Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:10 AM GMT

PDB ID	:	2FYS
Title	:	Crystal structure of Erk2 complex with KIM peptide derived from MKP3
Authors	:	Liu, S.; Sun, J.P.; Zhou, B.; Zhang, Z.Y.
Deposited on	:	2006-02-08
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:

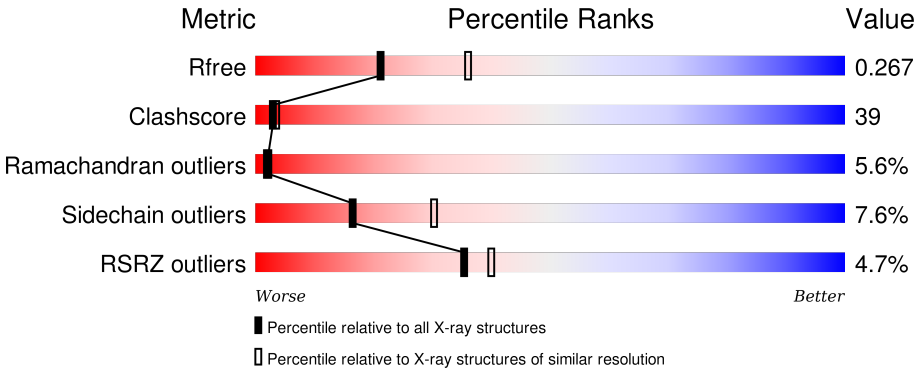
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	364	4% 39% 48% 8% •
1	B	364	2% 40% 47% 5% • 7%
2	C	17	29% 12% 35% 12% 6% 35%
2	D	17	41% 18% 29% 12% 6% 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6253 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 Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	338	Total	C	N	O	S	0	0	0
			2744	1762	470	498	14			
1	A	348	Total	C	N	O	S	0	0	0
			2835	1820	484	516	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP P63086
B	-4	HIS	-	EXPRESSION TAG	UNP P63086
B	-3	HIS	-	EXPRESSION TAG	UNP P63086
B	-2	HIS	-	EXPRESSION TAG	UNP P63086
B	-1	HIS	-	EXPRESSION TAG	UNP P63086
B	0	HIS	-	EXPRESSION TAG	UNP P63086
B	1	MET	-	EXPRESSION TAG	UNP P63086
A	-5	HIS	-	EXPRESSION TAG	UNP P63086
A	-4	HIS	-	EXPRESSION TAG	UNP P63086
A	-3	HIS	-	EXPRESSION TAG	UNP P63086
A	-2	HIS	-	EXPRESSION TAG	UNP P63086
A	-1	HIS	-	EXPRESSION TAG	UNP P63086
A	0	HIS	-	EXPRESSION TAG	UNP P63086
A	1	MET	-	EXPRESSION TAG	UNP P63086

- Molecule 2 is a protein called Dual specificity protein phosphatase 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			93	57	23	13			
2	C	11	Total	C	N	O	0	0	0
			93	57	23	13			

- Molecule 3 is water.

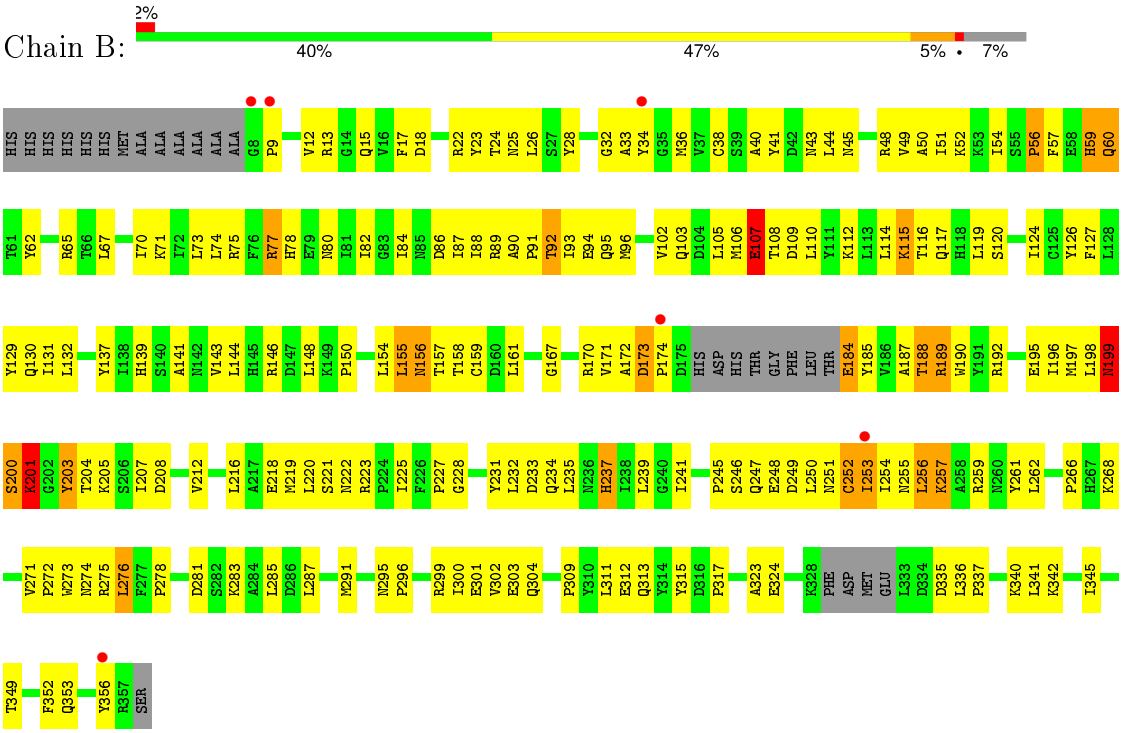
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	229	Total O 229 229	0	0
3	B	247	Total O 247 247	0	0
3	C	4	Total O 4 4	0	0
3	D	8	Total O 8 8	0	0

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.

