	2.00	0.43
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.53	0.43
3:G:19:ASN:ND2	3:G:27:GLN:OE1	2.46	0.43
2:B:35:TRP:CD2	2:B:73:LEU:HB2	2.54	0.43
2:L:2:ILE:HD11	2:L:93:ILE:CG2	2.49	0.43
2:L:49:TYR:O	2:L:53:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:VAL:HG23	3:G:155:ILE:HB	1.99	0.43
2:B:19:VAL:HG21	2:B:78:LEU:HD22	2.01	0.43
2:B:108:ARG:NE	2:B:109:THR:O	2.49	0.43
1:C:214:LYS:NZ	2:D:123:GLU:OE1	2.49	0.43
3:E:13:VAL:H	3:E:38:ALA:HB3	1.82	0.43
3:F:37:LEU:HD12	3:F:37:LEU:HA	1.87	0.43
1:C:158:SER:OG	1:C:202:ASN:HB2	2.18	0.43
2:B:117:ILE:HD13	2:B:208:SER:HA	2.01	0.43
1:C:50:TRP:CZ3	1:C:101:ARG:HG3	2.53	0.43
1:C:164:LEU:HD12	1:C:165:THR:N	2.34	0.43
3:F:61:GLN:HB3	3:F:151:TYR:CZ	2.54	0.43
1:A:124:PRO:HD3	1:A:205:HIS:ND1	2.34	0.43
1:C:76:LYS:HA	1:C:76:LYS:HD3	1.88	0.43
2:L:123:GLU:HA	2:L:126:LYS:HE2	2.00	0.43
3:F:53:GLU:HA	3:F:126:LEU:O	2.18	0.43
2:L:145:LYS:HD3	2:L:145:LYS:HA	1.81	0.42
3:F:80:ILE:HA	3:F:133:SER:O	2.19	0.42
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.85	0.42
1:H:210:THR:HG22	1:H:212:VAL:HG23	2.01	0.42
1:H:160:ASN:HB3	1:H:163:ALA:HB3	2.01	0.42
3:E:138:ARG:HE	3:E:138:ARG:HB3	1.59	0.42
2:B:151:ASP:N	2:B:191:VAL:HG12	2.10	0.42
2:D:145:LYS:HG2	2:D:197:THR:HG23	2.02	0.42
2:L:125:LEU:O	2:L:183:LYS:HD2	2.19	0.42
3:G:43:LEU:O	3:G:44:ARG:HB2	2.20	0.42
2:B:203:SER:O	2:B:205:VAL:HG23	2.19	0.42
1:C:164:LEU:HD21	1:C:187:VAL:HG21	2.01	0.42
2:D:107:LYS:HA	2:D:140:TYR:OH	2.19	0.42
3:E:23:GLU:HG2	3:E:24:GLY:H	1.84	0.42
3:E:69:CYS:HA	3:E:70:PRO:HD3	1.88	0.42
1:C:2:VAL:HG22	1:C:27:TYR:HB3	2.01	0.42
2:D:22:THR:HG22	2:D:72:THR:HG22	2.02	0.42
2:B:61:ARG:HD2	2:B:77:SER:O	2.20	0.42
2:B:93:ILE:HG12	2:B:94:TYR:N	2.33	0.42
2:B:106:ILE:HB	2:B:166:GLN:NE2	2.35	0.42
2:B:186:TYR:CE2	2:B:187:GLU:HB3	2.55	0.42
3:E:142:LEU:HD23	3:E:142:LEU:HA	1.89	0.42
2:L:105:GLU:HG3	2:L:166:GLN:OE1	2.19	0.42
3:G:49:VAL:HG22	3:G:131:ARG:HG2	2.01	0.42
2:L:2:ILE:HD11	2:L:93:ILE:HG22	2.01	0.42
2:B:124:GLN:O	2:B:127:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ASN:OD1	1:C:54:TYR:N	2.51	0.42
2:D:36:TYR:HD1	2:D:46:ALA:HA	1.84	0.42
1:H:206:LYS:HB3	1:H:207:PRO:HD3	2.02	0.42
3:F:143:ASP:OD1	3:F:149:GLN:NE2	2.52	0.42
3:G:13:VAL:HG12	3:G:38:ALA:HB3	2.02	0.42
2:B:120:PRO:HB3	2:B:131:SER:O	2.20	0.41
