



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:24 PM GMT

PDB ID : 3ZDP
Title : R416A Monomeric nucleoprotein of influenza A virus
Authors : Chenavas, S.; Ruigrok, R.W.H.; Crepin, T.
Deposited on : 2012-11-29
Resolution : 2.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

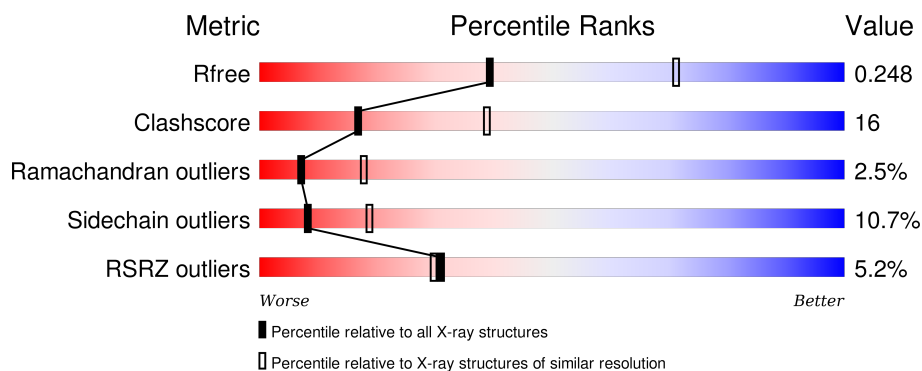
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	498	<div> <div>6%</div> <div>58% 28% 7% 7%</div> </div>
1	B	498	<div> <div>5%</div> <div>65% 24% • 6%</div> </div>
1	C	498	<div> <div>4%</div> <div>63% 25% • • 7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11113 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 NUCLEOCAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3670	2275	681	688	26			
1	B	467	Total	C	N	O	S	0	0	0
			3703	2294	688	695	26			
1	C	462	Total	C	N	O	S	0	0	0
			3677	2279	683	689	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	ALA	ARG	ENGINEERED MUTATION	UNP Q1K9H2
B	416	ALA	ARG	ENGINEERED MUTATION	UNP Q1K9H2
C	416	ALA	ARG	ENGINEERED MUTATION	UNP Q1K9H2

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

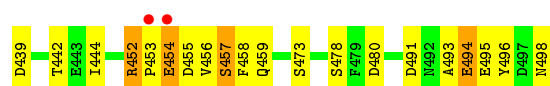
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	21	Total	O	0	0
			21	21		

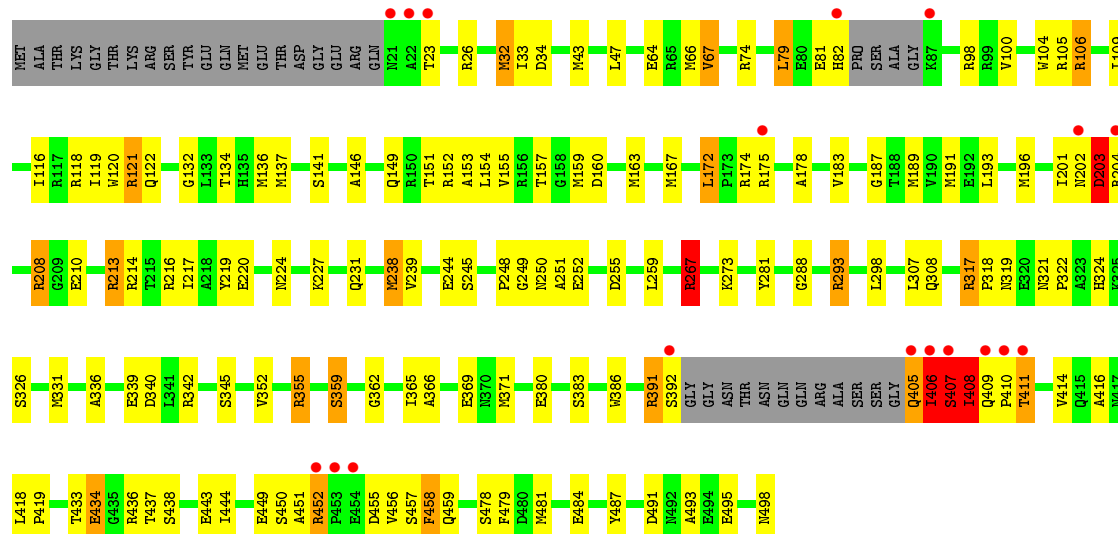
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	17	Total	O	0	0
			17	17		



● Molecule 1: NUCLEOCAPSID PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.42Å 285.44Å 118.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.12 – 2.69 39.89 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (143.12-2.69) 99.4 (39.89-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.198 , 0.250 0.197 , 0.248	Depositor DCC
R_{free} test set	3914 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.8	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 77393 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11113	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
K

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	0.76	0/3734	0.84	4/5022 (0.1%)
1	B	0.84	3/3768 (0.1%)	0.88	3/5070 (0.1%)
1	C	0.83	3/3740 (0.1%)	0.90	8/5030 (0.2%)
All	All	0.81	6/11242 (0.1%)	0.87	15/15122 (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	B	0	2
1	C	0	3
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	TRP	CD2-CE2	6.80	1.49	1.41
1	B	104	TRP	CD2-CE2	6.22	1.48	1.41
1	C	386	TRP	CD2-CE2	5.68	1.48	1.41
1	B	120	TRP	CD2-CE2	5.63	1.48	1.41
1	B	393	GLY	N-CA	5.10	1.53	1.46
1	C	104	TRP	CD2-CE2	5.04	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	167	MET	CG-SD-CE	-7.41	88.34	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	355	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	317	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	317	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	340	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	267	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	150	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	99	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	382	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	491	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	348	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	145	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	391	ARG	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	210	GLU	Peptide
1	B	411	THR	Peptide
1	C	288	GLY	Peptide
1	C	411	THR	Peptide
1	C	450	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3670	0	3630	132	0
1	B	3703	0	3661	95	0
1	C	3677	0	3637	137	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	0	1	0
3	B	21	0	0	1	0
3	C	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11113	0	10928	361	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 16.

