Full wwPDB X-ray Structure Validation Report

Dec 15, 2016 – 06:01 PM EST

PDB ID	:	1OKW
Title	:	Cyclin A binding groove inhibitor Ac-Arg-Arg-Leu-Asn-(m-Cl-Phe)-NH2
Authors	:	Kontopidis, G.; Andrews, M.; McInnes, C.; Cowan, A.; Powers, H.; Innes, L.; Plater, A.; Griffiths, G.; Paterson, D.; Zheleva, D.; Lane, D.; Green, S.; Walkinshaw, M.; Fischer, P.
Deposited on	:	2003-07-31
Resolution	:	2.50 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 (1)) were used in the production of this report:

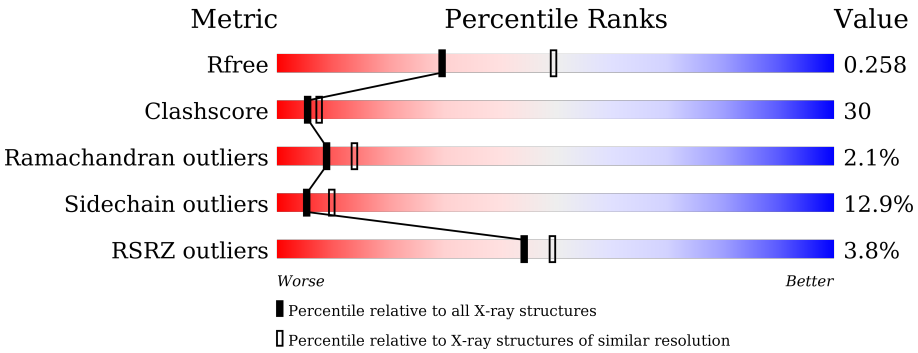
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	298	3% 50% 41% 7%
1	C	298	5% 60% 28% 10%
2	B	260	5% 63% 28% 7%
2	D	260	2% 62% 27% 8%
3	E	7	29% 43% 14% 14%
3	F	7	14% 29% 43% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9569 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called ACE-ARG-ARG-LEU-ASN-FCL-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	Cl	N	O	0	0	1
			54	33	1	13	7			
3	F	7	Total	C	Cl	N	O	0	0	1
			54	33	1	13	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	115	Total	O	0	0
			115	115		
4	C	146	Total	O	0	0
			146	146		
4	D	131	Total	O	0	0
			131	131		

Continued on next page...

Continued from previous page...

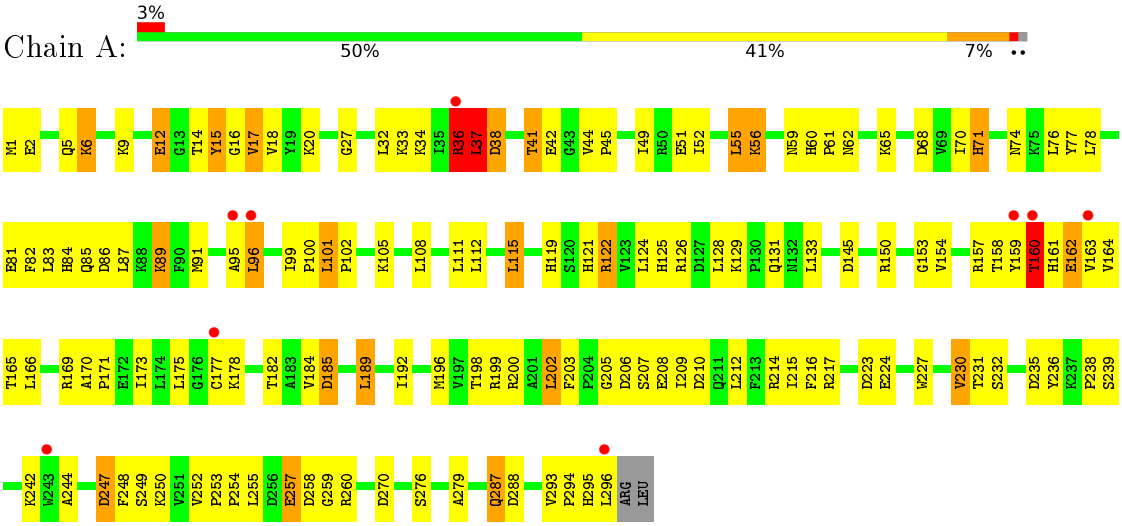
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	6	Total O 6 6	0	0
4	F	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

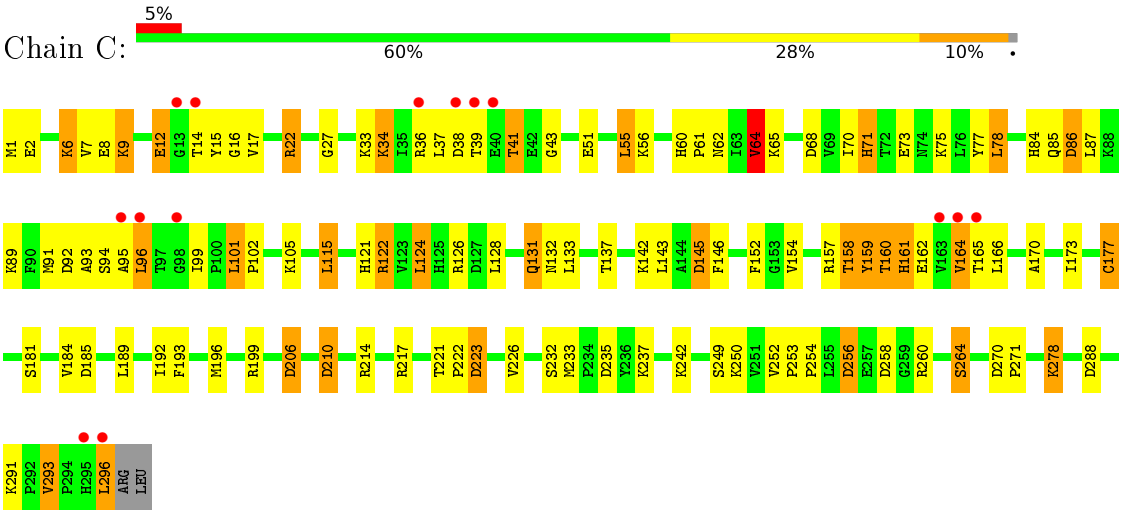
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



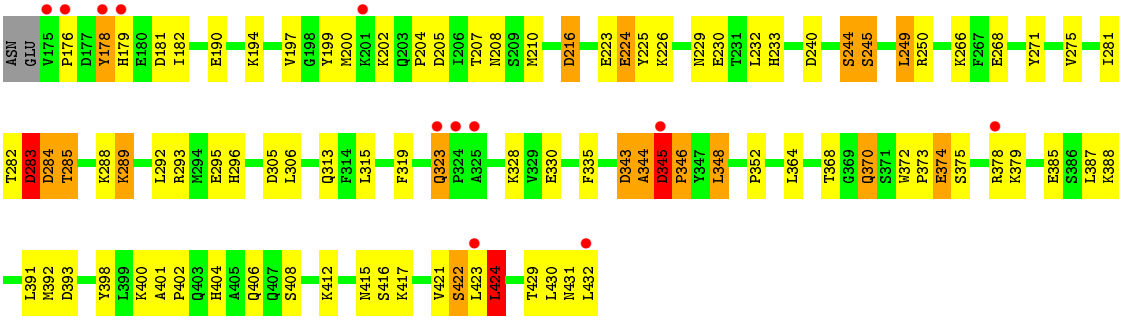
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:

