Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:41 PM GMT

PDB ID	:	1URC
Title	:	Cyclin A binding groove inhibitor Ace-Arg-Lys-Leu-Phe-Gly
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	:	2003-10-28
Resolution	:	2.60 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 ⓘ symbol.

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

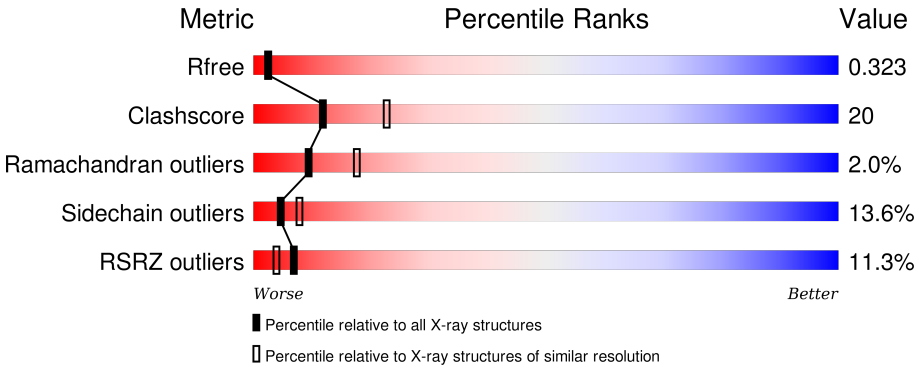
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	4% 60% 30% 6%
1	C	298	27% 60% 30% 7%
2	B	260	6% 62% 30% 6%
2	D	260	6% 63% 29% 6%
3	E	6	17% 67% 33%

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Mol	Chain	Length	Quality of chain
3	F	6	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9357 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	297	Total	C	N	O	S	0	0	1
			2379	1547	404	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	1	0
			2087	1352	339	384	12			

- Molecule 3 is a protein called PEPTIDE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			46	31	9	6			
3	F	6	Total	C	N	O	0	0	0
			46	31	9	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	75	Total	O	0	0
			75	75		
4	C	82	Total	O	0	0
			82	82		
4	D	95	Total	O	0	0
			95	95		

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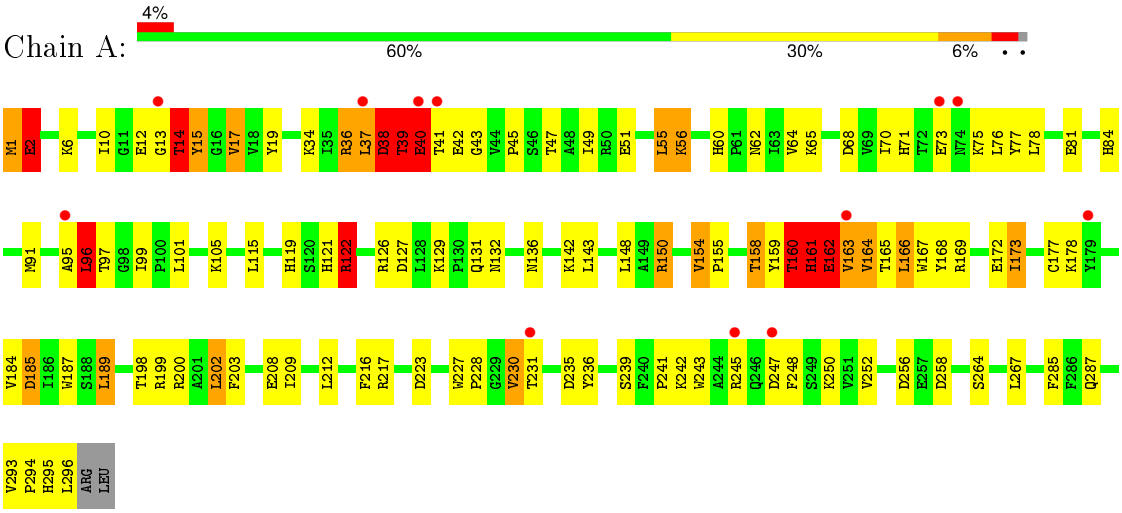
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O 1 1	0	0
4	F	4	Total O 4 4	0	0

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.

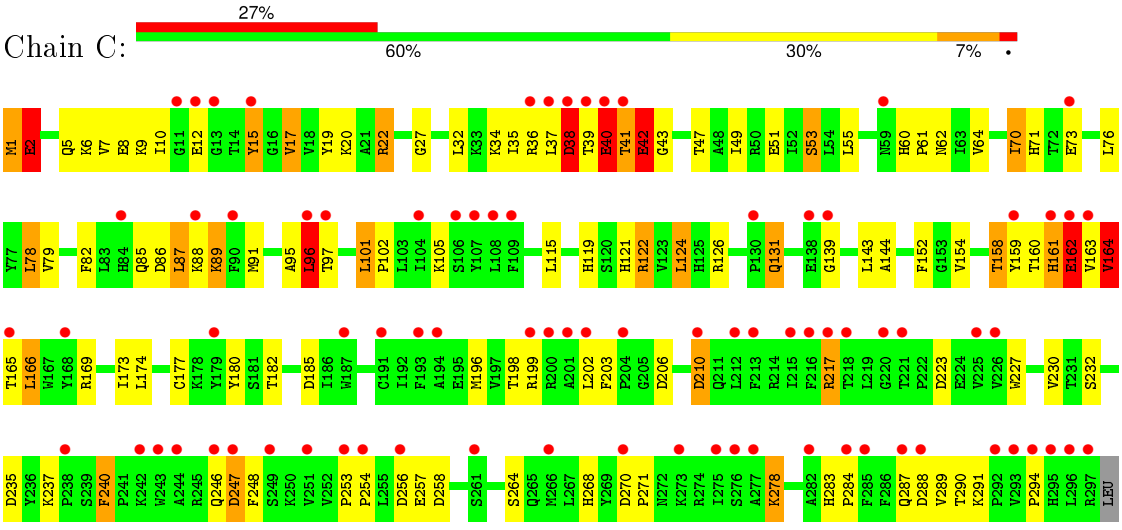
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



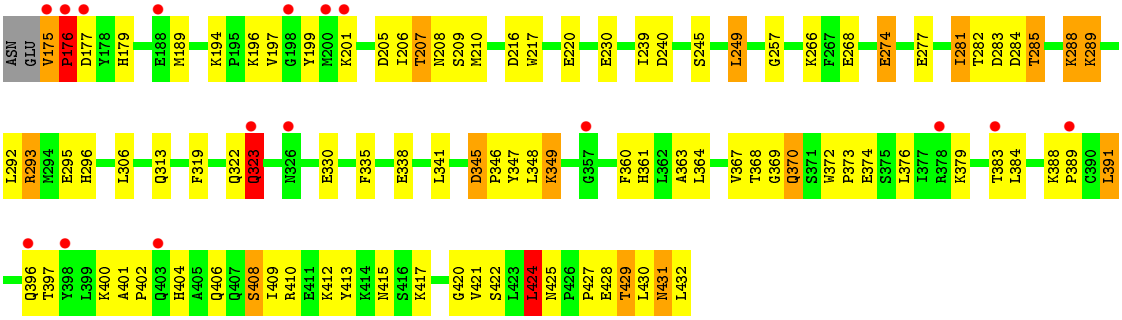
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:



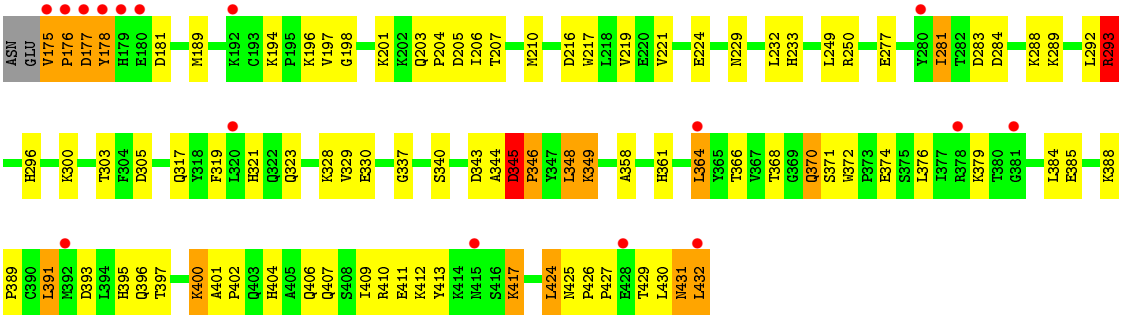
- Molecule 2: CYCLIN A2

Chain B:



- Molecule 2: CYCLIN A2

Chain D:



- Molecule 3: PEPTIDE INHIBITOR

Chain E:

- Molecule 3: PEPTIDE INHIBITOR

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.63Å 113.51Å 155.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.60 17.84 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (14.00-2.60) 96.4 (17.84-2.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.56Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.254 0.288 , 0.323	Depositor DCC
R_{free} test set	1257 reflections (3.24%)	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	3 of 40801 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.67	0/2440	1.13	15/3313 (0.5%)
1	C	0.66	0/2441	1.12	12/3315 (0.4%)
2	B	0.63	0/2133	1.04	5/2896 (0.2%)
2	D	0.65	0/2142	1.08	11/2907 (0.4%)
3	E	13.37	2/44 (4.5%)	16.51	6/56 (10.7%)
3	F	13.29	2/44 (4.5%)	16.64	7/56 (12.5%)
All	All	1.45	4/9244 (0.0%)	1.91	56/12543 (0.4%)

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	7
1	C	0	6
2	B	0	1
2	D	0	2
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	505	PHE	CG-CD2	68.72	2.41	1.38
3	E	504	PHE	CG-CD2	68.23	2.41	1.38
3	E	504	PHE	CE2-CZ	56.52	2.44	1.37
3	F	505	PHE	CE2-CZ	55.12	2.42	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	505	PHE	CG-CD2-CE2	-82.91	29.60	120.80
3	E	504	PHE	CG-CD2-CE2	-82.15	30.44	120.80
3	E	504	PHE	CZ-CE2-CD2	-75.90	29.02	120.10
3	F	505	PHE	CZ-CE2-CD2	-75.76	29.19	120.10
3	F	505	PHE	CB-CG-CD2	43.11	150.97	120.80
3	E	504	PHE	CB-CG-CD2	41.45	149.81	120.80
3	F	505	PHE	CD1-CG-CD2	-22.70	88.79	118.30
3	E	504	PHE	CD1-CG-CD2	-22.54	89.00	118.30
3	F	505	PHE	CE1-CZ-CE2	-17.81	87.94	120.00
3	E	504	PHE	CE1-CZ-CE2	-16.90	89.59	120.00
2	D	343	ASP	CB-CG-OD2	9.56	126.90	118.30
1	A	38	ASP	CB-CG-OD2	9.53	126.88	118.30
1	A	247	ASP	CB-CG-OD2	8.97	126.38	118.30
1	C	210	ASP	CB-CG-OD2	8.95	126.36	118.30
2	D	393	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	39	THR	N-CA-C	-7.88	89.73	111.00
2	B	205	ASP	CB-CG-OD2	7.87	125.38	118.30
2	B	345	ASP	CB-CG-OD2	7.58	125.12	118.30
1	C	166	LEU	CA-CB-CG	7.32	132.12	115.30
2	B	284	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	15	TYR	CB-CA-C	-7.05	96.31	110.40
1	C	164	VAL	CB-CA-C	-6.98	98.13	111.40
1	C	247	ASP	CB-CG-OD2	6.91	124.52	118.30
1	C	258	ASP	CB-CG-OD1	6.83	124.45	118.30
2	D	216	ASP	CB-CG-OD2	6.79	124.41	118.30
2	D	175	VAL	CB-CA-C	-6.64	98.78	111.40
1	A	235	ASP	CB-CG-OD2	6.57	124.21	118.30
2	D	205	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	122	ARG	NE-CZ-NH2	6.35	123.48	120.30
3	E	501	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	38	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	256	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	240	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	256	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	258	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	150	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	235	ASP	CB-CG-OD2	5.88	123.59	118.30
2	D	283	ASP	CB-CG-OD2	5.84	123.56	118.30
2	D	305	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	14	THR	N-CA-C	-5.61	95.84	111.00
2	D	181	ASP	CB-CG-OD2	5.61	123.34	118.30
2	B	176	PRO	N-CA-C	5.60	126.65	112.10
1	A	127	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	68	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	87	LEU	CB-CG-CD2	5.40	120.18	111.00
1	C	206	ASP	CB-CG-OD2	5.31	123.08	118.30
3	F	502	ARG	CG-CD-NE	-5.31	100.65	111.80
1	A	223	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	267	LEU	CB-CG-CD1	-5.25	102.07	111.00
2	D	177	ASP	CB-CG-OD2	5.12	122.91	118.30
2	D	178	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	C	240	PHE	N-CA-C	-5.05	97.38	111.00
2	D	293	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	42	GLU	N-CA-C	5.02	124.55	111.00
3	F	502	ARG	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	160	THR	Peptide
1	A	161	HIS	Peptide
1	A	162	GLU	Peptide
1	A	163	VAL	Peptide
1	A	38	ASP	Peptide
1	A	39	THR	Peptide
2	B	323	GLN	Peptide
1	C	161	HIS	Peptide
1	C	162	GLU	Peptide
1	C	164	VAL	Peptide
1	C	38	ASP	Peptide
1	C	40	GLU	Peptide
1	C	70	ILE	Peptide
2	D	194	LYS	Peptide
2	D	345	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2426	106	1
1	C	2379	0	2426	114	9
2	B	2083	0	2107	77	8
2	D	2087	0	2112	85	0
3	E	46	0	50	0	0
3	F	46	0	50	1	0
4	A	81	0	0	7	0
4	B	75	0	0	14	0
4	C	82	0	0	14	0
4	D	95	0	0	23	0
4	E	1	0	0	0	0
4	F	4	0	0	0	0
All	All	9357	0	9171	366	9