All (361) 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:355:ARG:HD3	1:C:493:ALA:HB2	1.26	1.13
1:C:208:ARG:HH11	1:C:208:ARG:HG2	0.98	1.13
1:C:324:HIS:CD2	1:C:359:SER:H	1.67	1.12
1:B:78:TYR:HA	1:B:137:MET:CE	1.80	1.10
1:A:369:GLU:C	1:A:370:ASN:CA	2.19	1.08
1:A:369:GLU:O	1:A:370:ASN:CA	2.01	1.07
1:A:167:MET:CE	1:A:187:GLY:HA3	1.85	1.06
1:B:78:TYR:HA	1:B:137:MET:HE2	1.10	1.06
1:C:267:ARG:HH11	1:C:267:ARG:HG3	1.17	1.04
1:C:167:MET:HE2	1:C:187:GLY:HA3	1.42	1.01
1:A:324:HIS:CD2	1:A:359:SER:H	1.81	0.97
1:A:324:HIS:HD2	1:A:359:SER:H	1.03	0.96
1:A:167:MET:HE1	1:A:187:GLY:HA3	1.43	0.96
1:C:160:ASP:H	1:C:163:MET:CE	1.78	0.95
1:A:118:ARG:HH21	1:A:122:GLN:HE22	1.10	0.95
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.31	0.94
1:B:355:ARG:HD3	1:B:493:ALA:HB2	1.46	0.94
1:A:82:HIS:HB2	1:A:84:SER:H	1.32	0.94
1:C:106:ARG:HH11	1:C:106:ARG:HG2	1.31	0.94
1:A:368:ASN:H	1:A:368:ASN:HD22	1.13	0.94
1:C:202:ASN:O	1:C:203:ASP:HB3	1.65	0.93
1:C:159:MET:HB3	1:C:163:MET:CE	1.96	0.93
1:C:167:MET:CE	1:C:187:GLY:HA3	1.99	0.93
1:C:159:MET:HB3	1:C:163:MET:HE3	1.53	0.91
1:C:324:HIS:HD2	1:C:359:SER:H	1.05	0.91
1:A:355:ARG:HD3	1:A:493:ALA:HB2	1.54	0.90
1:B:167:MET:HE2	1:B:187:GLY:HA3	1.52	0.90
1:A:196:MET:HE1	1:A:219:TYR:HB2	1.54	0.90
1:C:189:MET:HE2	1:C:189:MET:HA	1.55	0.89
1:C:317:ARG:HD3	1:C:369:GLU:OE1	1.73	0.88
1:C:160:ASP:N	1:C:163:MET:HE2	1.89	0.88
1:C:208:ARG:HG2	1:C:208:ARG:NH1	1.78	0.88
1:A:157:THR:HG22	1:A:159:MET:HG3	1.55	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLU:HG2	1:B:455:ASP:N	1.89	0.86
1:B:78:TYR:CA	1:B:137:MET:HE2	2.01	0.85
1:C:238:MET:HE1	1:C:444:ILE:HD12	1.59	0.85
1:C:238:MET:CE	1:C:444:ILE:HD12	2.08	0.84
1:C:160:ASP:N	1:C:163:MET:CE	2.39	0.84
1:B:174:ARG:HD3	1:B:174:ARG:H	1.41	0.84
1:C:267:ARG:HG3	1:C:267:ARG:NH1	1.87	0.82
1:A:452:ARG:NH1	1:A:456:VAL:HG23	1.94	0.82
1:A:454:GLU:O	1:A:455:ASP:HB2	1.79	0.82
1:A:157:THR:HG21	1:A:159:MET:HE2	1.61	0.80
1:A:115:GLU:OE2	1:A:118:ARG:NH1	2.14	0.80
1:C:189:MET:CE	1:C:189:MET:HA	2.11	0.80
1:C:160:ASP:H	1:C:163:MET:HE1	1.44	0.80
1:C:208:ARG:HH11	1:C:208:ARG:CG	1.90	0.80
1:C:437:THR:O	1:C:438:SER:HB3	1.81	0.79
1:C:324:HIS:HD2	1:C:359:SER:N	1.81	0.79
1:B:321:ASN:HD22	1:B:321:ASN:C	1.87	0.79
1:B:167:MET:CE	1:B:187:GLY:HA3	2.13	0.78
1:B:408:ILE:C	1:B:409:GLN:HG2	2.04	0.78
1:B:430:THR:HG23	1:B:431:GLY:H	1.49	0.77
1:A:321:ASN:ND2	1:A:323:ALA:H	1.83	0.76
1:A:443:GLU:O	1:A:444:ILE:HB	1.85	0.76
1:C:81:GLU:HB2	1:C:82:HIS:HB2	1.68	0.76
1:A:196:MET:CE	1:A:219:TYR:HB2	2.16	0.76
1:A:213:ARG:HA	1:A:216:ARG:HB3	1.67	0.76
1:A:167:MET:HE1	1:A:187:GLY:CA	2.15	0.75
1:C:317:ARG:NH2	1:C:362:GLY:O	2.18	0.75
1:B:324:HIS:HD2	1:B:359:SER:H	1.31	0.75
1:B:324:HIS:CD2	1:B:359:SER:H	2.05	0.75
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.87	0.74
1:A:317:ARG:NH2	1:A:362:GLY:O	2.20	0.74
1:B:167:MET:O	1:B:170:SER:HB3	1.87	0.74
1:B:21:ASN:HA	1:B:24:GLU:HB3	1.70	0.74
1:C:434:GLU:OE1	1:C:434:GLU:HA	1.87	0.74