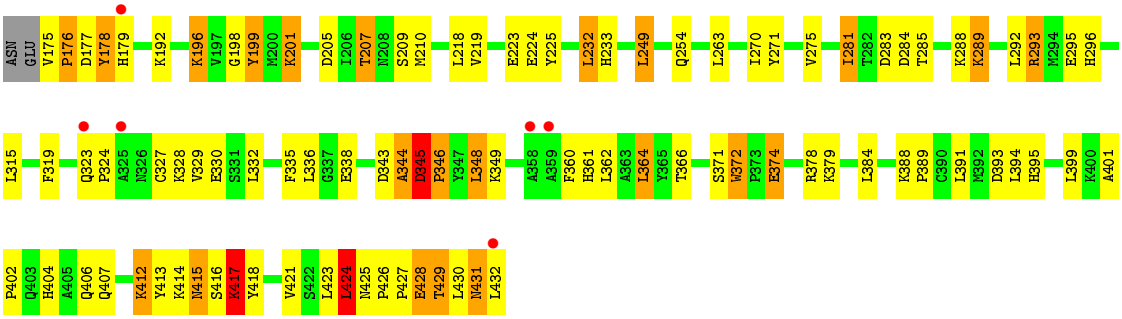


- Molecule 2: CYCLIN A2

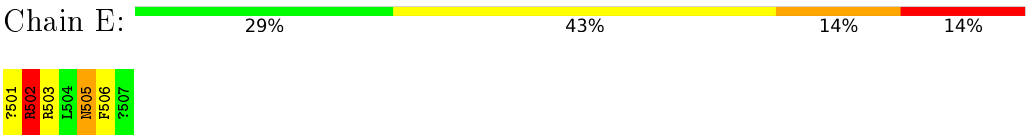
Chain B:



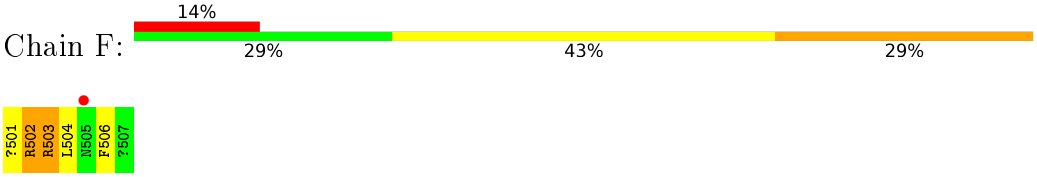
- Molecule 2: CYCLIN A2



- Molecule 3: ACE-ARG-ARG-LEU-ASN-FCL-NH2



- Molecule 3: ACE-ARG-ARG-LEU-ASN-FCL-NH2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.54Å 114.05Å 156.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.50) 99.1 (19.70-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.173 , 0.253 0.182 , 0.258	Depositor DCC
R_{free} test set	1430 reflections (3.20%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	1.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9569	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FCL, ACE, NH2

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	0.53	0/2440	0.91	11/3313 (0.3%)
1	C	0.52	0/2440	0.90	9/3313 (0.3%)
2	B	0.53	0/2133	0.88	8/2897 (0.3%)
2	D	0.55	0/2133	0.85	4/2895 (0.1%)
3	E	1.37	1/38 (2.6%)	1.98	2/49 (4.1%)
3	F	1.26	1/38 (2.6%)	2.45	2/49 (4.1%)
All	All	0.54	2/9222 (0.0%)	0.91	36/12516 (0.3%)

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	2
1	C	0	2
2	B	0	2
2	D	0	2
3	E	0	1
3	F	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	ARG	CB-CG	-7.10	1.33	1.52
3	F	502	ARG	CB-CG	-6.92	1.33	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	502	ARG	NE-CZ-NH2	8.51	124.56	120.30
1	A	235	ASP	CB-CG-OD2	8.09	125.58	118.30
1	C	210	ASP	CB-CG-OD2	7.93	125.44	118.30
3	F	502	ARG	NE-CZ-NH1	-7.83	116.39	120.30
2	D	393	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	185	ASP	CB-CG-OD2	6.96	124.57	118.30
2	B	345	ASP	CB-CG-OD2	6.88	124.49	118.30
2	B	305	ASP	CB-CG-OD2	6.73	124.36	118.30
2	B	216	ASP	CB-CG-OD2	6.67	124.30	118.30
2	B	284	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	86	ASP	CB-CG-OD2	6.48	124.13	118.30
3	E	502	ARG	NE-CZ-NH2	6.32	123.46	120.30
2	B	393	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	205	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	64	VAL	CB-CA-C	-5.97	100.06	111.40
1	C	223	ASP	CB-CG-OD2	5.97	123.67	118.30
2	B	181	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	256	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	68	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	210	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	68	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	145	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	38	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	124	LEU	CB-CG-CD1	-5.47	101.71	111.00
2	D	345	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	206	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	247	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	86	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	235	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	283	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	206	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	145	ASP	CB-CG-OD2	5.20	122.97	118.30
2	B	343	ASP	CB-CG-OD2	5.15	122.94	118.30
3	E	502	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	D	284	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	124	LEU	CB-CA-C	-5.04	100.62	110.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	ARG	Peptide
1	A	83	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	344	ALA	Peptide
2	B	345	ASP	Peptide
1	C	159	TYR	Peptide
1	C	164	VAL	Peptide
2	D	344	ALA	Peptide
2	D	345	ASP	Peptide
3	E	502	ARG	Sidechain
3	F	503	ARG	Sidechain

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	2378	0	2426	188	0
1	C	2378	0	2426	136	1
2	B	2083	0	2107	102	1
2	D	2083	0	2107	127	0
3	E	54	0	53	10	0
3	F	54	0	53	5	0
4	A	137	0	0	69	0
4	B	115	0	0	24	0
4	C	146	0	0	42	0
4	D	131	0	0	54	0
4	E	6	0	0	3	0
4	F	4	0	0	1	0
All	All	9569	0	9172	540	1

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 30.

