Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 10:06 am BST

PDB ID	:	1HHS
Title	:	RNA dependent RNA polymerase from dsRNA bacteriophage phi6
Authors	:	Grimes, J.M.; Butcher, S.J.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.
Deposited on	:	2000-12-28
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

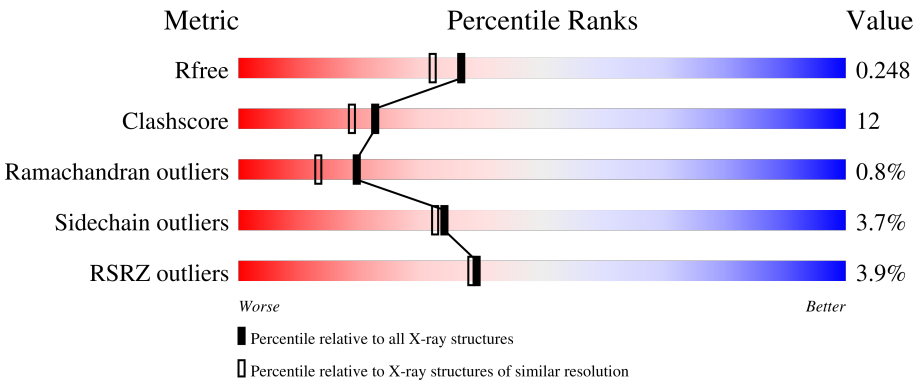
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	3% 82% 15% •
1	B	664	3% 83% 15% •
1	C	664	5% 81% 17% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18563 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 RNA-DIRECTED RNA POLYMERASE.

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

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	890	890	890	0	0
3	B	938	938	938	0	0

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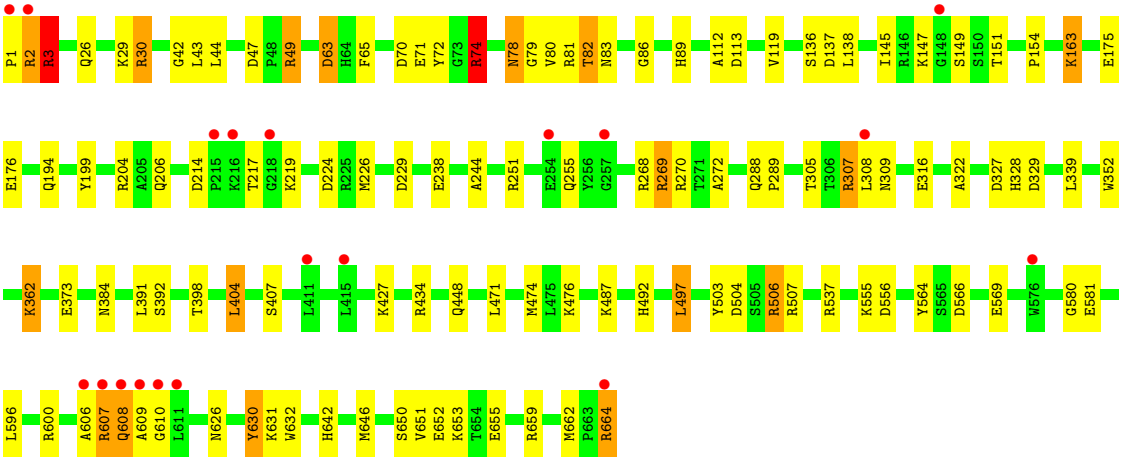
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	937	937	937	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

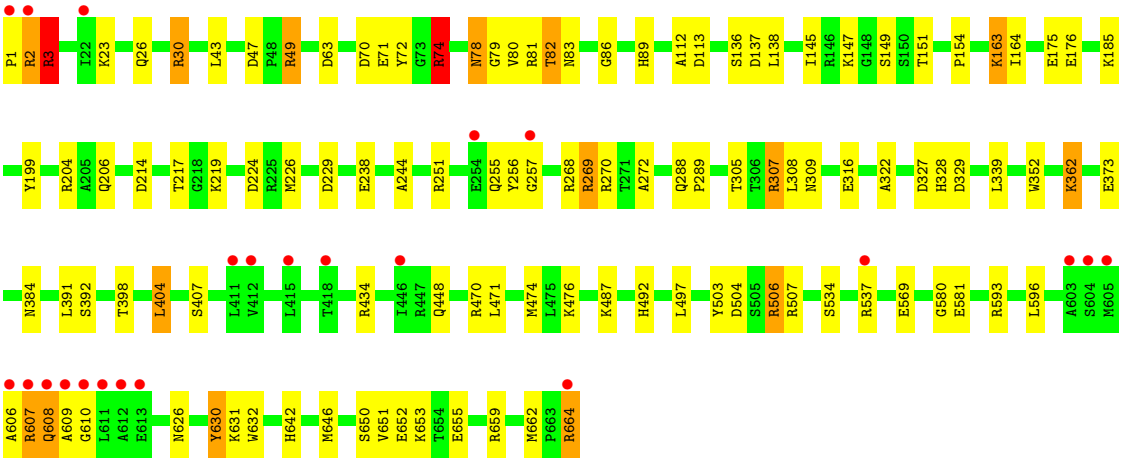
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain A:



