Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:49 PM GMT

PDB ID	:	1QSE
Title	:	STRUCTURE OF HUMAN A6-TCR BOUND TO HLA-A2 COMPLEXED WITH ALTERED HTLV-1 TAX PEPTIDE V7R
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

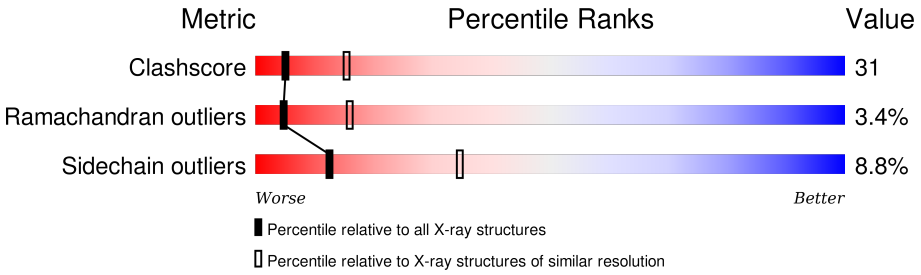
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	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	63% 32% 5%
2	B	100	58% 36% 6%
3	C	9	33% 56% 11%
4	D	200	45% 50% 6%
5	E	243	47% 45% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6500 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 PROTEIN (MHC class I HLA-A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2201	1377	398	417	9			

- Molecule 2 is a protein called PROTEIN (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 V7R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			81	57	12	12			

- Molecule 4 is a protein called PROTEIN (human T-Cell receptor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1502	941	246	309	6			

- Molecule 5 is a protein called PROTEIN (human T-Cell receptor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1879	1182	330	359	8			

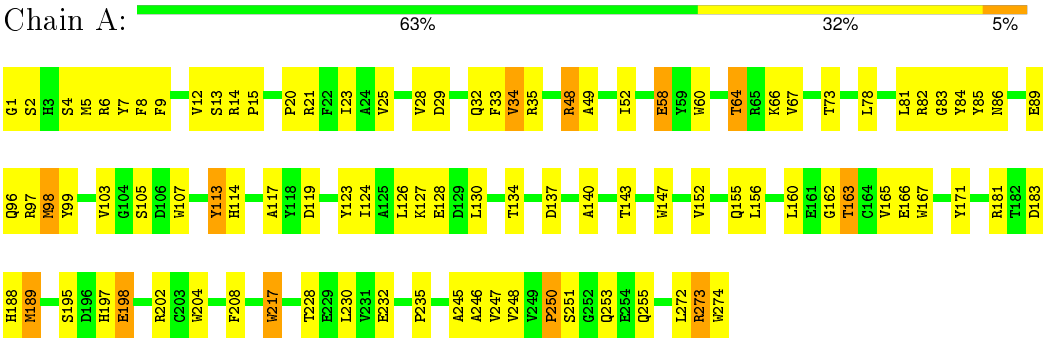
3 Residue-property plots (i)

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.

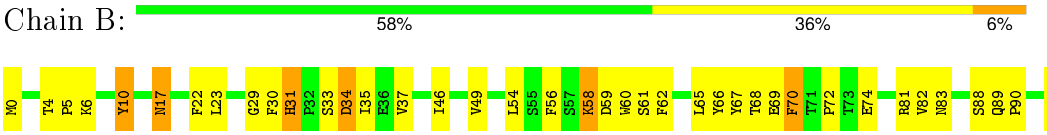
- Molecule 1: PROTEIN (MHC class I HLA-A)

Chain A:



- Molecule 2: PROTEIN (beta-2 microglobulin)

Chain B:

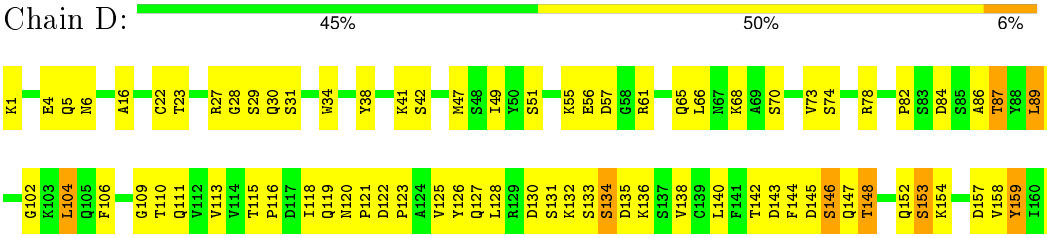


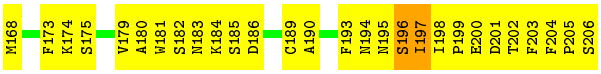
- Molecule 3: Tax Peptide V7R

Chain C:

- Molecule 4: PROTEIN (human T-Cell receptor)