All (540) 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:33:LYS:HE3	4:A:2033:HOH:O	1.27	1.32
1:C:199:ARG:HD3	4:C:2101:HOH:O	1.14	1.27
1:A:177:CYS:HB3	4:A:2093:HOH:O	1.29	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:HG2	4:B:2020:HOH:O	1.37	1.25
1:C:38:ASP:HB3	4:C:2028:HOH:O	1.34	1.24
2:D:421:VAL:HB	4:D:2125:HOH:O	1.04	1.18
1:C:164:VAL:HG12	1:C:165:THR:O	1.44	1.15
1:A:95:ALA:O	1:A:96:LEU:HB3	1.41	1.15
1:C:39:THR:HG22	4:D:2063:HOH:O	1.48	1.12
1:A:17:VAL:HG22	4:A:2020:HOH:O	1.50	1.08
1:A:38:ASP:OD1	1:A:41:THR:OG1	1.71	1.08
1:C:17:VAL:O	4:C:2013:HOH:O	1.70	1.08
2:D:430:LEU:O	2:D:431:ASN:HB2	1.50	1.06
2:B:374:GLU:HB3	4:B:2086:HOH:O	1.55	1.04
2:B:271:TYR:HB3	4:B:2054:HOH:O	1.58	1.03
2:B:282:THR:O	2:B:285:THR:HG22	1.58	1.03
2:D:292:LEU:HG	4:D:2068:HOH:O	1.56	1.02
2:D:407:GLN:N	4:D:2120:HOH:O	1.92	1.02
1:A:217:ARG:HA	4:A:2109:HOH:O	1.60	1.01
2:B:179:HIS:CE1	2:B:379:LYS:HZ2	1.78	1.00
2:B:374:GLU:CB	4:B:2086:HOH:O	2.08	1.00
1:C:95:ALA:O	1:C:96:LEU:HB3	1.63	0.98
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.46	0.98
1:A:15:TYR:HD2	1:A:33:LYS:HD3	1.26	0.98
2:D:404:HIS:HD2	2:D:406:GLN:H	1.06	0.97
2:B:179:HIS:CE1	2:B:379:LYS:NZ	2.32	0.97
2:D:270:ILE:HB	4:D:2054:HOH:O	1.65	0.97
2:B:282:THR:O	2:B:285:THR:CG2	2.12	0.96
2:B:374:GLU:CG	4:B:2086:HOH:O	2.13	0.96
2:D:327:CYS:HB2	4:D:2080:HOH:O	1.63	0.96
1:A:60:HIS:HD2	1:A:62:ASN:H	1.13	0.96
1:C:162:GLU:OE1	1:C:164:VAL:HG23	1.62	0.96
1:C:22:ARG:HD3	4:C:2014:HOH:O	1.63	0.96
1:A:91:MET:HE2	1:A:196:MET:HG2	1.47	0.96
1:C:60:HIS:HD2	1:C:62:ASN:H	1.14	0.96
1:A:91:MET:CE	1:A:196:MET:HG2	1.97	0.95
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.30	0.95
2:D:406:GLN:HA	4:D:2120:HOH:O	1.66	0.95
1:C:39:THR:CG2	4:D:2063:HOH:O	2.08	0.94
2:D:413:TYR:CE2	4:D:2082:HOH:O	2.20	0.93
2:B:245:SER:HB2	4:B:2045:HOH:O	1.67	0.93
2:B:404:HIS:HD2	2:B:406:GLN:H	1.16	0.93
1:C:160:THR:HA	4:C:2081:HOH:O	1.69	0.92
2:B:179:HIS:NE2	2:B:379:LYS:CE	2.34	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:HE2	4:C:2023:HOH:O	1.71	0.91
1:C:95:ALA:O	1:C:96:LEU:CB	2.19	0.90
1:A:236:TYR:CE2	4:A:2106:HOH:O	2.23	0.90
2:B:233:HIS:HD2	4:B:2069:HOH:O	1.54	0.89
2:D:179:HIS:CE1	2:D:379:LYS:HZ2	1.89	0.89
1:C:55:LEU:HD22	4:C:2032:HOH:O	1.72	0.89
1:A:276:SER:OG	4:A:2126:HOH:O	1.90	0.89
2:D:343:ASP:HB3	2:D:345:ASP:OD2	1.72	0.89
2:D:335:PHE:CA	4:D:2082:HOH:O	2.19	0.89
1:A:60:HIS:CD2	1:A:62:ASN:H	1.91	0.88
2:D:179:HIS:CE1	2:D:379:LYS:NZ	2.41	0.88
2:D:178:TYR:HE2	4:D:2009:HOH:O	1.55	0.88
2:D:430:LEU:HB3	2:D:432:LEU:HD21	1.56	0.88
1:A:236:TYR:CD2	4:A:2106:HOH:O	2.28	0.87
1:A:171:PRO:HB3	4:A:2092:HOH:O	1.75	0.86
1:C:162:GLU:OE1	1:C:164:VAL:CG2	2.23	0.86
2:D:178:TYR:CE2	4:D:2009:HOH:O	2.25	0.86
2:D:404:HIS:CD2	2:D:406:GLN:H	1.94	0.85
1:A:100:PRO:HD3	4:A:2065:HOH:O	1.77	0.85
1:A:91:MET:CE	1:A:196:MET:CG	2.54	0.84
2:B:207:THR:HG23	2:B:210:MET:H	1.42	0.84
1:A:95:ALA:O	1:A:96:LEU:CB	2.26	0.84
1:C:173:ILE:HD11	1:C:184:VAL:CG1	2.08	0.84
2:B:179:HIS:NE2	2:B:379:LYS:NZ	2.26	0.84
1:A:2:GLU:HG2	1:C:73:GLU:HG3	1.60	0.83
1:A:16:GLY:O	1:A:17:VAL:O	1.97	0.83
2:B:207:THR:HG21	4:B:2031:HOH:O	1.76	0.83
1:A:157:ARG:HD3	4:A:2083:HOH:O	1.80	0.82
1:C:91:MET:HE3	1:C:196:MET:HG2	1.60	0.82
2:B:430:LEU:HB3	2:B:432:LEU:HD21	1.60	0.82
2:D:395:HIS:ND1	4:D:2106:HOH:O	2.12	0.82
2:D:289:LYS:HD3	4:D:2064:HOH:O	1.78	0.81
1:C:131:GLN:HE21	1:C:131:GLN:H	1.22	0.81
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.15	0.81
1:C:71:HIS:CD2	4:C:2042:HOH:O	2.33	0.80
1:C:60:HIS:CD2	1:C:62:ASN:H	2.01	0.79
1:A:279:ALA:HB2	4:A:2126:HOH:O	1.82	0.79
2:D:196:LYS:HE3	4:D:2018:HOH:O	1.80	0.79
2:D:413:TYR:CZ	4:D:2082:HOH:O	2.34	0.78
2:D:430:LEU:HB3	2:D:432:LEU:CD2	2.13	0.78
2:D:210:MET:HA	3:F:506:FCL:HE2	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HD3	4:A:2092:HOH:O	1.81	0.78
2:D:179:HIS:NE2	2:D:379:LYS:NZ	2.32	0.78
2:B:190:GLU:OE1	2:B:352:PRO:HD2	1.84	0.78
1:C:39:THR:HG21	4:D:2065:HOH:O	1.83	0.78
2:B:205:ASP:OD2	2:B:250:ARG:HG3	1.84	0.78
1:C:164:VAL:CG1	1:C:165:THR:O	2.30	0.78
1:A:171:PRO:CD	4:A:2092:HOH:O	2.32	0.77
1:A:42:GLU:OE2	2:B:275:VAL:HG23	1.84	0.77
1:C:1:MET:N	4:C:2002:HOH:O	2.17	0.77
1:A:5:GLN:NE2	1:A:6:LYS:O	2.18	0.77
1:C:38:ASP:OD1	1:C:41:THR:OG1	2.03	0.76
2:B:179:HIS:NE2	2:B:379:LYS:HE3	1.99	0.76
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.67	0.76
2:B:423:LEU:CB	4:B:2112:HOH:O	2.34	0.75
1:A:287:GLN:HB3	4:A:2130:HOH:O	1.85	0.75
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.55	0.75
1:A:71:HIS:CE1	2:B:296:HIS:CE1	2.75	0.75
2:D:404:HIS:HD2	2:D:406:GLN:N	1.84	0.75
1:C:1:MET:CE	1:C:70:ILE:HD13	2.16	0.75
2:D:332:LEU:HD13	4:D:2125:HOH:O	1.87	0.75
1:A:15:TYR:HD2	1:A:33:LYS:CD	1.98	0.75
2:D:292:LEU:CD1	4:D:2068:HOH:O	2.35	0.75
1:A:71:HIS:CE1	2:B:296:HIS:NE2	2.55	0.74
2:D:293:ARG:CD	4:D:2064:HOH:O	2.34	0.74
1:A:163:VAL:O	1:A:163:VAL:HG13	1.88	0.74
1:A:17:VAL:CG2	4:A:2020:HOH:O	2.16	0.74
2:B:404:HIS:CD2	2:B:406:GLN:H	2.03	0.74
2:D:296:HIS:ND1	4:D:2070:HOH:O	2.19	0.74
2:D:349:LYS:CG	4:D:2093:HOH:O	2.35	0.74
2:D:335:PHE:N	4:D:2082:HOH:O	2.19	0.74
1:A:171:PRO:CB	4:A:2092:HOH:O	2.34	0.73
1:A:294:PRO:O	4:A:2134:HOH:O	2.07	0.73
1:A:121:HIS:O	1:A:122:ARG:HG3	1.89	0.73
1:C:73:GLU:HG2	4:D:2067:HOH:O	1.87	0.73
1:A:165:THR:HG23	4:A:2088:HOH:O	1.87	0.73
1:C:152:PHE:O	4:C:2075:HOH:O	2.07	0.73
2:D:323:GLN:O	2:D:323:GLN:HG2	1.87	0.73
2:B:424:LEU:N	4:B:2112:HOH:O	2.22	0.72
2:B:176:PRO:HB2	2:B:179:HIS:H	1.52	0.72
1:A:38:ASP:CG	1:A:41:THR:HG1	1.90	0.72
1:A:15:TYR:CD2	1:A:33:LYS:HD3	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:TYR:N	4:D:2020:HOH:O	2.23	0.72
1:C:91:MET:CE	1:C:196:MET:HG2	2.19	0.71
1:C:124:LEU:HD12	1:C:126:ARG:HG3	1.71	0.71
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.71	0.71
2:D:175:VAL:O	2:D:176:PRO:C	2.29	0.71
1:A:159:TYR:HB2	1:A:162:GLU:HB2	1.72	0.71
2:D:432:LEU:N	2:D:432:LEU:HD22	2.05	0.71
1:A:162:GLU:CD	1:A:164:VAL:HB	2.11	0.71
1:A:173:ILE:HD11	1:A:184:VAL:HG11	1.71	0.70
2:B:430:LEU:HB3	2:B:432:LEU:CD2	2.20	0.70
1:C:256:ASP:OD2	4:C:2117:HOH:O	2.08	0.70
1:C:1:MET:HE3	1:C:70:ILE:CD1	2.22	0.70
1:C:164:VAL:HG12	1:C:165:THR:N	2.06	0.70
1:C:51:GLU:O	1:C:55:LEU:HB2	1.91	0.70
1:A:101:LEU:N	1:A:102:PRO:CD	2.55	0.70
2:D:335:PHE:HA	4:D:2082:HOH:O	1.85	0.69
2:B:423:LEU:HB2	4:B:2112:HOH:O	1.91	0.69
2:D:179:HIS:NE2	2:D:379:LYS:CE	2.56	0.69
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.58	0.69
1:A:209:ILE:HB	4:A:2104:HOH:O	1.93	0.69
1:A:38:ASP:CG	1:A:41:THR:OG1	2.31	0.68
1:C:146:PHE:HB2	4:C:2032:HOH:O	1.92	0.68
2:D:349:LYS:HG2	4:D:2093:HOH:O	1.91	0.68
1:A:131:GLN:HG3	4:A:2074:HOH:O	1.92	0.68
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.11	0.68
2:B:343:ASP:HB3	2:B:345:ASP:HB2	1.76	0.68
1:C:278:LYS:NZ	2:D:177:ASP:O	2.25	0.68
2:D:414:LYS:HE2	2:D:423:LEU:HD21	1.76	0.68
1:A:33:LYS:HE2	4:A:2032:HOH:O	1.93	0.68
1:C:1:MET:CE	1:C:70:ILE:CD1	2.72	0.67
1:C:36:ARG:HG2	4:C:2026:HOH:O	1.95	0.67
2:B:285:THR:HB	3:E:503:ARG:NH2	2.09	0.67
1:C:95:ALA:HA	4:C:2101:HOH:O	1.93	0.67
1:A:257:GLU:HG3	1:A:260:ARG:NH2	2.09	0.67
2:D:198:GLY:N	4:D:2019:HOH:O	2.20	0.67
1:A:215:ILE:HD13	4:A:2092:HOH:O	1.94	0.67
2:B:374:GLU:HG2	4:B:2086:HOH:O	1.82	0.67
1:C:160:THR:OG1	4:C:2079:HOH:O	2.13	0.67
1:A:12:GLU:OE1	1:A:17:VAL:HG12	1.95	0.67
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.11	0.67
1:A:34:LYS:CD	4:A:2034:HOH:O	2.41	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:LYS:NZ	2:B:295:GLU:OE2	2.25	0.66
2:B:430:LEU:CB	2:B:432:LEU:CD2	2.74	0.66
1:C:160:THR:OG1	4:C:2080:HOH:O	2.12	0.66
1:A:150:ARG:NH1	4:A:2080:HOH:O	2.29	0.66
1:A:89:LYS:HE2	4:A:2062:HOH:O	1.95	0.66
1:C:71:HIS:CE1	2:D:296:HIS:CD2	2.84	0.66
1:A:171:PRO:CG	4:A:2092:HOH:O	2.44	0.66
1:A:238:PRO:HD2	4:A:2107:HOH:O	1.96	0.66
1:A:231:THR:HA	1:A:236:TYR:CD1	2.31	0.66
1:A:99:ILE:HA	4:A:2065:HOH:O	1.96	0.66
2:B:179:HIS:CD2	2:B:379:LYS:HE3	2.30	0.65
1:C:131:GLN:H	1:C:131:GLN:NE2	1.94	0.65
2:D:271:TYR:O	4:D:2053:HOH:O	2.13	0.65