1:A:308:GLN:HE22	1:A:383:SER:H	1.32	0.73
1:B:47:LEU:O	1:B:98:ARG:NH2	2.20	0.73
1:B:459:GLN:NE2	3:B:2020:HOH:O	2.21	0.73
1:C:267:ARG:CG	1:C:267:ARG:HH11	2.00	0.72
1:A:324:HIS:HD2	1:A:359:SER:N	1.85	0.72
1:B:174:ARG:HG2	1:B:175:ARG:HG2	1.70	0.72
1:A:167:MET:HE2	1:A:187:GLY:HA3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:O	1:A:239:VAL:HG23	1.90	0.71
1:A:452:ARG:HH12	1:A:456:VAL:HG23	1.54	0.71
1:C:251:ALA:HB1	1:C:436:ARG:NH1	2.05	0.71
1:A:167:MET:CE	1:A:187:GLY:CA	2.66	0.71
1:C:405:GLN:O	1:C:406:ILE:O	2.07	0.71
1:A:157:THR:HG21	1:A:159:MET:CE	2.21	0.71
1:A:171:THR:HG22	3:A:2005:HOH:O	1.89	0.70
1:A:21:ASN:N	1:A:23:THR:HG1	1.90	0.70
1:C:47:LEU:O	1:C:98:ARG:NH2	2.25	0.70
1:B:321:ASN:ND2	1:B:323:ALA:H	1.90	0.70
1:C:159:MET:CE	1:C:191:MET:HA	2.22	0.69
1:C:159:MET:HE1	1:C:191:MET:CA	2.21	0.69
1:B:321:ASN:HD22	1:B:322:PRO:N	1.90	0.69
1:A:144:ASN:HB2	1:A:171:THR:HG21	1.73	0.69
1:C:43:MET:HE2	1:C:119:ILE:CD1	2.23	0.69
1:C:160:ASP:H	1:C:163:MET:HE2	1.49	0.69
1:A:321:ASN:C	1:A:321:ASN:HD22	1.95	0.69
1:C:159:MET:HE1	1:C:191:MET:HA	1.75	0.69
1:A:141:SER:HB2	1:A:172:LEU:HD13	1.74	0.68
1:C:355:ARG:CD	1:C:493:ALA:HB2	2.16	0.68
1:A:192:GLU:HB3	1:A:222:MET:CE	2.24	0.68
1:C:273:LYS:HE2	1:C:405:GLN:HA	1.75	0.68
1:C:227:LYS:HB2	1:C:239:VAL:HG11	1.74	0.68
1:A:118:ARG:NH2	1:A:122:GLN:HE22	1.89	0.67
1:A:192:GLU:HB3	1:A:222:MET:HE3	1.76	0.67
1:B:355:ARG:HD3	1:B:493:ALA:CB	2.22	0.67
1:A:368:ASN:H	1:A:368:ASN:ND2	1.90	0.67
1:B:216:ARG:O	1:B:220:GLU:HG3	1.94	0.67
1:C:331:MET:HE1	1:C:487:TYR:CE1	2.29	0.67
1:C:298:LEU:H	1:C:406:ILE:HD13	1.59	0.66
1:A:422:ARG:HB3	1:A:423:PRO:HD3	1.77	0.66
1:C:238:MET:CE	1:C:444:ILE:CD1	2.73	0.66
1:C:118:ARG:NH1	1:C:122:GLN:HE22	1.94	0.65
1:C:106:ARG:HG2	1:C:106:ARG:NH1	2.10	0.65
1:B:174:ARG:H	1:B:174:ARG:CD	2.05	0.65
1:A:65:ARG:NH2	1:A:80:GLU:O	2.31	0.64
1:C:141:SER:HB2	1:C:172:LEU:HD13	1.77	0.64
1:B:407:SER:O	1:B:408:ILE:HB	1.96	0.64
1:B:74:ARG:HH11	1:B:89:PRO:HB3	1.63	0.64
1:A:152:ARG:HB3	1:A:495:GLU:CD	2.19	0.63
1:A:232:THR:OG1	1:A:235:GLN:HG2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:MET:HB3	1:C:163:MET:HE1	1.80	0.63
1:B:218:ALA:O	1:B:222:MET:HG3	1.99	0.62
1:B:454:GLU:HG2	1:B:455:ASP:H	1.63	0.62
1:C:43:MET:HE2	1:C:119:ILE:HD13	1.80	0.62
1:A:154:LEU:HD23	1:A:159:MET:CE	2.29	0.62
1:A:430:THR:O	1:A:432:ASN:N	2.28	0.61
1:C:160:ASP:N	1:C:163:MET:HE1	2.11	0.61
1:B:196:MET:HE1	1:B:219:TYR:HD1	1.66	0.61
1:A:245:SER:OG	1:A:246:ARG:N	2.34	0.61
1:C:331:MET:HG3	1:C:336:ALA:HB3	1.83	0.60
1:C:216:ARG:O	1:C:220:GLU:HG3	2.01	0.60
1:A:189:MET:HA	1:A:189:MET:CE	2.32	0.60
1:B:196:MET:CE	1:B:219:TYR:HB2	2.32	0.60
1:A:157:THR:CG2	1:A:157:THR:O	2.50	0.60
1:A:144:ASN:CB	1:A:171:THR:HG21	2.31	0.60
1:A:189:MET:HA	1:A:189:MET:HE3	1.82	0.60
1:A:432:ASN:C	1:A:434:GLU:H	2.04	0.60
1:B:26:ARG:NH1	1:B:295:GLY:HA3	2.17	0.59
1:C:308:GLN:HE22	1:C:383:SER:H	1.47	0.59
1:B:355:ARG:NH1	1:B:491:ASP:OD2	2.32	0.59