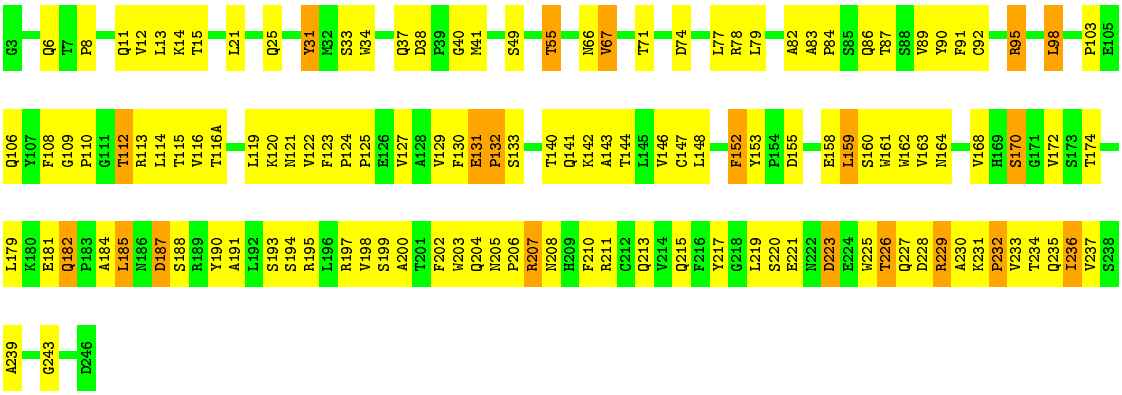
Chain D:





- Molecule 5: PROTEIN (human T-Cell receptor)

Chain E:



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	224.86Å 48.89Å 94.46Å 90.00° 90.49° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6500	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

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	0.52	0/2264	0.73	0/3076
2	B	0.61	0/860	0.75	0/1162
3	C	0.78	0/84	1.05	0/112
4	D	0.52	0/1535	0.76	0/2093
5	E	0.54	0/1932	0.78	1/2637 (0.0%)
All	All	0.54	0/6675	0.76	1/9080 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	187	ASP	N-CA-C	-5.46	96.26	111.00

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	2201	0	2037	105	0
2	B	837	0	803	52	0
3	C	81	0	83	8	0
4	D	1502	0	1363	118	0
5	E	1879	0	1755	151	0
All	All	6500	0	6041	386	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 31.