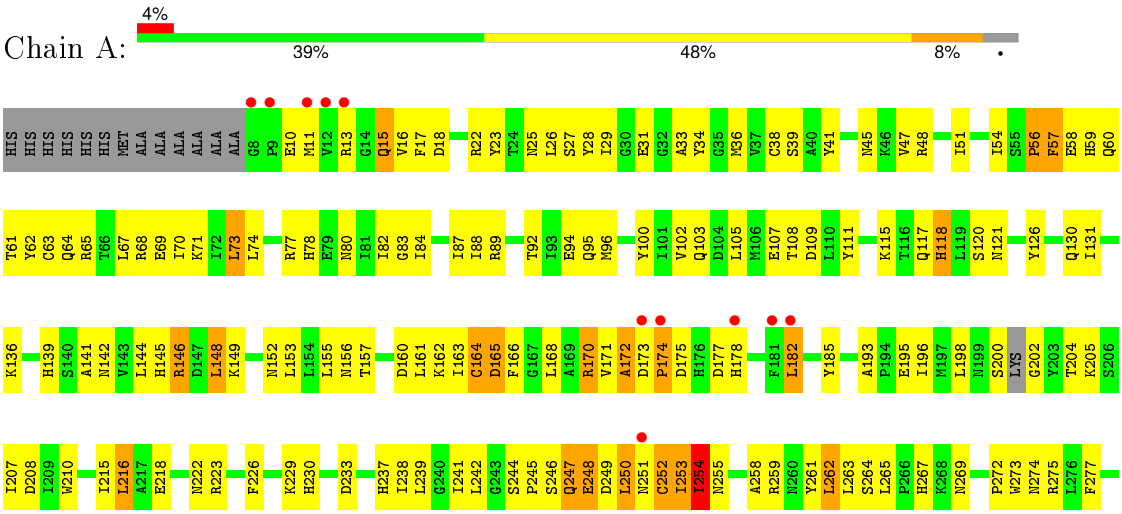
- Molecule 1: Mitogen-activated protein kinase 1

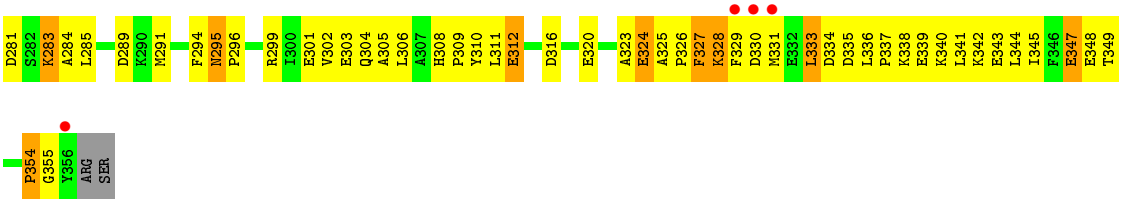
Chain B:



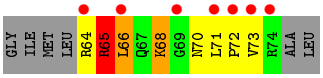
- Molecule 1: Mitogen-activated protein kinase 1

Chain A:

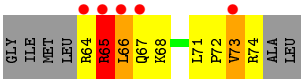




• Molecule 2: Dual specificity protein phosphatase 6



• Molecule 2: Dual specificity protein phosphatase 6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.38Å 67.48Å 86.61Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 28.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 84.2 (28.18-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.266 0.175 , 0.267	Depositor DCC
R_{free} test set	558 reflections (2.87%)	DCC
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	1 of 27999 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6253	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.87 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0761e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.32	0/2903	0.58	0/3934
1	B	0.30	0/2807	0.56	0/3803
2	C	0.30	0/93	0.66	0/122
2	D	0.32	0/93	0.63	0/122
All	All	0.31	0/5896	0.57	0/7981

There are no bond length outliers.

There are no bond angle outliers.

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	2835	0	2828	248	0
1	B	2744	0	2748	193	0
2	C	93	0	106	15	0
2	D	93	0	106	24	0
3	A	229	0	0	26	0
3	B	247	0	0	28	0
3	C	4	0	0	1	0
3	D	8	0	0	2	0
All	All	6253	0	5788	452	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 39.