1:A:216:ARG:O	1:A:220:GLU:HG3	2.01	0.59
1:B:193:LEU:HD21	1:B:222:MET:HB2	1.83	0.59
1:A:272:HIS:HD2	1:A:339:GLU:OE2	1.84	0.59
1:C:414:VAL:HG11	1:C:479:PHE:HZ	1.66	0.59
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.09	0.59
1:C:406:ILE:HG22	1:C:407:SER:H	1.67	0.58
1:C:248:PRO:HA	1:C:252:GLU:OE1	2.04	0.58
1:A:355:ARG:HA	1:A:358:LEU:HD22	1.84	0.58
1:A:234:ALA:HB1	1:A:444:ILE:HG13	1.84	0.58
1:A:152:ARG:HB3	1:A:495:GLU:OE2	2.04	0.58
1:C:267:ARG:NH2	1:C:418:LEU:O	2.37	0.58
1:B:98:ARG:HD2	1:B:107:GLU:OE1	2.04	0.57
1:C:167:MET:HE1	1:C:187:GLY:HA3	1.85	0.56
1:C:345:SER:HA	1:C:352:VAL:HG23	1.86	0.56
1:C:365:ILE:HG21	1:C:371:MET:CE	2.36	0.56
1:A:232:THR:OG1	1:A:235:GLN:CG	2.52	0.56
1:C:152:ARG:HG2	1:C:495:GLU:OE1	2.04	0.56
1:A:118:ARG:HH21	1:A:122:GLN:NE2	1.93	0.56
1:B:196:MET:HE1	1:B:219:TYR:HB2	1.88	0.56
1:C:452:ARG:HH22	1:C:456:VAL:HG23	1.70	0.56
1:C:452:ARG:NH2	1:C:456:VAL:HG23	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:HIS:CD2	1:C:359:SER:N	2.52	0.56
1:A:157:THR:CG2	1:A:159:MET:HG3	2.31	0.56
1:C:43:MET:CE	1:C:119:ILE:HD12	2.36	0.56
1:C:32:MET:HG3	1:C:33:ILE:N	2.20	0.56
1:A:29:VAL:HG12	1:A:296:TYR:HB3	1.88	0.56
1:A:321:ASN:HD22	1:A:322:PRO:N	2.04	0.56
1:A:321:ASN:ND2	1:A:321:ASN:C	2.60	0.56
1:A:56:LEU:HD21	1:A:315:LEU:HG	1.88	0.56
1:B:459:GLN:HG3	1:B:459:GLN:O	2.06	0.55
1:B:196:MET:HE1	1:B:219:TYR:CD1	2.41	0.55
1:B:261:ARG:HD3	1:B:430:THR:HG22	1.87	0.55
1:A:22:ALA:HA	1:A:25:ILE:HB	1.87	0.55
1:C:201:ILE:HD11	1:C:249:GLY:HA2	1.88	0.55
1:A:415:GLN:OE1	1:A:417:ASN:HB2	2.07	0.55
1:C:406:ILE:HD12	1:C:406:ILE:H	1.72	0.55
1:B:301:ILE:HD12	1:B:386:TRP:CE2	2.42	0.55
1:B:296:TYR:CE1	1:B:302:ASP:HB3	2.42	0.55
1:C:342:ARG:NH2	1:C:419:PRO:HG3	2.22	0.55
1:A:207:TRP:HZ3	1:A:216:ARG:HD2	1.72	0.54
1:B:321:ASN:ND2	1:B:321:ASN:C	2.58	0.54
1:A:157:THR:HG22	1:A:157:THR:O	2.08	0.54
1:B:392:SER:H	1:B:408:ILE:HG21	1.72	0.54
1:C:255:ASP:OD2	1:C:436:ARG:NH2	2.40	0.54
1:A:66:MET:CG	1:A:93:GLY:HA2	2.38	0.54
1:B:115:GLU:OE1	1:B:118:ARG:NH2	2.40	0.54
1:C:458:PHE:O	1:C:459:GLN:HB3	2.07	0.54
1:C:238:MET:HE3	1:C:444:ILE:CD1	2.37	0.53
1:C:153:ALA:O	1:C:157:THR:HG23	2.09	0.53
1:C:43:MET:HE2	1:C:119:ILE:HD12	1.89	0.53
1:A:77:LYS:HA	1:A:175:ARG:O	2.08	0.53
1:B:238:MET:O	1:B:242:VAL:HG23	2.09	0.53
1:C:391:ARG:HG3	1:C:458:PHE:HD2	1.74	0.53
1:C:339:GLU:HA	1:C:416:ALA:O	2.09	0.53
1:B:203:ASP:O	1:B:204:ARG:HB2	2.09	0.53
1:B:203:ASP:O	1:B:206:PHE:HB2	2.09	0.53
1:C:324:HIS:HD2	1:C:359:SER:HB2	1.73	0.52
1:A:441:ARG:O	1:A:445:ILE:HG13	2.08	0.52
1:C:433:THR:HG23	1:C:434:GLU:HB2	1.91	0.52
1:B:430:THR:HG23	1:B:431:GLY:N	2.23	0.52
1:C:273:LYS:HE2	1:C:405:GLN:CA	2.39	0.52
1:C:213:ARG:HH21	1:C:214:ARG:HH12	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:HE2	1:A:187:GLY:CA	2.35	0.52
1:C:159:MET:CB	1:C:163:MET:HE1	2.41	0.51
1:B:250:ASN:ND2	1:B:254:GLU:OE2	2.37	0.51
1:B:186:VAL:HG11	1:B:263:ALA:CB	2.41	0.51
1:C:407:SER:O	1:C:408:ILE:HG22	2.10	0.51
1:C:106:ARG:HH11	1:C:106:ARG:CG	2.13	0.51