All (386) 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)
4:D:119:GLN:O	4:D:121:PRO:HD3	1.54	1.07
4:D:197:ILE:HD13	4:D:197:ILE:H	1.06	1.06
5:E:55:THR:HG21	5:E:67:VAL:HG13	1.40	1.04
1:A:202:ARG:HH12	2:B:99:MET:HG2	1.24	1.02
1:A:188:HIS:HB3	1:A:204:TRP:HB2	1.41	1.02
1:A:202:ARG:HG2	1:A:246:ALA:HB2	1.42	1.01
2:B:81:ARG:HH21	2:B:90:PRO:HG2	1.25	1.00
5:E:163:VAL:HG12	5:E:210:PHE:HD1	1.28	0.98
1:A:33:PHE:HD2	1:A:52:ILE:HD12	1.27	0.98
1:A:204:TRP:HH2	2:B:99:MET:OXT	1.50	0.95
4:D:193:PHE:HB3	4:D:198:ILE:HD11	1.49	0.94
5:E:84:PRO:HA	5:E:116:VAL:HG23	1.50	0.92
5:E:225:TRP:HZ2	5:E:229:ARG:HB2	1.33	0.92
5:E:181:GLU:O	5:E:182:GLN:HG2	1.71	0.91
1:A:187:THR:HG21	1:A:272:LEU:HD11	1.51	0.91
4:D:152:GLN:HG2	4:D:153:SER:H	1.35	0.90
1:A:250:PRO:HB2	1:A:253:GLN:NE2	1.86	0.90
4:D:34:TRP:HB2	4:D:47:MET:HB2	1.53	0.89
4:D:202:THR:HB	4:D:204:PHE:CE1	2.07	0.88
4:D:203:PHE:HE2	4:D:205:PRO:HG3	1.37	0.88
1:A:32:GLN:NE2	1:A:48:ARG:HG2	1.89	0.87
4:D:197:ILE:H	4:D:197:ILE:CD1	1.83	0.87
4:D:115:THR:CG2	4:D:146:SER:HB3	2.04	0.87
4:D:93:THR:HG21	4:D:104:LEU:HD22	1.56	0.86
4:D:197:ILE:N	4:D:197:ILE:HD13	1.88	0.85
1:A:204:TRP:CH2	2:B:99:MET:OXT	2.28	0.85
2:B:81:ARG:NH2	2:B:90:PRO:HG2	1.91	0.85
5:E:159:LEU:HD12	5:E:160:SER:N	1.90	0.85
4:D:131:SER:O	4:D:133:SER:N	2.10	0.84
4:D:118:ILE:CD1	4:D:145:ASP:HA	2.08	0.84
4:D:168:MET:HE3	5:E:197:ARG:HB3	1.60	0.83
4:D:203:PHE:CE2	4:D:205:PRO:HG3	2.12	0.83
4:D:199:PRO:O	4:D:202:THR:HG23	1.79	0.82
1:A:113:TYR:CD1	1:A:113:TYR:N	2.48	0.81
4:D:118:ILE:HD13	4:D:145:ASP:HA	1.62	0.81
5:E:163:VAL:HG12	5:E:210:PHE:CD1	2.15	0.79
1:A:32:GLN:HE21	1:A:48:ARG:HG2	1.46	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.50	0.79
4:D:190:ALA:HA	4:D:204:PHE:CE2	2.17	0.78
5:E:143:ALA:O	5:E:197:ARG:HA	1.83	0.78
2:B:58:LYS:HG2	2:B:59:ASP:N	2.00	0.77
4:D:173:PHE:CE2	5:E:142:LYS:HE2	2.21	0.76
5:E:181:GLU:O	5:E:182:GLN:CG	2.34	0.75
5:E:233:VAL:O	5:E:235:GLN:HG3	1.87	0.74
1:A:202:ARG:NH1	2:B:99:MET:HG2	2.01	0.74
5:E:142:LYS:HA	5:E:199:SER:HA	1.70	0.73
4:D:152:GLN:HG2	4:D:153:SER:N	2.04	0.72
2:B:81:ARG:HH21	2:B:90:PRO:CG	2.01	0.72
5:E:205:ASN:HB3	5:E:208:ASN:HD21	1.55	0.72
5:E:164:ASN:HD21	5:E:208:ASN:CB	2.03	0.72
5:E:225:TRP:HZ2	5:E:229:ARG:CB	2.03	0.71
1:A:167:TRP:CE2	3:C:1:LEU:HD22	2.25	0.71
5:E:122:VAL:HG21	5:E:219:LEU:HD21	1.70	0.71
4:D:157:ASP:OD2	4:D:184:LYS:NZ	2.24	0.71
5:E:55:THR:HG21	5:E:67:VAL:CG1	2.20	0.71
1:A:188:HIS:HB3	1:A:204:TRP:CB	2.18	0.71
4:D:115:THR:HG23	4:D:146:SER:HB3	1.73	0.71
1:A:6:ARG:NH2	1:A:113:TYR:HE1	1.88	0.71
5:E:131:GLU:HG3	5:E:203:TRP:CH2	2.27	0.70
5:E:83:ALA:O	5:E:116:VAL:HG21	1.91	0.70
4:D:128:LEU:HD23	5:E:133:SER:HB2	1.73	0.70
5:E:205:ASN:HB3	5:E:208:ASN:ND2	2.06	0.69
5:E:225:TRP:CZ2	5:E:229:ARG:HB2	2.23	0.69
4:D:38:TYR:HB2	4:D:41:LYS:HD2	1.74	0.69
1:A:187:THR:CG2	1:A:272:LEU:HD11	2.22	0.69
5:E:164:ASN:ND2	5:E:208:ASN:HB2	2.08	0.69
5:E:164:ASN:HD21	5:E:208:ASN:HB2	1.58	0.68
5:E:21:LEU:HD12	5:E:77:LEU:HD23	1.75	0.68
1:A:187:THR:HG22	1:A:188:HIS:H	1.58	0.68
4:D:1:LYS:HD3	4:D:4:GLU:OE2	1.93	0.67
2:B:81:ARG:NH2	2:B:90:PRO:CG	2.58	0.67
1:A:6:ARG:HH21	1:A:113:TYR:HE1	1.40	0.67
4:D:154:LYS:CB	4:D:195:ASN:ND2	2.58	0.67
5:E:225:TRP:HH2	5:E:229:ARG:CZ	2.08	0.66
5:E:116(A):THR:HG22	5:E:153:TYR:OH	1.94	0.66
5:E:185:LEU:O	5:E:188:SER:HB2	1.94	0.66
5:E:66:ASN:HD22	5:E:78:ARG:NE	1.93	0.66
5:E:143:ALA:N	5:E:198:VAL:O	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:THR:HB	4:D:204:PHE:CD1	2.30	0.66