1:C:71:HIS:ND1	2:D:296:HIS:NE2	2.44	0.65
2:B:285:THR:HB	3:E:503:ARG:CZ	2.26	0.65
1:A:227:TRP:O	1:A:230:VAL:CG2	2.44	0.65
1:A:236:TYR:CZ	4:A:2106:HOH:O	2.45	0.64
2:B:210:MET:HG2	3:E:506:FCL:CD2	2.27	0.64
1:A:236:TYR:CG	4:A:2106:HOH:O	2.50	0.64
1:A:65:LYS:HD2	4:A:2046:HOH:O	1.97	0.63
1:C:157:ARG:HD3	4:D:2038:HOH:O	1.99	0.63
1:A:91:MET:CE	1:A:196:MET:HG3	2.28	0.63
1:C:159:TYR:CB	1:C:162:GLU:HB3	2.28	0.63
2:B:240:ASP:O	2:B:244:SER:OG	2.16	0.63
1:C:91:MET:CE	1:C:196:MET:CG	2.77	0.63
2:B:289:LYS:O	2:B:293:ARG:HG3	1.98	0.63
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.79	0.63
2:B:282:THR:HB	2:B:285:THR:HG23	1.81	0.63
1:C:162:GLU:CD	1:C:164:VAL:HG23	2.19	0.63
2:D:361:HIS:CE1	2:D:384:LEU:CD1	2.81	0.63
1:C:164:VAL:CG1	1:C:165:THR:N	2.61	0.63
2:D:349:LYS:CB	4:D:2093:HOH:O	2.47	0.63
2:B:216:ASP:OD1	2:B:408:SER:HB2	1.98	0.62
1:C:160:THR:O	1:C:161:HIS:C	2.38	0.61
2:B:385:GLU:O	2:B:388:LYS:HB2	2.00	0.61
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.82	0.61
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.82	0.61
1:A:258:ASP:OD1	4:A:2121:HOH:O	2.15	0.61
2:B:194:LYS:NZ	4:B:2026:HOH:O	2.34	0.61
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.36	0.60
2:D:175:VAL:O	2:D:175:VAL:HG13	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:C	1:A:122:ARG:HG3	2.22	0.60
1:C:124:LEU:HD12	1:C:126:ARG:CG	2.30	0.60
1:A:227:TRP:O	1:A:230:VAL:HG23	1.99	0.60
1:A:34:LYS:HD3	4:A:2034:HOH:O	2.01	0.60
2:D:207:THR:HG22	2:D:210:MET:H	1.65	0.60
2:D:349:LYS:NZ	4:D:2094:HOH:O	2.34	0.60
2:D:233:HIS:HD2	4:D:2074:HOH:O	1.83	0.60
1:A:2:GLU:HG3	4:C:2044:HOH:O	2.01	0.60
1:A:34:LYS:HE3	4:A:2058:HOH:O	2.01	0.60
1:A:125:HIS:O	1:A:126:ARG:HB2	2.02	0.60
1:A:162:GLU:CG	1:A:164:VAL:HB	2.32	0.59
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.82	0.59
1:C:43:GLY:HA3	4:D:2068:HOH:O	2.02	0.59
2:D:198:GLY:C	4:D:2020:HOH:O	2.39	0.59
1:A:14:THR:O	1:A:15:TYR:CB	2.48	0.59
1:C:15:TYR:HD2	1:C:33:LYS:HD3	1.67	0.59
1:A:60:HIS:HD2	1:A:62:ASN:N	1.94	0.59
1:A:122:ARG:HB3	2:B:182:ILE:HG12	1.84	0.59
1:C:7:VAL:O	1:C:8:GLU:HB3	2.02	0.59
2:B:400:LYS:HE3	4:B:2096:HOH:O	2.03	0.59
2:D:418:TYR:O	2:D:421:VAL:HG13	2.03	0.59
1:C:15:TYR:CE2	1:C:33:LYS:HD2	2.38	0.58
2:D:198:GLY:CA	4:D:2019:HOH:O	2.50	0.58
1:A:164:VAL:HG12	1:A:165:THR:O	2.02	0.58
1:A:244:ALA:HB3	4:A:2110:HOH:O	2.03	0.58
2:D:207:THR:HG22	2:D:210:MET:HG3	1.84	0.58
1:C:159:TYR:HB3	1:C:162:GLU:HB3	1.84	0.58
1:A:162:GLU:OE1	1:A:164:VAL:HB	2.03	0.58
1:A:164:VAL:CG1	1:A:165:THR:N	2.67	0.58
1:A:101:LEU:HB3	4:A:2067:HOH:O	2.03	0.58
2:D:179:HIS:CE1	2:D:379:LYS:HZ1	2.22	0.58
1:A:14:THR:O	1:A:15:TYR:HB2	2.02	0.58
1:A:287:GLN:CB	4:A:2130:HOH:O	2.45	0.58
1:A:1:MET:HG3	1:A:77:TYR:CE1	2.38	0.58
1:A:198:THR:O	1:A:199:ARG:HB2	2.04	0.57
2:B:179:HIS:CE1	2:B:379:LYS:HZ1	2.22	0.57
1:C:1:MET:HE3	1:C:70:ILE:HD12	1.85	0.57
2:D:270:ILE:HD13	2:D:270:ILE:N	2.19	0.57
4:C:2072:HOH:O	2:D:270:ILE:CD1	2.53	0.57
1:C:164:VAL:HG12	1:C:165:THR:C	2.22	0.57
1:A:101:LEU:N	1:A:102:PRO:HD3	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HD3	1:A:173:ILE:HG21	1.86	0.56
2:B:283:ASP:OD2	3:E:501:ACE:H2	2.04	0.56
2:D:293:ARG:HD2	4:D:2064:HOH:O	2.01	0.56
2:D:415:ASN:OD1	2:D:417:LYS:HB3	2.05	0.56
1:A:51:GLU:O	1:A:55:LEU:HB2	2.05	0.56
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.69	0.56
2:D:362:LEU:CD1	2:D:430:LEU:HD21	2.35	0.56
1:A:1:MET:N	4:A:2002:HOH:O	1.90	0.56
1:A:33:LYS:CE	4:A:2033:HOH:O	2.09	0.56
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.41	0.56
1:C:177:CYS:HB3	1:C:233:MET:CE	2.36	0.56
1:A:27:GLY:HA3	2:D:249:LEU:HD22	1.87	0.55
1:C:41:THR:HA	4:C:2030:HOH:O	2.04	0.55
1:A:2:GLU:CG	4:C:2044:HOH:O	2.52	0.55
1:A:182:THR:HG1	2:B:178:TYR:HH	1.52	0.55
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.89	0.55
2:B:226:LYS:HE2	4:B:2040:HOH:O	2.06	0.55
1:C:1:MET:HE3	1:C:70:ILE:HD13	1.85	0.55
1:C:214:ARG:HG2	1:C:214:ARG:NH1	2.05	0.55
2:B:323:GLN:HA	4:B:2074:HOH:O	2.07	0.55
2:B:368:THR:OG1	2:B:370:GLN:HB2	2.07	0.55
1:A:244:ALA:N	4:A:2110:HOH:O	2.29	0.55
1:A:18:VAL:HG22	1:A:33:LYS:HG2	1.88	0.55
1:A:71:HIS:ND1	2:B:296:HIS:NE2	2.55	0.55
1:A:59:ASN:HB3	4:A:2049:HOH:O	2.07	0.54
1:C:206:ASP:HA	4:C:2104:HOH:O	2.06	0.54
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.37	0.54
2:D:198:GLY:HA3	4:D:2019:HOH:O	2.05	0.54
2:B:398:TYR:OH	4:B:2095:HOH:O	2.15	0.54
2:D:271:TYR:N	4:D:2054:HOH:O	2.37	0.54
1:A:16:GLY:O	1:A:17:VAL:C	2.45	0.54
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.42	0.54
2:B:178:TYR:O	2:B:179:HIS:C	2.45	0.54
1:A:1:MET:N	4:A:2003:HOH:O	2.40	0.54
1:A:84:HIS:CE1	1:A:296:LEU:HG	2.43	0.54
1:C:15:TYR:CD2	1:C:33:LYS:HD3	2.44	0.53
2:D:332:LEU:O	2:D:335:PHE:HB3	2.09	0.53
1:A:163:VAL:O	1:A:163:VAL:CG1	2.56	0.53
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.90	0.53
1:A:108:LEU:HG	1:A:112:LEU:HD12	1.91	0.53
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HE2	1:A:196:MET:CG	2.27	0.53
1:C:78:LEU:N	1:C:78:LEU:HD23	2.23	0.53
2:B:283:ASP:OD2	3:E:501:ACE:CH3	2.57	0.53
2:D:430:LEU:O	2:D:431:ASN:CB	2.35	0.53
2:B:404:HIS:HD2	2:B:406:GLN:N	1.97	0.53
1:A:217:ARG:HG2	4:A:2109:HOH:O	2.09	0.52
1:C:15:TYR:CD2	1:C:33:LYS:CD	2.92	0.52
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.91	0.52
1:A:91:MET:HE3	1:A:196:MET:CG	2.40	0.52
2:D:198:GLY:HA3	2:D:201:LYS:NZ	2.24	0.52
1:A:1:MET:CE	1:A:70:ILE:CD1	2.88	0.52
2:B:345:ASP:CB	2:B:346:PRO:CD	2.88	0.52
2:D:401:ALA:N	2:D:402:PRO:CD	2.73	0.52
1:C:223:ASP:OD1	1:C:226:VAL:HG23	2.09	0.52
1:A:15:TYR:CD2	1:A:33:LYS:CD	2.88	0.52
2:D:323:GLN:CG	4:D:2078:HOH:O	2.58	0.52
2:B:388:LYS:O	2:B:392:MET:HG3	2.10	0.52
2:B:423:LEU:C	4:B:2112:HOH:O	2.48	0.52
2:D:335:PHE:HB2	4:D:2082:HOH:O	2.08	0.52
1:C:9:LYS:HE3	1:C:12:GLU:OE1	2.10	0.52
2:D:371:SER:O	2:D:372:TRP:C	2.48	0.52
2:D:432:LEU:N	2:D:432:LEU:CD2	2.71	0.52
1:A:165:THR:C	4:A:2088:HOH:O	2.48	0.51
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.45	0.51
1:A:14:THR:O	1:A:15:TYR:CG	2.63	0.51
1:A:169:ARG:NH1	4:A:2091:HOH:O	2.43	0.51
2:B:289:LYS:O	2:B:293:ARG:CG	2.59	0.51
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.41	0.51
1:C:170:ALA:HB3	1:C:173:ILE:HD12	1.91	0.51
4:C:2072:HOH:O	2:D:270:ILE:HD11	2.09	0.51
1:A:159:TYR:HD1	1:A:159:TYR:N	2.09	0.51
1:C:15:TYR:HD2	1:C:33:LYS:CD	2.24	0.51
1:C:165:THR:HB	4:C:2085:HOH:O	2.11	0.51
2:B:416:SER:O	2:B:417:LYS:C	2.49	0.50
2:D:338:GLU:OE1	2:D:412:LYS:NZ	2.44	0.50
1:A:169:ARG:CZ	4:A:2091:HOH:O	2.59	0.50
1:A:71:HIS:ND1	2:B:296:HIS:CE1	2.80	0.50
2:D:323:GLN:HG3	4:D:2078:HOH:O	2.12	0.50
1:C:165:THR:N	4:C:2085:HOH:O	2.43	0.50
1:C:55:LEU:HD13	4:C:2032:HOH:O	2.11	0.50
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:MET:HE3	1:C:196:MET:CG	2.35	0.50
1:C:1:MET:HG3	1:C:77:TYR:CE1	2.46	0.50
2:D:401:ALA:N	2:D:402:PRO:HD3	2.26	0.50
2:D:404:HIS:HA	4:D:2113:HOH:O	2.12	0.50
2:B:387:LEU:HD23	4:B:2090:HOH:O	2.11	0.50
2:B:430:LEU:HB2	2:B:432:LEU:CD2	2.41	0.50
1:C:162:GLU:OE1	1:C:164:VAL:HG21	2.09	0.50
2:B:421:VAL:HA	4:B:2109:HOH:O	2.12	0.50
1:C:71:HIS:CG	4:C:2042:HOH:O	2.60	0.50
1:C:65:LYS:HE2	4:C:2009:HOH:O	2.11	0.49
1:A:295:HIS:NE2	4:A:2135:HOH:O	2.34	0.49
1:C:258:ASP:OD2	4:C:2123:HOH:O	2.20	0.49
2:D:343:ASP:C	2:D:345:ASP:H	2.14	0.49
1:A:162:GLU:HG3	1:A:164:VAL:N	2.26	0.49
1:A:279:ALA:CB	4:A:2126:HOH:O	2.50	0.49
2:B:204:PRO:HG2	4:B:2004:HOH:O	2.11	0.49
1:C:214:ARG:NH1	1:C:214:ARG:CG	2.74	0.49
3:F:503:ARG:HD3	4:F:2003:HOH:O	2.10	0.49
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.48	0.49
1:A:223:ASP:HB2	4:A:2105:HOH:O	2.12	0.49
1:A:1:MET:CE	1:A:70:ILE:HD13	2.43	0.49
2:D:413:TYR:CD2	4:D:2082:HOH:O	2.58	0.49
1:C:121:HIS:O	1:C:122:ARG:HG3	2.13	0.49
1:C:41:THR:O	2:D:288:LYS:HE2	2.12	0.49
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.93	0.49
1:A:37:LEU:N	4:A:2038:HOH:O	2.45	0.49
2:D:428:GLU:HG2	4:D:2127:HOH:O	2.13	0.49
1:A:15:TYR:HE2	1:A:51:GLU:OE1	1.96	0.48
1:A:236:TYR:CE1	4:A:2106:HOH:O	2.64	0.48
2:D:293:ARG:NE	4:D:2064:HOH:O	2.44	0.48
2:D:431:ASN:HB3	4:D:2130:HOH:O	2.13	0.48