1:A:72:ASP:OD1	1:A:77:LYS:N	2.37	0.50
1:A:214:ARG:O	1:A:217:ILE:HG22	2.10	0.50
1:C:159:MET:CA	1:C:163:MET:HE1	2.42	0.50
1:C:121:ARG:HH11	1:C:121:ARG:CG	2.13	0.50
1:B:21:ASN:HA	1:B:24:GLU:CB	2.39	0.50
1:C:244:GLU:OE1	1:C:244:GLU:HA	2.12	0.50
1:A:149:GLN:HG2	1:A:151:THR:HB	1.93	0.50
1:C:324:HIS:CD2	1:C:359:SER:HB2	2.47	0.50
1:A:297:SER:OG	1:A:299:VAL:HG22	2.12	0.50
1:A:359:SER:OG	1:B:480:ASP:OD1	2.29	0.50
1:C:391:ARG:HG3	1:C:458:PHE:CD2	2.47	0.50
1:A:68:LEU:HG	1:A:78:TYR:HB3	1.94	0.49
1:C:159:MET:HE3	1:C:191:MET:HG3	1.93	0.49
1:B:166:LEU:HB3	1:B:187:GLY:H	1.77	0.49
1:A:168:GLN:HG3	1:A:338:PHE:CD1	2.47	0.49
1:B:291:PHE:O	1:B:295:GLY:N	2.45	0.49
1:A:368:ASN:N	1:A:368:ASN:HD22	1.92	0.49
1:B:353:VAL:HG13	1:B:357:LYS:HB2	1.94	0.49
1:C:355:ARG:HD2	1:C:491:ASP:OD1	2.11	0.49
1:C:118:ARG:HH12	1:C:122:GLN:HE22	1.60	0.49
1:A:207:TRP:CZ3	1:A:216:ARG:HD2	2.47	0.49
1:C:244:GLU:O	1:C:245:SER:C	2.50	0.49
1:A:193:LEU:HD21	1:A:222:MET:HB3	1.94	0.48
1:A:465:GLU:HG2	1:A:475:ILE:HD11	1.95	0.48
1:A:311:GLN:NE2	1:A:313:TYR:OH	2.42	0.48
1:C:392:SER:C	1:C:408:ILE:HD13	2.33	0.48
1:A:432:ASN:C	1:A:434:GLU:N	2.66	0.48
1:C:293:ARG:HD3	1:C:293:ARG:HA	1.54	0.48
1:C:189:MET:CE	1:C:189:MET:CA	2.90	0.48
1:A:43:MET:CE	1:A:119:ILE:HG21	2.44	0.48
1:A:276:LEU:HB3	1:A:277:PRO:HD2	1.95	0.48
1:A:177:GLY:O	1:A:178:ALA:C	2.53	0.47
1:C:134:THR:O	1:C:137:MET:HB3	2.14	0.47
1:A:442:THR:C	1:A:443:GLU:O	2.48	0.47
1:B:495:GLU:HB2	1:B:498:ASN:HD22	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:HA	1:C:26:ARG:HB2	1.97	0.47
1:B:26:ARG:NH1	1:B:294:GLU:O	2.47	0.47
1:A:149:GLN:HE21	1:A:151:THR:HB	1.80	0.47
1:C:100:VAL:HB	1:C:105:ARG:HG3	1.97	0.47
1:A:88:ASP:HA	1:A:89:PRO:HD3	1.73	0.47
1:A:159:MET:CE	1:A:191:MET:HB2	2.45	0.47
1:C:238:MET:HG2	1:C:259:LEU:HD11	1.97	0.47
1:C:324:HIS:HD2	1:C:359:SER:CB	2.28	0.46
1:B:78:TYR:HD1	1:B:137:MET:CE	2.28	0.46
1:A:159:MET:HE2	1:A:191:MET:CB	2.45	0.46
1:B:454:GLU:O	1:B:455:ASP:HB2	2.16	0.46
1:B:452:ARG:HB3	1:B:455:ASP:H	1.80	0.46
1:C:47:LEU:HD21	1:C:109:ILE:HD13	1.96	0.46
1:C:208:ARG:CG	1:C:208:ARG:NH1	2.60	0.46
1:A:226:LEU:HD22	1:A:230:PHE:CE2	2.51	0.46
1:A:154:LEU:HD23	1:A:159:MET:HE3	1.96	0.46
1:C:132:GLY:O	1:C:136:MET:HE2	2.16	0.46
1:B:226:LEU:HD22	1:B:230:PHE:CE2	2.51	0.46
1:B:290:ASP:OD1	1:B:293:ARG:HB3	2.16	0.46
1:A:43:MET:HE3	1:A:119:ILE:HG21	1.98	0.46
1:A:167:MET:O	1:A:170:SER:HB3	2.16	0.45
1:B:452:ARG:HA	1:B:453:PRO:HD2	1.87	0.45
1:A:454:GLU:O	1:A:455:ASP:CB	2.56	0.45
1:C:231:GLN:HG3	1:C:457:SER:OG	2.17	0.45
1:B:361:ARG:HD2	1:C:481:MET:HE3	1.99	0.45
1:C:79:LEU:HA	1:C:79:LEU:HD22	1.58	0.45
1:A:236:ARG:HH11	1:A:236:ARG:HG2	1.82	0.45
1:C:160:ASP:CA	1:C:163:MET:HE2	2.46	0.45
1:A:159:MET:HE2	1:A:191:MET:HG3	1.99	0.45
1:A:291:PHE:O	1:A:295:GLY:N	2.43	0.45
1:C:116:ILE:HA	1:C:116:ILE:HD13	1.77	0.45
1:B:213:ARG:NH1	1:B:246:ARG:HH22	2.14	0.45
1:C:437:THR:O	1:C:438:SER:CB	2.55	0.45
1:C:64:GLU:O	1:C:67:VAL:HG23	2.17	0.45
