Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:43 PM GMT

PDB ID	:	1UVJ
Title	:	THE STRUCTURAL BASIS FOR RNA SPECIFICITY AND CA2 INHIBITION OF AN RNA-DEPENDENT RNA POLYMERASE PHI6P2 WITH 7NT RNA
Authors	:	Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.
Deposited on	:	2004-01-21
Resolution	:	1.90 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:

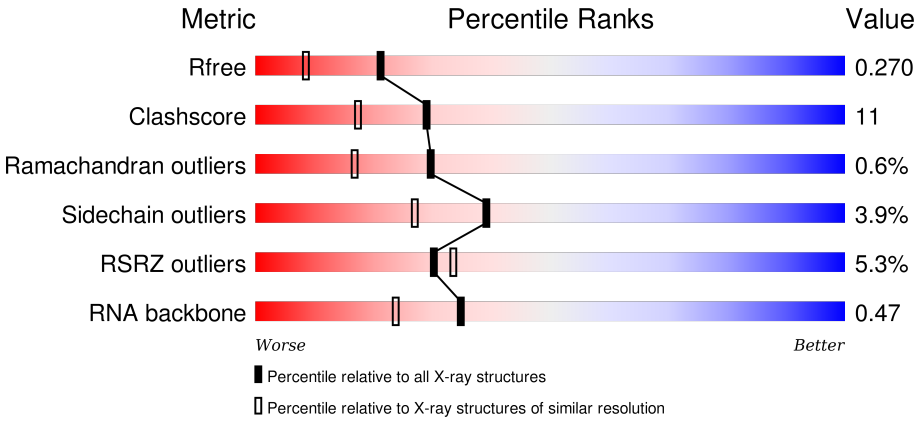
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)
RNA backbone	2183	1028 (2.70-1.10)

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	664	4% 81% 17% •
1	B	664	3% 80% 18% •
1	C	664	7% 79% 19% •
2	D	7	43% 43% 14% 43%

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Mol	Chain	Length	Quality of chain
2	E	7	57% 43% 14% 43%
2	F	7	57% 43% 14% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16633 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 P2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	CONFLICT	UNP P11124
B	456	MET	ILE	CONFLICT	UNP P11124
C	456	MET	ILE	CONFLICT	UNP P11124

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			
2	E	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			
2	F	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is water.

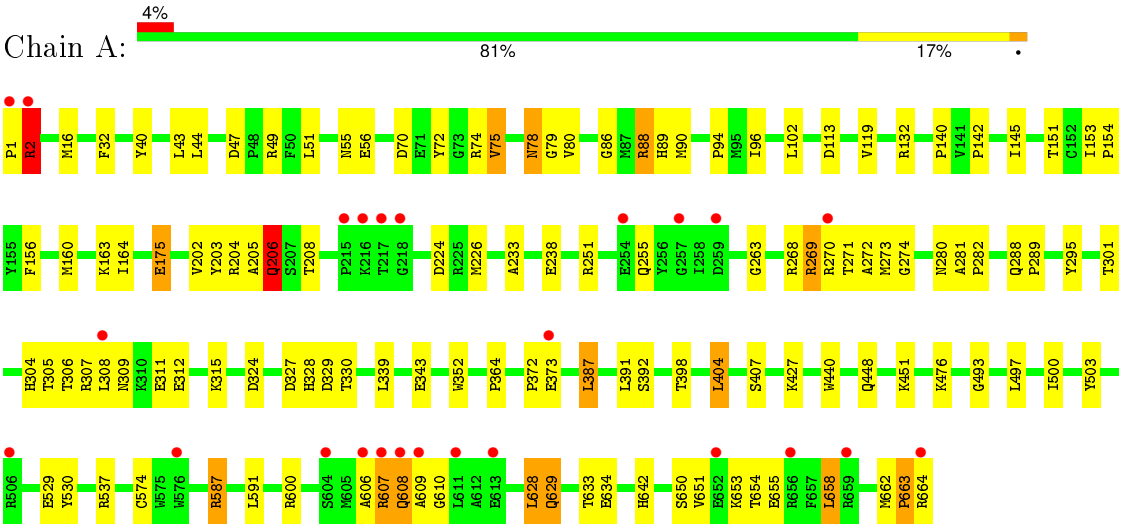
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	179	Total O 179 179	0	0
4	B	271	Total O 271 271	0	0
4	C	151	Total O 151 151	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

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.

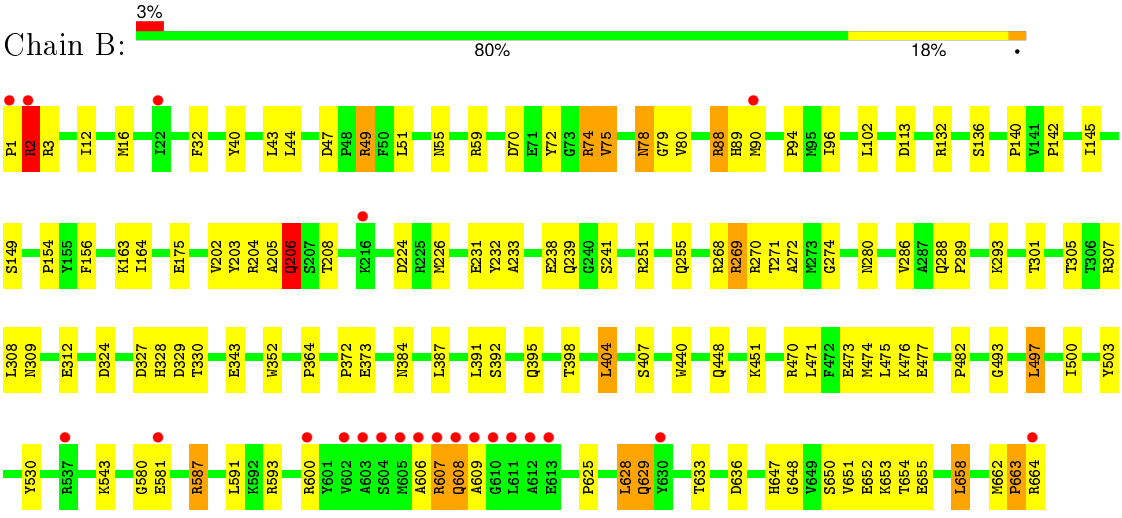
- Molecule 1: P2 PROTEIN

Chain A:



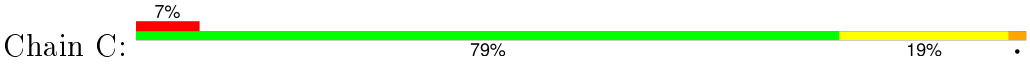
- Molecule 1: P2 PROTEIN

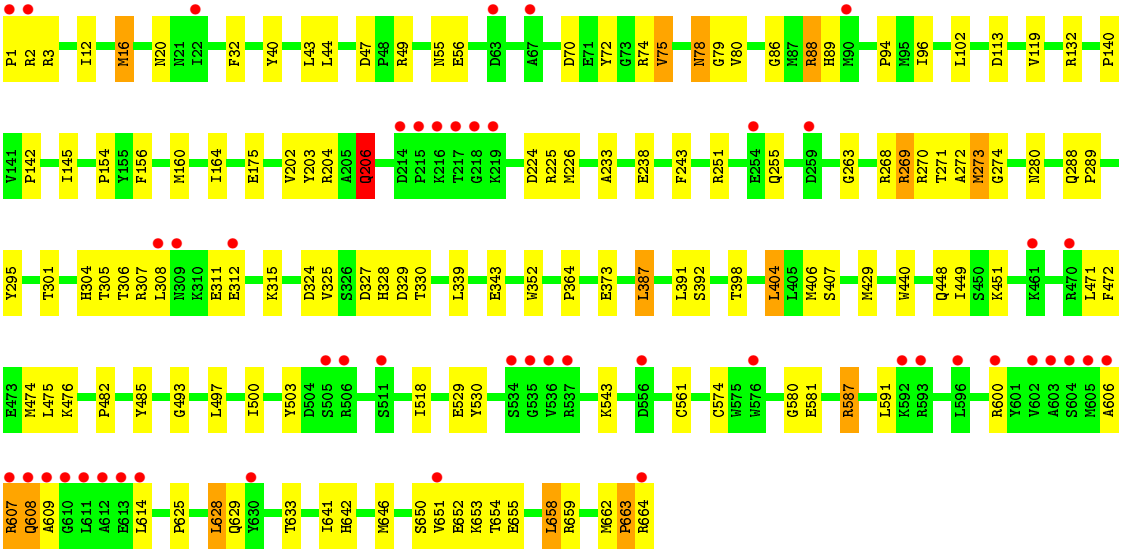
Chain B:



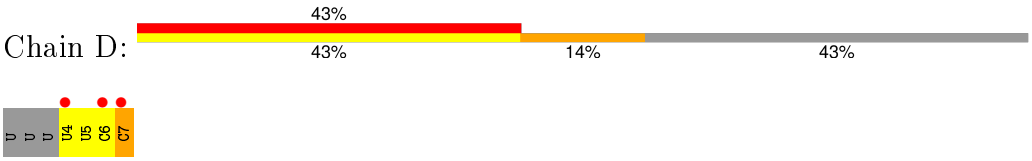
- Molecule 1: P2 PROTEIN

Chain C:

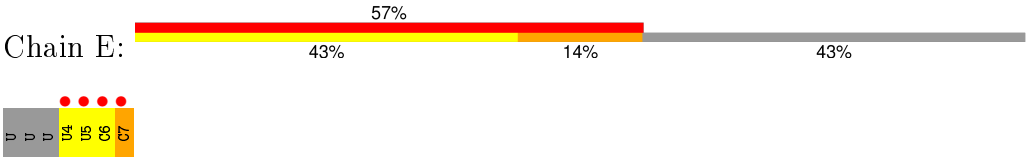




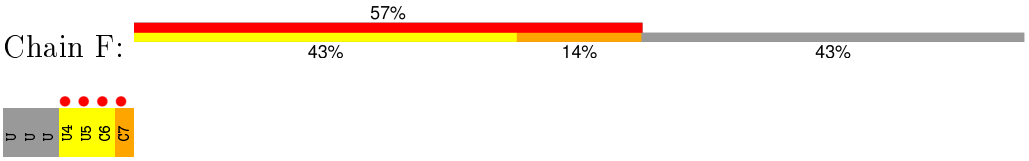
- Molecule 2: 5'-R(*UP*UP*CP*CP)-3'



- Molecule 2: 5'-R(*UP*UP*CP*CP)-3'



- Molecule 2: 5'-R(*UP*UP*CP*CP)-3'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.06Å 93.51Å 140.71Å 90.00° 101.19° 90.00°	Depositor
Resolution (Å)	18.74 – 1.90 18.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (18.74-1.90) 99.8 (18.73-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.271 0.241 , 0.270	Depositor DCC
R_{free} test set	10430 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 209435 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16633	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MN

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	0.57	0/5396	0.74	5/7297 (0.1%)
1	B	0.59	0/5396	0.76	6/7297 (0.1%)
1	C	0.56	0/5396	0.74	4/7297 (0.1%)
2	D	0.40	0/84	0.71	0/128
2	E	0.44	0/84	0.72	0/128
2	F	0.35	0/84	0.72	0/128
All	All	0.57	0/16440	0.75	15/22275 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	GLN	N-CA-C	-8.19	88.89	111.00
1	B	206	GLN	N-CA-C	-7.62	90.43	111.00
1	B	88	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	206	GLN	N-CA-C	-7.21	91.53	111.00
1	A	587	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	3	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	404	LEU	CA-CB-CG	6.33	129.85	115.30
1	A	404	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	88	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	404	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	49	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	175	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	C	88	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	587	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	587	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5265	0	5165	117	0
1	B	5265	0	5165	122	0
1	C	5265	0	5165	125	0
2	D	77	0	44	16	0
2	E	77	0	44	18	0
2	F	77	0	44	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	179	0	0	5	0
4	B	271	0	0	10	0
4	C	151	0	0	2	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	16633	0	15627	360	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 11.

