



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:21 PM GMT

PDB ID : 1HHS
Title : RNA DEPENDENT RNA POLYMERASE FROM DSRNA BACTERIO-
PHAGE 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 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/ValidationPDFNotes.html>

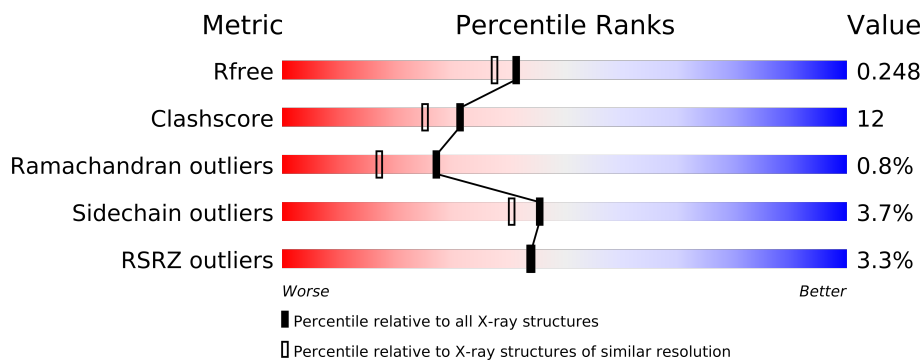
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	664	
1	B	664	
1	C	664	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18563 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

- Molecule 3 is water.

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

Continued on next page...

Continued from previous page...

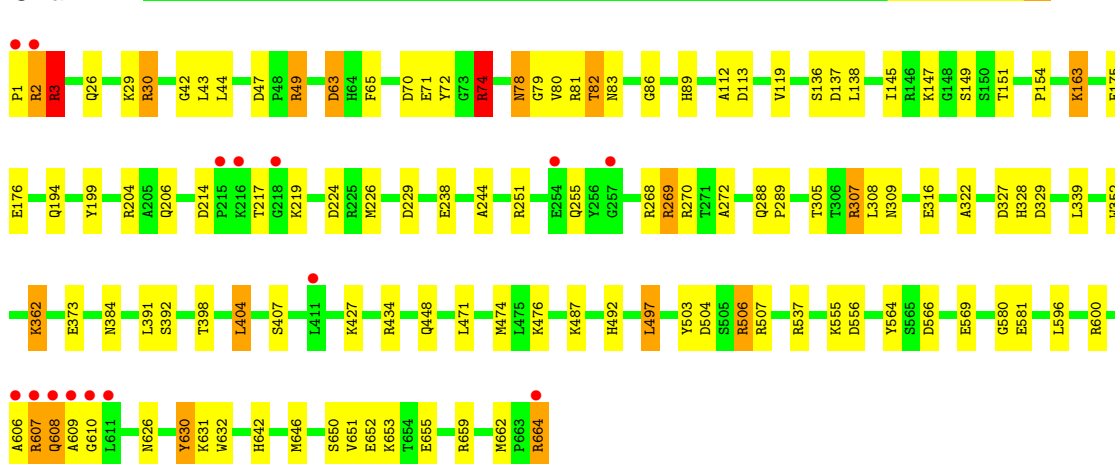
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	937	Total 937	O 937	0	0

3 Residue-property plots

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.

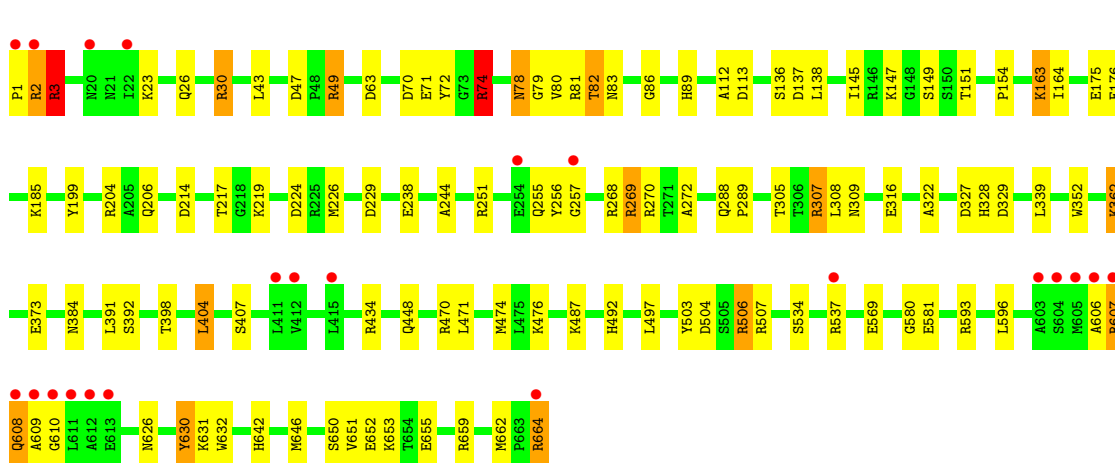
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain A:



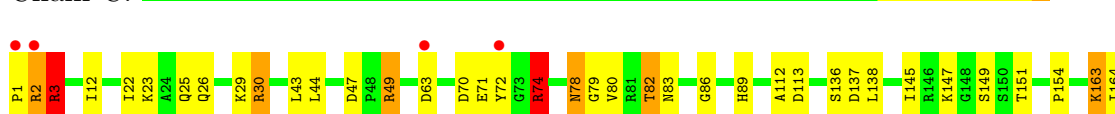
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

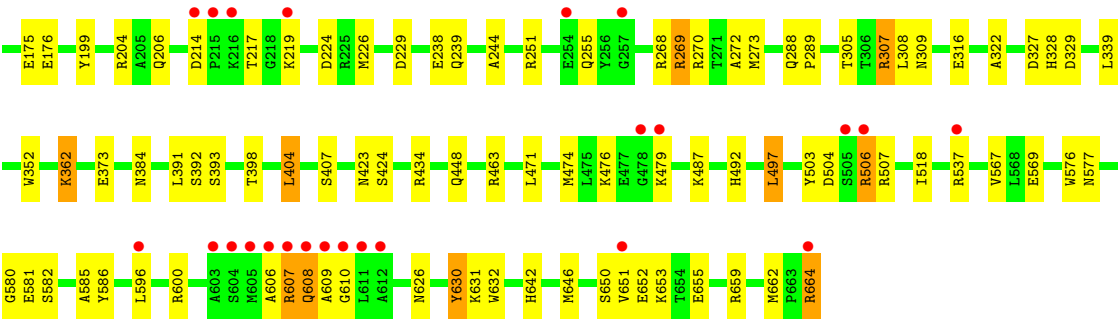
Chain B:



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain C:





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 181067 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

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	0.72	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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	937	0	0	61	7
All	All	18563	0	15495	364	21

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (364) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:664:ARG:HB3	3:C:2932:HOH:O	1.15	1.25
1:C:576:TRP:CE3	3:C:2822:HOH:O	1.87	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:664:ARG:CB	3:C:2932:HOH:O	1.78	1.05
1:C:44:LEU:HD22	3:C:2120:HOH:O	1.47	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:C:576:TRP:NE1	3:C:2824:HOH:O	2.11	0.81
1:B:217:THR:HG23	1:B:219:LYS:H	1.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:C:586:TYR:N	3:C:2831:HOH:O	1.86	0.78
1:C:307:ARG:HG2	3:C:2552:HOH:O	1.81	0.78
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.31	0.78
1:C:609:ALA:HA	3:C:2875:HOH:O	1.84	0.78
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.31	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:HB2	1:B:506:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:C:149:SER:O	1:C:163:LYS:HE2	1.94	0.67
1:A:569:GLU:HG2	3:A:2402:HOH:O	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:C:569:GLU:HG2	3:C:2435:HOH:O	1.94	0.65
1:B:581:GLU:OE1	3:B:2829:HOH:O	2.14	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:C:537:ARG:HD3	3:C:2769:HOH:O	1.96	0.64
1:B:70:ASP:OD1	1:B:74:ARG:HD2	1.97	0.64
1:A:537:ARG:HD3	3:A:2734:HOH:O	1.95	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:C:664:ARG:OXT	3:C:2932:HOH:O	2.15	0.63
1:B:650:SER:HB2	1:B:652:GLU:OE1	1.98	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:214:ASP:HB3	1:B:217:THR:CG2	2.28	0.63
1:B:3:ARG:O	3:B:2009:HOH:O	0.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:ARG:HD3	3:A:2021:HOH:O	1.99	0.62
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:B:492:HIS:HD2	3:B:2721:HOH:O	1.88	0.56
1:B:328:HIS:HD2	1:B:329:ASP:OD1	1.89	0.56
1:C:30:ARG:HD2	3:C:2106:HOH:O	2.05	0.56
1:A:328:HIS:HD2	1:A:329:ASP:OD1	1.89	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:B:470:ARG:CD	3:B:2700:HOH:O	2.26	0.56
1:B:362:LYS:HD2	3:B:2627:HOH:O	2.05	0.56
1:B:147:LYS:HD3	3:B:2785:HOH:O	2.06	0.56
1:A:30:ARG:HD2	3:A:2096:HOH:O	2.05	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:C:585:ALA:CA	3:C:2831:HOH:O	2.54	0.55
1:A:407:SER:HA	1:A:448:GLN:HE22	1.71	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:506:ARG:HH11	1:C:506:ARG:CB	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:492:HIS:HD2	3:C:2718:HOH:O	1.88	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:HD22	1:C:78:ASN:C	2.12	0.53
1:C:78:ASN:HD22	1:C:79:GLY:N	2.07	0.53
1:B:2:ARG:CA	3:B:2012:HOH:O	1.97	0.53
1:A:78:ASN:HD22	1:A:79:GLY:N	2.07	0.53
1:C:25:GLN:NE2	3:C:2086:HOH:O	2.37	0.53
1:B:78:ASN:ND2	1:B:80:VAL:H	2.06	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: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:29:LYS:CE	3:A:2091:HOH:O	2.57	0.53
1:C:585:ALA:HB3	3:C:2831:HOH:O	2.08	0.53
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.44	0.53
1:A:650:SER:OG	1:A:653:LYS:HG3	2.09	0.53
1:B:650:SER:OG	1:B:653:LYS:HG3	2.09	0.53
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.53
1:A:650:SER:HB2	1:A:652:GLU:CD	2.30	0.52
1:A:78:ASN:ND2	1:A:80:VAL:H	2.06	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:HD22	1:B:78:ASN:C	2.12	0.52
1:A:70:ASP:OD1	1:A:74:ARG:CD	2.58	0.52
1:B:664:ARG:HH11	1:B:664:ARG:HG2	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:C:650:SER:HB2	1:C:652:GLU:CD	2.30	0.52
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.91	0.52
1:A:474:MET:HE1	3:A:2614:HOH:O	2.09	0.52
1:A:78:ASN:C	1:A:78:ASN:HD22	2.12	0.51
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.03	0.51
1:C:664:ARG:HA	3:C:2933:HOH:O	2.11	0.51
1:C:70:ASP:OD1	1:C:74:ARG:CD	2.58	0.51
1:A:664:ARG:HH11	1:A:664:ARG:HG2	1.75	0.51