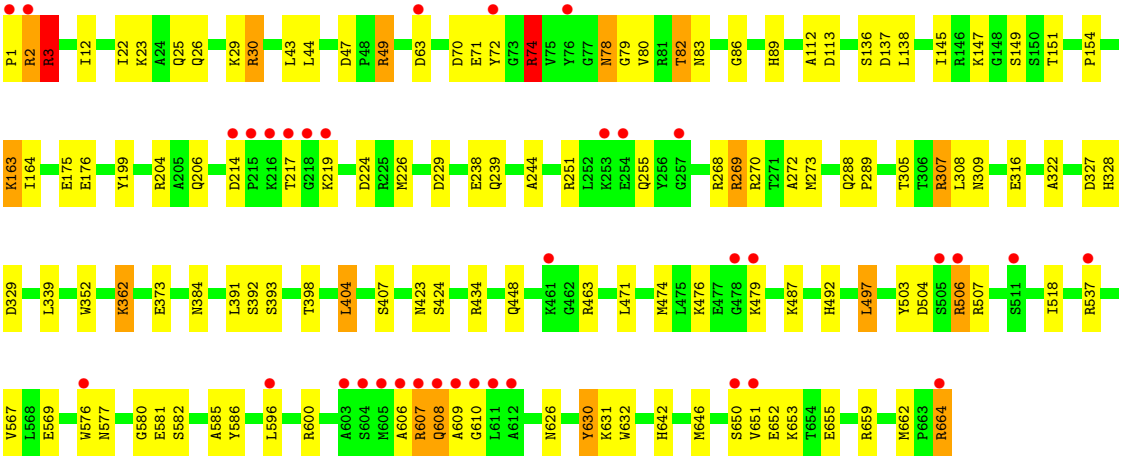
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain B:



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain C:


P1 R2 R3 I12 I22 K23 A24 Q25 Q26 K29 R30 L43 L44 D47 P48 R49 D63 D70 E71 Y72 G73 R74 V75 Y76 G77 N78 G79 V80 R81 T82 N83 G86 H89 A112 D113 S136 D137 L138 I145 R146 K147 G148 S149 S150 T151 P154
K163 I164 E175 E176 Y199 R204 A205 Q206 D214 P215 K216 T217 G218 K219 D224 R225 M226 D229 E238 Q239 A244 R251 L252 K253 E254 Q255 Y256 G257 R268 R269 R270 T271 A272 M273 Q288 P289 T305 T306 R307 L308 N309 E316 A322 D327 H328
D329 L339 W352 K362 E373 N384 L391 S392 S393 T398 L404 S407 N423 S424 R434 Q448 K461 G462 R463 L471 M474 L475 K476 E477 G478 K479 K487 H492 L497 Y503 D504 S505 R506 R507 S511 I518 R537
V567 L568 E569 W576 N577 G580 E581 S582 A585 Y586 L596 R600 A603 S604 M605 A606 R607 Q608 A609 G610 L611 A612 N626 Y630 K631 W632 H642 M646 S650 V651 E652 K653 T654 E655 R659 M662 P663 R664

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.41Å 93.36Å 141.20Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 29.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.00) 99.9 (29.86-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.249 0.220 , 0.248	Depositor DCC
R_{free} test set	9067 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18563	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.72	0/5396	0.81	8/7297 (0.1%)
1	B	0.72	0/5396	0.81	8/7297 (0.1%)
1	C	0.72	0/5396	0.81	8/7297 (0.1%)
All	All	0.72	0/16188	0.81	24/21891 (0.1%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	LEU	CA-CB-CG	7.32	132.14	115.30
1	C	404	LEU	CA-CB-CG	7.31	132.11	115.30
1	B	404	LEU	CA-CB-CG	7.30	132.10	115.30
1	C	3	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	3	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	206	GLN	N-CA-C	-6.78	92.71	111.00
1	C	206	GLN	N-CA-C	-6.77	92.72	111.00
1	A	3	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	206	GLN	N-CA-C	-6.76	92.75	111.00
1	B	362	LYS	CD-CE-NZ	-6.28	97.25	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	362	LYS	CD-CE-NZ	-6.28	97.27	111.70
1	C	362	LYS	CD-CE-NZ	-6.26	97.29	111.70
1	A	74	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	74	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	3	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	74	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	3	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	3	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	49	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	229	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	49	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	49	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	229	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	229	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	B	199	TYR	Sidechain
1	C	199	TYR	Sidechain

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	119	3
1	B	5265	0	5165	116	2
1	C	5265	0	5165	142	13
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	890	0	0	35	3
3	B	938	0	0	39	5
3	C	937	0	0	61	7
All	All	18563	0	15495	364	21

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 12.