All (360) 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:269:ARG:HH11	1:A:269:ARG:HG2	1.15	1.09
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.45	0.98
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.11	0.97
1:A:142:PRO:HG3	1:A:651:VAL:HG22	1.46	0.96
1:B:142:PRO:HG3	1:B:651:VAL:HG22	1.48	0.95
1:C:142:PRO:HG3	1:C:651:VAL:HG22	1.46	0.94
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.50	0.94
1:B:2:ARG:NH1	4:B:2003:HOH:O	2.00	0.93
1:C:269:ARG:HH11	1:C:269:ARG:HG2	1.32	0.93
1:A:47:ASP:OD1	1:A:49:ARG:HD3	1.71	0.90
1:A:269:ARG:NH1	1:A:269:ARG:HG2	1.82	0.87
1:B:451:LYS:HE2	2:E:7:C:N4	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ALA:HB3	1:A:609:ALA:HB2	1.57	0.85
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.22	0.83
1:C:451:LYS:HE2	2:F:7:C:N4	1.95	0.81
1:C:47:ASP:OD1	1:C:49:ARG:HD3	1.81	0.81
1:A:451:LYS:HE2	2:D:7:C:N4	1.97	0.80
1:C:301:THR:HG23	1:C:440:TRP:O	1.82	0.80
1:B:269:ARG:HD2	4:B:2146:HOH:O	1.82	0.79
1:B:269:ARG:HH11	1:B:269:ARG:HG2	1.48	0.79
1:A:608:GLN:HE22	1:B:593:ARG:CZ	1.96	0.78
1:C:629:GLN:HG2	2:F:6:C:C4	2.17	0.78
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.32	0.77
1:A:608:GLN:HE22	1:B:593:ARG:NH1	1.83	0.77
1:C:269:ARG:HG2	1:C:269:ARG:NH1	1.94	0.76
1:B:47:ASP:OD1	1:B:49:ARG:HD3	1.85	0.76
1:C:251:ARG:HH11	1:C:255:GLN:NE2	1.85	0.74
1:B:12:ILE:O	1:B:16:MET:HG2	1.88	0.74
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.69	0.74
1:B:658:LEU:HD21	4:B:2149:HOH:O	1.88	0.73
1:A:629:GLN:HG2	2:D:6:C:C4	2.24	0.73
1:C:75:VAL:HG21	1:C:500:ILE:HG21	1.69	0.72
1:A:301:THR:HG23	1:A:440:TRP:O	1.90	0.72
1:A:203:TYR:HB3	1:A:269:ARG:HD3	1.72	0.72
1:B:451:LYS:HE2	2:E:7:C:H41	1.55	0.71
1:A:75:VAL:HG21	1:A:500:ILE:HG21	1.73	0.70
1:A:607:ARG:O	1:A:608:GLN:HG3	1.91	0.70
1:B:607:ARG:O	1:B:608:GLN:HG3	1.92	0.70
1:C:140:PRO:HB3	1:C:658:LEU:HD23	1.72	0.70
1:B:301:THR:HG23	1:B:440:TRP:O	1.91	0.70
1:B:75:VAL:HG21	1:B:500:ILE:HG21	1.74	0.70
1:C:301:THR:HG22	4:C:2114:HOH:O	1.92	0.70
1:C:269:ARG:HD2	4:C:2082:HOH:O	1.91	0.70
1:B:269:ARG:NH1	1:B:269:ARG:HG2	2.05	0.70
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.73	0.69
1:B:55:ASN:OD1	1:B:88:ARG:NH2	2.23	0.69
1:C:633:THR:HA	2:F:7:C:H2'	1.73	0.69
1:B:51:LEU:HD13	1:B:90:MET:HE1	1.74	0.68
1:B:301:THR:HG22	4:B:2202:HOH:O	1.94	0.68
1:C:132:ARG:NH1	1:C:343:GLU:OE2	2.25	0.68
1:C:600:ARG:HB2	1:C:600:ARG:NH1	2.09	0.68
1:A:55:ASN:OD1	1:A:88:ARG:NH2	2.25	0.68
1:A:392:SER:O	1:A:398:THR:HG21	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:O	1:B:2:ARG:HD3	1.94	0.67
1:A:651:VAL:O	1:A:655:GLU:HB2	1.95	0.67
1:A:140:PRO:HB3	1:A:658:LEU:HD23	1.77	0.67
1:C:607:ARG:O	1:C:608:GLN:HG3	1.95	0.66
1:B:364:PRO:HA	1:B:387:LEU:HD22	1.75	0.66
1:C:600:ARG:HB2	1:C:600:ARG:HH11	1.60	0.66
1:B:59:ARG:HD3	4:B:2044:HOH:O	1.95	0.66
1:B:140:PRO:HB3	1:B:658:LEU:HD23	1.76	0.66
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.30	0.66
1:C:451:LYS:CE	2:F:7:C:N4	2.58	0.66
1:B:224:ASP:HB3	1:B:226:MET:HE1	1.78	0.66
1:B:75:VAL:HG21	1:B:500:ILE:CG2	2.26	0.66
1:A:308:LEU:O	1:A:312:GLU:HG3	1.96	0.66
1:B:132:ARG:NH1	1:B:343:GLU:OE2	2.29	0.65
1:C:203:TYR:HB3	1:C:269:ARG:HD3	1.78	0.65
1:A:251:ARG:HH11	1:A:255:GLN:NE2	1.92	0.65
1:B:629:GLN:HG2	2:E:6:C:C4	2.32	0.65
1:C:75:VAL:HG21	1:C:500:ILE:CG2	2.26	0.65
1:A:156:PHE:HD1	2:D:4:U:H5	1.45	0.65
1:A:274:GLY:HA2	2:D:5:U:H1'	1.78	0.65
1:C:202:VAL:HG11	2:F:4:U:C4'	2.27	0.65
1:A:600:ARG:HB2	1:A:600:ARG:HH11	1.62	0.65
1:A:1:PRO:HD2	1:A:238:GLU:OE1	1.97	0.64
1:C:392:SER:O	1:C:398:THR:HG21	1.98	0.64
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.32	0.64
1:C:78:ASN:HD22	1:C:79:GLY:N	1.96	0.64
1:C:308:LEU:O	1:C:312:GLU:HG3	1.98	0.63
1:A:451:LYS:HE2	2:D:7:C:H41	1.63	0.63
1:C:206:GLN:HE21	1:C:268:ARG:HH11	1.46	0.63
1:C:251:ARG:NH1	1:C:255:GLN:HE22	1.92	0.63
1:B:392:SER:O	1:B:398:THR:HG21	1.98	0.63
1:A:537:ARG:HD3	4:A:2143:HOH:O	1.98	0.63
1:A:658:LEU:HB3	1:A:662:MET:CE	2.28	0.63
1:C:55:ASN:OD1	1:C:88:ARG:NH2	2.27	0.62
1:B:606:ALA:CB	1:B:609:ALA:HB2	2.24	0.62
1:B:650:SER:OG	1:B:653:LYS:HG3	2.00	0.62
1:B:651:VAL:O	1:B:655:GLU:HB2	1.99	0.61
1:A:392:SER:O	1:A:398:THR:CG2	2.48	0.61
1:A:451:LYS:CE	2:D:7:C:N4	2.63	0.61
1:A:650:SER:OG	1:A:653:LYS:HG3	2.00	0.61