All (452) 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:202:GLY:HA2	2:D:72:PRO:HD3	1.26	1.12
1:A:251:ASN:HB2	1:A:259:ARG:HE	1.13	1.11
1:B:54:ILE:HG22	1:B:56:PRO:HD3	1.42	1.00
1:B:170:ARG:HE	1:B:171:VAL:H	1.05	0.97
1:A:202:GLY:HA3	2:D:70:ASN:HB3	1.48	0.95
1:B:170:ARG:HH21	1:B:171:VAL:HG23	1.33	0.94
1:A:246:SER:OG	1:A:249:ASP:HB2	1.67	0.93
1:B:117:GLN:HE21	1:A:254:ILE:HG23	1.36	0.90
1:A:202:GLY:CA	2:D:72:PRO:HD3	2.01	0.89
1:A:337:PRO:HG2	1:A:340:LYS:HG2	1.55	0.88
1:A:152:ASN:O	1:A:164:CYS:HB2	1.74	0.88
1:A:107:GLU:HG2	1:A:157:THR:HG23	1.55	0.88
1:A:253:ILE:HG23	1:A:254:ILE:H	1.36	0.87
1:A:295:ASN:HD22	1:A:296:PRO:HD2	1.37	0.87
1:A:251:ASN:HB2	1:A:259:ARG:NE	1.88	0.87
1:A:111:TYR:O	1:A:115:LYS:HD3	1.73	0.86
1:B:120:SER:HB3	1:A:252:CYS:HA	1.58	0.86
1:B:189:ARG:N	1:B:189:ARG:HD3	1.90	0.85
1:B:283:LYS:HE2	1:B:309:PRO:HB2	1.57	0.85
2:C:65:ARG:HE	2:C:65:ARG:HA	1.42	0.82
1:A:54:ILE:HG22	1:A:56:PRO:HD3	1.62	0.81
1:B:170:ARG:HE	1:B:171:VAL:N	1.77	0.81
1:B:336:LEU:HD12	1:B:336:LEU:H	1.45	0.81
1:B:239:LEU:HD22	1:B:245:PRO:HD3	1.63	0.79
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.63	0.79
1:A:247:GLN:O	1:A:251:ASN:HB3	1.82	0.79
1:A:251:ASN:HD22	1:A:259:ARG:HH21	1.30	0.77
1:A:251:ASN:HD22	1:A:259:ARG:NH2	1.83	0.77
1:A:324:GLU:H	1:A:324:GLU:CD	1.88	0.76
1:A:146:ARG:HD3	1:A:168:LEU:O	1.87	0.75
1:B:203:TYR:H	1:B:203:TYR:HD2	1.34	0.75
1:A:202:GLY:HA2	2:D:72:PRO:CD	2.14	0.74
1:B:187:ALA:HA	3:B:472:HOH:O	1.88	0.74
1:A:255:ASN:HD22	1:A:258:ALA:HB3	1.52	0.73
1:A:230:HIS:CE1	1:A:233:ASP:HB2	2.24	0.73
1:A:70:ILE:O	1:A:74:LEU:HB2	1.89	0.72
1:B:114:LEU:HD11	1:B:219:MET:HG2	1.70	0.72
1:A:336:LEU:HA	3:A:428:HOH:O	1.88	0.72
1:B:300:ILE:HG13	1:B:304:GLN:HE21	1.54	0.72
1:A:205:LYS:HG3	3:A:429:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:PRO:HG2	3:C:499:HOH:O	1.89	0.71
1:A:161:LEU:HD23	1:A:162:LYS:N	2.05	0.71
1:A:251:ASN:ND2	1:A:259:ARG:HH21	1.89	0.70
1:A:200:SER:HB3	1:A:253:ILE:HD11	1.72	0.70
1:A:200:SER:HB3	1:A:253:ILE:CG1	2.21	0.69
1:A:354:PRO:HG3	3:A:378:HOH:O	1.91	0.69
1:B:257:LYS:HA	1:B:257:LYS:NZ	2.07	0.69
1:A:272:PRO:HG2	1:A:275:ARG:HB2	1.75	0.69
1:B:158:THR:O	1:B:159:CYS:HB2	1.93	0.69
1:B:93:ILE:HG13	1:B:342:LYS:HE2	1.74	0.69
1:A:156:ASN:O	2:C:71:LEU:HD23	1.93	0.68
1:A:121:ASN:HB2	3:A:462:HOH:O	1.94	0.67
1:A:250:LEU:HD13	1:A:296:PRO:CD	2.24	0.67
1:A:251:ASN:C	1:A:253:ILE:H	1.97	0.67
1:B:54:ILE:HG22	1:B:56:PRO:CD	2.23	0.67
2:D:64:ARG:HA	2:D:64:ARG:HE	1.59	0.67
1:A:146:ARG:HH21	1:A:182:LEU:HD22	1.59	0.67
1:A:13:ARG:HB2	1:A:15:GLN:OE1	1.95	0.67
1:B:78:HIS:HD2	1:B:80:ASN:H	1.42	0.66
1:A:71:LYS:HG2	1:A:327:PHE:HZ	1.61	0.66
1:A:144:LEU:HD22	1:A:205:LYS:HA	1.77	0.66
1:A:82:ILE:HG21	3:A:459:HOH:O	1.96	0.66
1:B:207:ILE:HG13	1:B:208:ASP:N	2.09	0.66
1:B:117:GLN:HE21	1:A:254:ILE:CG2	2.06	0.66
1:B:70:ILE:O	1:B:74:LEU:HB2	1.96	0.66
1:A:195:GLU:HA	1:A:253:ILE:HD12	1.75	0.66
1:B:272:PRO:HB2	1:B:274:ASN:ND2	2.10	0.66
1:B:189:ARG:HD3	1:B:189:ARG:H	1.59	0.65
2:C:64:ARG:HA	2:C:64:ARG:HE	1.61	0.65
1:A:253:ILE:HG12	1:A:254:ILE:N	2.12	0.65
1:B:56:PRO:CB	1:B:62:TYR:HB3	2.27	0.65
1:B:233:ASP:HA	3:B:573:HOH:O	1.97	0.65
1:A:295:ASN:HD22	1:A:296:PRO:CD	2.09	0.64
1:B:170:ARG:NE	1:B:171:VAL:H	1.87	0.64
2:C:65:ARG:NE	2:C:65:ARG:HA	2.12	0.64
1:A:117:GLN:HG2	1:A:118:HIS:N	2.11	0.64
1:A:89:ARG:HH11	1:A:89:ARG:HG3	1.63	0.64
1:A:57:PHE:O	1:A:338:LYS:HD2	1.98	0.64
1:A:157:THR:HA	2:C:73:VAL:CG1	2.28	0.63
1:B:59:HIS:HB2	1:B:62:TYR:HB2	1.80	0.63
1:B:247:GLN:HB3	3:B:441:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:N	1:A:15:GLN:NE2	2.46	0.63
1:B:141:ALA:HB2	1:B:323:ALA:HB2	1.80	0.62
1:A:200:SER:HB3	1:A:253:ILE:CD1	2.29	0.62
1:B:93:ILE:CG1	1:B:342:LYS:HE2	2.29	0.62
1:B:203:TYR:CD2	1:B:203:TYR:N	2.67	0.62
1:B:89:ARG:NH1	1:B:353:GLN:HE21	1.98	0.62
1:A:78:HIS:CD2	1:A:80:ASN:H	2.17	0.62
1:B:129:TYR:HB2	1:B:311:LEU:HD22	1.80	0.62
1:A:316:ASP:O	1:A:320:GLU:HG3	2.00	0.61
1:B:246:SER:O	1:B:250:LEU:HG	2.00	0.61
1:A:168:LEU:HD23	3:A:517:HOH:O	1.99	0.61
1:B:248:GLU:O	1:B:252:CYS:HB2	1.99	0.61
1:A:28:TYR:OH	1:A:31:GLU:HG2	2.01	0.61
1:B:23:TYR:HE2	1:B:88:ILE:HD11	1.66	0.61
1:B:108:THR:HG22	2:D:73:VAL:HG21	1.83	0.61
1:B:25:ASN:HD21	1:A:337:PRO:HB3	1.66	0.61
2:D:65:ARG:HA	2:D:65:ARG:CZ	2.29	0.61
1:B:22:ARG:HA	3:B:432:HOH:O	2.01	0.61
1:A:92:THR:OG1	1:A:95:GLN:HG3	1.99	0.60
1:B:336:LEU:N	1:B:336:LEU:HD12	2.15	0.60
1:B:251:ASN:HA	1:B:259:ARG:NH1	2.16	0.60
1:A:308:HIS:CG	1:A:309:PRO:HD2	2.36	0.60
1:A:68:ARG:HD2	3:A:407:HOH:O	2.00	0.60
1:A:29:ILE:HD13	1:A:39:SER:HB3	1.81	0.60
1:B:247:GLN:H	1:B:247:GLN:CD	2.05	0.60
1:B:77:ARG:O	1:B:77:ARG:HG2	2.02	0.60
1:A:218:GLU:HG3	1:A:223:ARG:C	2.21	0.60
1:A:136:LYS:HD2	1:A:306:LEU:CD1	2.31	0.60
1:B:203:TYR:N	1:B:203:TYR:HD2	1.98	0.59
1:B:336:LEU:CD1	1:B:336:LEU:H	2.15	0.59
1:A:301:GLU:HB2	1:A:304:GLN:HE21	1.67	0.59
1:A:26:LEU:HD23	1:A:38:CYS:SG	2.43	0.59