1:C:121:HIS:C	1:C:122:ARG:HG3	2.33	0.48
2:D:296:HIS:CG	4:D:2070:HOH:O	2.64	0.48
2:D:423:LEU:O	2:D:424:LEU:O	2.30	0.48
1:C:291:LYS:HD3	4:C:2140:HOH:O	2.12	0.48
3:E:505:ASN:ND2	4:E:2005:HOH:O	2.45	0.48
2:B:249:LEU:O	2:B:250:ARG:C	2.52	0.48
1:C:71:HIS:HB2	4:C:2042:HOH:O	2.13	0.48
1:C:7:VAL:C	4:C:2006:HOH:O	2.52	0.48
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.95	0.48
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.49	0.48
1:C:38:ASP:CB	4:C:2028:HOH:O	2.16	0.48
1:C:64:VAL:HG22	1:C:143:LEU:O	2.14	0.48
1:A:129:LYS:CE	4:A:2073:HOH:O	2.62	0.47
1:A:131:GLN:CG	4:A:2074:HOH:O	2.55	0.47
1:A:247:ASP:HB3	4:A:2116:HOH:O	2.14	0.47
1:A:159:TYR:N	1:A:159:TYR:CD1	2.82	0.47
1:A:15:TYR:CE2	1:A:51:GLU:OE1	2.67	0.47
2:D:323:GLN:HA	2:D:324:PRO:HA	1.61	0.47
1:A:162:GLU:HB3	4:A:2091:HOH:O	2.15	0.47
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.95	0.47
1:A:52:ILE:O	1:A:56:LYS:HB2	2.14	0.47
1:C:15:TYR:OH	1:C:51:GLU:OE1	2.23	0.47
1:C:22:ARG:CD	4:C:2014:HOH:O	2.37	0.47
1:A:159:TYR:O	1:A:160:THR:C	2.52	0.47
1:A:198:THR:O	1:A:199:ARG:CB	2.63	0.47
1:A:36:ARG:O	1:A:38:ASP:N	2.47	0.47
1:A:162:GLU:HG2	4:A:2091:HOH:O	2.14	0.47
1:A:217:ARG:CB	4:A:2109:HOH:O	2.63	0.47
1:C:132:ASN:HA	4:C:2068:HOH:O	2.15	0.47
3:F:501:ACE:H1	3:F:502:ARG:HB2	1.96	0.47
1:A:236:TYR:CD1	4:A:2106:HOH:O	2.68	0.47
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.47	0.47
1:C:84:HIS:HD2	1:C:85:GLN:HG2	1.80	0.47
2:D:176:PRO:HB3	2:D:178:TYR:CE2	2.50	0.47
1:A:42:GLU:HG2	4:A:2041:HOH:O	2.15	0.46
2:D:431:ASN:N	2:D:432:LEU:HD22	2.30	0.46
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.98	0.46
1:C:6:LYS:CE	4:C:2023:HOH:O	2.47	0.46
2:D:179:HIS:NE2	2:D:379:LYS:HE3	2.27	0.46
2:D:263:LEU:HD21	2:D:295:GLU:HG3	1.97	0.46
1:C:15:TYR:CD2	1:C:33:LYS:HD2	2.51	0.46
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.98	0.46
2:B:207:THR:CG2	2:B:210:MET:H	2.21	0.46
3:E:505:ASN:HD22	3:E:505:ASN:C	2.19	0.46
1:A:2:GLU:HG2	1:C:73:GLU:CG	2.39	0.46
2:B:245:SER:CB	4:B:2045:HOH:O	2.43	0.46
1:A:166:LEU:HD23	1:A:205:GLY:O	2.16	0.46
2:D:428:GLU:HB3	4:D:2007:HOH:O	2.15	0.46
1:A:159:TYR:HB2	1:A:162:GLU:CB	2.44	0.45
1:A:164:VAL:HG13	1:A:165:THR:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.80	0.45
1:A:125:HIS:CE1	1:A:128:LEU:HD23	2.52	0.45
2:B:224:GLU:HG3	2:B:224:GLU:O	2.16	0.45
1:A:131:GLN:CD	4:A:2074:HOH:O	2.54	0.45
2:D:346:PRO:O	2:D:349:LYS:HB2	2.16	0.45
1:A:270:ASP:OD1	1:A:270:ASP:C	2.54	0.45
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.97	0.45
1:A:119:HIS:CE1	1:A:182:THR:HB	2.52	0.45
1:A:1:MET:CE	1:A:70:ILE:HD12	2.47	0.45
1:A:244:ALA:CA	4:A:2110:HOH:O	2.63	0.45
1:C:15:TYR:HE2	1:C:33:LYS:HD2	1.80	0.45
2:B:319:PHE:CD2	2:B:330:GLU:HG2	2.52	0.45
1:C:159:TYR:N	1:C:159:TYR:HD1	2.15	0.45
1:C:92:ASP:C	1:C:94:SER:H	2.20	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD3	1.82	0.44
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.79	0.44
2:B:179:HIS:NE2	2:B:379:LYS:CD	2.80	0.44
1:C:71:HIS:CG	2:D:296:HIS:HE2	2.36	0.44
1:C:91:MET:CE	1:C:196:MET:HG3	2.47	0.44
2:B:207:THR:HG22	2:B:210:MET:CG	2.47	0.44
2:B:225:TYR:HE1	2:B:281:ILE:CG2	2.30	0.44
2:D:429:THR:OG1	2:D:430:LEU:N	2.47	0.44
1:A:227:TRP:O	1:A:230:VAL:HG22	2.16	0.44
1:C:131:GLN:HE21	1:C:131:GLN:N	2.03	0.44
1:C:165:THR:HG23	4:C:2084:HOH:O	2.16	0.44
2:D:374:GLU:HB2	4:D:2098:HOH:O	2.17	0.44
1:A:71:HIS:HD2	4:B:2009:HOH:O	2.01	0.44
2:D:421:VAL:O	2:D:424:LEU:HB2	2.18	0.44
1:C:34:LYS:NZ	4:C:2023:HOH:O	2.49	0.44
1:C:95:ALA:O	1:C:96:LEU:HB2	2.13	0.44
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.99	0.44
1:C:161:HIS:N	4:C:2081:HOH:O	2.41	0.44
2:D:210:MET:HG2	3:F:506:FCL:CE2	2.48	0.44
1:A:163:VAL:HG22	4:A:2087:HOH:O	2.17	0.43
2:B:282:THR:CB	2:B:285:THR:HG23	2.46	0.43
2:B:423:LEU:O	2:B:424:LEU:C	2.56	0.43
1:A:227:TRP:CG	1:A:230:VAL:HG22	2.53	0.43
1:A:108:LEU:O	1:A:112:LEU:HD12	2.18	0.43
2:B:229:ASN:HB3	4:B:2078:HOH:O	2.17	0.43
2:B:345:ASP:CB	2:B:346:PRO:HD3	2.47	0.43
1:C:99:ILE:HA	4:C:2050:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:LEU:HD23	2:D:315:LEU:HA	1.87	0.43
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.90	0.43
1:A:65:LYS:N	1:A:81:GLU:OE1	2.50	0.43
1:C:158:THR:HG21	4:C:2090:HOH:O	2.17	0.43
1:C:159:TYR:N	1:C:159:TYR:CD1	2.86	0.43
2:D:404:HIS:CA	4:D:2113:HOH:O	2.66	0.43
2:B:268:GLU:HG3	2:B:268:GLU:O	2.19	0.43
2:B:345:ASP:HB3	2:B:346:PRO:HD3	2.00	0.43
2:B:430:LEU:O	2:B:431:ASN:HB2	2.18	0.43
2:D:275:VAL:HG21	2:D:292:LEU:HD11	2.00	0.43
2:D:417:LYS:HG2	2:D:418:TYR:CD2	2.54	0.43
1:A:231:THR:HA	4:A:2106:HOH:O	2.19	0.43
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.39	0.43
2:D:343:ASP:C	2:D:345:ASP:N	2.71	0.43
2:D:362:LEU:HD11	2:D:430:LEU:HD21	1.99	0.43
1:A:207:SER:O	1:A:208:GLU:C	2.56	0.43
1:A:60:HIS:CG	1:A:61:PRO:CD	3.02	0.43
1:A:84:HIS:HB3	4:A:2060:HOH:O	2.18	0.43
1:A:212:LEU:HD22	1:A:216:PHE:CE1	2.54	0.42
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.55	0.42
2:B:372:TRP:HA	2:B:373:PRO:HD3	1.85	0.42
1:C:137:THR:HA	1:C:296:LEU:HD21	2.01	0.42
1:C:146:PHE:CB	4:C:2032:HOH:O	2.59	0.42
3:E:505:ASN:ND2	4:E:2006:HOH:O	2.52	0.42
1:A:1:MET:HE2	1:A:70:ILE:HD13	2.00	0.42
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.85	0.42
1:C:101:LEU:N	1:C:102:PRO:CD	2.82	0.42
1:C:61:PRO:O	1:C:142:LYS:HD3	2.20	0.42
1:A:129:LYS:HA	1:A:192:ILE:HD11	2.01	0.42
1:A:175:LEU:HD12	1:A:227:TRP:CH2	2.55	0.42
1:C:16:GLY:O	1:C:17:VAL:C	2.57	0.42
2:D:176:PRO:HB2	2:D:179:HIS:H	1.84	0.42
2:D:366:THR:OG1	2:D:427:PRO:HD3	2.19	0.42
3:E:502:ARG:NE	4:E:2001:HOH:O	2.51	0.42
1:A:239:SER:N	4:A:2107:HOH:O	2.49	0.42
2:D:225:TYR:CE1	2:D:281:ILE:HG21	2.47	0.42
1:C:160:THR:N	4:C:2079:HOH:O	2.51	0.42
1:C:221:THR:HA	1:C:222:PRO:HD2	1.89	0.42
1:A:20:LYS:HD3	1:A:82:PHE:CE2	2.55	0.42
1:A:217:ARG:CG	4:A:2109:HOH:O	2.68	0.42
2:B:176:PRO:HB3	2:B:178:TYR:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:CG2	1:C:293:VAL:O	2.67	0.42
1:A:248:PHE:N	4:A:2115:HOH:O	2.52	0.42
1:C:105:LYS:NZ	1:C:288:ASP:OD1	2.51	0.42
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.77	0.42
1:A:42:GLU:OE2	2:B:275:VAL:N	2.39	0.41
2:D:198:GLY:HA3	2:D:201:LYS:HZ1	1.85	0.41
2:D:360:PHE:O	2:D:361:HIS:C	2.57	0.41
2:D:417:LYS:HG2	2:D:418:TYR:CE2	2.54	0.41
2:D:335:PHE:CB	4:D:2082:HOH:O	2.54	0.41
2:D:404:HIS:N	4:D:2113:HOH:O	2.53	0.41
2:B:401:ALA:HB3	2:B:402:PRO:HD3	2.02	0.41
1:C:65:LYS:HE3	1:C:65:LYS:HB3	1.83	0.41
2:D:218:LEU:HD23	2:D:218:LEU:HA	1.78	0.41
2:D:285:THR:O	2:D:285:THR:HG22	2.21	0.41
3:E:501:ACE:H2	3:E:502:ARG:HA	1.92	0.41
1:A:111:LEU:HD22	1:A:133:LEU:HD22	2.02	0.41
2:B:282:THR:O	2:B:285:THR:HG21	2.12	0.41
1:A:170:ALA:HB1	1:A:171:PRO:HD2	2.01	0.41
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.86	0.41
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.84	0.41
2:B:283:ASP:O	2:B:284:ASP:C	2.58	0.41
2:D:271:TYR:HB2	4:D:2055:HOH:O	2.21	0.41
1:A:177:CYS:SG	1:A:178:LYS:N	2.94	0.41
1:A:253:PRO:CD	1:A:254:PRO:HD3	2.50	0.41
2:B:207:THR:HG22	2:B:210:MET:HG3	2.02	0.41
1:C:253:PRO:HB2	1:C:254:PRO:HD3	2.03	0.41
1:A:173:ILE:HA	4:A:2093:HOH:O	2.20	0.41
1:A:288:ASP:OD1	1:A:288:ASP:N	2.49	0.41
1:A:84:HIS:HE1	1:A:296:LEU:HG	1.86	0.41
1:C:86:ASP:C	1:C:86:ASP:OD1	2.59	0.41
2:B:335:PHE:CZ	2:B:422:SER:HB2	2.56	0.40
1:C:1:MET:CE	1:C:70:ILE:HD12	2.46	0.40
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.88	0.40
2:D:254:GLN:NE2	3:F:504:LEU:HG	2.36	0.40
1:A:162:GLU:HB3	4:A:2086:HOH:O	2.21	0.40
1:A:2:GLU:H	1:A:2:GLU:CD	2.24	0.40
2:B:249:LEU:HD22	1:C:27:GLY:HA3	2.04	0.40
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.75	0.40
1:A:1:MET:HE3	1:A:70:ILE:CD1	2.52	0.40
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.77	0.40
1:C:260:ARG:O	1:C:264:SER:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:ALA:N	2:B:402:PRO:CD	2.84	0.40
1:C:152:PHE:CD2	1:C:152:PHE:O	2.75	0.40
2:D:399:LEU:HD23	2:D:399:LEU:HA	1.82	0.40
2:D:223:GLU:CD	2:D:412:LYS:HG3	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.96	0.24