1:A:387:ALA:HA	1:A:462:GLY:O	2.18	0.44
1:A:316:ILE:N	1:A:375:GLU:O	2.43	0.44
1:A:102:GLY:O	1:A:103:LYS:HE2	2.18	0.44
1:C:456:VAL:CG1	1:C:457:SER:N	2.80	0.44
1:A:177:GLY:O	1:A:179:ALA:N	2.49	0.44
1:A:236:ARG:NH1	1:A:236:ARG:HG2	2.31	0.44
1:C:443:GLU:OE1	1:C:443:GLU:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:HB1	1:B:444:ILE:HG13	1.98	0.44
1:C:167:MET:CE	1:C:187:GLY:CA	2.84	0.44
1:B:204:ARG:O	1:B:205:ASN:HB2	2.17	0.44
1:B:327:GLN:HE21	1:B:331:MET:CE	2.31	0.44
1:B:78:TYR:HD1	1:B:137:MET:HE3	1.83	0.44
1:A:43:MET:HE1	1:A:46:GLU:HG3	1.99	0.44
1:C:43:MET:CE	1:C:119:ILE:CD1	2.93	0.44
1:A:241:GLN:NE2	1:A:440:MET:HG3	2.33	0.44
1:A:128:ASP:O	1:A:129:ALA:C	2.56	0.43
1:A:324:HIS:CD2	1:A:359:SER:N	2.65	0.43
1:C:380:GLU:O	1:C:380:GLU:HG3	2.18	0.43
1:A:434:GLU:OE1	1:A:434:GLU:HA	2.19	0.43
1:A:388:ILE:HG21	1:A:409:GLN:HG3	2.01	0.43
1:A:422:ARG:N	1:A:423:PRO:CD	2.82	0.43
1:B:55:ARG:NH1	1:B:311:GLN:HB3	2.33	0.43
1:C:160:ASP:O	1:C:163:MET:HB2	2.19	0.43
1:C:33:ILE:HD12	1:C:281:TYR:CE1	2.54	0.43
1:B:196:MET:HE2	1:B:207:TRP:HH2	1.83	0.43
1:B:75:ARG:CG	1:B:75:ARG:HH11	2.32	0.43
1:B:68:LEU:HD22	1:B:78:TYR:HB3	2.01	0.43
1:A:320:GLU:HG2	1:A:360:THR:HA	2.00	0.43
1:C:159:MET:HE1	1:C:191:MET:N	2.34	0.42
1:A:366:ALA:HB1	1:A:368:ASN:ND2	2.33	0.42
1:B:415:GLN:OE1	1:B:458:PHE:O	2.36	0.42
1:B:494:GLU:H	1:B:494:GLU:HG3	1.46	0.42
1:A:445:ILE:O	1:A:449:GLU:HG3	2.19	0.42
1:A:456:VAL:HG13	1:A:457:SER:N	2.34	0.42
1:B:267:ARG:HH11	1:B:267:ARG:CG	2.33	0.42
1:B:418:LEU:HA	1:B:419:PRO:HD3	1.93	0.42
1:A:167:MET:CE	1:A:187:GLY:C	2.87	0.42
1:A:451:ALA:O	1:A:452:ARG:HB2	2.20	0.42
1:B:74:ARG:NH1	1:B:89:PRO:HB3	2.31	0.42
1:A:169:GLY:C	1:A:171:THR:H	2.23	0.42
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.75	0.42
1:B:196:MET:HE3	1:B:219:TYR:HB2	2.00	0.42
1:B:496:TYR:O	1:B:498:ASN:N	2.48	0.42
1:C:196:MET:HE1	1:C:219:TYR:HB2	2.01	0.42
1:C:317:ARG:O	1:C:318:PRO:C	2.58	0.42
1:A:308:GLN:NE2	1:A:383:SER:H	2.08	0.42
1:C:267:ARG:CG	1:C:267:ARG:NH1	2.66	0.41
1:A:422:ARG:N	1:A:423:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:HG22	1:B:496:TYR:CE2	2.54	0.41
1:B:38:ARG:NH1	1:B:123:ALA:O	2.52	0.41
1:A:186:VAL:HG11	1:A:263:ALA:HB2	2.02	0.41
1:B:293:ARG:HG3	1:B:294:GLU:N	2.33	0.41
1:A:71:PHE:CZ	1:A:117:ARG:HG2	2.55	0.41
1:C:307:LEU:HA	1:C:307:LEU:HD23	1.86	0.41
1:A:422:ARG:HB3	1:A:423:PRO:CD	2.46	0.41
1:B:72:ASP:O	1:B:75:ARG:HG3	2.19	0.41
1:B:58:GLN:NE2	1:B:363:VAL:HG13	2.35	0.41
1:A:370:ASN:OD1	1:A:372:GLU:HB2	2.20	0.41
1:A:210:GLU:O	1:A:214:ARG:HG2	2.20	0.41
1:A:41:ILE:CD1	1:A:285:VAL:HG12	2.50	0.41
1:C:146:ALA:C	1:C:355:ARG:HH21	2.24	0.41
1:A:251:ALA:HB1	1:A:436:ARG:HH11	1.85	0.41
1:A:150:ARG:HE	1:A:170:SER:HG	1.67	0.41
1:B:196:MET:HE1	1:B:219:TYR:CB	2.50	0.41
1:C:238:MET:HE2	1:C:238:MET:HB2	1.83	0.41
1:B:392:SER:N	1:B:408:ILE:HG21	2.36	0.41
1:B:35:GLY:HA3	1:B:124:ASN:ND2	2.36	0.41
1:B:231:GLN:HG3	1:B:457:SER:OG	2.21	0.41
1:C:224:ASN:HA	1:C:224:ASN:HD22	1.72	0.41