1:A:302:VAL:HG13	1:A:303:GLU:N	2.18	0.59
1:A:253:ILE:HG23	1:A:254:ILE:N	2.12	0.59
1:B:139:HIS:CE1	1:B:205:LYS:HB3	2.38	0.59
1:B:335:ASP:H	1:B:336:LEU:HD12	1.67	0.59
1:B:208:ASP:O	1:B:212:VAL:HG23	2.02	0.59
1:A:337:PRO:HG2	1:A:340:LYS:CG	2.29	0.58
1:A:56:PRO:O	1:A:58:GLU:N	2.36	0.58
1:A:185:TYR:HA	3:A:554:HOH:O	2.03	0.58
1:B:254:ILE:N	1:B:254:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HH21	1:A:182:LEU:CD2	2.17	0.58
1:A:29:ILE:HG12	1:A:38:CYS:HA	1.85	0.58
1:A:73:LEU:HD11	1:A:166:PHE:CD1	2.39	0.58
1:A:200:SER:HB3	1:A:253:ILE:HG13	1.86	0.57
1:B:304:GLN:HG3	3:B:395:HOH:O	2.05	0.57
2:D:64:ARG:HA	2:D:64:ARG:NE	2.19	0.57
1:A:139:HIS:CE1	1:A:205:LYS:HB3	2.40	0.57
1:B:301:GLU:HB2	3:B:395:HOH:O	2.05	0.57
1:A:238:ILE:HG23	1:A:242:LEU:HD12	1.86	0.57
1:B:65:ARG:HG3	1:B:167:GLY:O	2.05	0.57
1:A:80:ASN:ND2	1:A:130:GLN:HB3	2.20	0.57
1:B:107:GLU:HA	1:B:107:GLU:OE1	2.05	0.57
1:A:247:GLN:O	1:A:251:ASN:CB	2.51	0.56
1:A:284:ALA:HB2	1:A:310:TYR:CE1	2.40	0.56
1:B:56:PRO:HB3	1:B:62:TYR:HB3	1.87	0.56
1:B:112:LYS:HA	1:B:115:LYS:HE3	1.87	0.56
1:A:335:ASP:HB2	3:A:458:HOH:O	2.05	0.56
1:B:159:CYS:SG	2:D:70:ASN:N	2.78	0.56
1:A:171:VAL:HG21	1:A:174:PRO:HB2	1.86	0.56
1:A:57:PHE:CE1	1:A:342:LYS:HG3	2.40	0.56
1:A:126:TYR:O	1:A:130:GLN:HG3	2.05	0.56
1:B:119:LEU:HA	3:B:537:HOH:O	2.05	0.56
2:D:68:LYS:NZ	2:D:68:LYS:HB2	2.20	0.56
1:A:261:TYR:O	1:A:265:LEU:HD13	2.06	0.56
1:A:254:ILE:CD1	2:D:71:LEU:HD22	2.36	0.56
1:A:22:ARG:HB2	3:A:535:HOH:O	2.05	0.56
1:A:27:SER:O	1:A:38:CYS:HB2	2.06	0.56
1:A:11:MET:HA	1:A:16:VAL:HG23	1.88	0.56
1:B:114:LEU:HD11	1:B:219:MET:CG	2.36	0.56
1:B:257:LYS:HZ1	1:B:257:LYS:HA	1.69	0.56
1:B:146:ARG:NH2	1:B:201:LYS:HG3	2.22	0.55
1:B:157:THR:OG1	2:D:72:PRO:HA	2.05	0.55
1:A:87:ILE:HG21	1:A:349:THR:CG2	2.37	0.55
1:B:78:HIS:CD2	1:B:80:ASN:H	2.22	0.55
1:A:78:HIS:HD2	1:A:80:ASN:H	1.54	0.55
1:A:146:ARG:NH2	1:A:182:LEU:HD13	2.21	0.55
1:B:73:LEU:HD13	3:B:383:HOH:O	2.06	0.55
1:B:50:ALA:HB2	1:B:105:LEU:HD13	1.88	0.55
1:B:192:ARG:HD3	3:B:485:HOH:O	2.07	0.55
1:A:89:ARG:NH1	1:A:89:ARG:HG3	2.23	0.54
1:B:223:ARG:HG2	3:B:512:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HE3	1:A:152:ASN:OD1	2.06	0.54
1:B:228:GLY:HA2	1:B:233:ASP:OD2	2.07	0.54
1:B:51:ILE:HG12	1:B:102:VAL:HG22	1.89	0.54
1:A:152:ASN:C	1:A:164:CYS:HB2	2.26	0.54
1:A:170:ARG:HG2	1:A:170:ARG:HH11	1.73	0.54
2:C:64:ARG:NE	2:C:64:ARG:HA	2.22	0.54
1:A:60:GLN:HG3	3:A:370:HOH:O	2.06	0.54
1:B:287:LEU:HG	1:B:291:MET:CE	2.37	0.54
1:B:199:ASN:N	1:B:199:ASN:HD22	2.04	0.54
1:B:105:LEU:HA	3:B:507:HOH:O	2.07	0.54
1:B:57:PHE:CD1	1:B:342:LYS:HG3	2.42	0.54
1:A:108:THR:HB	2:C:74:ARG:O	2.07	0.53
1:A:87:ILE:HG21	1:A:349:THR:HG21	1.90	0.53
1:B:192:ARG:NH2	1:B:196:ILE:HG21	2.22	0.53
1:A:155:LEU:HD23	1:A:161:LEU:HA	1.90	0.53
1:B:199:ASN:N	1:B:199:ASN:ND2	2.57	0.53
1:A:226:PHE:CE1	1:A:241:ILE:HD12	2.44	0.53
1:A:117:GLN:HG2	1:A:118:HIS:H	1.73	0.53
3:B:407:HOH:O	1:A:337:PRO:HG3	2.08	0.53
1:B:303:GLU:H	1:B:303:GLU:CD	2.10	0.53
1:A:61:THR:O	1:A:65:ARG:HG3	2.09	0.53
1:A:83:GLY:O	1:A:103:GLN:HG2	2.09	0.53
1:B:337:PRO:HG2	1:B:340:LYS:HB2	1.90	0.53
1:A:177:ASP:O	1:A:178:HIS:HB3	2.08	0.53
1:A:325:ALA:HB2	3:A:500:HOH:O	2.08	0.53
1:B:257:LYS:C	1:B:259:ARG:H	2.11	0.53
1:B:287:LEU:HG	1:B:291:MET:HE2	1.91	0.53
1:B:204:THR:O	1:B:207:ILE:HG12	2.08	0.53
1:B:44:LEU:C	1:B:45:ASN:HD22	2.13	0.53
1:B:41:TYR:OH	1:A:336:LEU:HD23	2.08	0.52
1:A:283:LYS:HA	3:A:480:HOH:O	2.09	0.52
1:B:249:ASP:O	1:B:254:ILE:HD13	2.09	0.52
1:B:86:ASP:HA	1:B:352:PHE:CE1	2.44	0.52
1:A:248:GLU:HA	1:A:251:ASN:OD1	2.09	0.52
1:A:67:LEU:O	1:A:67:LEU:HD23	2.10	0.52
2:D:65:ARG:HG3	2:D:66:LEU:N	2.25	0.52
1:A:121:ASN:ND2	1:A:281:ASP:HB2	2.24	0.52
1:A:13:ARG:HD3	3:A:409:HOH:O	2.10	0.52
1:B:271:VAL:HG13	1:B:275:ARG:HD2	1.91	0.52
1:B:9:PRO:HB3	1:B:18:ASP:OD2	2.10	0.52
1:A:250:LEU:HD13	1:A:296:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:HD22	1:A:41:TYR:HB3	1.74	0.51
1:A:195:GLU:OE2	1:A:299:ARG:NH2	2.44	0.51
1:B:324:GLU:HA	1:B:324:GLU:OE1	2.11	0.51
1:A:249:ASP:HA	3:A:427:HOH:O	2.11	0.51
1:B:105:LEU:HD12	3:B:507:HOH:O	2.11	0.51
1:B:92:THR:HB	1:B:94:GLU:OE1	2.11	0.51
1:A:69:GLU:O	1:A:73:LEU:HB2	2.11	0.51
1:A:255:ASN:HD22	1:A:258:ALA:CB	2.23	0.51
1:A:157:THR:HA	2:C:73:VAL:HG13	1.92	0.51
1:A:251:ASN:CB	1:A:259:ARG:HE	2.03	0.51
1:A:109:ASP:OD1	1:A:111:TYR:HB3	2.11	0.51
1:B:137:TYR:CE1	1:B:323:ALA:HA	2.46	0.51
1:A:202:GLY:HA3	2:D:70:ASN:CB	2.32	0.50
1:B:25:ASN:ND2	1:A:337:PRO:HB3	2.25	0.50
1:A:57:PHE:HA	1:A:63:CYS:SG	2.51	0.50
1:A:171:VAL:CG2	1:A:174:PRO:HB2	2.41	0.50
1:B:251:ASN:HA	1:B:259:ARG:HH12	1.76	0.50
2:D:68:LYS:HG3	3:D:77:HOH:O	2.11	0.50
1:A:58:GLU:HG2	3:A:463:HOH:O	2.11	0.50
1:A:272:PRO:HD3	3:A:474:HOH:O	2.12	0.50
1:A:218:GLU:HA	1:A:223:ARG:O	2.11	0.50
1:A:170:ARG:HD3	1:A:171:VAL:N	2.27	0.50
1:B:26:LEU:HD23	1:B:40:ALA:HB2	1.94	0.49
1:A:250:LEU:C	1:A:252:CYS:N	2.64	0.49
1:B:256:LEU:O	1:B:257:LYS:HB3	2.12	0.49