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 20.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:VAL:HG22	2:B:176:PRO:CD	1.03	1.48
2:B:175:VAL:CG2	2:B:176:PRO:HD2	0.92	1.39
2:B:175:VAL:HG22	2:B:176:PRO:CG	1.55	1.34
2:B:175:VAL:CB	2:B:176:PRO:HD2	1.58	1.29
2:D:175:VAL:N	2:D:176:PRO:HD2	1.19	1.25
1:A:38:ASP:OD1	1:A:40:GLU:HG2	1.05	1.19
1:C:15:TYR:HB3	4:C:2009:HOH:O	1.36	1.19
1:A:164:VAL:HG12	1:A:165:THR:N	1.49	1.18
2:D:175:VAL:N	2:D:176:PRO:CD	2.03	1.17
1:C:164:VAL:HB	1:C:165:THR:HA	1.29	1.15
1:A:38:ASP:OD1	1:A:40:GLU:CG	1.96	1.13
1:A:164:VAL:CG1	1:A:165:THR:H	1.60	1.12
1:A:38:ASP:HA	1:A:39:THR:HG22	1.38	1.02
2:D:361:HIS:CE1	4:D:2069:HOH:O	2.14	1.00
1:C:51:GLU:O	1:C:55:LEU:HB2	1.63	0.98
2:B:175:VAL:CG2	2:B:176:PRO:CD	1.79	0.97
2:D:404:HIS:HD2	2:D:406:GLN:H	1.06	0.96
1:C:39:THR:O	1:C:40:GLU:CD	2.04	0.96
1:A:95:ALA:O	1:A:96:LEU:HB3	1.67	0.95
2:B:175:VAL:HG23	2:B:176:PRO:HD2	1.47	0.94
1:C:268:HIS:HD2	4:C:2065:HOH:O	1.50	0.93
1:C:161:HIS:O	1:C:162:GLU:O	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:NZ	1:C:34:LYS:HZ2	1.67	0.92
1:C:41:THR:HG22	2:D:288:LYS:HZ1	1.36	0.91
1:A:209:ILE:HG22	4:A:2060:HOH:O	1.71	0.91
1:C:6:LYS:NZ	1:C:34:LYS:NZ	2.19	0.91
1:C:15:TYR:CD1	1:C:15:TYR:N	2.39	0.90
2:D:296:HIS:CD2	4:D:2054:HOH:O	2.25	0.90
1:C:41:THR:O	1:C:43:GLY:N	2.06	0.89
1:C:41:THR:HG22	2:D:288:LYS:NZ	1.88	0.88
1:C:15:TYR:CB	4:C:2009:HOH:O	1.99	0.87
1:C:40:GLU:O	1:C:40:GLU:HG2	1.71	0.87
2:B:175:VAL:HG22	2:B:176:PRO:HG2	1.54	0.86
1:C:15:TYR:CE1	1:C:47:THR:OG1	2.29	0.85
1:C:9:LYS:HD3	4:C:2004:HOH:O	1.77	0.85
1:C:164:VAL:CB	1:C:165:THR:HA	2.08	0.84
1:C:278:LYS:NZ	2:D:177:ASP:O	2.10	0.83
2:D:404:HIS:CD2	2:D:406:GLN:H	1.93	0.83
2:D:323:GLN:O	2:D:323:GLN:HG2	1.79	0.82
2:B:216:ASP:OD1	2:B:408:SER:HB2	1.79	0.81
1:A:245:ARG:HD3	4:A:2068:HOH:O	1.80	0.80
1:A:241:PRO:HG2	1:A:243:TRP:CZ3	2.16	0.80
1:C:95:ALA:O	1:C:96:LEU:HB3	1.80	0.80
1:A:38:ASP:HA	1:A:39:THR:CG2	2.13	0.79
1:C:164:VAL:HB	1:C:165:THR:CA	2.10	0.79
1:A:164:VAL:HG12	1:A:165:THR:H	1.14	0.78
2:B:379:LYS:HE2	4:B:2052:HOH:O	1.83	0.78
1:A:1:MET:HE2	1:A:70:ILE:HD13	1.66	0.77
1:C:1:MET:CE	1:C:70:ILE:HD13	2.14	0.76
1:A:37:LEU:O	1:A:39:THR:HG22	1.85	0.76
2:D:323:GLN:O	2:D:323:GLN:CG	2.32	0.76
1:A:250:LYS:HD2	4:A:2037:HOH:O	1.85	0.76
2:B:430:LEU:HB3	2:B:432:LEU:CD2	2.15	0.76
1:A:252:VAL:HG23	1:A:252:VAL:O	1.83	0.76
1:A:1:MET:CE	1:A:70:ILE:HD13	2.15	0.76
2:B:277:GLU:O	2:B:281:ILE:HG23	1.86	0.75
1:C:6:LYS:HZ2	1:C:34:LYS:NZ	1.81	0.75
1:A:40:GLU:HG3	1:A:41:THR:N	2.01	0.75
1:A:158:THR:HG21	1:A:177:CYS:O	1.86	0.74
2:D:217:TRP:HZ2	2:D:281:ILE:HG13	1.50	0.74
2:B:249:LEU:HD22	1:C:27:GLY:HA3	1.67	0.74
1:A:115:LEU:HD22	1:A:119:HIS:CE1	2.23	0.74
1:A:231:THR:HA	1:A:236:TYR:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:O	1:A:14:THR:O	2.06	0.73
1:A:13:GLY:C	1:A:14:THR:O	2.21	0.73
1:C:64:VAL:HG23	1:C:143:LEU:O	1.88	0.73
1:A:164:VAL:HG13	1:A:165:THR:H	1.52	0.73
1:A:198:THR:O	1:A:199:ARG:HB2	1.88	0.72
1:C:60:HIS:CD2	1:C:62:ASN:H	2.08	0.72
1:C:91:MET:HE3	1:C:196:MET:HG2	1.70	0.72
1:A:121:HIS:O	1:A:122:ARG:HG3	1.88	0.72
2:B:176:PRO:HD3	2:B:179:HIS:CE1	2.25	0.72
2:D:349:LYS:HE2	4:D:2068:HOH:O	1.88	0.72
1:A:60:HIS:HD2	1:A:62:ASN:H	1.39	0.71
1:C:15:TYR:CE1	1:C:47:THR:CB	2.75	0.70
1:A:95:ALA:O	1:A:96:LEU:CB	2.39	0.69
2:D:346:PRO:O	2:D:349:LYS:HG3	1.92	0.69
1:C:39:THR:O	1:C:40:GLU:OE2	2.10	0.69
2:B:217:TRP:HZ2	2:B:281:ILE:HG13	1.57	0.69
2:B:322:GLN:HG3	4:B:2043:HOH:O	1.92	0.69
1:A:115:LEU:HD12	1:A:189:LEU:CD2	2.22	0.69
2:D:361:HIS:ND1	4:D:2069:HOH:O	2.18	0.68
2:D:221:VAL:HG21	2:D:281:ILE:HD12	1.75	0.68
1:C:37:LEU:C	1:C:39:THR:H	1.95	0.68
1:A:241:PRO:HG2	1:A:243:TRP:CH2	2.27	0.68
1:C:1:MET:HE3	1:C:70:ILE:HD13	1.75	0.68
2:D:277:GLU:O	2:D:281:ILE:HG23	1.93	0.68
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.94	0.68
2:D:175:VAL:O	2:D:175:VAL:HG13	1.94	0.67
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.77	0.67
2:B:274:GLU:HG2	4:B:2035:HOH:O	1.96	0.66
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.31	0.66
2:B:266:LYS:NZ	2:B:295:GLU:OE2	2.27	0.66
1:C:169:ARG:HD3	1:C:173:ILE:HG22	1.77	0.66
2:B:346:PRO:O	2:B:349:LYS:HG3	1.97	0.65
2:B:363:ALA:O	2:B:367:VAL:HG23	1.95	0.65
2:B:197:VAL:HG22	4:B:2018:HOH:O	1.97	0.65
1:A:15:TYR:CD2	1:A:47:THR:OG1	2.49	0.65
2:D:404:HIS:HD2	2:D:406:GLN:N	1.88	0.65
2:D:400:LYS:HE3	4:D:2083:HOH:O	1.96	0.65
2:B:206:ILE:HA	2:B:210:MET:HE3	1.79	0.64
1:A:227:TRP:O	1:A:230:VAL:HG22	1.97	0.64
1:A:164:VAL:CG1	1:A:165:THR:N	2.15	0.64
1:C:39:THR:O	1:C:40:GLU:CG	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:CG2	2:D:288:LYS:HZ1	2.10	0.64
1:C:7:VAL:HG12	1:C:8:GLU:HG2	1.81	0.63
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.27	0.63
2:D:432:LEU:N	2:D:432:LEU:HD23	2.14	0.63
1:A:51:GLU:O	1:A:55:LEU:HB2	1.98	0.63
1:C:41:THR:CG2	2:D:288:LYS:NZ	2.62	0.62
2:D:217:TRP:CZ2	2:D:281:ILE:HG13	2.34	0.62
1:A:73:GLU:HG3	1:C:2:GLU:HG2	1.82	0.62
1:C:41:THR:HA	2:D:288:LYS:HE3	1.80	0.62
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.35	0.62
1:C:95:ALA:O	1:C:96:LEU:CB	2.46	0.62
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.35	0.62
2:D:207:THR:HG23	2:D:210[B]:MET:CE	2.30	0.62
1:A:81:GLU:OE1	1:A:142:LYS:NZ	2.29	0.62
1:C:119:HIS:CE1	1:C:182:THR:HB	2.35	0.62
2:D:300:LYS:HB2	4:D:2055:HOH:O	1.99	0.61
2:D:207:THR:HG23	2:D:210[B]:MET:HE3	1.81	0.61
1:C:20:LYS:HD2	1:C:82:PHE:CZ	2.36	0.61
1:A:231:THR:HG22	1:A:236:TYR:CE1	2.36	0.60