1:C:148:LYS:HA	1:C:182:SER:HB2	2.01	0.41
1:H:68:PHE:CD1	1:H:83:MET:HB3	2.54	0.41
3:G:30:ASN:C	3:G:32:ARG:H	2.21	0.41
3:G:56:TYR:O	3:G:123:VAL:HA	2.20	0.41
3:G:58:ILE:HG22	3:G:80:ILE:HD13	2.02	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.54	0.41
3:F:132:LEU:CD1	3:F:154:ILE:HG21	2.50	0.41
3:G:48:LEU:HD23	3:G:48:LEU:HA	1.89	0.41
1:C:127:PHE:CE2	2:D:124:GLN:HB2	2.55	0.41
2:L:107:LYS:HE2	2:L:107:LYS:HB3	1.84	0.41
1:C:48:MET:HE1	1:C:94:TYR:HD2	1.85	0.41
2:D:195:GLU:HG3	2:D:206:THR:OG1	2.21	0.41
3:E:14:ALA:HB3	3:E:154:ILE:HG13	2.01	0.41
3:F:31:ARG:HD2	3:F:31:ARG:HA	1.96	0.41
2:D:113:PRO:HA	2:D:139:PHE:HB3	2.02	0.41
2:D:192:TYR:HB2	2:D:208:SER:HA	2.01	0.41
1:H:73:ASP:OD2	1:H:76:LYS:HB2	2.20	0.41
2:L:140:TYR:CG	2:L:141:PRO:HA	2.56	0.41
3:E:80:ILE:HA	3:E:133:SER:O	2.21	0.41
2:L:25:ALA:HB3	2:L:69:THR:HG22	2.03	0.41
2:L:32:ASN:HB3	2:L:91:TYR:CE1	2.56	0.41
2:L:112:ALA:HA	2:L:113:PRO:HD3	1.97	0.41
3:E:98:LYS:HZ3	3:F:98:LYS:HZ1	1.69	0.41
1:A:167:GLY:C	1:A:187:VAL:HG23	2.41	0.41
2:D:60:TYR:OH	3:G:24:GLY:HA2	2.21	0.41
1:H:39:GLN:HG3	1:H:44:GLY:O	2.21	0.41
3:E:13:VAL:HG23	3:E:155:ILE:HB	2.03	0.41
3:E:122:GLY:HA2	3:G:59:TYR:CE2	2.56	0.41
2:D:62:PHE:CE1	2:D:75:ILE:HG12	2.56	0.40
1:H:157:VAL:HG22	1:H:203:VAL:HG22	2.02	0.40
3:E:19:ASN:HA	3:E:20:PRO:HD3	1.88	0.40
3:F:30:ASN:HD22	3:F:30:ASN:H	1.70	0.40
3:G:37:LEU:HD21	3:G:43:LEU:H	1.86	0.40
3:G:51:PRO:C	3:G:128:LYS:HD2	2.41	0.40
3:G:58:ILE:HD13	3:G:132:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:SER:OG	3:E:90:LYS:HD3	2.21	0.40
1:H:24:ALA:HB3	1:H:29:PHE:HD1	1.87	0.40
3:F:146:GLU:HG3	3:F:149:GLN:OE1	2.20	0.40
3:F:151:TYR:CZ	3:G:94:LEU:HD22	2.56	0.40
1:A:148:LYS:HE3	2:B:131:SER:OG	2.21	0.40
2:D:63:SER:HB2	3:G:138:ARG:NH1	2.36	0.40
1:H:215:LYS:HG3	1:H:215:LYS:O	2.21	0.40
3:F:78:HIS:HB3	3:F:118:ILE:HG21	2.04	0.40
3:G:40:GLY:C	3:G:51:PRO:HB3	2.42	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	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	29	61
1	C	196/224 (88%)	189 (96%)	6 (3%)	1 (0%)	29	61
1	H	208/224 (93%)	198 (95%)	10 (5%)	0	100	100
2	B	210/214 (98%)	197 (94%)	12 (6%)	1 (0%)	29	61
2	D	197/214 (92%)	184 (93%)	11 (6%)	2 (1%)	15	45
2	L	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