1:A:251:ASN:C	1:A:253:ILE:N	2.64	0.49
1:B:232:LEU:HD22	1:B:261:TYR:CD2	2.47	0.49
1:B:276:LEU:C	1:B:278:PRO:HD3	2.32	0.49
1:A:153:LEU:HD11	1:A:215:ILE:HD13	1.95	0.49
1:A:250:LEU:HD23	1:A:294:PHE:CE2	2.48	0.49
1:A:309:PRO:O	1:A:312:GLU:HB3	2.13	0.49
1:B:24:THR:HG23	1:B:43:ASN:HD21	1.76	0.49
1:A:247:GLN:O	1:A:249:ASP:N	2.46	0.49
1:B:56:PRO:HB2	1:B:62:TYR:HB3	1.93	0.49
1:A:336:LEU:HB3	1:A:337:PRO:HD2	1.95	0.49
1:B:107:GLU:HB2	1:B:156:ASN:HA	1.95	0.49
1:B:192:ARG:NH2	1:B:196:ILE:CG2	2.75	0.49
1:B:189:ARG:N	1:B:189:ARG:CD	2.69	0.49
1:A:326:PRO:O	1:A:328:LYS:N	2.46	0.49
2:C:74:ARG:HH11	2:C:74:ARG:HG2	1.77	0.49
1:B:12:VAL:HG11	1:B:38:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:O	1:A:249:ASP:HB3	2.13	0.49
2:D:65:ARG:HG3	2:D:66:LEU:H	1.78	0.49
2:D:68:LYS:HA	3:D:78:HOH:O	2.13	0.48
1:B:172:ALA:O	1:B:173:ASP:CB	2.61	0.48
1:B:110:LEU:HB3	1:B:150:PRO:O	2.13	0.48
2:C:71:LEU:HD12	2:C:72:PRO:HD2	1.95	0.48
1:B:157:THR:HB	1:A:175:ASP:O	2.12	0.48
1:B:127:PHE:O	1:B:131:ILE:HG13	2.13	0.48
1:A:34:TYR:HB3	1:A:54:ILE:HG12	1.94	0.48
1:A:170:ARG:HH21	1:A:178:HIS:HB2	1.78	0.48
1:A:277:PHE:HB2	1:A:285:LEU:HD11	1.95	0.48
1:A:251:ASN:HB2	1:A:259:ARG:CZ	2.44	0.48
1:B:84:ILE:HG12	1:B:103:GLN:HE21	1.79	0.48
1:B:154:LEU:C	1:B:155:LEU:HG	2.35	0.48
1:B:112:LYS:O	1:B:115:LYS:HB3	2.13	0.48
1:B:124:ILE:HD13	1:B:220:LEU:HD23	1.96	0.48
1:A:146:ARG:HH11	1:A:170:ARG:HB2	1.79	0.47
1:B:89:ARG:NH1	1:B:353:GLN:NE2	2.61	0.47
1:B:253:ILE:HG22	1:B:253:ILE:O	2.14	0.47
1:A:196:ILE:HD11	1:A:207:ILE:CD1	2.44	0.47
3:B:454:HOH:O	2:D:73:VAL:HB	2.15	0.47
1:B:94:GLU:HA	3:B:590:HOH:O	2.14	0.47
1:A:250:LEU:O	1:A:253:ILE:HG22	2.13	0.47
1:A:141:ALA:HB2	1:A:323:ALA:HB2	1.95	0.47
1:A:204:THR:HB	3:A:429:HOH:O	2.13	0.47
1:A:89:ARG:HD3	1:A:349:THR:OG1	2.14	0.47
1:B:23:TYR:HA	1:B:41:TYR:O	2.15	0.47
1:B:239:LEU:HD22	1:B:245:PRO:CD	2.40	0.47
1:A:15:GLN:H	1:A:15:GLN:NE2	2.11	0.47
1:B:250:LEU:C	1:B:252:CYS:N	2.67	0.47
1:B:222:ASN:HB2	3:B:417:HOH:O	2.14	0.47
1:A:341:LEU:O	1:A:345:ILE:HG13	2.15	0.47
1:B:108:THR:HG23	1:B:109:ASP:N	2.28	0.47
1:A:200:SER:C	2:D:72:PRO:HD2	2.34	0.47
1:B:204:THR:O	1:B:207:ILE:HG23	2.15	0.47
1:B:200:SER:O	1:B:201:LYS:O	2.33	0.46
1:A:196:ILE:HD11	1:A:207:ILE:HD12	1.97	0.46
1:B:126:TYR:CE2	1:B:130:GLN:NE2	2.83	0.46
1:B:252:CYS:SG	1:B:253:ILE:HG12	2.54	0.46
1:B:172:ALA:O	1:B:173:ASP:HB3	2.16	0.46
1:B:251:ASN:N	1:B:251:ASN:HD22	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HG2	1:B:268:LYS:HE2	1.97	0.46
1:A:15:GLN:N	1:A:15:GLN:HE21	2.12	0.46
1:A:347:GLU:HG2	1:A:348:GLU:N	2.29	0.46
1:B:199:ASN:HD22	1:B:199:ASN:H	1.64	0.46
1:A:207:ILE:HG13	1:A:208:ASP:N	2.30	0.46
1:A:45:ASN:O	1:A:47:VAL:HG13	2.16	0.46
1:B:106:MET:HG3	1:B:154:LEU:HB3	1.97	0.46
1:A:59:HIS:HB2	1:A:62:TYR:HB2	1.98	0.46
1:A:164:CYS:O	1:A:165:ASP:O	2.33	0.46
1:A:328:LYS:HB3	1:A:330:ASP:OD1	2.16	0.46
1:A:178:HIS:ND1	1:A:178:HIS:O	2.48	0.46
1:A:89:ARG:NE	1:A:349:THR:OG1	2.49	0.46
1:A:218:GLU:HG3	1:A:223:ARG:O	2.16	0.46
1:A:51:ILE:HG12	1:A:102:VAL:HG22	1.97	0.46
1:A:60:GLN:HE22	1:A:64:GLN:HE21	1.64	0.46
1:A:11:MET:HB3	3:A:376:HOH:O	2.15	0.46
1:A:305:ALA:O	1:A:311:LEU:HD12	2.16	0.46
1:A:107:GLU:HB3	2:C:73:VAL:HB	1.98	0.45
1:A:302:VAL:HG13	1:A:303:GLU:H	1.81	0.45
1:A:239:LEU:HD22	1:A:245:PRO:HD3	1.98	0.45
2:C:67:GLN:O	2:C:68:LYS:HB2	2.17	0.45
1:B:161:LEU:C	1:B:161:LEU:HD23	2.37	0.45
1:B:117:GLN:HG3	1:A:254:ILE:HG12	1.96	0.45
1:B:195:GLU:HG2	1:B:196:ILE:N	2.32	0.45
1:B:106:MET:HG3	1:B:154:LEU:CB	2.47	0.45
1:B:34:TYR:CB	1:B:54:ILE:HG23	2.46	0.45
1:B:23:TYR:CE2	1:B:88:ILE:HD11	2.50	0.45
1:B:65:ARG:HG3	1:B:167:GLY:C	2.37	0.45
1:A:48:ARG:HG3	1:A:105:LEU:HD12	1.99	0.45
1:A:254:ILE:HG23	1:A:255:ASN:N	2.30	0.45
1:B:252:CYS:C	1:B:254:ILE:H	2.20	0.45
1:B:15:GLN:HG3	1:B:36:MET:CE	2.46	0.45
1:A:254:ILE:HG13	2:D:71:LEU:HD22	1.99	0.45
1:A:173:ASP:HB3	1:A:174:PRO:HD3	1.99	0.45
1:A:142:ASN:ND2	1:A:172:ALA:HB3	2.32	0.45
1:B:273:TRP:HB3	1:B:285:LEU:HD22	1.99	0.45
1:A:145:HIS:CG	1:A:148:LEU:HD13	2.52	0.45
1:A:249:ASP:OD1	1:A:294:PHE:HB3	2.17	0.44
1:A:131:ILE:HG13	1:A:161:LEU:CD1	2.47	0.44
1:B:45:ASN:N	1:B:45:ASN:HD22	2.15	0.44
1:B:154:LEU:HD22	3:B:566:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:C	1:A:336:LEU:HD12	2.38	0.44
1:B:48:ARG:HG2	1:B:48:ARG:HH11	1.83	0.44
1:B:341:LEU:O	1:B:345:ILE:HG13	2.18	0.44
1:B:49:VAL:HA	3:B:458:HOH:O	2.18	0.44
1:B:295:ASN:HA	3:B:452:HOH:O	2.16	0.44
1:A:89:ARG:HD2	1:A:96:MET:SD	2.57	0.44
2:D:68:LYS:HZ3	2:D:68:LYS:HB2	1.81	0.44
1:A:244:SER:HA	1:A:245:PRO:HD3	1.86	0.44
1:A:253:ILE:O	1:A:254:ILE:HG13	2.18	0.44
1:A:273:TRP:NE1	1:A:289:ASP:HB2	2.33	0.44
1:B:250:LEU:C	1:B:252:CYS:H	2.21	0.44
1:B:87:ILE:HG21	1:B:349:THR:HG22	1.99	0.44
1:B:259:ARG:C	1:B:261:TYR:N	2.71	0.44
2:D:70:ASN:O	2:D:71:LEU:HG	2.18	0.43
1:B:257:LYS:C	1:B:259:ARG:N	2.72	0.43
1:A:202:GLY:CA	2:D:70:ASN:HB3	2.33	0.43