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	294/298 (99%)	277 (94%)	11 (4%)	6 (2%)	9 15
1	C	294/298 (99%)	272 (92%)	17 (6%)	5 (2%)	11 19
2	B	256/260 (98%)	238 (93%)	13 (5%)	5 (2%)	9 15
2	D	256/260 (98%)	235 (92%)	14 (6%)	7 (3%)	6 9
3	E	4/7 (57%)	4 (100%)	0	0	100 100
3	F	4/7 (57%)	4 (100%)	0	0	100 100
All	All	1108/1130 (98%)	1030 (93%)	55 (5%)	23 (2%)	9 14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	17	VAL
1	A	37	LEU
1	A	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	345	ASP
2	B	346	PRO
2	B	424	LEU
1	C	96	LEU
2	D	415	ASN
2	D	431	ASN
1	A	160	THR
1	C	161	HIS
1	C	249	SER
2	D	346	PRO
2	D	417	LYS
1	C	160	THR
2	D	176	PRO
2	D	424	LEU
2	B	370	GLN
2	B	415	ASN
1	C	93	ALA
2	D	372	TRP
1	A	153	GLY

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	261/263 (99%)	226 (87%)	35 (13%)	5 9
1	C	261/263 (99%)	222 (85%)	39 (15%)	4 6
2	B	232/234 (99%)	207 (89%)	25 (11%)	8 15
2	D	232/234 (99%)	205 (88%)	27 (12%)	7 13
3	E	4/4 (100%)	2 (50%)	2 (50%)	0 0
3	F	4/4 (100%)	4 (100%)	0	100 100
All	All	994/1002 (99%)	866 (87%)	128 (13%)	5 10