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:504:ASP:HB2	3:C:2735:HOH:O	2.14	0.48
1:C:423:ASN:HB2	3:C:2654:HOH:O	2.11	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:B:112:ALA:HB1	1:B:487:LYS:HE2	1.94	0.48
1:A:269:ARG:NH2	3:A:2488:HOH:O	2.43	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:B:214:ASP:CB	1:B:217:THR:HG22	2.41	0.47
1:A:651:VAL:O	1:A:655:GLU:HB2	2.14	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:C:424:SER:N	3:C:2654:HOH:O	2.40	0.47
1:B:269:ARG:NH2	3:B:2520:HOH:O	2.43	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: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:642:HIS:CE1	1:A:646:MET:HG3	2.50	0.47
1:A:339:LEU:C	1:A:339:LEU:HD23	2.35	0.47
1:B:339:LEU:HD23	1:B:339:LEU:C	2.35	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:HD23	1:C:339:LEU:C	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:C:651:VAL:O	1:C:655:GLU:HB2	2.14	0.46
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: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
1:A:471:LEU:HD12	1:A:474:MET:HE2	1.98	0.46
1:B:492:HIS:HE1	3:B:2213:HOH:O	1.99	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:492:HIS:HE1	3:C:2223:HOH:O	1.98	0.45
1:C:434:ARG:NH1	3:C:2663:HOH:O	2.50	0.45
1:C:86:GLY:O	1:C:89:HIS:HD2	1.99	0.45
1:C:29:LYS:HE3	3:C:2098:HOH:O	2.12	0.45
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.52	0.45
1:C:305:THR:H	1:C:309:ASN:ND2	2.15	0.45
1:C:268:ARG:HH12	1:C:270:ARG:HH21	1.62	0.45
1:A:305:THR:H	1:A:309:ASN:ND2	2.15	0.45
1:C:82:THR:HG22	1:C:83:ASN:N	2.28	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:497:LEU:HD12	1:A:497:LEU:HA	1.87	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:B:74:ARG:HD3	1:B:507:ARG:HD2	2.01	0.43
1:A:74:ARG:HD3	1:A: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:HA	1:C:497:LEU:HD12	1.87	0.43
1:B:607:ARG:NH1	3:B:2868:HOH:O	2.52	0.43
1:B:204:ARG:HG3	1:B:272:ALA:CB	2.49	0.43
1:B:71:GLU:H	1:B:71:GLU:CD	2.23	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:175:GLU:HA	1:B: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:C	1:C:630:TYR:CD1	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:HE	1:C:607:ARG:H	1.68	0.41
1:C:145:ILE:HD12	1:C:164:ILE:HD13	2.02	0.41
1:A:506:ARG:CG	1:A:506:ARG:NH1	2.84	0.41
1:B:596:LEU:CD2	1:B:608:GLN:HG2	2.51	0.41
1:C:226:MET:HE3	3:C:2473:HOH:O	2.19	0.41
1:B:86:GLY:O	1:B:89:HIS:CD2	2.74	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:C:664:ARG:HB2	3:C:2932:HOH:O	1.77	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: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:C:664:ARG:HG2	1:C:664:ARG:NH1	2.36	0.40
1:B:664:ARG:HG2	1:B:664:ARG:NH1	2.36	0.40
1:A:630:TYR:C	1:A:630:TYR:CD1	2.94	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	Distance(Å)	Clash(Å)
1:C:479:LYS:NZ	1:C:607:ARG:C[2_445]	0.93	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

