WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID	:	1QSF
Title	:	STRUCTURE OF A6-TCR BOUND TO HLA-A2 COMPLEXED WITH AL-TERED HTLV-1 TAX PEPTIDE Y8A
Authors	:	Ding, Y.H.; Baker, B.M.; Garboczi, D.N.; Biddison, W.E.; Wiley, D.C.
Deposited on	:	1999-06-21
Resolution	:	2.80 Å(reported)

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

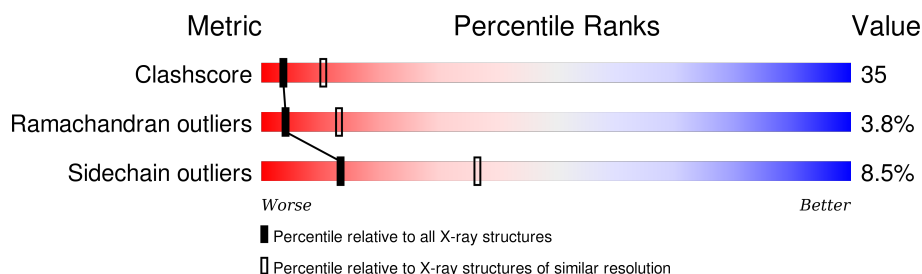|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		3.8%
Sidechain outliers		8.5%

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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	A	274	55% 40% 5%
2	B	100	61% 33% 5% •
3	C	9	33% 67%
4	D	200	44% 49% 7% •
5	E	243	40% 53% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6486 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 MHC CLASS I HLA-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	1	0	0
			2179	1364	391	415	9			

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	ALA	engineered	UNP P61769

- Molecule 3 is a protein called TAX PEPTIDE Y8A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			70	50	9	11			

- Molecule 4 is a protein called HUMAN T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1497	938	245	308	6			

- Molecule 5 is a protein called HUMAN T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1882	1184	328	362	8			

- Molecule 6 is water.

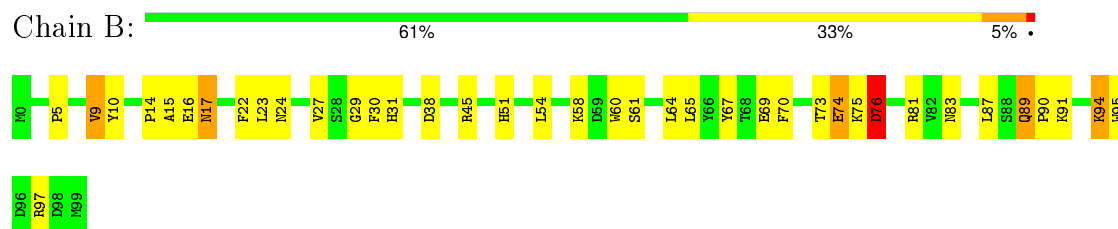| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total 10	O 10	0	0
6	B	6	Total 6	O 6	0	0
6	C	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	E	3	Total 3	O 3	0	0

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.

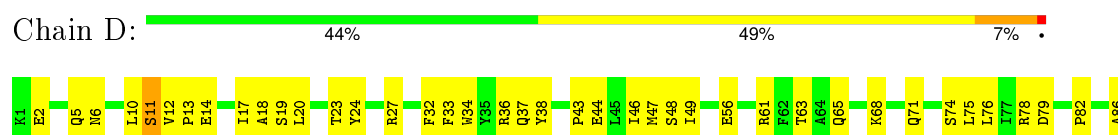Note EDS was not executed.

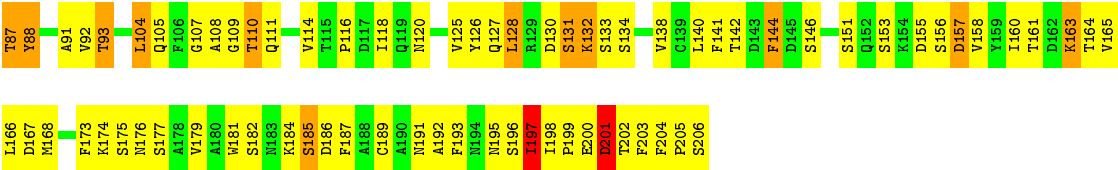- Molecule 1: MHC CLASS I HLA-A

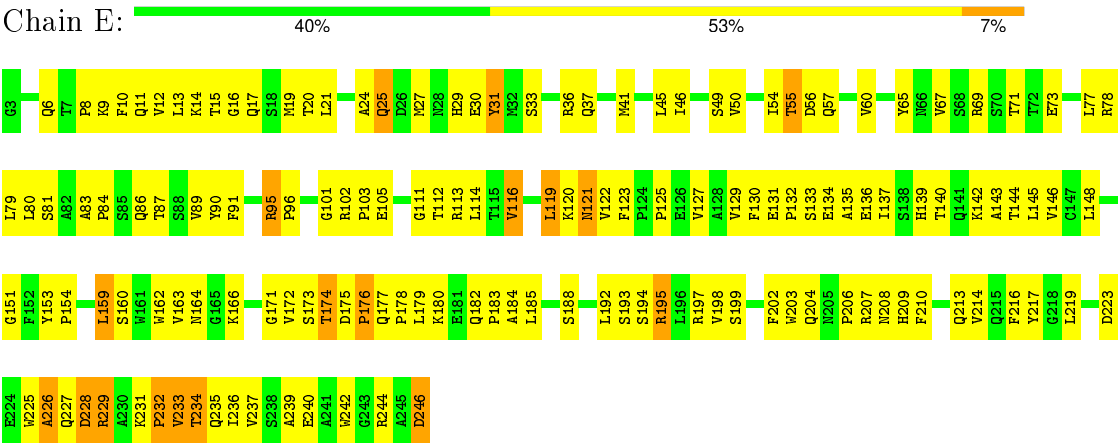- Molecule 2: BETA-2 MICROGLOBULIN

- Molecule 3: TAX PEPTIDE Y8A

- Molecule 4: HUMAN T-CELL RECEPTOR

T87 Y88 A91 V92 T93 L104 Q105 F106 G107 A108 G109 T110 Q111 V114 T115 P116 D117 I118 Q119 N120 V125 Y126 Q127 L128 R129 D130 S131 K132 S133 S134 V138 C139 L140 F141 T142 D143 F144 D145 S146 S151 Q152 S153 K154 D155 S156 D157 V158 Y159 I160 T161 D162 K163 T164 V165