All (364) 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:C:576:TRP:CE3	3:C:2822:HOH:O	1.87	1.25
1:C:664:ARG:HB3	3:C:2932:HOH:O	1.15	1.25
1:C:44:LEU:CD2	3:C:2120:HOH:O	1.83	1.24
1:C:463:ARG:HD2	3:C:2691:HOH:O	1.37	1.24
1:B:2:ARG:HA	3:B:2012:HOH:O	1.10	1.23
1:C:239:GLN:HG2	3:C:2494:HOH:O	1.41	1.21
1:B:470:ARG:HD2	3:B:2700:HOH:O	1.49	1.12
1:A:137:ASP:N	3:A:2284:HOH:O	1.86	1.09
1:C:137:ASP:N	3:C:2306:HOH:O	1.86	1.09
1:B:137:ASP:N	3:B:2301:HOH:O	1.86	1.09
1:A:564:TYR:OH	3:A:2767:HOH:O	1.71	1.07
1:C:44:LEU:HD22	3:C:2120:HOH:O	1.47	1.05
1:C:664:ARG:CB	3:C:2932:HOH:O	1.78	1.05
1:C:2:ARG:HD3	3:C:2005:HOH:O	1.58	1.02
1:A:564:TYR:CZ	3:A:2767:HOH:O	2.10	1.01
1:A:555:LYS:HD3	3:A:2767:HOH:O	1.58	0.99
1:A:316:GLU:HG2	3:A:2529:HOH:O	1.67	0.95
1:C:316:GLU:HG2	3:C:2563:HOH:O	1.67	0.95
1:A:608:GLN:HE22	1:B:593:ARG:CZ	1.80	0.94
1:B:316:GLU:HG2	3:B:2561:HOH:O	1.67	0.92
1:A:608:GLN:HE22	1:B:593:ARG:NH1	1.67	0.91
1:A:555:LYS:CD	3:A:2767:HOH:O	2.17	0.91
1:C:2:ARG:NH1	3:C:2008:HOH:O	2.08	0.87
1:A:427:LYS:HE3	1:C:12:ILE:HG21	1.58	0.85
1:C:82:THR:HG23	3:C:2102:HOH:O	1.78	0.83
1:A:82:THR:HG23	3:A:2092:HOH:O	1.78	0.83
1:A:556:ASP:OD2	3:A:2759:HOH:O	1.96	0.83
1:C:217:THR:HG23	1:C:219:LYS:H	1.43	0.82
1:B:82:THR:HG23	3:B:2096:HOH:O	1.78	0.82
1:B:217:THR:HG23	1:B:219:LYS:H	1.43	0.81
1:C:576:TRP:NE1	3:C:2824:HOH:O	2.11	0.81
1:A:217:THR:HG23	1:A:219:LYS:H	1.43	0.81
1:A:307:ARG:HG2	3:A:2518:HOH:O	1.81	0.80
1:A:564:TYR:CE1	3:A:2767:HOH:O	2.28	0.80
1:A:63:ASP:HA	3:A:2165:HOH:O	1.79	0.80
1:B:307:ARG:HG2	3:B:2549:HOH:O	1.81	0.79
1:A:427:LYS:HE3	1:C:12:ILE:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:TYR:N	3:C:2831:HOH:O	1.86	0.78
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.31	0.78
1:C:307:ARG:HG2	3:C:2552:HOH:O	1.81	0.78
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.31	0.78
1:C:609:ALA:HA	3:C:2875:HOH:O	1.84	0.78
1:A:26:GLN:HG2	3:A:2038:HOH:O	1.85	0.77
1:B:163:LYS:HD3	3:B:2318:HOH:O	1.85	0.77
1:A:163:LYS:HD3	3:A:2302:HOH:O	1.85	0.76
1:C:26:GLN:HG2	3:C:2047:HOH:O	1.84	0.76
1:C:82:THR:HG21	3:C:2107:HOH:O	1.86	0.76
1:B:26:GLN:HG2	3:B:2041:HOH:O	1.85	0.75
1:B:47:ASP:OD2	1:B:49:ARG:HD3	1.87	0.75
1:C:163:LYS:HD3	3:C:2324:HOH:O	1.85	0.75
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.31	0.75
1:C:47:ASP:OD2	1:C:49:ARG:HD3	1.87	0.74
1:A:82:THR:HG21	3:A:2097:HOH:O	1.86	0.74
1:B:82:THR:HG21	3:B:2102:HOH:O	1.86	0.74
1:C:214:ASP:HB3	1:C:217:THR:HG22	1.70	0.74
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.23	0.73
1:A:47:ASP:OD2	1:A:49:ARG:HD3	1.86	0.73
1:B:72:TYR:CE1	1:B:476:LYS:HD3	2.23	0.73
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.23	0.73
1:B:214:ASP:HB3	1:B:217:THR:HG22	1.70	0.73
1:A:214:ASP:HB3	1:A:217:THR:HG22	1.70	0.73
1:B:268:ARG:NH1	1:B:270:ARG:HH21	1.88	0.72
1:B:506:ARG:HH11	1:B:506:ARG:HB2	1.55	0.72
1:A:506:ARG:HH11	1:A:506:ARG:HB2	1.55	0.71
1:C:609:ALA:CB	3:C:2875:HOH:O	2.38	0.71
1:C:82:THR:HG22	1:C:83:ASN:H	1.54	0.71
1:A:82:THR:HG22	1:A:83:ASN:H	1.54	0.71
1:A:194:GLN:OE1	3:A:2391:HOH:O	2.08	0.71
1:B:82:THR:HG22	1:B:83:ASN:H	1.54	0.71
1:C:268:ARG:NH1	1:C:270:ARG:HH21	1.88	0.71
1:A:608:GLN:NE2	1:B:593:ARG:NH1	2.39	0.71
1:A:268:ARG:NH1	1:A:270:ARG:HH21	1.88	0.71
1:C:506:ARG:HH11	1:C:506:ARG:HB2	1.55	0.71
1:B:655:GLU:HG2	1:B:659:ARG:NH1	2.06	0.70
1:C:576:TRP:HE3	3:C:2822:HOH:O	1.44	0.70
1:A:655:GLU:HG2	1:A:659:ARG:NH1	2.06	0.70
1:B:534:SER:OG	3:B:2773:HOH:O	2.10	0.69
1:C:655:GLU:HG2	1:C:659:ARG:NH1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:HB3	3:C:2005:HOH:O	1.91	0.69
1:B:607:ARG:O	1:B:608:GLN:HG3	1.93	0.68
1:A:607:ARG:O	1:A:608:GLN:HG3	1.93	0.68
1:C:607:ARG:O	1:C:608:GLN:HG3	1.93	0.68
1:B:149:SER:O	1:B:163:LYS:HE2	1.94	0.68
1:A:149:SER:O	1:A:163:LYS:HE2	1.94	0.68
1:A:569:GLU:HG2	3:A:2402:HOH:O	1.94	0.67
1:C:149:SER:O	1:C:163:LYS:HE2	1.94	0.67
1:C:176:GLU:OE1	3:C:2386:HOH:O	2.13	0.66
1:B:176:GLU:OE1	3:B:2378:HOH:O	2.13	0.66
1:A:176:GLU:OE1	3:A:2358:HOH:O	2.13	0.66
1:B:581:GLU:OE1	3:B:2829:HOH:O	2.14	0.65
1:C:569:GLU:HG2	3:C:2435:HOH:O	1.94	0.65