1:A:2:GLU:HG2	1:C:73:GLU:HG3	1.83	0.60
1:A:39:THR:H	1:A:40:GLU:HB3	1.67	0.60
2:B:175:VAL:HG23	2:B:176:PRO:CD	2.14	0.60
1:A:6:LYS:HZ1	1:A:34:LYS:HD2	1.67	0.60
1:C:37:LEU:C	1:C:39:THR:N	2.50	0.60
1:A:60:HIS:CD2	1:A:62:ASN:H	2.18	0.60
2:D:210[A]:MET:CE	2:D:250:ARG:HB2	2.32	0.60
1:C:40:GLU:O	1:C:41:THR:O	2.19	0.60
2:B:288:LYS:HZ3	2:B:288:LYS:HB2	1.67	0.60
2:B:197:VAL:CG2	4:B:2018:HOH:O	2.51	0.59
2:B:293:ARG:HG3	2:B:293:ARG:HH11	1.67	0.59
2:D:296:HIS:CG	4:D:2054:HOH:O	2.52	0.59
1:C:253:PRO:N	1:C:254:PRO:CD	2.66	0.59
1:C:32:LEU:HD22	1:C:79:VAL:HG22	1.85	0.59
1:C:105:LYS:NZ	1:C:288:ASP:OD1	2.34	0.59
1:C:6:LYS:NZ	1:C:34:LYS:HZ1	2.01	0.58
2:B:217:TRP:CZ2	2:B:281:ILE:HG13	2.37	0.58
2:D:358:ALA:HA	2:D:391:LEU:HD13	1.84	0.58
1:A:39:THR:H	1:A:40:GLU:CB	2.16	0.58
1:A:15:TYR:HD2	1:A:47:THR:OG1	1.86	0.58
2:D:379:LYS:HE2	4:D:2073:HOH:O	2.03	0.58
1:A:159:TYR:O	1:A:160:THR:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:HIS:CG	4:D:2069:HOH:O	2.53	0.58
1:C:40:GLU:HB2	1:C:41:THR:OG1	2.03	0.58
2:B:430:LEU:HB3	2:B:432:LEU:HD23	1.86	0.58
1:C:53:SER:HB3	4:D:2058:HOH:O	2.03	0.58
1:C:41:THR:HG22	2:D:288:LYS:CE	2.35	0.57
2:B:175:VAL:CG2	2:B:176:PRO:HG2	2.29	0.57
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.87	0.57
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.40	0.57
1:A:164:VAL:HG12	1:A:165:THR:CA	2.33	0.56
2:B:293:ARG:HG3	2:B:293:ARG:NH1	2.20	0.56
1:A:17:VAL:CG1	1:A:19:TYR:CE2	2.88	0.56
1:C:159:TYR:HB3	1:C:162:GLU:HA	1.88	0.56
1:C:86:ASP:OD2	1:C:89:LYS:NZ	2.38	0.56
2:B:323:GLN:HE21	2:B:370:GLN:HE22	1.54	0.56
1:C:198:THR:O	1:C:199:ARG:HB2	2.06	0.55
1:C:64:VAL:CG2	1:C:143:LEU:O	2.55	0.55
2:D:395:HIS:HD2	4:D:2081:HOH:O	1.89	0.55
1:C:9:LYS:CD	4:C:2004:HOH:O	2.47	0.55
1:A:17:VAL:HG13	1:A:19:TYR:CE2	2.41	0.55
1:C:131:GLN:H	1:C:131:GLN:NE2	2.04	0.55
1:C:121:HIS:O	1:C:122:ARG:HG3	2.06	0.55
1:A:121:HIS:C	1:A:122:ARG:HG3	2.27	0.54
2:B:207:THR:CG2	2:B:210:MET:HG3	2.37	0.54
2:D:303:THR:HG23	4:D:2057:HOH:O	2.06	0.54
1:A:2:GLU:HG3	4:C:2023:HOH:O	2.08	0.54
1:C:60:HIS:HD2	1:C:62:ASN:H	1.52	0.54
1:C:6:LYS:HZ1	1:C:34:LYS:NZ	2.03	0.54
1:A:159:TYR:HD2	1:A:163:VAL:HG13	1.73	0.54
1:C:78:LEU:N	1:C:78:LEU:HD23	2.22	0.54
1:C:162:GLU:OE1	1:C:180:TYR:OH	2.26	0.53
1:A:217:ARG:HD3	4:A:2062:HOH:O	2.07	0.53
1:A:172:GLU:HG2	1:A:173:ILE:N	2.24	0.53
1:A:173:ILE:CD1	1:A:184:VAL:HG11	2.39	0.53
1:C:17:VAL:HG12	1:C:19:TYR:CE1	2.44	0.53
1:C:124:LEU:HD21	1:C:182:THR:HA	1.91	0.53
1:C:164:VAL:CB	1:C:165:THR:CA	2.80	0.52
1:C:22:ARG:HD3	4:C:2010:HOH:O	2.07	0.52
2:B:388:LYS:N	2:B:389:PRO:CD	2.73	0.52
1:A:6:LYS:NZ	1:A:34:LYS:HD2	2.24	0.52
1:A:1:MET:CE	1:A:70:ILE:CD1	2.87	0.52
2:D:345:ASP:OD2	2:D:346:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:CE1	2:B:296:HIS:CE1	2.98	0.52
1:A:198:THR:O	1:A:199:ARG:CB	2.55	0.52
1:A:169:ARG:HD3	1:A:173:ILE:HG22	1.90	0.52
2:B:404:HIS:CD2	2:B:406:GLN:HB2	2.45	0.52
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.45	0.51
2:D:289:LYS:HG2	2:D:293:ARG:HD2	1.92	0.51
2:D:289:LYS:HE3	4:D:2049:HOH:O	2.09	0.51
2:B:207:THR:HG22	2:B:210:MET:HE3	1.93	0.51
2:D:210[A]:MET:HE3	2:D:250:ARG:HB2	1.93	0.51
1:A:81:GLU:CD	1:A:142:LYS:HZ3	2.13	0.51
1:A:56:LYS:HD3	4:B:2040:HOH:O	2.10	0.51
2:B:347:TYR:HH	2:B:397:THR:HG1	1.57	0.51
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.79	0.51
1:C:9:LYS:CG	4:C:2004:HOH:O	2.58	0.50
1:A:56:LYS:CD	4:B:2040:HOH:O	2.59	0.50
1:A:294:PRO:HG2	1:A:296:LEU:HD13	1.93	0.50
1:C:290:THR:HG23	4:C:2073:HOH:O	2.12	0.50
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.47	0.50
2:D:361:HIS:CD2	4:D:2069:HOH:O	2.65	0.50
2:D:379:LYS:CE	4:D:2073:HOH:O	2.60	0.50
2:D:233:HIS:HD2	4:D:2060:HOH:O	1.95	0.50
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.94	0.50
2:D:371:SER:O	2:D:372:TRP:C	2.50	0.50
2:D:430:LEU:O	2:D:431:ASN:CB	2.60	0.49
1:A:166:LEU:O	1:A:167:TRP:HB2	2.12	0.49
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.48	0.49
2:B:208:ASN:HB3	4:B:2022:HOH:O	2.12	0.49
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.94	0.49
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.47	0.49
2:B:207:THR:HG22	2:B:210:MET:CE	2.43	0.49
1:C:64:VAL:HG21	1:C:144:ALA:CB	2.42	0.49
1:C:253:PRO:N	1:C:254:PRO:HD3	2.28	0.49
1:C:71:HIS:CE1	2:D:296:HIS:CD2	3.01	0.48
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.94	0.48
1:C:10:ILE:HG21	1:C:20:LYS:HB2	1.95	0.48
1:A:73:GLU:CG	1:C:2:GLU:HG2	2.43	0.48
1:A:159:TYR:CD2	1:A:163:VAL:HG13	2.49	0.48
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.42	0.48
2:B:401:ALA:N	2:B:402:PRO:CD	2.77	0.48
1:A:166:LEU:O	1:A:168:TYR:N	2.42	0.48
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:ASN:C	2:D:432:LEU:HD23	2.34	0.48
1:A:56:LYS:HE2	4:B:2040:HOH:O	2.14	0.48
2:B:323:GLN:HE21	2:B:370:GLN:NE2	2.11	0.48
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.44	0.47
2:D:379:LYS:NZ	4:D:2073:HOH:O	2.47	0.47
2:D:425:ASN:O	2:D:426:PRO:C	2.50	0.47
1:C:152:PHE:CD2	1:C:152:PHE:O	2.68	0.47
2:D:210[A]:MET:HE1	2:D:250:ARG:CB	2.44	0.47
1:A:150:ARG:NH2	2:B:268:GLU:O	2.47	0.47
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.44	0.47
2:D:345:ASP:OD2	2:D:346:PRO:CD	2.61	0.47
2:D:210[B]:MET:HG2	3:F:505:PHE:CD2	2.49	0.47
1:A:81:GLU:CD	1:A:142:LYS:NZ	2.68	0.47
2:B:293:ARG:CG	2:B:293:ARG:HH11	2.27	0.47
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.95	0.47
2:B:282:THR:O	2:B:283:ASP:HB3	2.15	0.47
1:A:13:GLY:O	1:A:14:THR:C	2.52	0.47
1:C:15:TYR:CE1	1:C:47:THR:HB	2.49	0.47