L166 D167 M168 F173 K174 S175 N176 S177 A178 V179 A180 W181 S182 N183 K184 S185 D186 F187 A188 C189 A190 N191 A192 F193 N194 N195 S196 I197 I198 P199 E200 D201 T202 F203 F204 P205 S206

• Molecule 5: HUMAN T-CELL RECEPTOR

Chain E:

40%　　　　53%　　　　7%

G3 Q6 I7 P8 K9 F10 Q11 V12 L13 K14 T15 G16 Q17 S18 M19 T20 L21 A24 Q25 D26 M27 N28 H29 E30 Y31 M32 S33 R36 Q37 M41 L45 I46 S49 V50 I54 T55 D56 Q57 V60 Y65 N66 V67 S68 R69 S70 T71 T72 E73 L77 R78

L79 L80 S81 A82 A83 P84 S85 Q86 T87 S88 V89 Y90 F91 R95 P96 G101 R102 P103 E105 G111 T112 R113 L114 T115 V116 L119 K120 N121 V122 F123 P124 P125 E126 V127 A128 V129 F130 E131 P132 S133 E134 A135 E136 I137 S138 H139 T140 Q141 K142 A143 T144 L145 V146 C147 L148

G151 F152 Y153 P154 I159 S160 W161 V162 V163 N164 G165 K166 G171 V172 S173 T174 D175 P176 Q177 P178 L179 K180 E181 Q182 P183 A184 L185 S188 L192 S193 S194 R195 L196 R197 V198 S199 F202 W203 Q204 N205 P206 R207 N208 H209 F210 Q213 V214 Q215 F216 Y217 G218 L219 D223

E224 W225 A226 Q227 D228 R229 A230 K231 P232 V233 T234 Q235 I236 V237 S238 A239 E240 A241 W242 G243 R244 A245 D246

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.66Å 48.46Å 93.74Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.47	0/2241	0.74	0/3043
2	B	0.50	0/860	0.79	1/1162 (0.1%)
3	C	0.75	0/72	0.98	0/97
4	D	0.47	0/1530	0.81	0/2084
5	E	0.44	0/1935	0.75	0/2641
All	All	0.47	0/6638	0.77	1/9027 (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
4	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	76	ASP	N-CA-C	-5.92	95.03	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	88	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	A	2179	0	2015	119	0
2	B	837	0	803	32	0
3	C	70	0	75	9	0
4	D	1497	0	1363	150	0
5	E	1882	0	1763	171	0
6	A	10	0	0	0	0
6	B	6	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	1	0
All	All	6486	0	6019	440	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 35.