1:B:255:ASN:C	1:B:257:LYS:H	2.21	0.43
1:A:31:GLU:HG3	3:A:452:HOH:O	2.17	0.43
1:B:94:GLU:HB2	1:B:95:GLN:OE1	2.19	0.43
1:A:251:ASN:O	1:A:253:ILE:N	2.51	0.43
1:B:281:ASP:HA	3:B:520:HOH:O	2.18	0.43
1:B:272:PRO:HG2	1:B:275:ARG:CB	2.48	0.43
1:B:223:ARG:HG3	3:B:417:HOH:O	2.17	0.43
1:B:234:GLN:O	1:B:237:HIS:HB2	2.18	0.43
1:A:200:SER:O	2:D:72:PRO:HG2	2.19	0.43
1:A:80:ASN:HD22	1:A:130:GLN:HB3	1.82	0.43
1:A:308:HIS:CD2	1:A:309:PRO:HD2	2.53	0.43
1:B:281:ASP:OD1	1:B:283:LYS:N	2.47	0.43
1:A:60:GLN:O	1:A:63:CYS:HB2	2.18	0.43
1:B:13:ARG:NH1	3:B:460:HOH:O	2.51	0.43
1:A:160:ASP:OD2	2:C:66:LEU:HD21	2.18	0.43
1:A:253:ILE:CG2	1:A:254:ILE:H	2.13	0.43
1:A:67:LEU:HD11	1:A:344:LEU:CB	2.49	0.43
1:A:107:GLU:H	1:A:107:GLU:CD	2.21	0.43
1:B:112:LYS:HE3	3:B:404:HOH:O	2.18	0.43
1:B:192:ARG:CZ	1:B:196:ILE:HG21	2.49	0.43
1:B:218:GLU:O	1:B:222:ASN:N	2.43	0.43
1:A:251:ASN:HB2	1:A:259:ARG:HH21	1.83	0.43
1:B:132:LEU:HD12	1:B:311:LEU:HD11	2.01	0.43
1:B:311:LEU:O	1:B:315:TYR:HB2	2.18	0.43
1:A:142:ASN:OD1	1:A:172:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:HA	1:A:210:TRP:CD1	2.54	0.43
1:B:231:TYR:O	1:B:235:LEU:HB2	2.19	0.43
1:A:262:LEU:C	1:A:264:SER:H	2.21	0.43
1:A:246:SER:H	1:A:249:ASP:CB	2.31	0.43
1:B:249:ASP:O	1:B:252:CYS:HB3	2.18	0.43
1:A:247:GLN:C	1:A:249:ASP:N	2.71	0.43
1:B:187:ALA:O	1:B:188:THR:HB	2.19	0.43
1:A:342:LYS:HB2	3:A:440:HOH:O	2.18	0.43
1:B:250:LEU:O	1:B:252:CYS:N	2.52	0.43
1:B:184:GLU:N	1:B:199:ASN:HB3	2.34	0.43
1:A:200:SER:CB	1:A:253:ILE:HG13	2.49	0.42
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.83	0.42
1:A:121:ASN:HD21	1:A:281:ASP:HB2	1.83	0.42
1:A:339:GLU:O	1:A:343:GLU:HG3	2.19	0.42
1:B:304:GLN:NE2	3:B:527:HOH:O	2.52	0.42
1:B:252:CYS:SG	1:B:253:ILE:N	2.89	0.42
1:A:33:ALA:HB1	1:A:65:ARG:HH22	1.84	0.42
1:B:190:TRP:CD1	1:B:227:PRO:HA	2.55	0.42
1:A:267:HIS:HE1	1:A:269:ASN:OD1	2.03	0.42
1:A:262:LEU:C	1:A:264:SER:N	2.71	0.42
1:A:146:ARG:NH2	1:A:178:HIS:NE2	2.68	0.42
1:A:88:ILE:HB	1:A:100:TYR:HB2	2.02	0.42
1:B:146:ARG:HH11	1:B:170:ARG:HB2	1.84	0.42
1:B:315:TYR:CZ	1:B:317:PRO:HD3	2.55	0.42
1:A:223:ARG:HG3	3:A:436:HOH:O	2.18	0.42
1:B:40:ALA:O	1:B:48:ARG:HA	2.18	0.42
1:A:295:ASN:ND2	1:A:296:PRO:HD2	2.18	0.42
1:B:157:THR:HB	1:A:175:ASP:HB3	2.02	0.42
1:A:238:ILE:CG2	1:A:242:LEU:HD12	2.48	0.42
1:A:216:LEU:HD12	1:A:291:MET:CE	2.50	0.42
1:A:23:TYR:CE2	1:A:88:ILE:HD11	2.54	0.42
1:A:273:TRP:C	1:A:275:ARG:H	2.23	0.41
1:A:195:GLU:HA	1:A:253:ILE:CD1	2.47	0.41
1:A:291:MET:O	1:A:299:ARG:HD2	2.20	0.41
1:B:18:ASP:HA	3:B:379:HOH:O	2.18	0.41
1:B:60:GLN:OE1	1:B:341:LEU:HD11	2.20	0.41
1:A:281:ASP:OD1	1:A:283:LYS:HB2	2.20	0.41
1:B:52:LYS:HE3	3:B:367:HOH:O	2.19	0.41
1:B:272:PRO:HG2	1:B:275:ARG:HB3	2.02	0.41
1:A:163:ILE:HG22	1:A:164:CYS:N	2.34	0.41
1:B:67:LEU:O	1:B:67:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:C	1:A:331:MET:H	2.23	0.41
1:A:170:ARG:HD2	3:A:365:HOH:O	2.21	0.41
1:B:13:ARG:NH1	1:B:28:TYR:HB3	2.35	0.41
1:B:235:LEU:HG	1:B:262:LEU:HD21	2.03	0.41
1:A:77:ARG:NH1	1:A:77:ARG:HG3	2.35	0.41
1:A:84:ILE:HG22	1:A:84:ILE:O	2.20	0.41
1:B:143:VAL:CG1	1:B:144:LEU:N	2.84	0.41
1:A:17:PHE:HE1	1:A:36:MET:HG2	1.86	0.41
1:A:120:SER:HB2	3:A:406:HOH:O	2.20	0.41
1:A:247:GLN:O	1:A:248:GLU:C	2.58	0.41
1:A:340:LYS:O	1:A:344:LEU:HG	2.20	0.41
1:B:207:ILE:CG1	1:B:208:ASP:N	2.80	0.41
1:B:295:ASN:HA	1:B:296:PRO:HD2	1.85	0.41
1:A:251:ASN:HB2	1:A:259:ARG:NH2	2.36	0.41
1:A:251:ASN:ND2	3:A:369:HOH:O	2.53	0.41
1:B:78:HIS:HE1	3:B:363:HOH:O	2.04	0.41
1:A:246:SER:HG	1:A:249:ASP:HB2	1.75	0.41
1:A:152:ASN:O	1:A:164:CYS:N	2.54	0.41
1:B:251:ASN:N	1:B:251:ASN:ND2	2.69	0.41
1:A:273:TRP:O	1:A:275:ARG:N	2.54	0.41
1:A:283:LYS:NZ	1:A:283:LYS:HB2	2.36	0.41
1:A:308:HIS:CE1	1:A:310:TYR:H	2.39	0.41
1:A:142:ASN:CG	1:A:172:ALA:HB3	2.41	0.41
1:B:71:LYS:HE3	1:B:75:ARG:NH2	2.35	0.41
1:B:116:THR:HA	3:B:412:HOH:O	2.21	0.41
2:C:71:LEU:HA	2:C:72:PRO:HD2	1.96	0.41
1:A:155:LEU:HD21	1:A:161:LEU:HB2	2.02	0.41
1:B:302:VAL:HG12	1:B:303:GLU:OE2	2.21	0.41
1:B:225:ILE:HD11	1:B:241:ILE:HD13	2.01	0.41
1:A:15:GLN:H	1:A:15:GLN:CD	2.24	0.40
1:A:64:GLN:HB3	1:A:68:ARG:NH1	2.37	0.40
1:B:17:PHE:CZ	1:B:38:CYS:HB2	2.56	0.40
1:A:237:HIS:HA	3:A:546:HOH:O	2.21	0.40
1:A:333:LEU:O	1:A:336:LEU:HD11	2.21	0.40
1:A:67:LEU:CD2	1:A:71:LYS:HE3	2.51	0.40
1:A:273:TRP:C	1:A:275:ARG:N	2.75	0.40
1:B:272:PRO:HD2	1:B:275:ARG:CZ	2.51	0.40
1:A:222:ASN:O	1:A:223:ARG:HG2	2.21	0.40
1:A:161:LEU:HD23	1:A:161:LEU:C	2.42	0.40
1:A:218:GLU:O	1:A:222:ASN:N	2.54	0.40
1:B:221:SER:O	1:B:222:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:O	1:B:278:PRO:HD3	2.22	0.40
1:B:90:ALA:HA	1:B:91:PRO:HD3	1.91	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	344/364 (94%)	274 (80%)	52 (15%)	18 (5%)	2	2
1	B	332/364 (91%)	281 (85%)	35 (10%)	16 (5%)	3	3
2	C	9/17 (53%)	3 (33%)	3 (33%)	3 (33%)	0	0
2	D	9/17 (53%)	4 (44%)	3 (33%)	2 (22%)	0	0
All	All	694/762 (91%)	562 (81%)	93 (13%)	39 (6%)	2	2