1:C:206:GLN:HG3	1:C:270:ARG:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TYR:CE1	1:B:476:LYS:HD3	2.36	0.61
1:C:651:VAL:O	1:C:655:GLU:HB2	2.00	0.61
1:A:224:ASP:HB3	1:A:226:MET:HE1	1.83	0.61
1:B:224:ASP:HB3	1:B:226:MET:CE	2.31	0.61
1:B:658:LEU:HB3	1:B:662:MET:CE	2.31	0.60
1:B:606:ALA:HB3	1:B:609:ALA:CB	2.27	0.60
1:A:629:GLN:NE2	2:D:7:C:H5"	2.15	0.60
1:A:600:ARG:NH1	1:A:600:ARG:HB2	2.16	0.60
1:C:600:ARG:CB	1:C:600:ARG:HH11	2.15	0.60
1:A:280:ASN:ND2	4:A:2082:HOH:O	2.35	0.59
1:A:2:ARG:HD3	1:A:2:ARG:O	2.01	0.59
1:C:269:ARG:HH11	1:C:269:ARG:CG	2.10	0.59
1:B:308:LEU:O	1:B:312:GLU:HG3	2.01	0.59
1:A:202:VAL:HG11	2:D:4:U:H4'	1.83	0.59
1:B:633:THR:HA	2:E:7:C:H2'	1.83	0.59
1:B:629:GLN:NE2	2:E:7:C:H5"	2.17	0.58
1:C:543:LYS:NZ	2:F:5:U:OP2	2.36	0.58
1:B:206:GLN:HE21	1:B:268:ARG:HH11	1.51	0.58
1:B:202:VAL:HG23	1:B:272:ALA:HB3	1.86	0.58
1:B:1:PRO:HD2	1:B:238:GLU:OE1	2.03	0.58
1:A:269:ARG:CG	1:A:269:ARG:NH1	2.61	0.58
1:A:119:VAL:HG23	1:C:20:ASN:OD1	2.04	0.58
1:B:600:ARG:NH1	1:B:600:ARG:HB2	2.19	0.57
1:B:51:LEU:HD13	1:B:90:MET:CE	2.33	0.57
1:A:132:ARG:NH1	1:A:343:GLU:OE2	2.35	0.57
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.67	0.57
1:B:628:LEU:O	2:E:7:C:H3'	2.04	0.57
1:A:301:THR:HG22	4:A:2117:HOH:O	2.04	0.57
1:C:12:ILE:O	1:C:16:MET:HG3	2.04	0.57
1:A:633:THR:HA	2:D:7:C:H2'	1.85	0.57
1:A:202:VAL:HG11	2:D:4:U:C4'	2.35	0.57
1:C:202:VAL:HG11	2:F:4:U:H4'	1.87	0.57
1:B:606:ALA:C	1:B:608:GLN:H	2.08	0.56
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.86	0.56
1:B:274:GLY:HA2	2:E:5:U:H1'	1.86	0.56
1:B:205:ALA:HB2	1:B:269:ARG:HH12	1.70	0.56
1:C:32:PHE:CZ	1:C:96:ILE:HD11	2.40	0.56
1:A:78:ASN:ND2	1:A:80:VAL:H	2.02	0.56
1:A:606:ALA:C	1:A:608:GLN:H	2.08	0.56
1:C:1:PRO:O	1:C:2:ARG:HB3	2.06	0.56
1:B:451:LYS:CE	2:E:7:C:N4	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ALA:O	1:A:608:GLN:N	2.39	0.56
1:C:328:HIS:HD2	1:C:329:ASP:OD1	1.89	0.56
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.88	0.56
1:A:251:ARG:NH1	1:A:255:GLN:HE22	1.99	0.55
1:A:156:PHE:HD1	2:D:4:U:C5	2.24	0.55
1:C:1:PRO:HD2	1:C:238:GLU:OE1	2.06	0.55
1:A:327:ASP:CG	1:A:330:THR:OG1	2.44	0.55
1:A:75:VAL:HG21	1:A:500:ILE:CG2	2.35	0.55
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.88	0.55
1:B:600:ARG:HH11	1:B:600:ARG:HB2	1.70	0.55
1:B:40:TYR:OH	1:B:587:ARG:NH2	2.39	0.55
1:C:156:PHE:HD1	2:F:4:U:H5	1.54	0.54
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.43	0.54
1:A:78:ASN:HD22	1:A:79:GLY:N	2.05	0.54
1:C:392:SER:O	1:C:398:THR:CG2	2.54	0.54
1:B:328:HIS:HD2	1:B:329:ASP:OD1	1.90	0.54
1:C:295:TYR:HH	2:F:7:C:H5	1.54	0.54
1:C:451:LYS:CE	2:F:7:C:H41	2.21	0.54
1:A:206:GLN:HG3	1:A:270:ARG:HD2	1.90	0.54
1:C:606:ALA:C	1:C:608:GLN:H	2.11	0.54
1:C:606:ALA:HB3	1:C:609:ALA:CB	2.31	0.54
1:B:600:ARG:HH11	1:B:600:ARG:CB	2.20	0.54
1:A:269:ARG:CG	1:A:269:ARG:HH11	1.99	0.53
1:A:628:LEU:O	2:D:7:C:O2	2.26	0.53
1:C:606:ALA:CB	1:C:609:ALA:HB2	2.30	0.53
1:A:608:GLN:NE2	1:B:593:ARG:NH1	2.53	0.53
1:B:94:PRO:HB2	1:B:269:ARG:HG3	1.90	0.53
1:B:606:ALA:O	1:B:608:GLN:N	2.42	0.53
1:C:94:PRO:HB2	1:C:269:ARG:HG3	1.91	0.53
1:A:90:MET:HA	1:A:90:MET:HE2	1.91	0.53
1:C:663:PRO:O	1:C:664:ARG:CZ	2.57	0.53
1:A:51:LEU:HD21	1:A:90:MET:HE1	1.90	0.52
1:A:451:LYS:CE	2:D:7:C:H41	2.22	0.52
1:C:274:GLY:HA2	2:F:5:U:H1'	1.90	0.52
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.91	0.52
1:A:94:PRO:HB2	1:A:269:ARG:HG3	1.91	0.52
1:B:392:SER:O	1:B:398:THR:CG2	2.58	0.52
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.52
1:C:301:THR:HG21	1:C:440:TRP:HA	1.92	0.52
1:B:156:PHE:HD1	2:E:4:U:H5	1.57	0.51
1:B:32:PHE:CZ	1:B:96:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:HH	2:D:7:C:H5	1.55	0.51
1:C:204:ARG:HD2	1:C:530:TYR:OH	2.10	0.51
1:A:407:SER:HA	1:A:448:GLN:HE22	1.76	0.51
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.46	0.51
1:C:658:LEU:HB3	1:C:662:MET:CE	2.40	0.51
1:A:663:PRO:O	1:A:664:ARG:CZ	2.58	0.51
1:A:70:ASP:OD2	1:A:74:ARG:HD3	2.11	0.51
1:B:628:LEU:O	2:E:7:C:O2	2.29	0.51
1:C:339:LEU:HD23	1:C:339:LEU:C	2.31	0.51
1:C:78:ASN:HD22	1:C:78:ASN:C	2.14	0.50
1:A:86:GLY:O	1:A:89:HIS:HD2	1.94	0.50
1:A:204:ARG:HD2	1:A:530:TYR:OH	2.11	0.50
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.46	0.50