All (440) 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:228:THR:HG22	1:A:229:GLU:H	1.21	1.04
4:D:168:MET:CE	5:E:197:ARG:HG2	1.92	0.98
2:B:17:ASN:OD1	2:B:73:THR:HA	1.66	0.96
5:E:6:GLN:HE21	5:E:112:THR:HG23	1.35	0.91
4:D:197:ILE:HD13	4:D:197:ILE:H	1.34	0.90
4:D:153:SER:HB3	4:D:160:ILE:HG23	1.52	0.89
1:A:228:THR:HG22	1:A:229:GLU:N	1.89	0.88
4:D:168:MET:HE1	5:E:197:ARG:HG2	1.54	0.87
4:D:182:SER:HB3	4:D:187:PHE:CZ	2.11	0.86
1:A:197:HIS:O	1:A:250:PRO:HA	1.75	0.86
5:E:159:LEU:HD12	5:E:160:SER:N	1.91	0.85
1:A:252:GLY:O	1:A:254:GLU:N	2.09	0.85
5:E:233:VAL:O	5:E:235:GLN:HG3	1.77	0.85
5:E:122:VAL:HG21	5:E:219:LEU:HD21	1.60	0.84
4:D:168:MET:HE2	5:E:197:ARG:CG	2.08	0.84
4:D:193:PHE:HB2	4:D:198:ILE:HD11	1.61	0.82
4:D:138:VAL:HG12	4:D:181:TRP:HB3	1.64	0.79
4:D:125:VAL:HG11	4:D:189:CYS:HB3	1.64	0.79
5:E:231:LYS:HB2	5:E:233:VAL:HG23	1.65	0.78
5:E:178:PRO:HG3	5:E:192:LEU:HD13	1.66	0.78
5:E:12:VAL:HG22	5:E:154:PRO:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:ALA:HB1	4:D:104:LEU:HD12	1.65	0.77
4:D:198:ILE:CG2	4:D:202:THR:HG21	2.16	0.76
2:B:54:LEU:HD12	2:B:64:LEU:HD13	1.68	0.75
5:E:198:VAL:HG11	5:E:202:PHE:HD2	1.51	0.75
4:D:168:MET:HE2	5:E:197:ARG:HG2	1.66	0.75
5:E:65:TYR:CE1	5:E:79:LEU:HD21	2.22	0.75
5:E:12:VAL:O	5:E:13:LEU:HD23	1.87	0.74
1:A:194:VAL:HG22	1:A:198:GLU:O	1.88	0.74
4:D:93:THR:HG21	4:D:104:LEU:HD22	1.70	0.74
4:D:193:PHE:CB	4:D:198:ILE:HD11	2.19	0.73
1:A:32:GLN:HE21	1:A:48:ARG:HG3	1.54	0.73
2:B:17:ASN:HD21	2:B:74:GLU:H	1.37	0.73
1:A:127:LYS:HE2	1:A:134:THR:OG1	1.89	0.72
4:D:168:MET:CE	5:E:197:ARG:CG	2.63	0.72
5:E:136:GLU:HG3	5:E:142:LYS:O	1.88	0.72
4:D:157:ASP:O	4:D:182:SER:OG	2.07	0.72
2:B:17:ASN:HD21	2:B:74:GLU:N	1.87	0.71
4:D:17:ILE:CG2	4:D:76:LEU:HD12	2.20	0.71
4:D:153:SER:HB3	4:D:160:ILE:CG2	2.20	0.71
1:A:189:MET:CE	1:A:201:LEU:HB3	2.20	0.71
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.71	0.71
1:A:228:THR:CG2	1:A:229:GLU:H	1.98	0.71
4:D:27:ARG:HG3	4:D:71:GLN:OE1	1.90	0.70
4:D:198:ILE:HG21	4:D:202:THR:HG21	1.73	0.70
4:D:32:PHE:HD1	4:D:92:VAL:HG22	1.57	0.70
5:E:119:LEU:HD11	5:E:219:LEU:CD2	2.22	0.70
1:A:250:PRO:O	1:A:252:GLY:N	2.25	0.69
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.74	0.69
5:E:122:VAL:HG12	5:E:232:PRO:HB2	1.73	0.69
4:D:65:GLN:HB2	4:D:74:SER:HB2	1.74	0.69
4:D:140:LEU:HG	4:D:142:THR:HG23	1.74	0.68
2:B:73:THR:OG1	2:B:76:ASP:HB2	1.93	0.68
4:D:127:GLN:C	4:D:128:LEU:HD23	2.14	0.68
1:A:11:SER:HA	1:A:21:ARG:O	1.93	0.68
1:A:189:MET:HE2	1:A:201:LEU:HB3	1.76	0.68
4:D:128:LEU:HB3	5:E:131:GLU:O	1.95	0.67
4:D:118:ILE:HD11	4:D:176:ASN:ND2	2.10	0.67
4:D:166:LEU:HA	5:E:173:SER:OG	1.95	0.67
4:D:56:GLU:HG3	4:D:63:THR:OG1	1.95	0.66
5:E:132:PRO:HG3	5:E:143:ALA:HB1	1.78	0.66
4:D:166:LEU:HD21	5:E:197:ARG:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:THR:HG22	4:D:177:SER:HB3	1.77	0.66
4:D:166:LEU:HD12	4:D:167:ASP:N	2.11	0.65
4:D:116:PRO:O	4:D:146:SER:HB3	1.96	0.65
4:D:10:LEU:HG	4:D:11:SER:H	1.61	0.65
4:D:156:SER:C	4:D:158:VAL:H	1.98	0.65
1:A:197:HIS:O	1:A:251:SER:N	2.29	0.65
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.12	0.65
5:E:163:VAL:HG12	5:E:210:PHE:HD1	1.61	0.65
1:A:198:GLU:HA	1:A:250:PRO:HA	1.79	0.65
4:D:168:MET:HE2	5:E:197:ARG:HB3	1.78	0.65
5:E:8:PRO:O	5:E:112:THR:HG22	1.95	0.65
4:D:141:PHE:HB2	4:D:193:PHE:CE1	2.32	0.65
4:D:203:PHE:CD2	4:D:205:PRO:HD3	2.32	0.65
5:E:122:VAL:O	5:E:232:PRO:HB3	1.97	0.64
4:D:61:ARG:HG3	4:D:78:ARG:HH21	1.63	0.64
5:E:119:LEU:HD11	5:E:219:LEU:HD21	1.77	0.64
4:D:82:PRO:HG2	4:D:174:LYS:NZ	2.12	0.64
5:E:130:PHE:HB2	5:E:146:VAL:HG23	1.79	0.64
1:A:133:TRP:O	1:A:144:LYS:HE2	1.98	0.64
1:A:197:HIS:CD2	1:A:198:GLU:HB2	2.33	0.64
4:D:36:ARG:HB2	4:D:46:ILE:HD13	1.80	0.63
5:E:159:LEU:C	5:E:159:LEU:HD12	2.19	0.63
5:E:204:GLN:O	5:E:206:PRO:HD3	1.98	0.63
1:A:218:GLN:HB3	1:A:258:THR:OG1	1.99	0.62
4:D:44:GLU:O	4:D:46:ILE:HG23	1.99	0.62
1:A:217:TRP:CZ3	1:A:259:CYS:HB2	2.34	0.62