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%)	27	17
1	B	662/664 (100%)	645 (97%)	12 (2%)	5 (1%)	27	17
1	C	662/664 (100%)	645 (97%)	12 (2%)	5 (1%)	27	17
All	All	1986/1992 (100%)	1935 (97%)	36 (2%)	15 (1%)	27	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	44	39
1	B	557/557 (100%)	536 (96%)	21 (4%)	44	39
1	C	557/557 (100%)	537 (96%)	20 (4%)	47	42
All	All	1671/1671 (100%)	1609 (96%)	62 (4%)	45	40

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
1	A	81	ARG
1	A	82	THR
1	A	113	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	C	82	THR
1	C	113	ASP
1	C	154	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Some 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
1	B	448	GLN
1	B	525	GLN
1	B	626	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

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.

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, 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%)	-0.11	15 (2%) 57 57	25, 37, 72, 159	0
1	B	664/664 (100%)	-0.03	22 (3%) 44 44	25, 37, 72, 159	0
1	C	664/664 (100%)	0.06	28 (4%) 35 34	25, 37, 72, 159	0
All	All	1992/1992 (100%)	-0.03	65 (3%) 44 44	25, 37, 72, 159	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	ARG	10.5
1	C	606	ALA	10.4
1	C	607	ARG	10.4
1	C	608	GLN	9.3
1	B	608	GLN	8.4
1	C	603	ALA	8.2
1	C	610	GLY	7.9
1	C	609	ALA	7.8
1	B	606	ALA	7.4
1	A	607	ARG	5.9
1	C	612	ALA	5.9
1	C	664	ARG	5.8
1	B	603	ALA	5.8
1	B	609	ALA	5.8
1	C	604	SER	5.6
1	A	1	PRO	5.4
1	A	606	ALA	5.4
1	B	610	GLY	5.3
1	B	604	SER	5.1
1	B	611	LEU	4.4
1	A	609	ALA	4.4
1	A	608	GLN	4.2
1	C	215	PRO	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	612	ALA	4.1
1	B	664	ARG	4.0
1	A	2	ARG	4.0
1	B	22	ILE	4.0
1	C	596	LEU	3.9
1	B	2	ARG	3.9
1	C	2	ARG	3.8
1	A	664	ARG	3.5
1	A	216	LYS	3.5
1	B	605	MET	3.5
1	A	610	GLY	3.5
1	C	605	MET	3.4
1	B	1	PRO	3.4
1	C	254	GLU	3.3
1	A	257	GLY	3.3
1	B	257	GLY	3.1
1	A	611	LEU	3.1
1	C	216	LYS	3.1
1	C	651	VAL	3.1
1	B	411	LEU	2.9
1	C	1	PRO	2.8
1	C	72	TYR	2.7
1	A	254	GLU	2.7
1	C	63	ASP	2.6
1	C	537	ARG	2.6
1	C	611	LEU	2.5
1	B	415	LEU	2.5
1	C	479	LYS	2.5
1	A	218	GLY	2.5
1	C	257	GLY	2.5
1	A	411	LEU	2.4
1	C	478	GLY	2.4
1	B	537	ARG	2.3
1	B	613	GLU	2.3
1	B	20	ASN	2.3
1	C	219	LYS	2.2
1	C	506	ARG	2.2
1	C	214	ASP	2.2
1	A	215	PRO	2.2
1	B	254	GLU	2.1
1	B	412	VAL	2.1
1	C	505	SER	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	A	665	1/1	0.07	-1.87	32,32,32,32	0
2	MN	B	665	1/1	0.05	-2.98	32,32,32,32	0
2	MN	C	665	1/1	0.04	-5.67	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.