1:B:70:ASP:OD2	1:B:74:ARG:HD3	2.12	0.50
1:B:75:VAL:HG12	1:B:493:GLY:HA2	1.93	0.50
1:A:427:LYS:HE3	1:C:12:ILE:HG21	1.93	0.50
1:A:224:ASP:HB3	1:A:226:MET:CE	2.40	0.50
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.07	0.49
1:C:224:ASP:HB3	1:C:226:MET:HE1	1.92	0.49
1:C:311:GLU:O	1:C:315:LYS:HG2	2.12	0.49
1:A:206:GLN:HE21	1:A:268:ARG:HH11	1.61	0.49
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.95	0.49
1:C:652:GLU:CD	1:C:652:GLU:H	2.16	0.49
1:B:580:GLY:C	1:B:581:GLU:HG2	2.33	0.49
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.78	0.49
1:B:203:TYR:HB3	1:B:269:ARG:HD3	1.93	0.49
1:A:339:LEU:C	1:A:339:LEU:HD23	2.33	0.49
1:C:451:LYS:HE2	2:F:7:C:H41	1.73	0.49
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.48	0.49
1:A:40:TYR:OH	1:A:587:ARG:NH2	2.46	0.49
1:B:301:THR:HG21	1:B:440:TRP:HA	1.94	0.49
1:B:471:LEU:HD12	1:B:474:MET:HE2	1.95	0.49
1:C:327:ASP:CG	1:C:330:THR:OG1	2.51	0.49
1:C:88:ARG:HD3	1:C:263:GLY:O	2.13	0.48
1:C:78:ASN:ND2	1:C:80:VAL:H	2.10	0.48
1:C:650:SER:O	1:C:654:THR:HG23	2.14	0.48
1:C:224:ASP:HB3	1:C:226:MET:CE	2.43	0.48
1:B:395:GLN:O	1:B:398:THR:HG23	2.13	0.48
1:A:311:GLU:O	1:A:315:LYS:HG2	2.13	0.48
1:B:633:THR:HG22	1:B:636:ASP:OD2	2.14	0.48
1:A:600:ARG:HH11	1:A:600:ARG:CB	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:LYS:CE	2:E:7:C:H41	2.25	0.48
1:B:475:LEU:HD21	1:B:482:PRO:HG3	1.96	0.48
1:C:580:GLY:C	1:C:581:GLU:HG2	2.33	0.48
1:C:40:TYR:OH	1:C:587:ARG:NH2	2.47	0.47
1:C:650:SER:OG	1:C:653:LYS:HG3	2.14	0.47
2:F:7:C:H3'	2:F:7:C:O2	2.14	0.47
1:B:78:ASN:ND2	1:B:80:VAL:H	2.12	0.47
1:C:119:VAL:HG22	1:C:485:TYR:OH	2.15	0.47
1:B:663:PRO:O	1:B:664:ARG:CZ	2.63	0.47
1:C:629:GLN:NE2	2:F:7:C:H5"	2.30	0.47
1:B:51:LEU:CD1	1:B:90:MET:HE1	2.41	0.47
1:A:88:ARG:HD3	1:A:263:GLY:O	2.15	0.47
1:A:78:ASN:C	1:A:78:ASN:HD22	2.15	0.47
1:A:32:PHE:CD2	1:A:372:PRO:HG3	2.50	0.47
1:B:231:GLU:HG2	4:B:2122:HOH:O	2.15	0.47
1:C:628:LEU:O	2:F:7:C:O2	2.33	0.47
1:B:650:SER:O	1:B:654:THR:HG23	2.15	0.47
1:B:202:VAL:HG11	2:E:4:U:H4'	1.96	0.47
1:A:160:MET:O	1:A:164:ILE:HG12	2.14	0.47
1:A:654:THR:O	1:A:658:LEU:HD22	2.15	0.47
1:B:280:ASN:ND2	4:B:2148:HOH:O	2.47	0.47
1:A:610:GLY:HA3	4:A:2169:HOH:O	2.14	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.97	0.47
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.51	0.47
2:E:7:C:O2	2:E:7:C:H3'	2.15	0.46
1:C:295:TYR:OH	2:F:7:C:H5	1.97	0.46
1:C:518:ILE:HB	1:C:561:CYS:SG	2.55	0.46
1:C:327:ASP:CG	1:C:330:THR:HG1	2.17	0.46
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.50	0.46
1:B:206:GLN:HG3	1:B:270:ARG:HD2	1.96	0.46
1:C:70:ASP:OD2	1:C:74:ARG:HD3	2.15	0.46
1:B:652:GLU:CD	1:B:652:GLU:H	2.18	0.46
1:C:56:GLU:HG2	1:C:574:CYS:SG	2.56	0.46
1:B:204:ARG:NE	2:E:5:U:O4	2.48	0.46
1:C:474:MET:HE2	1:C:474:MET:HB3	1.84	0.46
1:B:327:ASP:CG	1:B:330:THR:HG1	2.19	0.46
1:A:274:GLY:HA2	2:D:5:U:C1'	2.43	0.46
1:B:51:LEU:CD1	1:B:90:MET:CE	2.94	0.46
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.51	0.46
1:A:102:LEU:HD12	1:A:233:ALA:HA	1.97	0.46
1:A:205:ALA:HB2	1:A:269:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD21	1:A:90:MET:CE	2.46	0.45
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.51	0.45
1:C:102:LEU:HD12	1:C:233:ALA:HA	1.98	0.45
1:B:658:LEU:HB3	1:B:662:MET:HE1	1.97	0.45
1:A:32:PHE:CZ	1:A:96:ILE:HD11	2.51	0.45
1:C:471:LEU:HD12	1:C:474:MET:HE2	1.98	0.45
1:B:327:ASP:CG	1:B:330:THR:OG1	2.55	0.45
1:A:56:GLU:HG2	1:A:574:CYS:SG	2.57	0.45
1:C:140:PRO:CB	1:C:658:LEU:HD23	2.43	0.45
1:C:1:PRO:HD2	1:C:238:GLU:CD	2.37	0.45
1:C:606:ALA:O	1:C:608:GLN:N	2.49	0.45
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.98	0.45
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.51	0.45
1:B:286:VAL:C	1:B:289:PRO:HD2	2.37	0.45
1:C:625:PRO:O	1:C:628:LEU:HB2	2.17	0.45
1:A:327:ASP:CG	1:A:330:THR:HG1	2.19	0.45
1:A:606:ALA:C	1:A:608:GLN:N	2.70	0.44
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.81	0.44
1:C:407:SER:HA	1:C:448:GLN:HE22	1.83	0.44
1:C:614:LEU:HD21	1:C:641:ILE:HD11	2.00	0.44
1:C:325:VAL:HG21	1:C:406:MET:HE2	1.98	0.44
1:B:606:ALA:C	1:B:608:GLN:N	2.70	0.44
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.99	0.44
1:B:239:GLN:NE2	4:B:2128:HOH:O	2.51	0.44