5:E:20:THR:HG22	5:E:78:ARG:HG2	1.82	0.62
1:A:223:ASP:C	1:A:225:THR:H	2.01	0.62
5:E:136:GLU:OE2	5:E:144:THR:N	2.32	0.62
1:A:137:ASP:O	1:A:141:GLN:HG2	2.00	0.61
5:E:244:ARG:C	5:E:246:ASP:H	2.03	0.61
5:E:227:GLN:O	5:E:228:ASP:C	2.38	0.61
5:E:145:LEU:N	5:E:145:LEU:HD12	2.16	0.61
1:A:143:THR:HG23	3:C:9:VAL:HA	1.83	0.61
4:D:168:MET:HE2	5:E:197:ARG:CB	2.29	0.61
5:E:174:THR:HB	5:E:194:SER:HB2	1.82	0.61
4:D:198:ILE:CG2	4:D:202:THR:CG2	2.78	0.61
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.84	0.61
4:D:151:SER:OG	4:D:195:ASN:HB2	2.01	0.61
1:A:217:TRP:CE3	1:A:217:TRP:HA	2.36	0.61
5:E:137:ILE:HD11	5:E:204:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:THR:HG22	6:E:248:HOH:O	2.00	0.60
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.16	0.60
4:D:130:ASP:OD1	4:D:131:SER:N	2.34	0.60
4:D:91:ALA:HB1	4:D:104:LEU:CD1	2.30	0.60
5:E:179:LEU:HG	5:E:180:LYS:N	2.17	0.60
5:E:244:ARG:C	5:E:246:ASP:N	2.53	0.60
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.83	0.60
5:E:123:PHE:HB3	5:E:151:GLY:O	2.02	0.59
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.82	0.59
4:D:158:VAL:HA	4:D:182:SER:HB2	1.83	0.59
5:E:20:THR:HG22	5:E:78:ARG:CG	2.32	0.59
5:E:129:VAL:HG23	5:E:239:ALA:CB	2.33	0.59
1:A:187:THR:HA	1:A:204:TRP:O	2.03	0.58
5:E:132:PRO:HD3	5:E:145:LEU:HG	1.85	0.58
4:D:19:SER:HB3	4:D:76:LEU:HD11	1.84	0.58
1:A:201:LEU:O	1:A:246:ALA:HA	2.02	0.58
4:D:199:PRO:O	4:D:202:THR:HG23	2.02	0.58
3:C:5:TYR:CE2	5:E:103:PRO:HB3	2.38	0.58
4:D:10:LEU:HG	4:D:11:SER:N	2.18	0.58
5:E:174:THR:HA	5:E:194:SER:HA	1.84	0.58
1:A:167:TRP:CE2	3:C:1:LEU:HD22	2.38	0.58
5:E:244:ARG:HB3	5:E:246:ASP:HB2	1.85	0.58
5:E:225:TRP:O	5:E:226:ALA:HB2	2.04	0.58
5:E:122:VAL:HG12	5:E:122:VAL:O	2.04	0.58
1:A:24:ALA:O	1:A:35:ARG:HA	2.04	0.58
4:D:32:PHE:CD1	4:D:92:VAL:HG22	2.39	0.57
4:D:182:SER:HB3	4:D:187:PHE:CE2	2.38	0.57
5:E:136:GLU:OE2	5:E:144:THR:HG23	2.05	0.57
1:A:165:VAL:O	1:A:169:ARG:HG3	2.04	0.57
4:D:163:LYS:HA	4:D:177:SER:O	2.05	0.57
5:E:121:ASN:O	5:E:153:TYR:CD1	2.57	0.57
5:E:203:TRP:HE3	5:E:210:PHE:CE2	2.23	0.57
4:D:167:ASP:OD1	4:D:168:MET:N	2.38	0.57
4:D:82:PRO:HG2	4:D:174:LYS:HZ3	1.69	0.57
1:A:111:ARG:HD3	1:A:113:TYR:OH	2.04	0.57
5:E:198:VAL:CG1	5:E:202:PHE:HB3	2.34	0.57
4:D:141:PHE:O	4:D:144:PHE:HZ	1.88	0.57
1:A:63:GLU:OE2	3:C:1:LEU:HD12	2.05	0.57
5:E:231:LYS:C	5:E:233:VAL:H	2.08	0.57
5:E:227:GLN:O	5:E:229:ARG:N	2.37	0.56
1:A:197:HIS:CD2	1:A:198:GLU:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ILE:HD12	4:D:144:PHE:O	2.05	0.56
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.36	0.56
4:D:61:ARG:HD3	4:D:79:ASP:CB	2.35	0.56
5:E:219:LEU:O	5:E:233:VAL:HA	2.05	0.56
4:D:131:SER:O	4:D:133:SER:N	2.38	0.56
5:E:182:GLN:C	5:E:184:ALA:H	2.08	0.56
5:E:134:GLU:HA	5:E:137:ILE:CG2	2.36	0.56
1:A:77:ASP:O	1:A:81:LEU:HG	2.06	0.56
5:E:143:ALA:N	5:E:198:VAL:O	2.31	0.56
4:D:141:PHE:O	4:D:144:PHE:CZ	2.59	0.55
5:E:19:MET:HG2	5:E:20:THR:N	2.21	0.55
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.87	0.55
5:E:209:HIS:NE2	5:E:240:GLU:HB2	2.22	0.55
4:D:158:VAL:HG22	4:D:187:PHE:CZ	2.41	0.55
5:E:11:GLN:HG2	5:E:19:MET:HE3	1.87	0.55
1:A:197:HIS:O	1:A:250:PRO:CA	2.52	0.55
4:D:182:SER:CB	4:D:187:PHE:CZ	2.87	0.54
5:E:25:GLN:HG2	5:E:27:MET:H	1.72	0.54
4:D:91:ALA:HA	4:D:105:GLN:O	2.07	0.54
5:E:134:GLU:HA	5:E:137:ILE:HG22	1.88	0.54
1:A:195:SER:OG	1:A:197:HIS:ND1	2.40	0.54
4:D:61:ARG:CG	4:D:78:ARG:HH21	2.21	0.54
5:E:79:LEU:HD22	5:E:86:GLN:OE1	2.07	0.54
1:A:27:TYR:CE2	1:A:32:GLN:HB2	2.43	0.54
2:B:9:VAL:CG2	2:B:95:TRP:HA	2.38	0.54
4:D:38:TYR:CD1	4:D:86:ALA:HB2	2.42	0.54
4:D:197:ILE:H	4:D:197:ILE:CD1	2.11	0.54
4:D:158:VAL:HG13	4:D:187:PHE:HE2	1.73	0.54
5:E:65:TYR:HB3	5:E:77:LEU:HD11	1.88	0.54
5:E:102:ARG:C	5:E:105:GLU:H	2.11	0.54
4:D:173:PHE:CZ	4:D:175:SER:HB3	2.43	0.54
5:E:21:LEU:HD12	5:E:77:LEU:HD23	1.89	0.54
4:D:93:THR:HG22	4:D:104:LEU:HD13	1.89	0.53