1:B:569:GLU:HG2	3:B:2429:HOH:O	1.94	0.65
1:C:70:ASP:OD1	1:C:74:ARG:HD2	1.97	0.65
1:A:204:ARG:HH22	1:A:626:ASN:HD21	1.45	0.65
1:C:650:SER:HB2	1:C:652:GLU:OE1	1.97	0.65
1:C:29:LYS:CE	3:C:2098:HOH:O	2.45	0.65
1:B:204:ARG:HH22	1:B:626:ASN:HD21	1.45	0.64
1:A:537:ARG:HD3	3:A:2734:HOH:O	1.95	0.64
1:B:70:ASP:OD1	1:B:74:ARG:HD2	1.97	0.64
1:C:537:ARG:HD3	3:C:2769:HOH:O	1.96	0.64
1:A:650:SER:HB2	1:A:652:GLU:OE1	1.97	0.64
1:C:151:THR:HG22	1:C:163:LYS:HG3	1.80	0.64
1:B:151:THR:HG22	1:B:163:LYS:HG3	1.80	0.64
1:C:204:ARG:HH22	1:C:626:ASN:HD21	1.45	0.64
1:B:650:SER:HB2	1:B:652:GLU:OE1	1.98	0.63
1:C:664:ARG:OXT	3:C:2932:HOH:O	2.15	0.63
1:A:70:ASP:OD1	1:A:74:ARG:HD2	1.97	0.63
1:A:392:SER:O	1:A:398:THR:HG21	1.99	0.63
1:C:392:SER:O	1:C:398:THR:HG21	1.98	0.63
1:C:22:ILE:HG12	3:C:2076:HOH:O	1.98	0.63
1:A:214:ASP:HB3	1:A:217:THR:CG2	2.29	0.63
1:A:427:LYS:CE	1:C:12:ILE:HG21	2.28	0.63
1:C:3:ARG:HD3	3:C:2028:HOH:O	1.99	0.63
1:B:3:ARG:O	3:B:2009:HOH:O	0.63	0.63
1:B:214:ASP:HB3	1:B:217:THR:CG2	2.28	0.63
1:C:214:ASP:HB3	1:C:217:THR:CG2	2.28	0.62
1:C:609:ALA:CA	3:C:2875:HOH:O	2.44	0.62
1:B:392:SER:O	1:B:398:THR:HG21	1.98	0.62
1:A:3:ARG:HD3	3:A:2021:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:ALA:N	3:C:2831:HOH:O	2.33	0.61
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.80	0.61
1:B:3:ARG:HD3	3:B:2021:HOH:O	1.99	0.60
1:B:581:GLU:HG3	3:B:2831:HOH:O	2.02	0.60
1:C:607:ARG:NH2	3:C:2869:HOH:O	1.98	0.60
1:A:655:GLU:HG2	1:A:659:ARG:HH12	1.67	0.59
1:C:655:GLU:HG2	1:C:659:ARG:HH12	1.67	0.59
1:B:288:GLN:HB3	1:B:289:PRO:HD3	1.85	0.59
1:A:606:ALA:H	1:A:609:ALA:HB2	1.69	0.58
1:B:606:ALA:H	1:B:609:ALA:HB2	1.68	0.58
1:C:577:ASN:OD1	3:C:2825:HOH:O	2.17	0.58
1:B:581:GLU:CG	3:B:2831:HOH:O	2.51	0.58
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.85	0.57
1:B:470:ARG:NH2	3:B:2695:HOH:O	2.37	0.57
1:C:606:ALA:H	1:C:609:ALA:HB2	1.69	0.57
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.85	0.57
1:B:655:GLU:HG2	1:B:659:ARG:HH12	1.67	0.57
1:A:362:LYS:HD2	3:A:2595:HOH:O	2.05	0.57
1:A:328:HIS:HD2	1:A:329:ASP:OD1	1.89	0.56
1:B:328:HIS:HD2	1:B:329:ASP:OD1	1.89	0.56
1:B:492:HIS:HD2	3:B:2721:HOH:O	1.88	0.56
1:C:30:ARG:HD2	3:C:2106:HOH:O	2.05	0.56
1:C:328:HIS:HD2	1:C:329:ASP:OD1	1.89	0.56
1:C:147:LYS:HD3	3:C:2780:HOH:O	2.06	0.56
1:A:30:ARG:HD2	3:A:2096:HOH:O	2.05	0.56
1:B:147:LYS:HD3	3:B:2785:HOH:O	2.06	0.56
1:B:362:LYS:HD2	3:B:2627:HOH:O	2.05	0.56
1:B:470:ARG:CD	3:B:2700:HOH:O	2.26	0.56
1:C:362:LYS:HD2	3:C:2630:HOH:O	2.05	0.56
1:B:30:ARG:HD2	3:B:2097:HOH:O	2.05	0.56
1:B:407:SER:HA	1:B:448:GLN:HE22	1.71	0.56
1:A:147:LYS:HD3	3:A:2743:HOH:O	2.06	0.55
1:C:407:SER:HA	1:C:448:GLN:HE22	1.72	0.55
1:A:407:SER:HA	1:A:448:GLN:HE22	1.71	0.55
1:C:585:ALA:CA	3:C:2831:HOH:O	2.54	0.55
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.03	0.55
1:A:44:LEU:HD21	1:B:257:GLY:HA3	1.89	0.55
1:C:576:TRP:CD2	3:C:2822:HOH:O	2.35	0.55
1:C:1:PRO:HG2	1:C:238:GLU:OE1	2.07	0.55
1:B:1:PRO:HG2	1:B:238:GLU:OE1	2.07	0.55
1:C:492:HIS:HD2	3:C:2718:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ARG:HH11	1:C:506:ARG:CB	2.20	0.55
1:C:251:ARG:HH11	1:C:255:GLN:NE2	2.03	0.54
1:B:474:MET:HE1	3:B:2646:HOH:O	2.06	0.54
1:A:492:HIS:HD2	3:A:2682:HOH:O	1.88	0.54
1:A:29:LYS:NZ	3:A:2091:HOH:O	2.27	0.54
1:A:1:PRO:HG2	1:A:238:GLU:OE1	2.07	0.54
1:A:119:VAL:HG22	1:C:22:ILE:HD11	1.90	0.53
1:C:78:ASN:C	1:C:78:ASN:HD22	2.12	0.53
1:C:78:ASN:HD22	1:C:79:GLY:N	2.07	0.53
1:A:78:ASN:HD22	1:A:79:GLY:N	2.07	0.53
1:B:2:ARG:CA	3:B:2012:HOH:O	1.97	0.53
1:B:78:ASN:ND2	1:B:80:VAL:H	2.06	0.53
1:C:25:GLN:NE2	3:C:2086:HOH:O	2.37	0.53
1:C:78:ASN:ND2	1:C:80:VAL:H	2.06	0.53
1:C:226:MET:HE2	1:C:244:ALA:HA	1.91	0.53
1:A:29:LYS:CE	3:A:2091:HOH:O	2.57	0.53
1:A:506:ARG:HH11	1:A:506:ARG:CB	2.20	0.53
1:C:650:SER:OG	1:C:653:LYS:HG3	2.09	0.53
1:A:650:SER:OG	1:A:653:LYS:HG3	2.09	0.53
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.44	0.53
1:C:585:ALA:HB3	3:C:2831:HOH:O	2.08	0.53
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.53
1:B:650:SER:OG	1:B:653:LYS:HG3	2.09	0.53