1:C:37:LEU:O	1:C:38:ASP:C	2.53	0.47
1:C:161:HIS:C	1:C:162:GLU:O	2.48	0.47
1:C:15:TYR:HE1	1:C:47:THR:CB	2.26	0.47
1:C:101:LEU:N	1:C:102:PRO:CD	2.77	0.47
2:D:388:LYS:N	2:D:389:PRO:CD	2.78	0.47
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.44	0.47
1:A:115:LEU:HD12	1:A:189:LEU:HD22	1.96	0.47
1:A:159:TYR:O	1:A:161:HIS:N	2.48	0.47
2:D:176:PRO:HB3	2:D:178:TYR:CZ	2.50	0.47
1:A:43:GLY:HA2	4:A:2014:HOH:O	2.15	0.47
2:D:385:GLU:HB3	4:D:2076:HOH:O	2.14	0.47
2:B:415:ASN:ND2	4:B:2069:HOH:O	1.91	0.46
2:B:383:THR:O	2:B:384:LEU:C	2.54	0.46
1:C:88:LYS:HD2	1:C:88:LYS:O	2.15	0.46
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.69	0.46
2:D:229:ASN:HB3	4:D:2067:HOH:O	2.14	0.46
1:A:227:TRP:O	1:A:228:PRO:C	2.51	0.46
1:A:173:ILE:CD1	1:A:184:VAL:CG1	2.94	0.46
2:B:175:VAL:CG2	2:B:176:PRO:CG	2.50	0.46
2:D:395:HIS:HE1	2:D:427:PRO:O	1.98	0.46
2:B:282:THR:O	2:B:285:THR:CG2	2.63	0.46
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.46
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:GLY:N	4:D:2015:HOH:O	2.48	0.46
2:B:430:LEU:O	2:B:432:LEU:HD22	2.16	0.46
2:D:303:THR:CG2	4:D:2057:HOH:O	2.64	0.46
1:C:91:MET:CE	1:C:196:MET:HG2	2.42	0.46
1:A:158:THR:HB	1:A:178:LYS:O	2.16	0.46
1:C:1:MET:CE	1:C:70:ILE:CD1	2.91	0.46
2:B:288:LYS:NZ	2:B:288:LYS:HB2	2.31	0.45
2:B:412:LYS:HE2	2:B:413:TYR:CE1	2.51	0.45
1:A:65:LYS:HD2	4:A:2030:HOH:O	2.16	0.45
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.97	0.45
1:A:129:LYS:HE2	1:A:132:ASN:ND2	2.31	0.45
1:A:252:VAL:CG2	1:A:252:VAL:O	2.56	0.45
2:B:175:VAL:CG2	2:B:176:PRO:HD3	2.19	0.45
2:B:421:VAL:O	2:B:424:LEU:HB2	2.17	0.45
1:A:173:ILE:HD13	1:A:184:VAL:CG1	2.47	0.45
2:D:321:HIS:CD2	2:D:376:LEU:HD21	2.52	0.45
2:B:207:THR:HG23	2:B:210:MET:HG3	1.99	0.45
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.77	0.44
1:A:78:LEU:HD23	1:A:78:LEU:N	2.31	0.44
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.98	0.44
2:B:206:ILE:HA	2:B:210:MET:CE	2.44	0.44
1:C:158:THR:HG21	4:C:2048:HOH:O	2.17	0.44
2:D:412:LYS:HE2	2:D:413:TYR:CE1	2.52	0.44
1:A:187:TRP:CD1	1:A:187:TRP:C	2.91	0.44
2:B:410:ARG:NE	4:B:2067:HOH:O	2.51	0.44
2:B:335:PHE:CE1	2:B:409:ILE:HG22	2.51	0.44
2:D:204:PRO:HG2	4:D:2019:HOH:O	2.17	0.44
1:A:159:TYR:HB3	1:A:162:GLU:HA	1.99	0.44
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.47	0.44
1:C:202:LEU:HD23	1:C:203:PHE:CE2	2.51	0.44
1:C:6:LYS:HZ2	1:C:34:LYS:HZ1	1.59	0.44
1:C:95:ALA:O	1:C:96:LEU:HD23	2.18	0.44
4:C:2044:HOH:O	2:D:317:GLN:HG2	2.17	0.44
1:C:15:TYR:CZ	1:C:47:THR:OG1	2.60	0.44
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.82	0.43
2:B:373:PRO:HG2	2:B:376:LEU:HD12	2.00	0.43
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.54	0.43
2:B:335:PHE:HE1	2:B:409:ILE:HG22	1.84	0.43
1:C:159:TYR:CB	1:C:162:GLU:HA	2.49	0.43
2:B:207:THR:OG1	2:B:208:ASN:N	2.52	0.43
2:D:361:HIS:CE1	2:D:384:LEU:CD1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:HIS:HD2	2:B:406:GLN:H	1.67	0.43
2:B:427:PRO:HA	4:B:2073:HOH:O	2.19	0.43
2:D:175:VAL:O	2:D:176:PRO:O	2.36	0.42
1:A:105:LYS:HE2	1:A:285:PHE:CZ	2.54	0.42
1:A:64:VAL:HG12	1:A:143:LEU:O	2.19	0.42
1:A:115:LEU:CD1	1:A:189:LEU:HD22	2.49	0.42
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.52	0.42
2:D:396:GLN:O	2:D:397:THR:C	2.58	0.42
1:A:241:PRO:CG	1:A:243:TRP:CH2	3.00	0.42
2:D:203:GLN:HB3	2:D:206:ILE:HG12	2.00	0.42
2:D:401:ALA:HB3	2:D:402:PRO:HD3	2.01	0.42
1:A:115:LEU:HD12	1:A:189:LEU:HD23	1.98	0.42
1:C:164:VAL:CG1	1:C:165:THR:HA	2.49	0.42
2:D:430:LEU:O	2:D:431:ASN:HB2	2.19	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.54	0.42
2:B:207:THR:HG22	2:B:210:MET:HG3	2.01	0.42
1:A:173:ILE:HD13	1:A:184:VAL:HG11	2.01	0.42
1:C:290:THR:CG2	4:C:2073:HOH:O	2.67	0.41
1:C:227:TRP:O	1:C:230:VAL:HG12	2.19	0.41
2:B:282:THR:O	2:B:283:ASP:CB	2.67	0.41
2:B:396:GLN:HG3	4:B:2060:HOH:O	2.20	0.41
1:C:257:GLU:OE2	4:C:2062:HOH:O	2.21	0.41
2:B:429:THR:HA	4:B:2075:HOH:O	2.19	0.41
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.35	0.41
1:A:77:TYR:C	1:A:78:LEU:HD23	2.41	0.41
1:C:270:ASP:OD1	1:C:271:PRO:HD2	2.19	0.41
2:B:289:LYS:HB2	2:B:289:LYS:HE2	1.62	0.41
2:D:175:VAL:O	2:D:175:VAL:HG22	2.20	0.41
2:B:372:TRP:HA	2:B:373:PRO:HD3	1.86	0.41
2:B:239:ILE:HD11	2:B:257:GLY:HA2	2.02	0.41
2:B:430:LEU:O	2:B:431:ASN:HB2	2.20	0.41
1:A:212:LEU:HD22	1:A:216:PHE:CE1	2.55	0.41
1:C:174:LEU:O	4:C:2049:HOH:O	2.22	0.41
1:A:115:LEU:HD11	1:A:185:ASP:HB3	2.03	0.41
2:D:407:GLN:O	2:D:411:GLU:HG2	2.21	0.41
1:A:36:ARG:HH11	1:A:36:ARG:HD3	1.73	0.41
1:A:154:VAL:O	1:A:155:PRO:C	2.56	0.41
1:C:223:ASP:C	1:C:223:ASP:OD1	2.59	0.41
2:B:338:GLU:O	2:B:341:LEU:HB2	2.21	0.41
1:A:15:TYR:CE2	1:A:45:PRO:HB3	2.56	0.41
1:C:105:LYS:HG2	1:C:289:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:THR:OG1	2:B:370:GLN:HG3	2.21	0.41
2:D:219:VAL:HG21	2:D:409:ILE:CG1	2.51	0.41
1:C:164:VAL:HG22	1:C:164:VAL:H	1.41	0.41
1:A:173:ILE:HD11	1:A:184:VAL:HG11	2.03	0.41
2:D:417:LYS:NZ	4:D:2090:HOH:O	2.53	0.41
1:A:136:ASN:C	1:A:136:ASN:OD1	2.59	0.41
1:C:15:TYR:CD2	1:C:35:ILE:HG12	2.56	0.40
2:D:388:LYS:N	2:D:389:PRO:HD2	2.37	0.40
2:D:410:ARG:O	2:D:411:GLU:C	2.59	0.40
1:A:239:SER:HB3	4:A:2067:HOH:O	2.21	0.40
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.83	0.40
1:C:49:ILE:HG23	1:C:49:ILE:HD12	1.72	0.40
1:C:17:VAL:CG1	1:C:19:TYR:CE1	3.05	0.40
2:D:206:ILE:HG21	2:D:206:ILE:HD13	1.71	0.40
2:B:360:PHE:O	2:B:364:LEU:HB2	2.21	0.40
1:C:60:HIS:HA	1:C:61:PRO:HD3	1.88	0.40