4:D:144:PHE:CD2	4:D:144:PHE:N	2.72	0.53
1:A:66:LYS:HE3	3:C:2:LEU:HB2	1.90	0.53
5:E:198:VAL:HG11	5:E:202:PHE:CD2	2.38	0.53
4:D:161:THR:OG1	4:D:179:VAL:N	2.32	0.53
5:E:176:PRO:HG2	5:E:177:GLN:H	1.74	0.53
5:E:37:GLN:NE2	5:E:91:PHE:HE2	2.07	0.53
5:E:13:LEU:HD12	5:E:114:LEU:HD11	1.91	0.53
4:D:132:LYS:C	4:D:134:SER:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:217:TYR:HA	5:E:234:THR:HG22	1.91	0.53
5:E:30:GLU:HB3	5:E:50:VAL:O	2.09	0.53
5:E:9:LYS:HD2	5:E:10:PHE:CE2	2.43	0.53
1:A:219:ALA:O	1:A:220:ASP:C	2.47	0.53
1:A:196:ASP:N	1:A:196:ASP:OD1	2.42	0.52
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.90	0.52
1:A:49:ALA:O	1:A:52:ILE:HG22	2.10	0.52
5:E:122:VAL:HG12	5:E:232:PRO:CB	2.38	0.52
4:D:130:ASP:HB2	5:E:129:VAL:O	2.10	0.52
4:D:142:THR:N	4:D:144:PHE:HE2	2.08	0.52
4:D:61:ARG:HD3	4:D:79:ASP:HB2	1.90	0.52
4:D:166:LEU:HD12	4:D:167:ASP:H	1.73	0.52
2:B:81:ARG:HH21	2:B:90:PRO:HB3	1.74	0.52
1:A:197:HIS:CD2	1:A:198:GLU:H	2.27	0.52
4:D:46:ILE:O	4:D:47:MET:HG2	2.09	0.52
5:E:159:LEU:HB2	5:E:214:VAL:HG22	1.92	0.52
5:E:120:LYS:O	5:E:122:VAL:N	2.40	0.52
4:D:11:SER:O	4:D:12:VAL:HG23	2.10	0.52
2:B:9:VAL:HG21	2:B:94:LYS:O	2.10	0.51
4:D:107:GLY:O	4:D:109:GLY:N	2.42	0.51
4:D:155:ASP:O	4:D:158:VAL:HB	2.11	0.51
5:E:182:GLN:O	5:E:184:ALA:N	2.44	0.51
5:E:209:HIS:HB2	5:E:242:TRP:CZ3	2.45	0.51
1:A:219:ALA:O	1:A:222:GLU:N	2.34	0.51
4:D:201:ASP:OD1	4:D:201:ASP:N	2.42	0.51
4:D:128:LEU:HD12	5:E:146:VAL:HG22	1.92	0.51
4:D:34:TRP:HB2	4:D:47:MET:HB2	1.92	0.51
4:D:20:LEU:HD12	4:D:75:LEU:HD23	1.92	0.51
5:E:30:GLU:HB2	5:E:96:PRO:O	2.10	0.51
1:A:21:ARG:CD	1:A:23:ILE:HD11	2.41	0.51
4:D:126:TYR:HD2	5:E:135:ALA:HB3	1.76	0.51
5:E:122:VAL:CG1	5:E:232:PRO:HB2	2.41	0.51
4:D:198:ILE:HG22	4:D:202:THR:CG2	2.40	0.51
1:A:133:TRP:HZ2	1:A:152:VAL:HB	1.74	0.51
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.45	0.51
5:E:119:LEU:HD11	5:E:219:LEU:HD22	1.90	0.51
4:D:17:ILE:HG22	4:D:76:LEU:HD12	1.94	0.50
5:E:198:VAL:HG12	5:E:199:SER:N	2.25	0.50
1:A:197:HIS:CG	1:A:198:GLU:N	2.79	0.50
5:E:185:LEU:HB3	5:E:188:SER:HB2	1.93	0.50
5:E:37:GLN:HE21	5:E:91:PHE:HE2	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:TYR:O	5:E:111:GLY:HA2	2.12	0.50
1:A:250:PRO:O	1:A:251:SER:C	2.50	0.50
5:E:89:VAL:HG22	5:E:113:ARG:HG3	1.92	0.50
1:A:217:TRP:HD1	1:A:228:THR:CG2	2.25	0.50
4:D:12:VAL:HG12	4:D:13:PRO:O	2.12	0.50
4:D:130:ASP:O	4:D:132:LYS:N	2.45	0.50
4:D:5:GLN:NE2	4:D:110:THR:N	2.59	0.50
1:A:107:TRP:HH2	1:A:180:GLN:NE2	2.09	0.50
1:A:217:TRP:CD1	1:A:228:THR:HG21	2.46	0.50
5:E:203:TRP:HE3	5:E:210:PHE:HE2	1.60	0.49
5:E:49:SER:OG	5:E:69:ARG:NH1	2.45	0.49
5:E:127:VAL:HG21	5:E:237:VAL:O	2.11	0.49
5:E:130:PHE:HB2	5:E:146:VAL:CG2	2.42	0.49
5:E:50:VAL:HG22	5:E:54:ILE:HG21	1.93	0.49
5:E:114:LEU:HD21	5:E:116:VAL:HG22	1.94	0.49
1:A:217:TRP:HD1	1:A:228:THR:HG21	1.76	0.49
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.47	0.49
2:B:54:LEU:HA	2:B:64:LEU:CD1	2.42	0.49
4:D:18:ALA:O	4:D:76:LEU:HA	2.13	0.49
1:A:228:THR:HG23	1:A:246:ALA:O	2.12	0.49
1:A:216:THR:O	1:A:259:CYS:HA	2.13	0.49
5:E:227:GLN:O	5:E:229:ARG:HB3	2.12	0.49
5:E:87:THR:OG1	5:E:116:VAL:HG23	2.12	0.49
4:D:19:SER:HA	4:D:76:LEU:HD13	1.95	0.49
4:D:12:VAL:O	4:D:114:VAL:HA	2.12	0.49
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.47	0.49
2:B:10:TYR:N	2:B:10:TYR:CD1	2.81	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
5:E:120:LYS:C	5:E:122:VAL:H	2.14	0.48
4:D:10:LEU:CG	4:D:11:SER:H	2.24	0.48
4:D:184:LYS:HD3	4:D:185:SER:H	1.78	0.48
5:E:122:VAL:HG11	5:E:219:LEU:HG	1.95	0.48
2:B:23:LEU:O	2:B:67:TYR:HA	2.14	0.48
5:E:225:TRP:HZ2	5:E:229:ARG:NE	2.12	0.48
4:D:141:PHE:HD2	4:D:193:PHE:CE2	2.32	0.48
4:D:158:VAL:HA	4:D:182:SER:CB	2.43	0.48
5:E:232:PRO:O	5:E:233:VAL:C	2.51	0.48
5:E:163:VAL:HG12	5:E:210:PHE:CD1	2.46	0.48
4:D:164:THR:OG1	5:E:195:ARG:NH2	2.47	0.48
4:D:140:LEU:CG	4:D:142:THR:HG23	2.41	0.48