1:A:78:ASN:ND2	1:A:80:VAL:H	2.06	0.52
1:A:650:SER:HB2	1:A:652:GLU:CD	2.30	0.52
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.44	0.52
1:B:226:MET:HE2	1:B:244:ALA:HA	1.91	0.52
1:B:70:ASP:OD1	1:B:74:ARG:CD	2.58	0.52
1:B:78:ASN:C	1:B:78:ASN:HD22	2.12	0.52
1:A:70:ASP:OD1	1:A:74:ARG:CD	2.58	0.52
1:B:664:ARG:HG2	1:B:664:ARG:HH11	1.75	0.52
1:B:78:ASN:HD22	1:B:79:GLY:N	2.07	0.52
1:B:650:SER:HB2	1:B:652:GLU:CD	2.30	0.52
1:C:474:MET:HE1	3:C:2647:HOH:O	2.09	0.52
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.91	0.52
1:C:650:SER:HB2	1:C:652:GLU:CD	2.30	0.52
1:A:474:MET:HE1	3:A:2614:HOH:O	2.09	0.52
1:A:78:ASN:HD22	1:A:78:ASN:C	2.12	0.51
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.03	0.51
1:C:70:ASP:OD1	1:C:74:ARG:CD	2.58	0.51
1:C:664:ARG:HA	3:C:2933:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ARG:HG2	1:A:664:ARG:HH11	1.75	0.51
1:A:138:LEU:HB2	1:A:662:MET:SD	2.51	0.51
1:A:204:ARG:HG3	1:A:272:ALA:HB2	1.92	0.50
1:C:576:TRP:HB3	3:C:2822:HOH:O	2.11	0.50
1:C:138:LEU:HB2	1:C:662:MET:SD	2.51	0.50
1:A:600:ARG:HD3	3:B:2832:HOH:O	2.11	0.50
1:A:112:ALA:HB1	1:A:487:LYS:HE2	1.94	0.50
1:B:138:LEU:HB2	1:B:662:MET:SD	2.51	0.50
1:B:492:HIS:CD2	3:B:2721:HOH:O	2.64	0.50
1:B:204:ARG:HG3	1:B:272:ALA:HB2	1.92	0.50
1:C:664:ARG:HG2	1:C:664:ARG:HH11	1.75	0.50
1:C:112:ALA:HB1	1:C:487:LYS:HE2	1.94	0.50
1:C:392:SER:O	1:C:398:THR:CG2	2.60	0.50
1:A:214:ASP:CB	1:A:217:THR:HG22	2.40	0.50
1:A:504:ASP:CG	1:A:506:ARG:HH12	2.15	0.50
1:B:506:ARG:HH11	1:B:506:ARG:CB	2.20	0.50
1:B:581:GLU:CB	3:B:2831:HOH:O	2.59	0.50
1:C:145:ILE:HG21	1:C:163:LYS:HD2	1.94	0.50
1:A:1:PRO:O	1:A:2:ARG:HB2	2.12	0.49
1:A:322:ALA:HB3	3:A:2685:HOH:O	2.12	0.49
1:A:392:SER:O	1:A:398:THR:CG2	2.60	0.49
1:C:504:ASP:CG	1:C:506:ARG:HH12	2.15	0.49
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.47	0.49
1:B:631:LYS:HE3	1:B:632:TRP:CZ2	2.47	0.49
1:A:506:ARG:HH11	1:A:506:ARG:CG	2.26	0.49
1:B:1:PRO:O	1:B:2:ARG:HB2	2.12	0.49
1:C:204:ARG:HG3	1:C:272:ALA:HB2	1.92	0.49
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.47	0.49
1:A:492:HIS:CD2	3:A:2682:HOH:O	2.64	0.49
1:B:392:SER:O	1:B:398:THR:CG2	2.60	0.49
1:C:1:PRO:O	1:C:2:ARG:HB2	2.12	0.49
1:A:226:MET:HE2	1:A:244:ALA:HA	1.94	0.49
1:A:608:GLN:NE2	1:B:593:ARG:CZ	2.62	0.49
1:B:504:ASP:CG	1:B:506:ARG:HH12	2.15	0.49
1:B:506:ARG:HH11	1:B:506:ARG:CG	2.26	0.49
1:C:226:MET:HE1	1:C:244:ALA:HB2	1.95	0.49
1:C:506:ARG:HH11	1:C:506:ARG:CG	2.26	0.49
1:C:580:GLY:C	1:C:581:GLU:HG2	2.34	0.49
1:A:145:ILE:HG21	1:A:163:LYS:HD2	1.94	0.49
1:B:322:ALA:HB3	3:B:2722:HOH:O	2.12	0.49
1:C:29:LYS:HE2	3:C:2101:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TYR:CZ	1:C:476:LYS:HD3	2.49	0.48
1:C:600:ARG:HD3	3:C:2861:HOH:O	2.11	0.48
1:C:610:GLY:HA3	3:C:2874:HOH:O	2.14	0.48
1:A:504:ASP:HB2	3:A:2701:HOH:O	2.14	0.48
1:A:610:GLY:HA3	3:A:2827:HOH:O	2.14	0.48
1:C:423:ASN:HB2	3:C:2654:HOH:O	2.11	0.48
1:C:504:ASP:HB2	3:C:2735:HOH:O	2.14	0.48
1:A:119:VAL:O	1:C:25:GLN:HG3	2.14	0.48
1:A:580:GLY:C	1:A:581:GLU:HG2	2.34	0.48
1:B:610:GLY:HA3	3:B:2873:HOH:O	2.14	0.48
1:A:269:ARG:NH2	3:A:2488:HOH:O	2.43	0.48
1:B:112:ALA:HB1	1:B:487:LYS:HE2	1.94	0.48
1:B:145:ILE:HG21	1:B:163:LYS:HD2	1.94	0.48
1:B:651:VAL:O	1:B:655:GLU:HB2	2.14	0.48
1:B:504:ASP:HB2	3:B:2739:HOH:O	2.14	0.48
1:A:651:VAL:O	1:A:655:GLU:HB2	2.14	0.47
1:B:214:ASP:CB	1:B:217:THR:HG22	2.41	0.47
1:C:322:ALA:HB3	3:C:2720:HOH:O	2.12	0.47
1:B:471:LEU:HD12	1:B:474:MET:HE2	1.95	0.47
1:A:72:TYR:CZ	1:A:476:LYS:HD3	2.49	0.47
1:B:269:ARG:NH2	3:B:2520:HOH:O	2.43	0.47
1:C:424:SER:N	3:C:2654:HOH:O	2.40	0.47
1:B:72:TYR:CZ	1:B:476:LYS:HD3	2.49	0.47
1:B:226:MET:HE1	1:B:244:ALA:HB2	1.95	0.47
1:B:384:ASN:HB3	3:B:2618:HOH:O	2.15	0.47
1:A:339:LEU:C	1:A:339:LEU:HD23	2.35	0.47
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.50	0.47
1:B:339:LEU:HD23	1:B:339:LEU:C	2.35	0.47
1:B:470:ARG:NH1	3:B:2699:HOH:O	2.47	0.47
1:C:214:ASP:CB	1:C:217:THR:HG22	2.41	0.47
1:A:42:GLY:O	1:B:256:TYR:HB3	2.15	0.47
1:B:642:HIS:CE1	1:B:646:MET:HG3	2.50	0.47