All (9) 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:CG	1:C:210:ASP:OD1[2_664]	1.25	0.95
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.46	0.74
2:B:428:GLU:OE2	1:C:237:LYS:NZ[2_664]	1.65	0.55
2:B:369:GLY:O	1:C:217:ARG:NE[2_664]	1.75	0.45
2:B:431:ASN:CB	1:C:210:ASP:OD1[2_664]	1.93	0.27
2:B:431:ASN:ND2	1:C:210:ASP:CA[2_664]	1.97	0.23
2:B:431:ASN:ND2	1:C:210:ASP:CG[2_664]	2.06	0.14
2:B:431:ASN:OD1	1:C:210:ASP:OD1[2_664]	2.07	0.13
1:A:84:HIS:ND1	1:C:287:GLN:O[1_455]	2.15	0.05

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%)	268 (91%)	19 (6%)	7 (2%)	7 13
1	C	295/298 (99%)	274 (93%)	12 (4%)	9 (3%)	5 8
2	B	256/260 (98%)	244 (95%)	9 (4%)	3 (1%)	16 33
2	D	257/260 (99%)	236 (92%)	18 (7%)	3 (1%)	16 33
3	E	4/6 (67%)	3 (75%)	1 (25%)	0	100 100
3	F	4/6 (67%)	4 (100%)	0	0	100 100
All	All	1110/1128 (98%)	1029 (93%)	59 (5%)	22 (2%)	9 18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	160	THR
1	A	162	GLU
2	B	176	PRO
2	B	424	LEU
1	C	38	ASP
1	C	41	THR
1	C	42	GLU
1	C	162	GLU
2	D	176	PRO
1	A	2	GLU
1	A	96	LEU
1	A	164	VAL
2	B	420	GLY
1	C	2	GLU
1	C	96	LEU
1	C	164	VAL
2	D	424	LEU
1	C	160	THR
1	A	14	THR
1	C	40	GLU
2	D	346	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	261/263 (99%)	223 (85%)	38 (15%)	4 6
1	C	261/263 (99%)	223 (85%)	38 (15%)	4 6
2	B	232/234 (99%)	198 (85%)	34 (15%)	4 6
2	D	233/234 (100%)	208 (89%)	25 (11%)	8 15
3	E	4/4 (100%)	4 (100%)	0	100 100
3	F	4/4 (100%)	4 (100%)	0	100 100
All	All	995/1002 (99%)	860 (86%)	135 (14%)	5 8