5:E:203:TRP:CE3	5:E:210:PHE:CE2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:HIS:HB3	5:E:95:ARG:O	2.14	0.48
1:A:197:HIS:CG	1:A:198:GLU:H	2.31	0.47
4:D:5:GLN:HG3	4:D:107:GLY:HA3	1.96	0.47
1:A:15:PRO:HG3	1:A:91:GLY:O	2.14	0.47
1:A:26:GLY:O	1:A:33:PHE:CD1	2.67	0.47
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.50	0.47
5:E:36:ARG:HB3	5:E:46:ILE:HD11	1.96	0.47
1:A:31:THR:HG23	1:A:209:TYR:OH	2.14	0.47
5:E:142:LYS:HD2	5:E:197:ARG:HH21	1.78	0.47
1:A:271:THR:O	1:A:272:LEU:HD23	2.15	0.47
5:E:172:VAL:HG12	5:E:173:SER:N	2.29	0.47
4:D:166:LEU:CD2	5:E:197:ARG:HB2	2.45	0.47
4:D:156:SER:C	4:D:158:VAL:N	2.66	0.47
1:A:194:VAL:CG2	1:A:195:SER:N	2.77	0.47
4:D:203:PHE:CE2	4:D:205:PRO:HG3	2.50	0.47
4:D:61:ARG:HD2	4:D:78:ARG:O	2.15	0.47
1:A:28:VAL:O	1:A:29:ASP:HB2	2.13	0.47
4:D:37:GLN:HB3	4:D:87:THR:HG23	1.97	0.47
2:B:87:LEU:HD21	2:B:91:LYS:HD2	1.97	0.47
1:A:63:GLU:OE2	3:C:1:LEU:CD1	2.62	0.47
5:E:122:VAL:O	5:E:232:PRO:CB	2.61	0.47
1:A:217:TRP:HE3	1:A:217:TRP:HA	1.77	0.46
4:D:141:PHE:C	4:D:144:PHE:CE2	2.88	0.46
1:A:107:TRP:CH2	1:A:180:GLN:NE2	2.83	0.46
4:D:107:GLY:C	4:D:109:GLY:N	2.68	0.46
1:A:108:ARG:HA	1:A:169:ARG:HH21	1.80	0.46
1:A:189:MET:HE3	1:A:201:LEU:HB3	1.97	0.46
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.50	0.46
5:E:15:THR:HG23	5:E:84:PRO:HD3	1.98	0.46
1:A:225:THR:O	1:A:225:THR:HG22	2.15	0.46
1:A:8:PHE:HB2	1:A:25:VAL:CG2	2.46	0.46
2:B:9:VAL:O	2:B:9:VAL:CG2	2.63	0.46
5:E:145:LEU:N	5:E:145:LEU:CD1	2.79	0.46
5:E:162:TRP:HA	5:E:166:LYS:O	2.16	0.46
5:E:139:HIS:HB3	5:E:140:THR:H	1.58	0.46
5:E:120:LYS:O	5:E:229:ARG:NH2	2.49	0.46
1:A:231:VAL:HG22	1:A:244:TRP:O	2.16	0.46
5:E:203:TRP:CE3	5:E:210:PHE:HE2	2.34	0.46
1:A:249:VAL:CG1	1:A:253:GLN:HB2	2.46	0.46
4:D:168:MET:CE	5:E:197:ARG:CD	2.95	0.45
5:E:6:GLN:NE2	5:E:111:GLY:HA2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:TYR:CE1	4:D:32:PHE:CE1	3.04	0.45
4:D:10:LEU:HB3	4:D:111:GLN:O	2.16	0.45
1:A:150:ALA:O	1:A:151:HIS:HB2	2.17	0.45
5:E:198:VAL:CG1	5:E:202:PHE:HD2	2.26	0.45
1:A:109:PHE:HD1	1:A:165:VAL:CG1	2.29	0.45
1:A:98:MET:O	1:A:114:HIS:HA	2.17	0.45
4:D:116:PRO:HG2	4:D:165:VAL:HG11	1.98	0.45
4:D:107:GLY:C	4:D:109:GLY:H	2.20	0.45
1:A:168:LEU:O	1:A:172:LEU:HG	2.17	0.45
4:D:166:LEU:HD11	5:E:171:GLY:O	2.17	0.45
4:D:138:VAL:HG21	5:E:146:VAL:HG21	1.98	0.45
5:E:225:TRP:CZ2	5:E:229:ARG:NE	2.85	0.45
5:E:232:PRO:O	5:E:233:VAL:O	2.35	0.45
5:E:16:GLY:HA2	5:E:81:SER:HB2	1.98	0.45
1:A:223:ASP:C	1:A:225:THR:N	2.68	0.45
5:E:144:THR:C	5:E:145:LEU:HD12	2.37	0.45
5:E:146:VAL:O	5:E:146:VAL:HG23	2.17	0.45
4:D:142:THR:HG22	4:D:177:SER:CB	2.46	0.45
4:D:14:GLU:OE2	4:D:116:PRO:HA	2.17	0.45
5:E:25:GLN:OE1	5:E:29:HIS:N	2.38	0.45
1:A:52:ILE:HA	1:A:52:ILE:HD12	1.79	0.45
5:E:213:GLN:HE21	5:E:236:ILE:CG2	2.30	0.45
2:B:73:THR:O	2:B:75:LYS:N	2.50	0.45
4:D:61:ARG:HD3	4:D:79:ASP:HB3	1.98	0.45
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.98	0.45
5:E:132:PRO:CG	5:E:143:ALA:HB1	2.47	0.44
1:A:129:ASP:O	1:A:131:ARG:HG2	2.17	0.44
5:E:25:GLN:HE21	5:E:25:GLN:HB3	1.62	0.44
1:A:115:GLN:HB3	2:B:60:TRP:CZ2	2.53	0.44
1:A:73:THR:HG23	1:A:74:HIS:H	1.82	0.44
1:A:36:PHE:CD1	1:A:67:VAL:HG11	2.53	0.44
4:D:138:VAL:O	4:D:138:VAL:HG23	2.17	0.44
5:E:159:LEU:HD21	5:E:194:SER:HB2	1.98	0.44
5:E:231:LYS:O	5:E:233:VAL:N	2.51	0.44
4:D:88:TYR:N	4:D:88:TYR:CD1	2.85	0.44
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.65	0.44
1:A:201:LEU:O	1:A:246:ALA:CA	2.65	0.44
1:A:24:ALA:HB3	1:A:36:PHE:HB3	1.98	0.44
1:A:95:VAL:HG11	1:A:116:TYR:OH	2.17	0.44
5:E:14:LYS:CB	5:E:17:GLN:NE2	2.81	0.44
4:D:141:PHE:CD2	4:D:193:PHE:CE2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:PRO:O	5:E:112:THR:CG2	2.63	0.44
5:E:45:LEU:O	5:E:60:VAL:HG22	2.17	0.44
4:D:173:PHE:CG	5:E:142:LYS:NZ	2.84	0.44
5:E:198:VAL:CG1	5:E:199:SER:N	2.81	0.43
1:A:6:ARG:HD3	1:A:98:MET:CE	2.48	0.43
4:D:10:LEU:CG	4:D:11:SER:N	2.80	0.43
5:E:25:GLN:CD	5:E:29:HIS:HB2	2.38	0.43
1:A:228:THR:CG2	1:A:229:GLU:N	2.60	0.43