1:A:113:TYR:HD1	1:A:113:TYR:N	1.94	0.66
1:A:33:PHE:CD2	1:A:52:ILE:HD12	2.19	0.65
5:E:236:ILE:N	5:E:236:ILE:HD13	2.12	0.65
1:A:230:LEU:HG	1:A:245:ALA:HB2	1.78	0.65
5:E:229:ARG:NH1	5:E:232:PRO:CG	2.59	0.65
4:D:199:PRO:C	4:D:201:ASP:H	2.01	0.64
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.13	0.64
1:A:189:MET:HE1	1:A:274:TRP:HB2	1.79	0.64
5:E:140:THR:O	5:E:141:GLN:HB2	1.96	0.64
5:E:229:ARG:NH1	5:E:232:PRO:HG3	2.12	0.64
4:D:5:GLN:NE2	4:D:90:CYS:H	1.95	0.64
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.80	0.64
5:E:121:ASN:HD21	5:E:187:ASP:CA	2.10	0.64
5:E:231:LYS:O	5:E:233:VAL:N	2.31	0.63
2:B:22:PHE:CE2	2:B:69:GLU:HG2	2.33	0.63
4:D:161:THR:HG21	5:E:193:SER:OG	1.98	0.63
4:D:131:SER:C	4:D:133:SER:H	2.01	0.63
5:E:174:THR:HG22	5:E:194:SER:OG	1.99	0.63
5:E:6:GLN:HG2	5:E:110:PRO:HD2	1.81	0.62
5:E:220:SER:O	5:E:223:ASP:HB2	2.00	0.62
2:B:49:VAL:HG22	2:B:68:THR:OG1	1.99	0.62
2:B:68:THR:HG22	2:B:69:GLU:O	2.00	0.62
1:A:197:HIS:O	1:A:197:HIS:CD2	2.52	0.62
4:D:118:ILE:HD11	4:D:145:ASP:HA	1.81	0.62
5:E:79:LEU:HD23	5:E:86:GLN:OE1	1.99	0.62
1:A:1:GLY:O	1:A:105:SER:HA	2.00	0.62
1:A:202:ARG:HH12	2:B:99:MET:CG	2.04	0.62
4:D:125:VAL:O	4:D:205:PRO:HD2	2.00	0.62
4:D:93:THR:CG2	4:D:104:LEU:HD22	2.29	0.62
5:E:206:PRO:HA	5:E:243:GLY:O	1.99	0.62
5:E:162:TRP:HE1	5:E:213:GLN:HB3	1.64	0.61
1:A:250:PRO:HB2	1:A:253:GLN:HE21	1.64	0.61
4:D:133:SER:O	4:D:134:SER:CB	2.49	0.61
1:A:99:TYR:HA	1:A:113:TYR:O	2.01	0.61
4:D:184:LYS:C	4:D:186:ASP:H	2.02	0.61
5:E:159:LEU:HD21	5:E:194:SER:HB2	1.82	0.61
1:A:96:GLN:OE1	2:B:60:TRP:HE3	1.84	0.61
5:E:120:LYS:O	5:E:229:ARG:NH2	2.33	0.61
1:A:127:LYS:HE2	1:A:134:THR:OG1	2.01	0.60
5:E:55:THR:CG2	5:E:67:VAL:HG13	2.25	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:LEU:CD2	5:E:144:THR:HG21	2.31	0.60
1:A:202:ARG:NH1	2:B:99:MET:HA	2.16	0.60
5:E:182:GLN:O	5:E:184:ALA:N	2.31	0.60
5:E:147:CYS:HB2	5:E:161:TRP:CZ2	2.37	0.60
5:E:11:GLN:HB3	5:E:114:LEU:HD13	1.83	0.60
1:A:181:ARG:HD2	1:A:183:ASP:OD2	2.02	0.59
5:E:143:ALA:HB3	5:E:198:VAL:O	2.01	0.59
4:D:90:CYS:O	4:D:106:PHE:HA	2.02	0.59
1:A:189:MET:CE	1:A:274:TRP:HB2	2.32	0.59
4:D:22:CYS:HB3	4:D:73:VAL:HB	1.85	0.59
1:A:147:TRP:CG	1:A:152:VAL:HG21	2.38	0.59
5:E:121:ASN:ND2	5:E:187:ASP:CB	2.66	0.59
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.85	0.59
4:D:93:THR:HG21	4:D:104:LEU:CD2	2.32	0.58
4:D:168:MET:HE3	5:E:197:ARG:CB	2.33	0.58
1:A:197:HIS:O	1:A:198:GLU:CB	2.49	0.58
5:E:127:VAL:HG21	5:E:237:VAL:O	2.02	0.58
5:E:158:GLU:HB2	5:E:215:GLN:HB3	1.85	0.58
1:A:58:GLU:H	1:A:58:GLU:CD	2.06	0.58
4:D:128:LEU:CD2	5:E:133:SER:HB2	2.32	0.58
1:A:113:TYR:H	1:A:113:TYR:HD1	1.51	0.58
1:A:73:THR:HG21	3:C:6:PRO:HB2	1.85	0.58
1:A:13:SER:HA	1:A:20:PRO:HB3	1.86	0.58
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.84	0.58
4:D:130:ASP:OD1	4:D:131:SER:N	2.35	0.58
2:B:17:ASN:HA	2:B:72:PRO:O	2.04	0.58
2:B:29:GLY:HA2	2:B:61:SER:CB	2.34	0.58
5:E:121:ASN:ND2	5:E:187:ASP:CA	2.67	0.58
4:D:198:ILE:CG2	4:D:202:THR:HG22	2.34	0.58
4:D:91:ALA:HB1	4:D:104:LEU:HD12	1.85	0.57
5:E:130:PHE:HB2	5:E:146:VAL:HG23	1.86	0.57
4:D:115:THR:CG2	4:D:146:SER:CB	2.82	0.57
4:D:106:PHE:CZ	5:E:108:PHE:HZ	2.22	0.57
1:A:197:HIS:O	1:A:197:HIS:CG	2.57	0.57
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.84	0.57
2:B:34:ASP:N	2:B:34:ASP:OD1	2.36	0.57
4:D:102:GLY:O	5:E:95:ARG:NH2	2.37	0.57
4:D:198:ILE:HG22	4:D:202:THR:HG22	1.87	0.57
1:A:147:TRP:CD1	1:A:152:VAL:HG21	2.39	0.57