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	9	LYS
1	A	12	GLU
1	A	36	ARG
1	A	37	LEU
1	A	41	THR
1	A	55	LEU
1	A	56	LYS
1	A	71	HIS
1	A	74	ASN
1	A	76	LEU
1	A	85	GLN
1	A	87	LEU
1	A	89	LYS
1	A	101	LEU
1	A	105	LYS
1	A	115	LEU
1	A	122	ARG
1	A	154	VAL
1	A	158	THR
1	A	160	THR
1	A	161	HIS
1	A	162	GLU
1	A	189	LEU
1	A	200	ARG
1	A	202	LEU
1	A	230	VAL
1	A	232	SER
1	A	242	LYS
1	A	249	SER
1	A	250	LYS
1	A	252	VAL
1	A	257	GLU
1	A	287	GLN
1	A	293	VAL
2	B	178	TYR
2	B	197	VAL
2	B	199	TYR
2	B	202	LYS
2	B	224	GLU
2	B	232	LEU
2	B	244	SER
2	B	245	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	249	LEU
2	B	283	ASP
2	B	285	THR
2	B	288	LYS
2	B	289	LYS
2	B	292	LEU
2	B	323	GLN
2	B	328	LYS
2	B	348	LEU
2	B	364	LEU
2	B	374	GLU
2	B	375	SER
2	B	378	ARG
2	B	391	LEU
2	B	422	SER
2	B	424	LEU
2	B	429	THR
1	C	2	GLU
1	C	6	LYS
1	C	9	LYS
1	C	12	GLU
1	C	14	THR
1	C	22	ARG
1	C	34	LYS
1	C	37	LEU
1	C	41	THR
1	C	55	LEU
1	C	56	LYS
1	C	64	VAL
1	C	71	HIS
1	C	75	LYS
1	C	78	LEU
1	C	87	LEU
1	C	89	LYS
1	C	101	LEU
1	C	115	LEU
1	C	122	ARG
1	C	124	LEU
1	C	131	GLN
1	C	145	ASP
1	C	154	VAL
1	C	158	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	166	LEU
1	C	177	CYS
1	C	181	SER
1	C	193	PHE
1	C	217	ARG
1	C	232	SER
1	C	237	LYS
1	C	242	LYS
1	C	250	LYS
1	C	252	VAL
1	C	264	SER
1	C	278	LYS
1	C	293	VAL
1	C	296	LEU
2	D	178	TYR
2	D	192	LYS
2	D	196	LYS
2	D	199	TYR
2	D	201	LYS
2	D	207	THR
2	D	209	SER
2	D	224	GLU
2	D	232	LEU
2	D	249	LEU
2	D	281	ILE
2	D	283	ASP
2	D	289	LYS
2	D	293	ARG
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	364	LEU
2	D	374	GLU
2	D	378	ARG
2	D	391	LEU
2	D	412	LYS
2	D	416	SER
2	D	417	LYS
2	D	424	LEU
2	D	428	GLU
2	D	429	THR
3	E	502	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	505	ASN