4:D:158:VAL:HG22	4:D:187:PHE:HZ	1.83	0.43
4:D:118:ILE:C	4:D:120:ASN:N	2.72	0.43
4:D:128:LEU:N	4:D:128:LEU:HD23	2.33	0.43
4:D:2:GLU:OE1	4:D:105:GLN:NE2	2.51	0.43
1:A:109:PHE:HD1	1:A:165:VAL:HG11	1.82	0.43
5:E:31:TYR:CE2	5:E:95:ARG:NH2	2.87	0.43
2:B:89:GLN:O	2:B:90:PRO:C	2.57	0.43
4:D:166:LEU:HD11	5:E:171:GLY:C	2.39	0.43
5:E:225:TRP:CD1	5:E:226:ALA:N	2.87	0.43
1:A:162:GLY:O	1:A:165:VAL:HG22	2.19	0.43
4:D:179:VAL:HG12	4:D:181:TRP:HD1	1.84	0.43
5:E:134:GLU:CA	5:E:137:ILE:HG22	2.48	0.43
1:A:73:THR:HG23	1:A:74:HIS:N	2.33	0.43
2:B:29:GLY:HA2	2:B:61:SER:CB	2.47	0.43
1:A:203:CYS:O	1:A:244:TRP:HB2	2.19	0.43
1:A:199:ALA:O	1:A:248:VAL:HA	2.19	0.43
1:A:217:TRP:CD1	1:A:228:THR:CG2	3.02	0.42
5:E:236:ILE:HG22	5:E:236:ILE:O	2.18	0.42
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.67	0.42
4:D:166:LEU:CD1	5:E:171:GLY:O	2.67	0.42
4:D:200:GLU:O	4:D:202:THR:N	2.49	0.42
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.42
4:D:5:GLN:NE2	4:D:110:THR:H	2.18	0.42
2:B:22:PHE:CE2	2:B:69:GLU:HB2	2.55	0.42
5:E:123:PHE:HD2	5:E:151:GLY:O	2.02	0.42
5:E:175:ASP:OD2	5:E:193:SER:HB3	2.19	0.42
5:E:11:GLN:HG2	5:E:19:MET:CE	2.48	0.42
1:A:6:ARG:NE	1:A:98:MET:HE1	2.35	0.42
5:E:133:SER:O	5:E:137:ILE:HG22	2.20	0.42
2:B:27:VAL:HG23	2:B:27:VAL:O	2.20	0.42
4:D:184:LYS:O	4:D:187:PHE:HD1	2.01	0.42
4:D:132:LYS:C	4:D:134:SER:N	2.73	0.42
1:A:109:PHE:CE1	1:A:161:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:MET:HE2	5:E:197:ARG:CD	2.49	0.42
4:D:166:LEU:HD11	5:E:171:GLY:HA2	2.02	0.42
1:A:103:VAL:HA	1:A:108:ARG:O	2.20	0.42
2:B:45:ARG:NH2	6:B:100:HOH:O	2.53	0.42
4:D:191:ASN:O	4:D:192:ALA:C	2.56	0.42
1:A:135:ALA:HB3	1:A:141:GLN:NE2	2.35	0.41
5:E:164:ASN:HD21	5:E:208:ASN:HB2	1.85	0.41
5:E:140:THR:O	5:E:142:LYS:HG3	2.20	0.41
2:B:16:GLU:O	2:B:17:ASN:C	2.56	0.41
5:E:177:GLN:HA	5:E:178:PRO:HD3	1.83	0.41
4:D:126:TYR:HB3	5:E:133:SER:OG	2.21	0.41
1:A:235:PRO:CG	2:B:65:LEU:HD22	2.50	0.41
4:D:43:PRO:O	4:D:43:PRO:HG2	2.20	0.41
1:A:13:SER:OG	1:A:92:SER:HA	2.20	0.41
1:A:166:GLU:OE1	4:D:68:LYS:HD2	2.20	0.41
5:E:24:ALA:HA	5:E:73:GLU:O	2.21	0.41
4:D:184:LYS:O	4:D:186:ASP:N	2.52	0.41
4:D:125:VAL:HG22	4:D:141:PHE:CD1	2.55	0.41
4:D:82:PRO:HG2	4:D:174:LYS:HZ2	1.85	0.41
5:E:125:PRO:HD3	5:E:216:PHE:CD1	2.55	0.41
3:C:3:PHE:CZ	3:C:5:TYR:HB2	2.56	0.41
1:A:150:ALA:O	5:E:101:GLY:HA2	2.21	0.41
1:A:217:TRP:HE3	1:A:258:THR:O	2.03	0.41
4:D:173:PHE:CE2	5:E:197:ARG:CZ	3.04	0.41
1:A:167:TRP:NE1	3:C:1:LEU:HD22	2.35	0.41
5:E:213:GLN:HE21	5:E:236:ILE:HG21	1.85	0.41
5:E:146:VAL:HG12	5:E:195:ARG:CD	2.50	0.41
4:D:193:PHE:O	4:D:198:ILE:HD11	2.20	0.41
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.89	0.41
2:B:81:ARG:HE	2:B:90:PRO:HB3	1.85	0.41
2:B:89:GLN:HG3	2:B:90:PRO:HD2	2.03	0.41
4:D:20:LEU:HD13	4:D:88:TYR:HB2	2.03	0.41
1:A:96:GLN:OE1	2:B:31:HIS:HE1	2.03	0.41
5:E:137:ILE:HD11	5:E:204:GLN:CD	2.40	0.41
5:E:213:GLN:NE2	5:E:236:ILE:HG21	2.36	0.41
4:D:33:PHE:HD1	4:D:48:SER:HG	1.67	0.41
5:E:11:GLN:O	5:E:114:LEU:HA	2.21	0.40
5:E:83:ALA:HA	5:E:84:PRO:HD3	1.88	0.40
5:E:129:VAL:HG23	5:E:239:ALA:HB1	2.02	0.40
1:A:235:PRO:O	2:B:10:TYR:OH	2.30	0.40
1:A:6:ARG:HB3	1:A:8:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:GLN:HE22	4:D:110:THR:H	1.69	0.40
4:D:181:TRP:O	4:D:182:SER:HB2	2.21	0.40
4:D:142:THR:CA	4:D:144:PHE:CE2	3.05	0.40
4:D:19:SER:CA	4:D:76:LEU:HD13	2.51	0.40
1:A:8:PHE:CD1	1:A:8:PHE:N	2.88	0.40
1:A:73:THR:HG21	3:C:6:PRO:HB2	2.03	0.40
1:A:121:LYS:O	1:A:122:ASP:C	2.60	0.40
5:E:83:ALA:O	5:E:116:VAL:HG21	2.21	0.40
5:E:121:ASN:O	5:E:153:TYR:HD1	2.03	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	272/274 (99%)	242 (89%)	22 (8%)	8 (3%)	6	19
2	B	98/100 (98%)	88 (90%)	7 (7%)	3 (3%)	5	17
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	198/200 (99%)	166 (84%)	22 (11%)	10 (5%)	2	8
5	E	241/243 (99%)	208 (86%)	23 (10%)	10 (4%)	3	11
All	All	816/826 (99%)	711 (87%)	74 (9%)	31 (4%)	4	13