1:C:202:ASN:O	1:C:203:ASP:CB	2.48	0.41
1:C:366:ALA:N	1:C:369:GLU:OE2	2.52	0.41
1:C:308:GLN:NE2	1:C:383:SER:H	2.18	0.41
1:A:211:ASN:O	1:A:214:ARG:HB2	2.21	0.41
1:B:361:ARG:HG3	1:C:481:MET:HG3	2.02	0.41
1:B:70:ALA:HA	1:B:113:LYS:HB3	2.02	0.41
1:B:235:GLN:HE21	1:B:235:GLN:HB2	1.76	0.41
1:C:149:GLN:HG2	1:C:151:THR:HG23	2.03	0.41
1:C:298:LEU:H	1:C:406:ILE:CD1	2.30	0.40
1:B:301:ILE:HD12	1:B:386:TRP:CD2	2.56	0.40
1:B:249:GLY:O	1:B:250:ASN:C	2.60	0.40
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.91	0.40
1:B:244:GLU:O	1:B:245:SER:C	2.58	0.40
1:C:66:MET:SD	1:C:109:ILE:HD11	2.62	0.40
1:A:66:MET:HG3	1:A:93:GLY:HA2	2.03	0.40
1:C:459:GLN:HG3	1:C:459:GLN:O	2.21	0.40
1:C:154:LEU:HD21	1:C:167:MET:SD	2.60	0.40
1:B:456:VAL:CG1	1:B:457:SER:N	2.85	0.40
1:C:321:ASN:HA	1:C:322:PRO:HD2	1.95	0.40
1:C:204:ARG:HG2	1:C:208:ARG:HD2	2.04	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	456/498 (92%)	398 (87%)	40 (9%)	18 (4%)	4	8
1	B	463/498 (93%)	423 (91%)	32 (7%)	8 (2%)	11	29
1	C	456/498 (92%)	419 (92%)	28 (6%)	9 (2%)	9	24
All	All	1375/1494 (92%)	1240 (90%)	100 (7%)	35 (2%)	7	18

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	PRO
1	A	455	ASP
1	B	87	LYS
1	B	211	ASN
1	B	408	ILE
1	B	410	PRO
1	C	406	ILE
1	C	407	SER
1	C	410	PRO
1	C	458	PHE
1	A	411	THR
1	A	431	GLY
1	A	433	THR
1	A	457	SER
1	B	203	ASP
1	B	407	SER
1	C	203	ASP
1	C	408	ILE
1	C	451	ALA
1	A	177	GLY
1	A	178	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	CYS
1	B	452	ARG
1	C	178	ALA
1	A	129	ALA
1	A	170	SER
1	A	203	ASP
1	A	245	SER
1	A	452	ARG
1	B	205	ASN
1	C	455	ASP
1	A	444	ILE
1	A	197	ILE
1	A	86	GLY
1	A	83	PRO

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	391/421 (93%)	345 (88%)	46 (12%)	6	15
1	B	395/421 (94%)	352 (89%)	43 (11%)	8	18
1	C	393/421 (93%)	356 (91%)	37 (9%)	11	25
All	All	1179/1263 (93%)	1053 (89%)	126 (11%)	8	19

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	58	GLN
1	A	68	LEU
1	A	79	LEU
1	A	80	GLU
1	A	81	GLU
1	A	90	LYS
1	A	96	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	GLU
1	A	130	THR
1	A	151	THR
1	A	152	ARG
1	A	156	ARG
1	A	157	THR
1	A	170	SER
1	A	171	THR
1	A	172	LEU
1	A	174	ARG
1	A	189	MET
1	A	195	ARG
1	A	201	ILE
1	A	213	ARG
1	A	217	ILE
1	A	226	LEU
1	A	235	GLN
1	A	245	SER
1	A	246	ARG
1	A	259	LEU
1	A	283	SER
1	A	321	ASN
1	A	331	MET
1	A	348	ARG
1	A	358	LEU
1	A	359	SER
1	A	368	ASN
1	A	391	ARG
1	A	409	GLN
1	A	413	SER
1	A	418	LEU
1	A	422	ARG
1	A	430	THR
1	A	436	ARG
1	A	439	ASP
1	A	454	GLU
1	A	456	VAL
1	A	498	ASN
1	B	67	VAL
1	B	75	ARG
1	B	79	LEU
1	B	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	82	HIS
1	B	87	LYS
1	B	108	LEU
1	B	115	GLU
1	B	130	THR
1	B	170	SER
1	B	174	ARG
1	B	175	ARG
1	B	199	ARG
1	B	201	ILE
1	B	202	ASN
1	B	213	ARG
1	B	214	ARG
1	B	217	ILE
1	B	226	LEU
1	B	243	ARG
1	B	246	ARG
1	B	267	ARG
1	B	283	SER
1	B	293	ARG
1	B	321	ASN
1	B	348	ARG
1	B	351	LYS
1	B	388	ILE
1	B	408	ILE
1	B	409	GLN
1	B	411	THR
1	B	414	VAL