3	E	130/157 (83%)	123 (95%)	6 (5%)	1 (1%)	19	51
3	F	137/157 (87%)	134 (98%)	3 (2%)	0	100	100
3	G	137/157 (87%)	128 (93%)	7 (5%)	2 (2%)	10	34
All	All	1632/1785 (91%)	1551 (95%)	73 (4%)	8 (0%)	29	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	209	ASN
2	D	191	VAL
3	G	31	ARG
1	A	210	THR
2	B	190	LYS
2	D	190	LYS
3	G	44	ARG
3	E	145	ALA

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	174/186 (94%)	159 (91%)	15 (9%)	10 30
1	C	168/186 (90%)	146 (87%)	22 (13%)	4 12
1	H	176/186 (95%)	152 (86%)	24 (14%)	3 11
2	B	185/187 (99%)	153 (83%)	32 (17%)	2 6
2	D	176/187 (94%)	142 (81%)	34 (19%)	1 4
2	L	186/187 (100%)	171 (92%)	15 (8%)	11 33
3	E	114/133 (86%)	94 (82%)	20 (18%)	2 6
3	F	119/133 (90%)	103 (87%)	16 (13%)	4 11
3	G	119/133 (90%)	100 (84%)	19 (16%)	2 7
All	All	1417/1518 (93%)	1220 (86%)	197 (14%)	3 10

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	38	ARG
1	A	62	ASP
1	A	67	ARG
1	A	69	THR
1	A	84	ASN
1	A	87	ARG

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Mol	Chain	Res	Type
1	A	117	SER
1	A	129	LEU
1	A	146	LEU
1	A	174	VAL
1	A	182	SER
1	A	183	LEU
1	A	201	CYS
1	A	202	ASN
2	B	7	SER
2	B	9	SER
2	B	14	SER
2	B	21	ILE
2	B	24	LYS
2	B	69	THR
2	B	76	SER
2	B	97	THR
2	B	109	THR
2	B	115	VAL
2	B	122	ASP
2	B	129	THR
2	B	134	CYS
2	B	142	ARG
2	B	143	GLU
2	B	145	LYS
2	B	151	ASP
2	B	154	LEU
2	B	163	VAL
2	B	165	GLU
2	B	175	LEU
2	B	176	SER
2	B	181	LEU
2	B	185	ASP
2	B	186	TYR
2	B	187	GLU
2	B	190	LYS
2	B	191	VAL
2	B	197	THR
2	B	203	SER
2	B	210	ASN
2	B	211	ARG
1	C	12	VAL
1	C	18	LEU

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Mol	Chain	Res	Type
1	C	67	ARG
1	C	69	THR
1	C	71	SER
1	C	87	ARG
1	C	122	LYS
1	C	143	LEU
1	C	155	VAL
1	C	166	SER
1	C	174	VAL
1	C	176	GLN
1	C	183	LEU
1	C	184	SER
1	C	188	THR
1	C	189	VAL
1	C	193	SER
1	C	200	ILE
1	C	201	CYS
1	C	209	ASN
1	C	211	LYS
1	C	215	LYS
2	D	5	THR
2	D	7	SER
2	D	9	SER
2	D	14	SER
2	D	21	ILE
2	D	27	GLN
2	D	42	LYS
2	D	48	ILE
2	D	63	SER
2	D	73	LEU
2	D	74	THR
2	D	75	ILE
2	D	97	THR
2	D	100	GLN
2	D	108	ARG
2	D	109	THR
2	D	124	GLN
2	D	126	LYS
2	D	127	SER
2	D	135	LEU
2	D	142	ARG
2	D	145	LYS

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Mol	Chain	Res	Type
2	D	168	SER
2	D	173	TYR
2	D	176	SER
2	D	177	SER
2	D	178	THR
2	D	179	LEU
2	D	190	LYS