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	SER
1	A	253	GLN
4	D	131	SER
4	D	132	LYS
4	D	201	ASP

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Mol	Chain	Res	Type
5	E	226	ALA
5	E	228	ASP
1	A	114	HIS
4	D	163	LYS
4	D	185	SER
4	D	197	ILE
5	E	121	ASN
5	E	233	VAL
1	A	177	GLU
1	A	220	ASP
2	B	74	GLU
4	D	108	ALA
5	E	229	ARG
1	A	40	ALA
1	A	122	ASP
1	A	176	LYS
2	B	15	ALA
4	D	6	ASN
4	D	157	ASP
5	E	119	LEU
5	E	183	PRO
4	D	204	PHE
5	E	176	PRO
5	E	234	THR
2	B	97	ARG
5	E	232	PRO

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	219/229 (96%)	203 (93%)	16 (7%)	17	44
2	B	95/95 (100%)	85 (90%)	10 (10%)	8	24
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	160/178 (90%)	147 (92%)	13 (8%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	200/207 (97%)	181 (90%)	19 (10%)	11	30
All	All	681/716 (95%)	623 (92%)	58 (8%)	13	36

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	35	ARG
1	A	67	VAL
1	A	73	THR
1	A	98	MET
1	A	131	ARG
1	A	157	ARG
1	A	181	ARG
1	A	190	THR
1	A	196	ASP
1	A	198	GLU
1	A	207	SER
1	A	217	TRP
1	A	223	ASP
1	A	247	VAL
1	A	269	PRO
2	B	9	VAL
2	B	14	PRO
2	B	17	ASN
2	B	38	ASP
2	B	58	LYS
2	B	70	PHE
2	B	76	ASP
2	B	83	ASN
2	B	89	GLN
2	B	94	LYS
4	D	11	SER
4	D	23	THR
4	D	49	ILE
4	D	87	THR
4	D	93	THR
4	D	104	LEU
4	D	110	THR
4	D	128	LEU
4	D	144	PHE
4	D	196	SER

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Mol	Chain	Res	Type
4	D	197	ILE
4	D	201	ASP
4	D	206	SER
5	E	25	GLN
5	E	31	TYR
5	E	33	SER
5	E	41	MET
5	E	55	THR
5	E	56	ASP
5	E	57	GLN
5	E	67	VAL
5	E	71	THR
5	E	80	LEU
5	E	95	ARG
5	E	116	VAL
5	E	148	LEU
5	E	159	LEU
5	E	174	THR
5	E	195	ARG
5	E	207	ARG
5	E	223	ASP
5	E	246	ASP

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	54	GLN
1	A	86	ASN
1	A	93	HIS
1	A	174	ASN
1	A	180	GLN
1	A	242	GLN
2	B	17	ASN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
4	D	37	GLN
4	D	176	ASN
5	E	22	GLN
5	E	37	GLN

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Mol	Chain	Res	Type
5	E	204	GLN
5	E	208	ASN
5	E	213	GLN
5	E	235	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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