1:A:4:SER:O	1:A:28:VAL:HA	2.04	0.57
5:E:131:GLU:HG3	5:E:203:TRP:CZ2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:TYR:HH	4:D:31:SER:HG	1.52	0.57
1:A:187:THR:HG22	1:A:188:HIS:N	2.19	0.56
5:E:31:TYR:HA	5:E:49:SER:O	2.04	0.56
4:D:168:MET:HE1	5:E:197:ARG:HG2	1.87	0.56
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.40	0.56
4:D:87:THR:HA	4:D:111:GLN:HA	1.86	0.56
1:A:250:PRO:HB2	1:A:253:GLN:HE22	1.67	0.56
2:B:10:TYR:N	2:B:10:TYR:CD1	2.73	0.56
1:A:12:VAL:CG2	1:A:21:ARG:HB3	2.36	0.56
4:D:140:LEU:HD22	5:E:144:THR:HG21	1.88	0.56
1:A:187:THR:HG21	1:A:272:LEU:CD1	2.31	0.55
5:E:95:ARG:HD2	5:E:106:GLN:HB2	1.87	0.55
4:D:202:THR:CB	4:D:204:PHE:CE1	2.86	0.55
4:D:152:GLN:CG	4:D:153:SER:H	2.15	0.55
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.42	0.55
1:A:7:TYR:O	1:A:98:MET:HA	2.08	0.54
1:A:248:VAL:HG23	1:A:248:VAL:O	2.08	0.54
5:E:179:LEU:O	5:E:190:TYR:HA	2.08	0.54
5:E:121:ASN:ND2	5:E:187:ASP:HA	2.23	0.54
4:D:179:VAL:HG12	4:D:180:ALA:N	2.21	0.54
5:E:229:ARG:NH1	5:E:232:PRO:HG2	2.23	0.54
5:E:6:GLN:HE22	5:E:92:CYS:H	1.56	0.54
1:A:15:PRO:HB3	1:A:89:GLU:O	2.08	0.54
5:E:11:GLN:O	5:E:114:LEU:HD12	2.08	0.54
1:A:60:TRP:O	1:A:64:THR:HB	2.08	0.54
1:A:103:VAL:HB	1:A:107:TRP:HA	1.90	0.54
1:A:25:VAL:HG13	1:A:32:GLN:HG3	1.89	0.54
2:B:46:ILE:HG21	2:B:68:THR:HG21	1.89	0.54
1:A:97:ARG:HG2	1:A:98:MET:N	2.23	0.53
1:A:28:VAL:O	1:A:29:ASP:HB2	2.08	0.53
5:E:55:THR:CG2	5:E:67:VAL:CG1	2.86	0.53
1:A:34:VAL:HG13	1:A:52:ILE:HD13	1.89	0.53
4:D:179:VAL:CG1	4:D:180:ALA:N	2.71	0.53
5:E:181:GLU:O	5:E:182:GLN:NE2	2.41	0.53
5:E:164:ASN:HD21	5:E:208:ASN:HB3	1.74	0.53
2:B:65:LEU:HD12	2:B:66:TYR:N	2.23	0.53
4:D:91:ALA:HB1	4:D:104:LEU:CD1	2.38	0.53
4:D:181:TRP:CH2	5:E:191:ALA:HB1	2.44	0.53
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.91	0.53
1:A:8:PHE:CE2	1:A:98:MET:HG3	2.43	0.53
5:E:219:LEU:N	5:E:219:LEU:HD23	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:VAL:HG22	5:E:168:VAL:HG13	1.91	0.53
4:D:104:LEU:HD23	5:E:95:ARG:CZ	2.38	0.52
4:D:184:LYS:C	4:D:186:ASP:N	2.62	0.52
5:E:130:PHE:HB2	5:E:146:VAL:CG2	2.39	0.52
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.27	0.52
1:A:232:GLU:OE2	2:B:6:LYS:HD2	2.07	0.52
1:A:230:LEU:HG	1:A:245:ALA:CB	2.40	0.52
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.40	0.52
4:D:184:LYS:O	4:D:186:ASP:N	2.43	0.52
1:A:97:ARG:NH1	1:A:114:HIS:NE2	2.53	0.51
5:E:8:PRO:O	5:E:112:THR:HB	2.09	0.51
5:E:164:ASN:ND2	5:E:208:ASN:CB	2.69	0.51
2:B:17:ASN:ND2	2:B:74:GLU:HG2	2.25	0.51
4:D:154:LYS:CB	4:D:195:ASN:HD22	2.23	0.51
4:D:82:PRO:HG3	4:D:174:LYS:NZ	2.26	0.51
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.92	0.51
5:E:217:TYR:HA	5:E:234:THR:HG23	1.93	0.51
1:A:202:ARG:HG2	1:A:246:ALA:CB	2.27	0.50
5:E:203:TRP:HE3	5:E:210:PHE:CE2	2.29	0.50
5:E:152:PHE:HD1	5:E:152:PHE:H	1.57	0.50
4:D:82:PRO:HG3	4:D:174:LYS:HZ2	1.74	0.50
2:B:96:ASP:O	2:B:98:ASP:N	2.45	0.50
5:E:132:PRO:HD2	5:E:203:TRP:CZ2	2.46	0.50
1:A:9:PHE:O	1:A:96:GLN:HA	2.12	0.50
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.41	0.50
1:A:96:GLN:NE2	2:B:31:HIS:HE1	2.10	0.50
4:D:193:PHE:O	4:D:196:SER:N	2.45	0.50
5:E:205:ASN:ND2	5:E:207:ARG:HE	2.09	0.50
1:A:162:GLY:O	1:A:165:VAL:HG22	2.12	0.50
4:D:126:TYR:HD2	4:D:205:PRO:HG2	1.76	0.50
4:D:91:ALA:HB2	4:D:106:PHE:CD2	2.47	0.50
5:E:155:ASP:HB3	5:E:190:TYR:CE1	2.47	0.50
1:A:66:LYS:HZ1	3:C:1:LEU:HG	1.76	0.50
1:A:250:PRO:O	1:A:251:SER:C	2.51	0.49