1:C:339:LEU:C	1:C:339:LEU:HD23	2.35	0.47
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.50	0.47
1:C:492:HIS:CD2	3:C:2718:HOH:O	2.64	0.47
1:A:492:HIS:HE1	3:A:2198:HOH:O	1.98	0.46
1:C:224:ASP:HB3	1:C:226:MET:CE	2.45	0.46
1:C:651:VAL:O	1:C:655:GLU:HB2	2.14	0.46
1:B:580:GLY:C	1:B:581:GLU:HG2	2.33	0.46
1:A:224:ASP:HB3	1:A:226:MET:CE	2.45	0.46
1:B:86:GLY:O	1:B:89:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LEU:HD12	1:A:474:MET:HE2	1.98	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.99	0.46
1:B:492:HIS:HE1	3:B:2213:HOH:O	1.99	0.46
1:A:384:ASN:HB3	3:A:2586:HOH:O	2.15	0.46
1:B:224:ASP:HB3	1:B:226:MET:CE	2.45	0.46
1:C:384:ASN:HB3	3:C:2620:HOH:O	2.15	0.46
1:A:268:ARG:HH12	1:A:270:ARG:HH21	1.62	0.46
1:C:606:ALA:N	1:C:609:ALA:HB2	2.31	0.45
1:A:151:THR:CG2	1:A:163:LYS:HG3	2.46	0.45
1:C:471:LEU:HD12	1:C:474:MET:HE2	1.97	0.45
1:C:86:GLY:O	1:C:89:HIS:HD2	1.99	0.45
1:C:434:ARG:NH1	3:C:2663:HOH:O	2.50	0.45
1:C:492:HIS:HE1	3:C:2223:HOH:O	1.98	0.45
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.52	0.45
1:C:29:LYS:HE3	3:C:2098:HOH:O	2.12	0.45
1:C:305:THR:H	1:C:309:ASN:ND2	2.15	0.45
1:A:305:THR:H	1:A:309:ASN:ND2	2.15	0.45
1:C:268:ARG:HH12	1:C:270:ARG:HH21	1.62	0.45
1:C:82:THR:HG22	1:C:83:ASN:N	2.28	0.44
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.87	0.44
1:A:606:ALA:N	1:A:609:ALA:HB2	2.31	0.44
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.52	0.44
1:A:434:ARG:NH1	3:A:2630:HOH:O	2.50	0.44
1:C:151:THR:CG2	1:C:163:LYS:HG3	2.46	0.44
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.52	0.44
1:B:305:THR:H	1:B:309:ASN:ND2	2.15	0.44
1:B:470:ARG:CZ	3:B:2699:HOH:O	2.65	0.44
1:B:434:ARG:NH1	3:B:2661:HOH:O	2.50	0.43
1:B:23:LYS:HB3	1:B:23:LYS:HE2	1.80	0.43
1:B:606:ALA:N	1:B:609:ALA:HB2	2.31	0.43
1:C:74:ARG:HD3	1:C:507:ARG:HD2	2.01	0.43
1:B:151:THR:CG2	1:B:163:LYS:HG3	2.46	0.43
1:A:74:ARG:HD3	1:A:507:ARG:HD2	2.01	0.43
1:B:74:ARG:HD3	1:B:507:ARG:HD2	2.01	0.43
1:C:269:ARG:NH2	3:C:2525:HOH:O	2.43	0.43
1:C:497:LEU:HD12	1:C:497:LEU:HA	1.87	0.43
1:B:71:GLU:H	1:B:71:GLU:CD	2.23	0.43
1:B:204:ARG:HG3	1:B:272:ALA:CB	2.49	0.43
1:B:607:ARG:NH1	3:B:2868:HOH:O	2.52	0.43
1:B:268:ARG:HH12	1:B:270:ARG:HH21	1.62	0.42
1:C:204:ARG:HG3	1:C:272:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:THR:HG22	1:B:83:ASN:N	2.28	0.42
1:A:204:ARG:HG3	1:A:272:ALA:CB	2.49	0.42
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.55	0.42
1:C:70:ASP:CG	1:C:74:ARG:HD2	2.40	0.42
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.55	0.42
1:A:70:ASP:CG	1:A:74:ARG:HD2	2.40	0.42
1:C:23:LYS:HE2	1:C:23:LYS:HB3	1.80	0.42
1:B:70:ASP:CG	1:B:74:ARG:HD2	2.40	0.42
1:A:119:VAL:HG13	1:C:22:ILE:HD13	2.02	0.42
1:C:71:GLU:CD	1:C:71:GLU:H	2.23	0.42
1:A:71:GLU:CD	1:A:71:GLU:H	2.23	0.41
1:C:630:TYR:CD1	1:C:630:TYR:C	2.94	0.41
1:A:163:LYS:HB2	1:A:163:LYS:HE3	1.74	0.41
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.55	0.41
1:B:185:LYS:HG2	3:B:2186:HOH:O	2.19	0.41
1:A:607:ARG:H	1:A:607:ARG:HE	1.68	0.41
1:C:607:ARG:H	1:C:607:ARG:HE	1.68	0.41
1:A:506:ARG:CG	1:A:506:ARG:NH1	2.84	0.41
1:B:86:GLY:O	1:B:89:HIS:CD2	2.74	0.41
1:B:596:LEU:CD2	1:B:608:GLN:HG2	2.51	0.41
1:C:145:ILE:HD12	1:C:164:ILE:HD13	2.02	0.41
1:C:226:MET:HE3	3:C:2473:HOH:O	2.19	0.41
1:A:86:GLY:O	1:A:89:HIS:CD2	2.74	0.41
1:C:273:MET:H	1:C:393:SER:HG	1.69	0.41
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.51	0.41
1:C:506:ARG:CG	1:C:506:ARG:NH1	2.84	0.41
1:C:664:ARG:HB2	3:C:2932:HOH:O	1.77	0.41
1:A:89:HIS:HE1	3:A:2466:HOH:O	2.04	0.41
1:C:2:ARG:CD	3:C:2005:HOH:O	2.39	0.41
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.51	0.41
1:B:145:ILE:HD12	1:B:164:ILE:HD13	2.03	0.40
1:C:89:HIS:HE1	3:C:2502:HOH:O	2.04	0.40
1:A:630:TYR:CD1	1:A:630:TYR:C	2.94	0.40
1:B:664:ARG:HG2	1:B:664:ARG:NH1	2.36	0.40
1:C:664:ARG:HG2	1:C:664:ARG:NH1	2.36	0.40
1:A:608:GLN:HE22	1:B:593:ARG:NE	2.16	0.40
1:B:163:LYS:HB2	1:B:163:LYS:HE3	1.74	0.40
1:C:86:GLY:O	1:C:89:HIS:CD2	2.74	0.40
1:C:518:ILE:HG12	1:C:567:VAL:HG21	2.03	0.40
1:B:630:TYR:CD1	1:B:630:TYR:C	2.94	0.40