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ALA
1	B	173	ASP
1	B	197	MET
1	B	199	ASN
1	B	201	LYS
1	B	252	CYS
1	A	57	PHE
1	A	165	ASP
1	A	328	LYS
2	C	73	VAL
1	B	32	GLY
1	B	115	LYS
1	B	174	PRO

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Mol	Chain	Res	Type
1	B	253	ILE
1	A	56	PRO
1	A	172	ALA
1	A	247	GLN
1	A	252	CYS
1	A	333	LEU
2	D	66	LEU
2	C	66	LEU
1	B	96	MET
1	B	200	SER
1	A	146	ARG
1	A	355	GLY
1	B	185	TYR
1	A	250	LEU
1	A	327	PHE
1	B	107	GLU
1	B	188	THR
1	A	174	PRO
1	A	248	GLU
1	A	253	ILE
1	A	274	ASN
2	C	65	ARG
1	A	354	PRO
2	D	65	ARG
1	A	254	ILE
1	B	82	ILE

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	313/324 (97%)	292 (93%)	21 (7%)	20 37
1	B	302/324 (93%)	278 (92%)	24 (8%)	15 28
2	C	10/14 (71%)	9 (90%)	1 (10%)	9 18
2	D	10/14 (71%)	8 (80%)	2 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	635/676 (94%)	587 (92%)	48 (8%)	16 30