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.48	0.44
1:B:205:ALA:CB	1:B:269:ARG:HH12	2.30	0.44
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.44	0.44
1:C:132:ARG:HD2	1:C:429:MET:HE2	2.00	0.43
1:C:202:VAL:HG23	1:C:272:ALA:HB3	2.00	0.43
1:B:32:PHE:CD2	1:B:372:PRO:HG3	2.52	0.43
1:A:305:THR:H	1:A:309:ASN:ND2	2.16	0.43
1:C:659:ARG:NH1	1:C:659:ARG:HB2	2.33	0.43
1:B:1:PRO:HD2	1:B:238:GLU:CD	2.38	0.43
1:B:78:ASN:HD22	1:B:79:GLY:N	2.15	0.43
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.76	0.43
1:B:202:VAL:HG11	2:E:4:U:C4'	2.47	0.43
1:C:650:SER:HB2	1:C:652:GLU:OE1	2.19	0.43
1:B:305:THR:H	1:B:309:ASN:ND2	2.15	0.43
1:C:628:LEU:O	2:F:7:C:H3'	2.18	0.43
1:B:286:VAL:O	1:B:289:PRO:HD2	2.19	0.43
1:A:301:THR:HG21	1:A:440:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:SER:HB2	1:B:652:GLU:OE1	2.19	0.43
1:B:274:GLY:HA2	2:E:5:U:C1'	2.48	0.43
1:B:78:ASN:HD22	1:B:78:ASN:C	2.20	0.43
1:C:529:GLU:O	1:C:529:GLU:HG2	2.18	0.43
1:C:12:ILE:O	1:C:16:MET:CG	2.65	0.43
1:C:475:LEU:HD21	1:C:482:PRO:HG3	2.00	0.43
1:A:151:THR:CG2	1:A:163:LYS:HG2	2.49	0.43
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.54	0.43
1:A:51:LEU:CD2	1:A:90:MET:CE	2.97	0.43
1:B:204:ARG:CZ	2:E:5:U:O4	2.67	0.43
1:B:149:SER:OG	1:B:163:LYS:HE3	2.19	0.43
1:A:634:GLU:HB2	1:A:642:HIS:NE2	2.34	0.43
1:A:658:LEU:HB3	1:A:662:MET:HE1	2.02	0.42
1:A:280:ASN:HA	1:A:280:ASN:HD22	1.62	0.42
1:B:204:ARG:HD3	2:E:5:U:O4	2.19	0.42
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.02	0.42
1:C:304:HIS:CE1	1:C:449:ILE:HB	2.54	0.42
1:C:606:ALA:C	1:C:608:GLN:N	2.72	0.42
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.55	0.42
1:B:140:PRO:CB	1:B:658:LEU:HD23	2.46	0.42
1:A:1:PRO:HD2	1:A:238:GLU:CD	2.39	0.42
1:A:206:GLN:OE1	1:A:208:THR:O	2.37	0.42
1:B:175:GLU:HG3	1:B:352:TRP:CD1	2.55	0.42
1:C:664:ARG:HG2	1:C:664:ARG:NH1	2.34	0.42
1:B:407:SER:HA	1:B:448:GLN:HE22	1.85	0.42
2:D:7:C:O2	2:D:7:C:H3'	2.19	0.42
1:B:470:ARG:HD2	4:B:2212:HOH:O	2.19	0.42
1:A:610:GLY:CA	4:A:2169:HOH:O	2.67	0.42
1:C:274:GLY:HA2	2:F:5:U:C1'	2.50	0.42
1:A:427:LYS:HE3	1:C:12:ILE:CG2	2.50	0.42
1:C:280:ASN:HD22	1:C:280:ASN:HA	1.64	0.42
1:A:153:ILE:HA	1:A:154:PRO:HA	1.78	0.41
1:A:119:VAL:CG2	1:C:20:ASN:OD1	2.67	0.41
1:B:204:ARG:HD2	1:B:530:TYR:OH	2.20	0.41
1:C:160:MET:O	1:C:164:ILE:HG12	2.20	0.41
1:C:86:GLY:O	1:C:89:HIS:CD2	2.73	0.41
1:C:156:PHE:HD1	2:F:4:U:C5	2.37	0.41
1:B:288:GLN:HB3	1:B:289:PRO:HD3	2.02	0.41
1:B:543:LYS:O	1:B:625:PRO:HD2	2.19	0.41
1:A:529:GLU:HG2	1:A:529:GLU:O	2.19	0.41
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLN:OE1	1:B:208:THR:O	2.38	0.41
1:C:273:MET:O	2:F:5:U:H1'	2.21	0.41
1:B:474:MET:HB3	1:B:474:MET:HE2	1.90	0.41
1:A:304:HIS:HA	1:A:309:ASN:HD21	1.86	0.41
1:B:89:HIS:HE1	4:B:2133:HOH:O	2.04	0.41
1:C:305:THR:OG1	1:C:306:THR:N	2.54	0.41
1:A:202:VAL:HG23	1:A:272:ALA:HB3	2.03	0.41
1:C:225:ARG:HD3	1:C:225:ARG:HA	1.84	0.41
1:B:232:TYR:HA	1:B:239:GLN:O	2.20	0.40
1:A:305:THR:OG1	1:A:306:THR:N	2.53	0.40
1:C:628:LEU:HD12	1:C:628:LEU:HA	1.96	0.40
1:B:647:HIS:ND1	1:B:648:GLY:N	2.68	0.40
1:B:473:GLU:O	1:B:477:GLU:HG3	2.21	0.40
1:A:175:GLU:HG3	1:A:352:TRP:CD1	2.57	0.40
1:C:70:ASP:OD2	1:C:74:ARG:CD	2.70	0.40
1:A:281:ALA:HB3	1:A:282:PRO:CD	2.52	0.40
1:B:102:LEU:HD12	1:B:233:ALA:HA	2.03	0.40
1:C:1:PRO:HD2	1:C:238:GLU:OE2	2.21	0.40
1:C:243:PHE:CD1	1:C:243:PHE:N	2.89	0.40
1:B:136:SER:OG	1:B:293:LYS:NZ	2.55	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	662/664 (100%)	638 (96%)	20 (3%)	4 (1%)	30	17
1	B	662/664 (100%)	635 (96%)	23 (4%)	4 (1%)	30	17
1	C	662/664 (100%)	634 (96%)	25 (4%)	3 (0%)	34	21
All	All	1986/1992 (100%)	1907 (96%)	68 (3%)	11 (1%)	30	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ARG
1	A	608	GLN
1	B	607	ARG
1	B	608	GLN
1	C	607	ARG
1	C	608	GLN
1	A	2	ARG
1	B	2	ARG
1	A	663	PRO
1	B	663	PRO
1	C	663	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	557/557 (100%)	536 (96%)	21 (4%)	40	28
1	B	557/557 (100%)	535 (96%)	22 (4%)	39	27
1	C	557/557 (100%)	535 (96%)	22 (4%)	39	27
All	All	1671/1671 (100%)	1606 (96%)	65 (4%)	39	27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	16	MET
1	A	43	LEU
1	A	44	LEU
1	A	75	VAL
1	A	78	ASN
1	A	113	ASP
1	A	206	GLN
1	A	269	ARG
1	A	273	MET