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	59	ASN
1	A	60	HIS
1	A	84	HIS
1	A	131	GLN
2	B	208	ASN
2	B	229	ASN
2	B	233	HIS
2	B	323	GLN
2	B	404	HIS
2	B	431	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	131	GLN
1	C	287	GLN
2	D	208	ASN
2	D	229	ASN
2	D	233	HIS
2	D	404	HIS
3	E	505	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FCL	E	506	3	10,12,13	0.75	1 (10%)	13,15,17	1.63	3 (23%)
3	FCL	F	506	3	10,12,13	0.77	0	13,15,17	2.39	5 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FCL	E	506	3	-	0/4/6/8	0/1/1/1
3	FCL	F	506	3	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	506	FCL	CE1-CL1	2.13	1.79	1.74

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	506	FCL	CB-CG-CD2	-4.25	112.32	120.91
3	F	506	FCL	CG-CB-CA	-4.06	104.76	114.12
3	E	506	FCL	CG-CB-CA	-3.50	106.06	114.12
3	F	506	FCL	O-C-CA	-2.97	117.75	125.72
3	E	506	FCL	O-C-CA	-2.91	117.92	125.72
3	F	506	FCL	CE1-CD1-CG	-2.89	116.88	119.71
3	E	506	FCL	CB-CG-CD2	-2.14	116.59	120.91
3	F	506	FCL	CB-CG-CD1	3.48	126.94	120.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	506	FCL	1	0
3	F	506	FCL	2	0

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

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	296/298 (99%)	-0.01	9 (3%) 54 59	25, 44, 88, 108	1 (0%)
1	C	296/298 (99%)	-0.02	14 (4%) 35 40	23, 42, 86, 122	0
2	B	258/260 (99%)	-0.10	12 (4%) 35 40	25, 42, 71, 116	0
2	D	258/260 (99%)	-0.04	6 (2%) 64 67	19, 43, 73, 111	0
3	E	4/7 (57%)	-0.03	0 100 100	30, 39, 52, 70	4 (100%)
3	F	4/7 (57%)	0.21	1 (25%) 1 1	41, 57, 59, 75	0
All	All	1116/1130 (98%)	-0.04	42 (3%) 44 49	19, 43, 83, 122	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	6.4
1	C	40	GLU	5.8
2	B	175	VAL	4.9
1	A	95	ALA	4.7
1	C	14	THR	4.2
1	C	163	VAL	4.1
1	A	296	LEU	4.1
2	B	325	ALA	3.8
1	A	96	LEU	3.7
2	B	176	PRO	3.6
2	D	323	GLN	3.5
1	A	159	TYR	3.4
2	B	324	PRO	3.0
2	D	325	ALA	3.0
2	D	432	LEU	2.9
1	C	95	ALA	2.8
1	C	165	THR	2.7
1	C	98	GLY	2.7
1	C	13	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	378	ARG	2.6
1	C	38	ASP	2.5
2	B	179	HIS	2.5
1	C	36	ARG	2.4
1	A	163	VAL	2.4
2	B	178	TYR	2.4
1	C	96	LEU	2.4
3	F	505	ASN	2.3
1	C	295	HIS	2.3
1	A	177	CYS	2.3
1	C	296	LEU	2.3
1	A	36	ARG	2.3
1	C	164	VAL	2.2
1	A	160	THR	2.2
2	B	423	LEU	2.2
2	B	201	LYS	2.2
2	B	323	GLN	2.1
2	D	358	ALA	2.1
2	D	359	ALA	2.1
2	D	179	HIS	2.1
2	B	432	LEU	2.1
2	B	345	ASP	2.0
1	A	243	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FCL	F	506	12/13	0.79	0.22	-	52,60,71,75	0
3	FCL	E	506	12/13	0.88	0.17	-	55,62,68,71	12

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.