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10	ILE
1	A	12	GLU
1	A	14	THR
1	A	17	VAL
1	A	36	ARG
1	A	37	LEU
1	A	39	THR
1	A	40	GLU
1	A	42	GLU
1	A	55	LEU
1	A	56	LYS
1	A	75	LYS
1	A	76	LEU
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	122	ARG
1	A	126	ARG
1	A	131	GLN
1	A	148	LEU
1	A	154	VAL
1	A	158	THR
1	A	160	THR
1	A	161	HIS
1	A	166	LEU
1	A	173	ILE

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	200	ARG
1	A	202	LEU
1	A	208	GLU
1	A	230	VAL
1	A	242	LYS
1	A	248	PHE
1	A	264	SER
1	A	287	GLN
1	A	293	VAL
1	A	295	HIS
2	B	175	VAL
2	B	177	ASP
2	B	189	MET
2	B	194	LYS
2	B	196	LYS
2	B	199	TYR
2	B	201	LYS
2	B	207	THR
2	B	209	SER
2	B	220	GLU
2	B	245	SER
2	B	249	LEU
2	B	274	GLU
2	B	281	ILE
2	B	285	THR
2	B	288	LYS
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	323	GLN
2	B	345	ASP
2	B	348	LEU
2	B	349	LYS
2	B	370	GLN
2	B	374	GLU
2	B	391	LEU
2	B	400	LYS
2	B	408	SER
2	B	417	LYS
2	B	422	SER
2	B	424	LEU