All (21) 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)
1:C:479:LYS:NZ	1:C:607:ARG:C[2_445]	0.93	1.27
1:C:479:LYS:CE	1:C:608:GLN:N[2_445]	1.13	1.07
3:A:2392:HOH:O	3:C:2828:HOH:O[1_655]	1.43	0.77
1:C:479:LYS:NZ	1:C:608:GLN:N[2_445]	1.47	0.73
1:A:652:GLU:CG	1:C:664:ARG:NH1[2_545]	1.52	0.68
3:B:2030:HOH:O	3:C:2317:HOH:O[2_555]	1.52	0.68
1:A:566:ASP:OD2	1:C:2:ARG:CG[2_555]	1.53	0.67
1:C:479:LYS:NZ	1:C:607:ARG:O[2_445]	1.69	0.51
1:C:479:LYS:NZ	1:C:607:ARG:CA[2_445]	1.79	0.41
3:B:2046:HOH:O	3:C:2283:HOH:O[2_555]	1.81	0.39
3:A:2773:HOH:O	3:C:2005:HOH:O[2_555]	1.90	0.30
1:B:537:ARG:NH2	1:C:582:SER:N[1_655]	1.95	0.25
1:C:479:LYS:CE	1:C:607:ARG:C[2_445]	1.96	0.24
3:B:2861:HOH:O	3:C:2067:HOH:O[1_655]	1.98	0.22
1:A:65:PHE:CE2	1:C:2:ARG:NH2[2_555]	2.03	0.17
1:C:479:LYS:CE	1:C:608:GLN:CA[2_445]	2.04	0.16
1:C:479:LYS:CD	1:C:608:GLN:CB[2_445]	2.05	0.15
1:B:537:ARG:CD	1:C:581:GLU:OE1[1_655]	2.06	0.14
3:C:2426:HOH:O	3:C:2472:HOH:O[2_455]	2.11	0.09
3:B:2038:HOH:O	3:C:2327:HOH:O[2_555]	2.14	0.06
3:A:2029:HOH:O	3:B:2263:HOH:O[2_646]	2.19	0.01