2	D	197	THR
2	D	199	GLN
2	D	202	SER
2	D	203	SER
2	D	206	THR
1	H	13	GLN
1	H	18	LEU
1	H	19	ARG
1	H	21	SER
1	H	30	THR
1	H	31	ASP
1	H	43	LYS
1	H	51	ILE
1	H	69	THR
1	H	71	SER
1	H	73	ASP
1	H	77	SER
1	H	83	MET
1	H	87	ARG
1	H	89	GLU
1	H	115	THR
1	H	121	THR
1	H	122	LYS
1	H	166	SER
1	H	176	GLN
1	H	182	SER
1	H	188	THR
1	H	191	SER
1	H	215	LYS
2	L	5	THR
2	L	9	SER
2	L	12	SER
2	L	18	ARG
2	L	29	VAL
2	L	39	LYS

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Mol	Chain	Res	Type
2	L	69	THR
2	L	72	THR
2	L	73	LEU
2	L	76	SER
2	L	122	ASP
2	L	143	GLU
2	L	187	GLU
2	L	188	LYS
2	L	199	GLN
3	E	34	ASN
3	E	36	LEU
3	E	39	ASN
3	E	45	ASP
3	E	53	GLU
3	E	62	VAL
3	E	67	GLN
3	E	69	CYS
3	E	79	THR
3	E	85	VAL
3	E	89	THR
3	E	90	LYS
3	E	101	CYS
3	E	112	LYS
3	E	116	GLU
3	E	131	ARG
3	E	137	ASN
3	E	147	SER
3	E	154	ILE
3	E	157	LEU
3	F	10	ASP
3	F	13	VAL
3	F	23	GLU
3	F	30	ASN
3	F	32	ARG
3	F	37	LEU
3	F	44	ARG
3	F	71	SER
3	F	85	VAL
3	F	99	SER
3	F	102	GLN
3	F	124	PHE
3	F	136	ILE

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Mol	Chain	Res	Type
3	F	140	ASP
3	F	142	LEU
3	F	146	GLU
3	G	11	LYS
3	G	25	GLN
3	G	26	LEU
3	G	29	LEU
3	G	42	GLU
3	G	44	ARG
3	G	50	VAL
3	G	53	GLU
3	G	85	VAL
3	G	91	VAL
3	G	123	VAL
3	G	128	LYS
3	G	135	GLU
3	G	140	ASP
3	G	144	PHE
3	G	146	GLU
3	G	147	SER
3	G	152	PHE
3	G	155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	176	GLN
2	B	166	GLN
1	C	13	GLN
3	E	39	ASN
3	E	67	GLN
3	E	137	ASN
3	F	39	ASN
3	F	102	GLN
3	G	25	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	210/224 (93%)	0.34	5 (2%) 59 56	54, 78, 128, 140	0
1	C	202/224 (90%)	0.63	22 (10%) 5 4	60, 92, 131, 149	0
1	H	212/224 (94%)	0.50	15 (7%) 16 12	54, 92, 123, 137	0
2	B	212/214 (99%)	0.52	17 (8%) 12 9	47, 80, 133, 166	0
2	D	201/214 (93%)	0.86	37 (18%) 1 0	57, 96, 157, 174	0
2	L	213/214 (99%)	0.21	7 (3%) 46 41	48, 72, 99, 122	0
3	E	136/157 (86%)	0.51	12 (8%) 10 7	54, 82, 128, 159	0
3	F	141/157 (89%)	0.52	9 (6%) 19 15	48, 72, 116, 146	0
3	G	141/157 (89%)	0.62	12 (8%) 10 8	54, 81, 119, 166	0
All	All	1668/1785 (93%)	0.52	136 (8%) 11 9	47, 83, 133, 174	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	71	SER	6.9
2	D	154	LEU	5.8
3	E	71	SER	5.8
1	C	199	TYR	5.5
2	B	184	ALA	5.2
2	D	204	PRO	5.1
2	D	201	LEU	4.8
3	G	102	GLN	4.7