5:E:34:TRP:CE2	5:E:77:LEU:HB2	2.48	0.49
4:D:166:LEU:HD21	4:D:175:SER:OG	2.12	0.49
5:E:205:ASN:OD1	5:E:207:ARG:HG3	2.12	0.49
5:E:14:LYS:HB3	5:E:119:LEU:HG	1.93	0.49
4:D:158:VAL:HG13	4:D:182:SER:HB2	1.93	0.49
5:E:89:VAL:HG22	5:E:113:ARG:HG3	1.94	0.49
2:B:59:ASP:O	2:B:60:TRP:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HA	3:C:8:TYR:CE1	2.48	0.49
5:E:13:LEU:HB2	5:E:116:VAL:HG12	1.94	0.49
1:A:202:ARG:HH12	2:B:99:MET:HA	1.77	0.49
4:D:138:VAL:HG23	5:E:130:PHE:CE2	2.48	0.49
5:E:143:ALA:HB3	5:E:198:VAL:HG23	1.94	0.48
4:D:51:SER:O	4:D:66:LEU:HD23	2.14	0.48
5:E:229:ARG:HH11	5:E:232:PRO:HG3	1.77	0.48
4:D:127:GLN:OE1	4:D:189:CYS:SG	2.71	0.48
5:E:87:THR:OG1	5:E:116:VAL:HG22	2.13	0.48
4:D:61:ARG:NH1	4:D:84:ASP:OD2	2.35	0.48
5:E:122:VAL:O	5:E:229:ARG:NH1	2.31	0.48
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.97	0.48
2:B:58:LYS:C	2:B:60:TRP:H	2.16	0.48
2:B:65:LEU:HD12	2:B:66:TYR:H	1.79	0.48
5:E:225:TRP:CD1	5:E:226:THR:N	2.82	0.47
1:A:6:ARG:HD3	1:A:98:MET:CE	2.44	0.47
1:A:73:THR:CG2	5:E:98:LEU:HG	2.44	0.47
4:D:126:TYR:HB3	5:E:133:SER:CB	2.44	0.47
5:E:40:GLY:C	5:E:41:MET:HG2	2.34	0.47
4:D:122:ASP:O	4:D:123:PRO:C	2.52	0.47
4:D:119:GLN:C	4:D:121:PRO:HD3	2.32	0.47
5:E:203:TRP:HE3	5:E:210:PHE:HE2	1.62	0.47
5:E:31:TYR:HB3	5:E:95:ARG:HB3	1.96	0.47
5:E:159:LEU:C	5:E:159:LEU:HD12	2.33	0.47
5:E:161:TRP:C	5:E:162:TRP:CD1	2.88	0.47
4:D:181:TRP:CZ2	5:E:191:ALA:HB1	2.49	0.47
4:D:193:PHE:O	4:D:195:ASN:N	2.47	0.46
5:E:14:LYS:O	5:E:15:THR:C	2.52	0.46
1:A:34:VAL:HG13	1:A:52:ILE:CD1	2.46	0.46
1:A:85:TYR:O	1:A:86:ASN:C	2.51	0.46
5:E:66:ASN:ND2	5:E:78:ARG:NE	2.62	0.46
4:D:116:PRO:HB2	4:D:174:LYS:HD2	1.96	0.46
4:D:193:PHE:CB	4:D:198:ILE:HD11	2.32	0.46
4:D:28:GLY:O	4:D:30:GLN:HG3	2.15	0.46
1:A:123:TYR:OH	1:A:143:THR:OG1	2.30	0.46
1:A:166:GLU:OE1	4:D:68:LYS:HD2	2.16	0.46
2:B:65:LEU:HG	2:B:67:TYR:HD2	1.79	0.46
4:D:173:PHE:CD2	5:E:142:LYS:HE2	2.50	0.46
4:D:38:TYR:CD1	4:D:86:ALA:HB2	2.50	0.46
5:E:162:TRP:CD1	5:E:162:TRP:N	2.84	0.46
4:D:193:PHE:C	4:D:195:ASN:N	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:LEU:HD12	4:D:109:GLY:HA3	1.98	0.46
4:D:145:ASP:O	4:D:148:THR:N	2.47	0.45
5:E:200:ALA:O	5:E:204:GLN:HG3	2.15	0.45
1:A:49:ALA:O	1:A:52:ILE:HG22	2.17	0.45
4:D:167:ASP:O	5:E:170:SER:O	2.34	0.45
5:E:168:VAL:O	5:E:172:VAL:HG21	2.17	0.45
5:E:230:ALA:O	5:E:231:LYS:C	2.55	0.45
4:D:5:GLN:HE22	4:D:89:LEU:HA	1.81	0.45
4:D:118:ILE:O	4:D:118:ILE:HG13	2.17	0.45
5:E:116(A):THR:CG2	5:E:153:TYR:OH	2.63	0.45
1:A:156:LEU:O	1:A:160:LEU:HG	2.17	0.45
5:E:203:TRP:CE3	5:E:210:PHE:HE2	2.34	0.45
4:D:42:SER:HA	5:E:91:PHE:CE1	2.51	0.45
5:E:225:TRP:HH2	5:E:229:ARG:NE	2.13	0.45
5:E:143:ALA:CB	5:E:198:VAL:O	2.65	0.45
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.98	0.45
4:D:61:ARG:HD2	4:D:78:ARG:O	2.17	0.45
5:E:202:PHE:HE2	5:E:210:PHE:CE1	2.35	0.44
5:E:119:LEU:C	5:E:121:ASN:H	2.19	0.44
1:A:217:TRP:HD1	1:A:228:THR:CG2	2.30	0.44
1:A:273:ARG:HE	1:A:273:ARG:H	1.65	0.44
4:D:93:THR:HG22	4:D:104:LEU:HD13	1.99	0.44
1:A:235:PRO:O	2:B:10:TYR:OH	2.25	0.44
4:D:5:GLN:NE2	4:D:109:GLY:HA2	2.32	0.44
5:E:90:TYR:HB2	5:E:112:THR:HG23	1.99	0.44
1:A:94:THR:HG22	1:A:95:VAL:N	2.33	0.44
4:D:106:PHE:CZ	5:E:108:PHE:CZ	3.05	0.44
2:B:69:GLU:O	2:B:70:PHE:HB3	2.17	0.44
5:E:123:PHE:CE1	5:E:229:ARG:CZ	3.01	0.44
1:A:25:VAL:CG1	1:A:32:GLN:HG3	2.47	0.44
3:C:6:PRO:O	3:C:7:ARG:HD2	2.18	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.44
4:D:183:ASN:C	4:D:184:LYS:HG3	2.39	0.43