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Mol	Chain	Res	Type
2	B	425	ASN
2	B	429	THR
2	B	431	ASN
1	C	1	MET
1	C	2	GLU
1	C	5	GLN
1	C	12	GLU
1	C	15	TYR
1	C	17	VAL
1	C	22	ARG
1	C	36	ARG
1	C	38	ASP
1	C	40	GLU
1	C	42	GLU
1	C	53	SER
1	C	76	LEU
1	C	78	LEU
1	C	87	LEU
1	C	89	LYS
1	C	96	LEU
1	C	97	THR
1	C	101	LEU
1	C	122	ARG
1	C	124	LEU
1	C	126	ARG
1	C	131	GLN
1	C	154	VAL
1	C	158	THR
1	C	163	VAL
1	C	164	VAL
1	C	166	LEU
1	C	177	CYS
1	C	217	ARG
1	C	232	SER
1	C	240	PHE
1	C	246	GLN
1	C	247	ASP
1	C	248	PHE
1	C	264	SER
1	C	278	LYS
1	C	291	LYS
2	D	189	MET

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Mol	Chain	Res	Type
2	D	196	LYS
2	D	197	VAL
2	D	201	LYS
2	D	224	GLU
2	D	232	LEU
2	D	249	LEU
2	D	281	ILE
2	D	284	ASP
2	D	292	LEU
2	D	293	ARG
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	349	LYS
2	D	364	LEU
2	D	370	GLN
2	D	374	GLU
2	D	391	LEU
2	D	400	LYS
2	D	417	LYS
2	D	424	LEU
2	D	429	THR
2	D	431	ASN
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	211	GLN
2	B	179	HIS
2	B	208	ASN
2	B	296	HIS
2	B	322	GLN
2	B	370	GLN
2	B	404	HIS
2	B	419	HIS
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN

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Mol	Chain	Res	Type
1	C	131	GLN
1	C	211	GLN
2	D	208	ASN
2	D	233	HIS
2	D	370	GLN
2	D	395	HIS
2	D	404	HIS
2	D	419	HIS

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

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%)	0.24	12 (4%) 41 33	23, 40, 83, 112	1 (0%)
1	C	297/298 (99%)	1.42	81 (27%) 1 0	21, 40, 84, 111	0
2	B	258/260 (99%)	0.80	16 (6%) 24 18	23, 42, 69, 101	0
2	D	258/260 (99%)	0.53	16 (6%) 24 18	25, 43, 70, 102	0
3	E	5/6 (83%)	0.96	1 (20%) 1 1	40, 41, 57, 76	0
3	F	5/6 (83%)	0.07	0 100 100	40, 43, 50, 58	0
All	All	1119/1128 (99%)	0.75	126 (11%) 7 4	21, 41, 79, 112	1 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	ARG	6.3
1	C	96	LEU	6.1
1	C	249	SER	6.0
2	B	175	VAL	5.8
1	C	39	THR	5.3
1	C	38	ASP	5.1
1	C	295	HIS	4.5
2	B	201	LYS	4.3
1	A	73	GLU	4.2
2	D	175	VAL	4.2
1	C	40	GLU	4.1
1	C	36	ARG	4.0
1	C	217	ARG	4.0
1	C	15	TYR	3.9
1	C	225	VAL	3.9
2	D	179	HIS	3.8
1	C	253	PRO	3.8
2	B	323	GLN	3.8
2	B	176	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	177	ASP	3.7
1	C	293	VAL	3.7
1	C	218	THR	3.7
2	D	176	PRO	3.6
1	C	12	GLU	3.6
1	C	97	THR	3.6
1	C	37	LEU	3.6
2	D	180	GLU	3.5
1	C	13	GLY	3.4
1	C	244	ALA	3.4
1	C	220	GLY	3.4
1	C	287	GLN	3.4
2	B	383	THR	3.4
2	B	200	MET	3.3
1	A	40	GLU	3.3
1	C	73	GLU	3.2
1	A	13	GLY	3.2
1	C	213	PHE	3.2
1	C	284	PRO	3.1
2	D	378	ARG	3.1
1	C	194	ALA	3.1
1	C	215	ILE	3.1
1	C	163	VAL	3.1
2	B	378	ARG	3.0
1	A	247	ASP	3.0
2	B	198	GLY	3.0
2	B	177	ASP	3.0
1	C	266	MET	2.9
1	C	243	TRP	2.9
2	B	403	GLN	2.9
1	C	288	ASP	2.9
2	B	389	PRO	2.9
2	D	415	ASN	2.9
1	C	276	SER	2.9
1	C	285	PHE	2.9
1	C	199	ARG	2.8
1	C	162	GLU	2.8
1	C	104	ILE	2.8
1	C	261	SER	2.7
1	C	256	ASP	2.7
1	C	216	PHE	2.7
1	C	159	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	254	PRO	2.7
1	A	74	ASN	2.6
1	A	231	THR	2.6
1	C	242	LYS	2.6
1	C	277	ALA	2.6
2	D	432	LEU	2.6
1	C	204	PRO	2.6
1	C	165	THR	2.6
2	B	188	GLU	2.6
2	D	428	GLU	2.6
1	C	106	SER	2.5
1	C	247	ASP	2.5
1	C	168	TYR	2.5
1	C	238	PRO	2.5
1	C	226	VAL	2.5
1	C	210	ASP	2.5
2	D	192	LYS	2.4
1	C	108	LEU	2.4
2	D	320	LEU	2.4
1	C	221	THR	2.4
1	C	90	PHE	2.4
1	C	187	TRP	2.4
1	C	107	TYR	2.4
1	A	245	ARG	2.4
2	D	392	MET	2.4
1	C	296	LEU	2.4
1	C	109	PHE	2.4
1	C	130	PRO	2.4
1	A	95	ALA	2.4
1	C	41	THR	2.4
1	C	200	ARG	2.4
1	C	139	GLY	2.3
1	C	294	PRO	2.3
3	E	504	PHE	2.3
1	C	202	LEU	2.3
1	C	273	LYS	2.3
1	C	251	VAL	2.2
2	D	280	TYR	2.2
2	B	396	GLN	2.2
1	A	41	THR	2.2
2	B	357	GLY	2.2
1	C	11	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	246	GLN	2.2
1	C	84	HIS	2.2
1	C	282	ALA	2.2
2	B	326	ASN	2.2
1	C	138	GLU	2.2
2	D	381	GLY	2.1
1	A	179	TYR	2.1
2	D	178	TYR	2.1
1	C	201	ALA	2.1
1	C	191	CYS	2.1
1	A	37	LEU	2.1
2	D	364	LEU	2.1
2	B	398	TYR	2.1
1	A	163	VAL	2.1
1	C	88	LYS	2.1
1	C	212	LEU	2.0
1	C	59	ASN	2.0
1	C	193	PHE	2.0
1	C	292	PRO	2.0
1	C	270	ASP	2.0
1	C	161	HIS	2.0
1	C	179	TYR	2.0
1	C	275	ILE	2.0

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

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

6.3 Carbohydrates

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.