1	B	425	ILE
1	B	434	GLU
1	B	436	ARG
1	B	438	SER
1	B	439	ASP
1	B	442	THR
1	B	454	GLU
1	B	457	SER
1	B	473	SER
1	B	478	SER
1	B	494	GLU
1	C	32	MET
1	C	34	ASP
1	C	67	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	74	ARG
1	C	79	LEU
1	C	106	ARG
1	C	121	ARG
1	C	155	VAL
1	C	172	LEU
1	C	174	ARG
1	C	175	ARG
1	C	183	VAL
1	C	193	LEU
1	C	203	ASP
1	C	208	ARG
1	C	210	GLU
1	C	213	ARG
1	C	217	ILE
1	C	238	MET
1	C	250	ASN
1	C	267	ARG
1	C	293	ARG
1	C	319	ASN
1	C	326	SER
1	C	359	SER
1	C	405	GLN
1	C	406	ILE
1	C	407	SER
1	C	408	ILE
1	C	409	GLN
1	C	411	THR
1	C	434	GLU
1	C	449	GLU
1	C	452	ARG
1	C	478	SER
1	C	484	GLU
1	C	498	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	122	GLN
1	A	149	GLN
1	A	231	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	GLN
1	A	272	HIS
1	A	308	GLN
1	A	311	GLN
1	A	321	ASN
1	A	324	HIS
1	A	368	ASN
1	B	124	ASN
1	B	235	GLN
1	B	272	HIS
1	B	308	GLN
1	B	321	ASN
1	B	324	HIS
1	B	409	GLN
1	B	459	GLN
1	B	498	ASN
1	C	76	ASN
1	C	122	GLN
1	C	144	ASN
1	C	149	GLN
1	C	224	ASN
1	C	308	GLN
1	C	324	HIS
1	C	370	ASN
1	C	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 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	462/498 (92%)	-0.17	29 (6%)	23 22	24, 45, 116, 153	0
1	B	467/498 (93%)	-0.24	26 (5%)	28 26	23, 40, 99, 156	0
1	C	462/498 (92%)	-0.25	18 (3%)	43 43	24, 41, 98, 161	0
All	All	1391/1494 (93%)	-0.22	73 (5%)	31 30	23, 42, 104, 161	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	453	PRO	7.7
1	A	453	PRO	7.2
1	C	22	ALA	6.0
1	A	86	GLY	5.9
1	C	407	SER	5.6
1	A	83	PRO	5.4
1	C	21	ASN	5.3
1	B	453	PRO	5.2
1	B	82	HIS	5.0
1	A	82	HIS	4.9
1	C	410	PRO	4.9
1	B	410	PRO	4.7
1	A	411	THR	4.6
1	C	87	LYS	4.5
1	A	206	PHE	4.4
1	A	21	ASN	4.3
1	B	204	ARG	4.2
1	B	22	ALA	4.2
1	B	83	PRO	4.2
1	A	207	TRP	4.2
1	B	406	ILE	4.2
1	A	22	ALA	4.1
1	C	454	GLU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	23	THR	4.0
1	C	411	THR	3.9
1	B	407	SER	3.9
1	A	410	PRO	3.9
1	A	204	ARG	3.8
1	A	454	GLU	3.8
1	A	205	ASN	3.8
1	B	454	GLU	3.7
1	B	411	THR	3.7
1	B	408	ILE	3.6
1	B	21	ASN	3.6
1	B	86	GLY	3.4
1	B	405	GLN	3.4
1	C	452	ARG	3.3
1	C	392	SER	3.1
1	B	87	LYS	3.1
1	A	412	PHE	3.1
1	C	204	ARG	3.0
1	A	23	THR	3.0
1	B	208	ARG	3.0
1	A	209	GLY	3.0
1	B	23	THR	2.9
1	A	208	ARG	2.8
1	B	434	GLU	2.8
1	B	205	ASN	2.8
1	A	210	GLU	2.7
1	A	452	ARG	2.7
1	B	392	SER	2.7
1	B	85	ALA	2.7
1	C	175	ARG	2.7
1	A	214	ARG	2.7
1	A	85	ALA	2.7
1	A	178	ALA	2.6
1	C	406	ILE	2.6
1	A	87	LYS	2.5
1	C	409	GLN	2.4
1	B	433	THR	2.3
1	C	82	HIS	2.3
1	A	247	ASN	2.3
1	C	405	GLN	2.3
1	B	412	PHE	2.2
1	A	246	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	211	ASN	2.1
1	A	434	GLU	2.1
1	C	202	ASN	2.1
1	B	84	SER	2.1
1	A	408	ILE	2.0
1	B	213	ARG	2.0
1	A	203	ASP	2.0
1	B	247	ASN	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	K	A	1499	1/1	0.95	0.08	-1.80	53,53,53,53	0
2	K	B	1499	1/1	0.99	0.08	-2.45	48,48,48,48	0
2	K	C	1499	1/1	0.97	0.06	-3.26	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.