1:A:84:TYR:HD2	1:A:123:TYR:HH	1.66	0.43
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.83	0.43
4:D:136:LYS:CB	4:D:182:SER:O	2.66	0.43
1:A:81:LEU:C	1:A:83:GLY:N	2.71	0.43
4:D:199:PRO:C	4:D:201:ASP:N	2.70	0.43
5:E:125:PRO:HB3	5:E:152:PHE:HB3	1.98	0.43
5:E:121:ASN:HD21	5:E:187:ASP:CB	2.30	0.43
1:A:107:TRP:CD1	1:A:107:TRP:N	2.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:ASN:OD1	5:E:208:ASN:HA	2.18	0.43
5:E:67:VAL:HG23	5:E:77:LEU:HA	2.00	0.43
4:D:128:LEU:HD12	5:E:146:VAL:HG22	2.00	0.43
4:D:140:LEU:HD22	5:E:144:THR:CG2	2.48	0.43
1:A:66:LYS:HE3	3:C:2:LEU:HB2	2.00	0.43
2:B:35:ILE:HD11	2:B:82:VAL:HG11	1.99	0.43
5:E:211:ARG:HG3	5:E:239:ALA:O	2.19	0.43
1:A:82:ARG:O	1:A:82:ARG:HG2	2.17	0.43
2:B:96:ASP:C	2:B:98:ASP:H	2.22	0.42
1:A:5:MET:SD	1:A:171:TYR:HE2	2.41	0.42
4:D:65:GLN:HB2	4:D:74:SER:HB2	2.01	0.42
1:A:185:PRO:HB3	1:A:208:PHE:HB3	2.01	0.42
4:D:118:ILE:HD13	4:D:144:PHE:O	2.19	0.42
5:E:203:TRP:CE3	5:E:210:PHE:CE2	3.07	0.42
1:A:52:ILE:O	1:A:52:ILE:HG12	2.19	0.42
5:E:152:PHE:N	5:E:152:PHE:CD1	2.84	0.42
4:D:183:ASN:O	4:D:184:LYS:HG3	2.19	0.42
1:A:14:ARG:NH1	1:A:21:ARG:HB2	2.34	0.42
1:A:185:PRO:CA	1:A:208:PHE:HB3	2.49	0.42
4:D:142:THR:OG1	4:D:143:ASP:N	2.53	0.42
5:E:119:LEU:C	5:E:121:ASN:N	2.73	0.42
5:E:226:THR:O	5:E:227:GLN:C	2.58	0.42
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.50	0.42
5:E:127:VAL:HG13	5:E:147:CYS:SG	2.60	0.42
4:D:140:LEU:HD21	5:E:144:THR:HG21	2.01	0.42
1:A:96:GLN:NE2	2:B:62:PHE:CZ	2.88	0.42
4:D:157:ASP:CB	4:D:184:LYS:NZ	2.83	0.42
1:A:163:THR:HG21	4:D:30:GLN:HG2	2.01	0.42
1:A:126:LEU:HD23	1:A:130:LEU:HD22	2.01	0.42
4:D:29:SER:HB3	4:D:92:VAL:CG1	2.50	0.42
4:D:145:ASP:O	4:D:147:GLN:N	2.53	0.41
4:D:161:THR:HG21	5:E:193:SER:HG	1.82	0.41
1:A:217:TRP:HD1	1:A:228:THR:HG21	1.85	0.41
5:E:84:PRO:HA	5:E:116:VAL:CG2	2.36	0.41
2:B:29:GLY:HA2	2:B:61:SER:OG	2.20	0.41
4:D:159:TYR:O	4:D:180:ALA:HA	2.21	0.41
2:B:88:SER:O	2:B:89:GLN:HG3	2.21	0.41
1:A:81:LEU:O	1:A:82:ARG:C	2.59	0.41
5:E:124:PRO:HD3	5:E:232:PRO:HB3	2.02	0.41
2:B:0:MET:O	2:B:0:MET:HG3	2.21	0.41
5:E:153:TYR:C	5:E:153:TYR:CD1	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:GLN:HE21	5:E:109:GLY:HA3	1.85	0.41
1:A:12:VAL:HG22	1:A:21:ARG:HB3	2.01	0.41
3:C:5:TYR:OH	4:D:31:SER:OG	2.25	0.41
4:D:158:VAL:HG22	4:D:182:SER:CB	2.50	0.41
5:E:38:ASP:HB2	5:E:41:MET:HG3	2.02	0.41
5:E:131:GLU:HG3	5:E:203:TRP:HH2	1.80	0.40
5:E:123:PHE:O	5:E:152:PHE:HA	2.21	0.40
5:E:231:LYS:HA	5:E:232:PRO:HD3	1.96	0.40
4:D:113:VAL:O	4:D:113:VAL:HG23	2.21	0.40
2:B:29:GLY:CA	2:B:61:SER:HB2	2.51	0.40
2:B:30:PHE:O	2:B:31:HIS:HB2	2.20	0.40
5:E:205:ASN:HD21	5:E:207:ARG:HE	1.67	0.40
5:E:37:GLN:NE2	5:E:91:PHE:HE2	2.20	0.40
4:D:198:ILE:HG22	4:D:202:THR:CG2	2.51	0.40
4:D:115:THR:HG21	4:D:146:SER:HB3	1.94	0.40
5:E:34:TRP:NE1	5:E:77:LEU:HB2	2.36	0.40
2:B:81:ARG:NE	2:B:90:PRO:HB3	2.37	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
5:E:204:GLN:O	5:E:206:PRO:HD3	2.22	0.40
1:A:126:LEU:CD2	1:A:130:LEU:HD22	2.52	0.40
4:D:55:LYS:HG2	4:D:56:GLU:N	2.37	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%)	245 (90%)	25 (9%)	2 (1%)	26 62
2	B	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	5 17
3	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0 1
4	D	198/200 (99%)	167 (84%)	19 (10%)	12 (6%)	2 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	241/243 (99%)	205 (85%)	26 (11%)	10 (4%)	3 11
All	All	816/826 (99%)	713 (87%)	75 (9%)	28 (3%)	5 16