2	D	184	ALA	4.6
2	D	144	ALA	4.6
1	C	189	VAL	4.5
3	E	101	CYS	4.3
1	C	190	PRO	4.3
1	C	119	ALA	4.2
1	C	198	THR	4.2

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Mol	Chain	Res	Type	RSRZ
3	F	23	GLU	4.2
1	C	164	LEU	3.8
2	D	93	ILE	3.8
2	D	25	ALA	3.7
2	D	26	SER	3.7
3	E	119	TYR	3.6
1	A	206	LYS	3.5
1	C	143	LEU	3.5
2	D	1	ASP	3.5
1	C	211	LYS	3.5
1	C	200	ILE	3.5
3	G	31	ARG	3.5
2	D	24	LYS	3.4
2	D	189	HIS	3.4
2	D	195	GLU	3.3
1	C	192	SER	3.3
2	B	191	VAL	3.3
2	B	189	HIS	3.3
1	H	117	SER	3.2
2	D	155	GLN	3.2
2	D	188	LYS	3.2
1	C	216	VAL	3.2
2	B	201	LEU	3.1
1	C	214	LYS	3.1
2	D	186	TYR	3.1
3	F	102	GLN	3.1
2	B	203	SER	3.0
2	D	196	VAL	3.0
2	L	213	GLU	3.0
2	B	190	LYS	3.0
1	A	117	SER	3.0
2	D	198	HIS	3.0
2	D	192	TYR	3.0
2	D	203	SER	2.9
2	D	107	LYS	2.9
3	E	121	GLY	2.9
2	B	186	TYR	2.9
2	D	194	CYS	2.9
2	D	193	ALA	2.9
2	D	169	LYS	2.9
2	B	169	LYS	2.8
1	H	11	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	3	GLN	2.8
1	H	207	PRO	2.8
2	L	184	ALA	2.7
3	G	119	TYR	2.7
3	E	111	ALA	2.7
1	H	206	LYS	2.7
1	H	75	SER	2.7
1	H	3	GLN	2.7
3	F	29	LEU	2.7
1	C	120	SER	2.7
1	H	54	TYR	2.6
2	L	2	ILE	2.6
2	D	208	SER	2.6
2	D	157	GLY	2.6
1	C	209	ASN	2.6
3	F	31	ARG	2.6
2	B	202	SER	2.5
3	E	35	ALA	2.5
3	G	81	SER	2.5
1	A	1	GLU	2.5
1	H	118	SER	2.5
1	C	204	ASN	2.5
3	G	72	THR	2.5
2	D	145	LYS	2.4
2	D	200	GLY	2.4
1	C	151	PHE	2.4
2	L	212	GLY	2.4
1	C	215	LYS	2.4
2	D	206	THR	2.4
2	D	205	VAL	2.4
2	B	126	LYS	2.4
3	G	79	THR	2.4
2	D	197	THR	2.3
1	A	163	ALA	2.3
2	D	2	ILE	2.3
3	G	60	SER	2.3
1	H	220	SER	2.3
1	C	207	PRO	2.3
3	G	134	ALA	2.3
3	F	119	TYR	2.3
2	D	181	LEU	2.3
3	F	21	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1	GLU	2.3
2	L	176	SER	2.3
1	H	97	ALA	2.3
3	F	121	GLY	2.3
3	F	112	LYS	2.3
1	C	191	SER	2.2
2	B	183	LYS	2.2
3	E	73	HIS	2.2
3	F	67	GLN	2.2
3	G	120	LEU	2.2
1	C	122	LYS	2.2
3	E	21	GLN	2.2
2	B	106	ILE	2.2
1	H	105	MET	2.2
2	D	108	ARG	2.2
1	H	122	LYS	2.1
3	E	59	TYR	2.1
2	L	27	GLN	2.1
2	B	152	ASN	2.1
1	A	192	SER	2.1
1	C	71	SER	2.1
3	E	67	GLN	2.1
1	H	204	ASN	2.1
2	B	24	LYS	2.1
2	B	1	ASP	2.1
1	H	76	LYS	2.1
3	G	27	GLN	2.0
3	E	44	ARG	2.0
3	G	70	PRO	2.0
2	L	1	ASP	2.0
2	D	109	THR	2.0
3	E	72	THR	2.0
1	H	86	LEU	2.0
2	B	185	ASP	2.0
2	D	50	SER	2.0
2	B	178	THR	2.0
2	D	69	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.