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Mol	Chain	Res	Type
1	A	307	ARG
1	A	324	ASP
1	A	373	GLU
1	A	387	LEU
1	A	391	LEU
1	A	404	LEU
1	A	497	LEU
1	A	591	LEU
1	A	628	LEU
1	A	629	GLN
1	A	658	LEU
1	B	2	ARG
1	B	43	LEU
1	B	44	LEU
1	B	74	ARG
1	B	75	VAL
1	B	78	ASN
1	B	113	ASP
1	B	154	PRO
1	B	206	GLN
1	B	241	SER
1	B	269	ARG
1	B	307	ARG
1	B	324	ASP
1	B	373	GLU
1	B	384	ASN
1	B	391	LEU
1	B	404	LEU
1	B	497	LEU
1	B	591	LEU
1	B	628	LEU
1	B	629	GLN
1	B	658	LEU
1	C	3	ARG
1	C	16	MET
1	C	43	LEU
1	C	44	LEU
1	C	75	VAL
1	C	78	ASN
1	C	113	ASP
1	C	154	PRO
1	C	206	GLN

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Mol	Chain	Res	Type
1	C	269	ARG
1	C	273	MET
1	C	307	ARG
1	C	324	ASP
1	C	373	GLU
1	C	387	LEU
1	C	391	LEU
1	C	404	LEU
1	C	472	PHE
1	C	497	LEU
1	C	591	LEU
1	C	628	LEU
1	C	658	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	191	GLN
1	A	206	GLN
1	A	255	GLN
1	A	280	ASN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	A	629	GLN
1	B	15	GLN
1	B	25	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	191	GLN
1	B	206	GLN
1	B	239	GLN