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	56	PRO
1	B	59	HIS
1	B	60	GLN
1	B	77	ARG
1	B	92	THR
1	B	107	GLU
1	B	148	LEU
1	B	155	LEU
1	B	156	ASN
1	B	184	GLU
1	B	189	ARG
1	B	198	LEU
1	B	199	ASN
1	B	201	LYS
1	B	203	TYR
1	B	216	LEU
1	B	237	HIS
1	B	256	LEU
1	B	257	LYS
1	B	276	LEU
1	B	299	ARG
1	B	312	GLU
1	B	313	GLN
1	B	356	TYR
1	A	10	GLU
1	A	15	GLN
1	A	18	ASP
1	A	73	LEU
1	A	94	GLU
1	A	118	HIS
1	A	148	LEU
1	A	164	CYS
1	A	170	ARG
1	A	182	LEU
1	A	198	LEU
1	A	216	LEU
1	A	229	LYS

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Mol	Chain	Res	Type
1	A	254	ILE
1	A	262	LEU
1	A	263	LEU
1	A	283	LYS
1	A	295	ASN
1	A	312	GLU
1	A	324	GLU
1	A	347	GLU
2	D	65	ARG
2	D	68	LYS
2	C	65	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	25	ASN
1	B	43	ASN
1	B	45	ASN
1	B	64	GLN
1	B	78	HIS
1	B	85	ASN
1	B	103	GLN
1	B	117	GLN
1	B	121	ASN
1	B	199	ASN
1	B	230	HIS
1	B	251	ASN
1	B	274	ASN
1	B	304	GLN
1	B	313	GLN
1	B	353	GLN
1	A	25	ASN
1	A	60	GLN
1	A	78	HIS
1	A	121	ASN
1	A	222	ASN
1	A	230	HIS
1	A	234	GLN
1	A	251	ASN
1	A	255	ASN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	267	HIS
1	A	295	ASN
1	A	297	HIS
1	A	304	GLN
1	A	313	GLN
1	A	353	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

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	348/364 (95%)	-0.17	15 (4%) 39 44	3, 17, 56, 75	0
1	B	338/364 (92%)	-0.23	6 (1%) 71 75	2, 19, 46, 59	0
2	C	11/17 (64%)	2.22	5 (45%) 0 0	54, 61, 69, 73	0
2	D	11/17 (64%)	3.52	7 (63%) 0 0	63, 67, 69, 69	0
All	All	708/762 (92%)	-0.11	33 (4%) 35 40	2, 18, 57, 75	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	71	LEU	9.0
1	A	329	PHE	7.1
2	D	69	GLY	6.3
2	D	73	VAL	6.1
1	A	330	ASP	4.9
2	C	64	ARG	4.3
1	A	9	PRO	4.1
1	A	12	VAL	4.0
2	D	74	ARG	3.9
1	A	331	MET	3.2
2	D	72	PRO	3.2
1	B	34	TYR	3.1
2	C	73	VAL	3.1
1	A	356	TYR	3.1
1	A	13	ARG	3.1
1	B	9	PRO	3.0
1	B	253	ILE	2.9
1	A	173	ASP	2.9
1	A	181	PHE	2.8
2	D	66	LEU	2.8
1	B	174	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	65	ARG	2.8
1	B	356	TYR	2.8
2	C	67	GLN	2.7
1	A	178	HIS	2.6
2	D	64	ARG	2.5
1	A	174	PRO	2.4
1	B	8	GLY	2.4
2	C	66	LEU	2.4
1	A	11	MET	2.2
1	A	251	ASN	2.2
1	A	182	LEU	2.1
1	A	8	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.