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
4	D	6	ASN
4	D	132	LYS
4	D	134	SER
4	D	135	ASP
5	E	82	ALA
5	E	221	GLU
5	E	226	THR
5	E	229	ARG
1	A	198	GLU
4	D	146	SER
5	E	182	GLN
2	B	97	ARG
4	D	120	ASN
4	D	185	SER
4	D	194	ASN
5	E	170	SER
4	D	16	ALA
4	D	153	SER
4	D	200	GLU
5	E	232	PRO
4	D	148	THR
5	E	228	ASP
2	B	17	ASN
3	C	8	TYR
2	B	31	HIS
5	E	103	PRO
5	E	132	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	222/230 (96%)	202 (91%)	20 (9%)	12 34
2	B	95/95 (100%)	90 (95%)	5 (5%)	28 61
3	C	8/8 (100%)	8 (100%)	0	100 100
4	D	160/178 (90%)	146 (91%)	14 (9%)	12 35
5	E	198/208 (95%)	177 (89%)	21 (11%)	8 24
All	All	683/719 (95%)	623 (91%)	60 (9%)	12 35

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	34	VAL
1	A	35	ARG
1	A	48	ARG
1	A	58	GLU
1	A	64	THR
1	A	67	VAL
1	A	98	MET
1	A	113	TYR
1	A	128	GLU
1	A	137	ASP
1	A	155	GLN
1	A	163	THR
1	A	187	THR
1	A	189	MET
1	A	217	TRP
1	A	247	VAL
1	A	250	PRO
1	A	255	GLN
1	A	273	ARG
2	B	10	TYR
2	B	34	ASP
2	B	58	LYS
2	B	70	PHE
2	B	83	ASN
4	D	23	THR
4	D	27	ARG
4	D	49	ILE
4	D	57	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	70	SER
4	D	87	THR
4	D	89	LEU
4	D	93	THR
4	D	104	LEU
4	D	110	THR
4	D	159	TYR
4	D	196	SER
4	D	197	ILE
4	D	206	SER
5	E	12	VAL
5	E	25	GLN
5	E	31	TYR
5	E	33	SER
5	E	55	THR
5	E	67	VAL
5	E	71	THR
5	E	74	ASP
5	E	95	ARG
5	E	98	LEU
5	E	112	THR
5	E	115	THR
5	E	131	GLU
5	E	148	LEU
5	E	152	PHE
5	E	159	LEU
5	E	185	LEU
5	E	195	ARG
5	E	207	ARG
5	E	223	ASP
5	E	236	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	86	ASN
1	A	93	HIS
1	A	96	GLN
1	A	155	GLN
1	A	197	HIS
1	A	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	242	GLN
1	A	253	GLN
2	B	31	HIS
2	B	83	ASN
4	D	5	GLN
4	D	37	GLN
4	D	71	GLN
4	D	127	GLN
4	D	195	ASN
5	E	6	GLN
5	E	11	GLN
5	E	37	GLN
5	E	66	ASN
5	E	121	ASN
5	E	139	HIS
5	E	208	ASN
5	E	215	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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