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Mol	Chain	Res	Type
1	B	255	GLN
1	B	280	ASN
1	B	309	ASN
1	B	328	HIS
1	B	384	ASN
1	B	448	GLN
1	B	525	GLN
1	B	629	GLN
1	C	15	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	191	GLN
1	C	206	GLN
1	C	255	GLN
1	C	280	ASN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	525	GLN
1	C	629	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	3/7 (42%)	1 (33%)	0
2	E	3/7 (42%)	1 (33%)	0
2	F	3/7 (42%)	1 (33%)	0
All	All	9/21 (42%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	7	C
2	E	7	C
2	F	7	C

There are no RNA pucker outliers to report.

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	664/664 (100%)	0.08	25 (3%) 44 48	18, 30, 50, 101	0
1	B	664/664 (100%)	0.10	22 (3%) 50 53	19, 28, 50, 101	0
1	C	664/664 (100%)	0.41	48 (7%) 18 20	19, 32, 52, 102	0
2	D	4/7 (57%)	3.34	3 (75%) 0 0	119, 122, 123, 127	0
2	E	4/7 (57%)	4.99	4 (100%) 0 0	119, 122, 124, 127	0
2	F	4/7 (57%)	2.91	4 (100%) 0 0	119, 122, 123, 127	0
All	All	2004/2013 (99%)	0.22	106 (5%) 30 33	18, 30, 52, 127	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	609	ALA	14.0
1	C	603	ALA	13.5
1	C	607	ARG	12.6
1	C	608	GLN	11.7
1	B	603	ALA	10.7
1	C	606	ALA	10.3
1	C	609	ALA	9.9
1	A	606	ALA	8.8
1	B	608	GLN	8.4
1	B	606	ALA	8.3
1	A	1	PRO	7.5
1	B	607	ARG	7.1
1	C	604	SER	6.7
1	A	664	ARG	6.7
1	C	664	ARG	6.7
1	C	612	ALA	6.4
1	C	610	GLY	6.4
1	C	215	PRO	6.3
1	A	607	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
2	E	6	C	5.6
1	B	664	ARG	5.6
2	E	7	C	5.3
1	C	537	ARG	5.2
2	E	4	U	5.0
1	C	611	LEU	5.0
1	B	1	PRO	4.9
1	C	254	GLU	4.9
1	B	610	GLY	4.9
1	C	216	LYS	4.8
1	B	604	SER	4.7
1	C	63	ASP	4.7
2	D	4	U	4.7
1	C	461	LYS	4.7
2	F	4	U	4.5
2	D	7	C	4.5
1	B	612	ALA	4.4
1	A	254	GLU	4.3
1	C	613	GLU	4.1
2	E	5	U	4.1
1	C	605	MET	4.1
1	C	596	LEU	4.0
1	C	470	ARG	3.8
1	A	576	TRP	3.7
1	C	602	VAL	3.7
1	A	216	LYS	3.7
1	C	1	PRO	3.6
1	C	217	THR	3.6
1	C	2	ARG	3.5
1	C	308	LEU	3.5
1	B	611	LEU	3.5
1	C	592	LYS	3.5
1	C	506	ARG	3.5
1	B	537	ARG	3.4
1	B	613	GLU	3.4
1	B	2	ARG	3.3
1	A	604	SER	3.3
1	C	505	SER	3.2
1	C	556	ASP	3.2
1	C	576	TRP	3.1
2	F	7	C	3.1
1	C	535	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	217	THR	3.0
1	A	659	ARG	2.9
1	B	216	LYS	2.9
1	B	602	VAL	2.9
1	C	67	ALA	2.9
1	A	308	LEU	2.8
1	A	608	GLN	2.8
1	B	605	MET	2.8
1	C	600	ARG	2.7
1	C	90	MET	2.7
1	A	373	GLU	2.7
1	B	22	ILE	2.6
1	C	259	ASP	2.6
1	C	309	ASN	2.6
1	A	652	GLU	2.6
1	C	214	ASP	2.6
1	B	90	MET	2.5
1	A	2	ARG	2.5
2	D	6	C	2.4
1	C	651	VAL	2.4
1	A	613	GLU	2.4
1	B	600	ARG	2.4
1	C	536	VAL	2.4
1	C	219	LYS	2.4
1	A	215	PRO	2.3
1	C	22	ILE	2.3
1	C	593	ARG	2.3
1	C	630	TYR	2.3
1	A	270	ARG	2.2
1	A	506	ARG	2.2
1	A	609	ALA	2.1
1	A	257	GLY	2.1
1	A	656	ARG	2.1
1	B	630	TYR	2.1
1	A	218	GLY	2.1
1	A	259	ASP	2.1
1	C	614	LEU	2.1
1	A	611	LEU	2.1
1	C	312	GLU	2.1
2	F	6	C	2.1
1	B	581	GLU	2.0
2	F	5	U	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	534	SER	2.0
1	C	218	GLY	2.0
1	C	511	SER	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)

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	MN	B	1665	1/1	0.99	0.04	-2.46	25,25,25,25	0
3	MN	C	1665	1/1	0.99	0.02	-2.87	30,30,30,30	0
3	MN	A	1665	1/1	0.99	0.06	-5.30	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.