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%)	645 (97%)	12 (2%)	5 (1%)	19	13
1	B	662/664 (100%)	645 (97%)	12 (2%)	5 (1%)	19	13
1	C	662/664 (100%)	645 (97%)	12 (2%)	5 (1%)	19	13
All	All	1986/1992 (100%)	1935 (97%)	36 (2%)	15 (1%)	19	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	607	ARG
1	B	136	SER
1	B	607	ARG
1	C	136	SER
1	C	607	ARG
1	A	630	TYR
1	B	630	TYR
1	C	608	GLN
1	C	630	TYR
1	A	2	ARG
1	A	608	GLN
1	B	2	ARG
1	B	608	GLN
1	C	2	ARG

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%)	33	31
1	B	557/557 (100%)	536 (96%)	21 (4%)	33	31
1	C	557/557 (100%)	537 (96%)	20 (4%)	35	34
All	All	1671/1671 (100%)	1609 (96%)	62 (4%)	34	32

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	43	LEU
1	A	63	ASP
1	A	74	ARG
1	A	78	ASN

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	82	THR
1	A	113	ASP
1	A	154	PRO
1	A	163	LYS
1	A	269	ARG
1	A	307	ARG
1	A	308	LEU
1	A	327	ASP
1	A	373	GLU
1	A	391	LEU
1	A	404	LEU
1	A	497	LEU
1	A	506	ARG
1	A	664	ARG
1	B	3	ARG
1	B	30	ARG
1	B	43	LEU
1	B	63	ASP
1	B	74	ARG
1	B	78	ASN
1	B	81	ARG
1	B	82	THR
1	B	113	ASP
1	B	154	PRO
1	B	163	LYS
1	B	269	ARG
1	B	307	ARG
1	B	308	LEU
1	B	327	ASP
1	B	373	GLU
1	B	391	LEU
1	B	404	LEU
1	B	497	LEU
1	B	506	ARG
1	B	664	ARG
1	C	3	ARG
1	C	30	ARG
1	C	43	LEU
1	C	63	ASP
1	C	74	ARG
1	C	78	ASN

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Mol	Chain	Res	Type
1	C	82	THR
1	C	113	ASP
1	C	154	PRO
1	C	163	LYS
1	C	269	ARG
1	C	307	ARG
1	C	308	LEU
1	C	327	ASP
1	C	373	GLU
1	C	391	LEU
1	C	404	LEU
1	C	497	LEU
1	C	506	ARG
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) 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	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
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	255	GLN
1	B	309	ASN
1	B	328	HIS

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Mol	Chain	Res	Type
1	B	448	GLN
1	B	525	GLN
1	B	626	ASN
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	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	525	GLN
1	C	626	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.10	19 (2%)	51	50	25, 37, 72, 159	0
1	B	664/664 (100%)	-0.02	23 (3%)	44	43	25, 37, 72, 159	0
1	C	664/664 (100%)	0.08	36 (5%)	25	24	25, 37, 72, 159	0
All	All	1992/1992 (100%)	-0.01	78 (3%)	39	38	25, 37, 72, 159	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	607	ARG	10.9
1	C	606	ALA	10.3
1	C	608	GLN	10.2
1	B	607	ARG	10.2
1	C	610	GLY	9.2
1	C	603	ALA	9.0
1	B	608	GLN	8.0
1	C	609	ALA	7.1
1	C	612	ALA	7.0
1	B	603	ALA	6.9
1	B	606	ALA	6.6
1	C	664	ARG	6.4
1	A	1	PRO	6.4
1	B	609	ALA	6.3
1	A	607	ARG	6.2
1	B	604	SER	5.8
1	C	604	SER	5.6
1	B	610	GLY	5.6
1	A	606	ALA	5.2
1	A	608	GLN	4.8
1	C	215	PRO	4.7
1	A	609	ALA	4.7
1	C	596	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	2	ARG	4.3
1	A	2	ARG	4.1
1	C	2	ARG	4.1
1	A	216	LYS	4.1
1	B	611	LEU	4.1
1	B	664	ARG	4.0
1	B	22	ILE	3.9
1	A	257	GLY	3.9
1	A	664	ARG	3.8
1	B	605	MET	3.8
1	B	612	ALA	3.8
1	C	216	LYS	3.7
1	C	605	MET	3.6
1	C	254	GLU	3.6
1	A	610	GLY	3.5
1	A	611	LEU	3.4
1	C	651	VAL	3.4
1	B	257	GLY	3.4
1	B	1	PRO	3.3
1	C	72	TYR	3.2
1	B	411	LEU	3.2
1	C	1	PRO	3.2
1	C	611	LEU	3.1
1	C	479	LYS	3.0
1	C	537	ARG	2.9
1	A	411	LEU	2.8
1	C	505	SER	2.8
1	A	215	PRO	2.8
1	A	254	GLU	2.8
1	C	506	ARG	2.8
1	C	63	ASP	2.7
1	B	537	ARG	2.7
1	C	214	ASP	2.7
1	C	257	GLY	2.6
1	B	613	GLU	2.5
1	A	218	GLY	2.5
1	C	217	THR	2.5
1	C	478	GLY	2.5
1	C	511	SER	2.4
1	B	415	LEU	2.4
1	C	219	LYS	2.4
1	C	218	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	76	TYR	2.4
1	A	576	TRP	2.3
1	B	418	THR	2.2
1	C	650	SER	2.2
1	B	446	ILE	2.2
1	B	412	VAL	2.1
1	A	415	LEU	2.1
1	C	461	LYS	2.1
1	C	576	TRP	2.1
1	B	254	GLU	2.1
1	A	148	GLY	2.0
1	C	253	LYS	2.0
1	A	308	LEU	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	MN	A	665	1/1	0.98	0.08	32,32,32,32	0
2	MN	B	665	1/1	0.98	0.06	32,32,32,32	0
2	MN	C	665	1/1	0.98	0.03	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.