



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 3ZDP / pdb_00003zdp
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

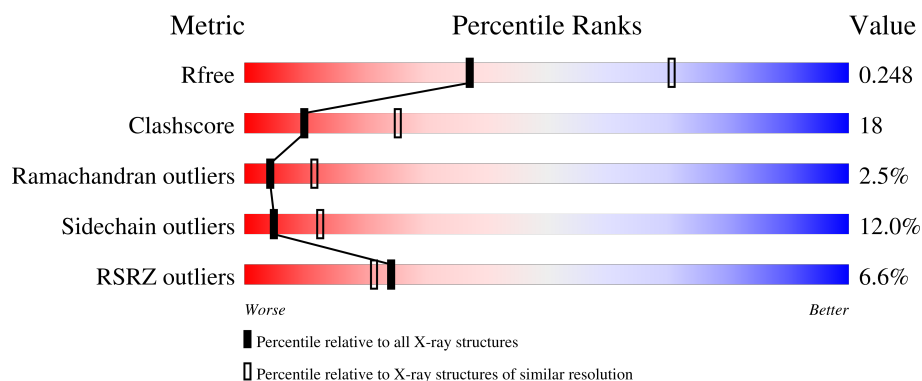
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	7% 55% 30% 7% • 7%
1	B	498	6% 62% 26% 5% 6%
1	C	498	5% 61% 25% 5% • 7%

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 (CCD ID: K) (formula: K).

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

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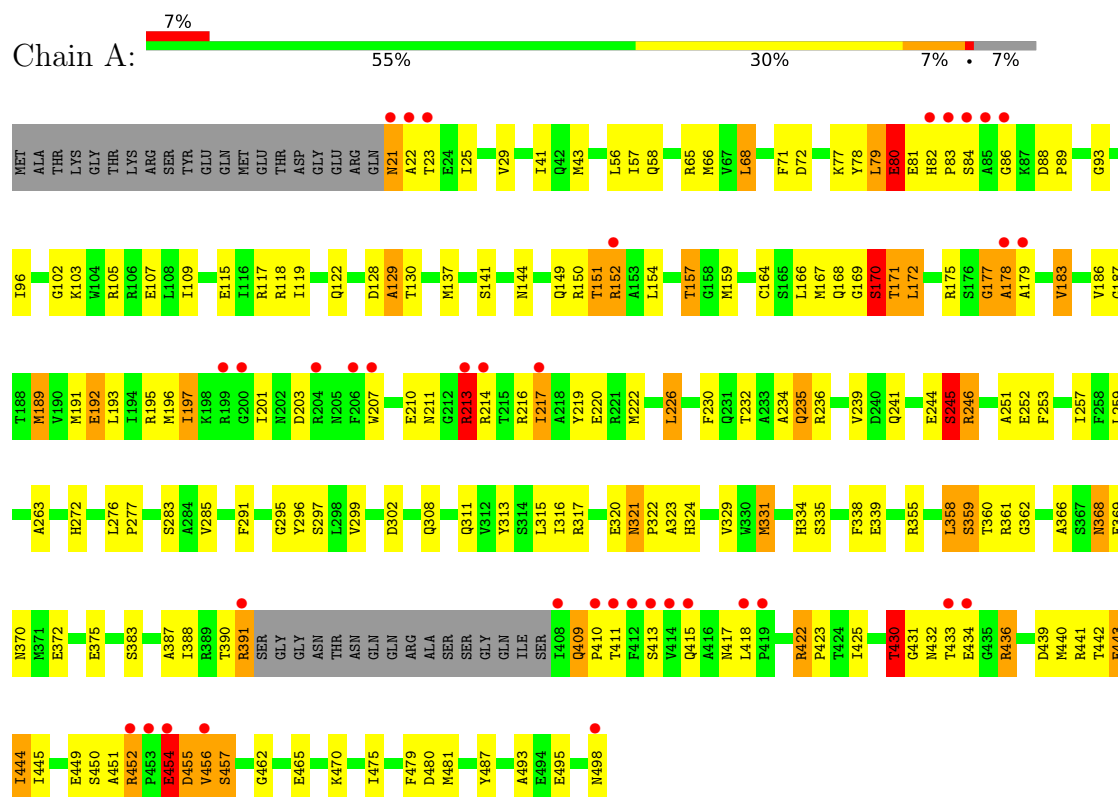
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	17	Total	O	0	0
			17	17		

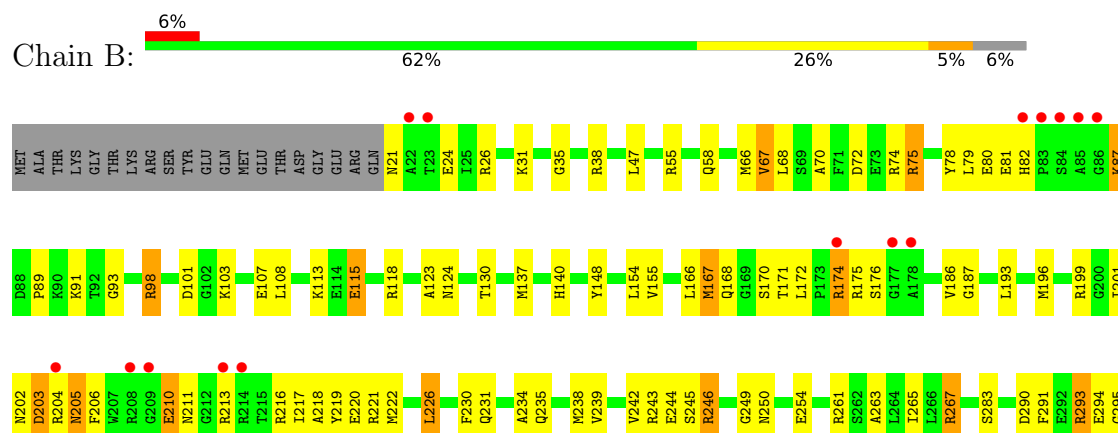
3 Residue-property plots

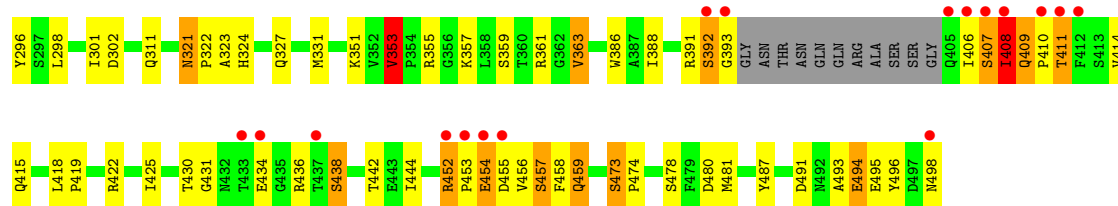
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NUCLEOCAPSID PROTEIN

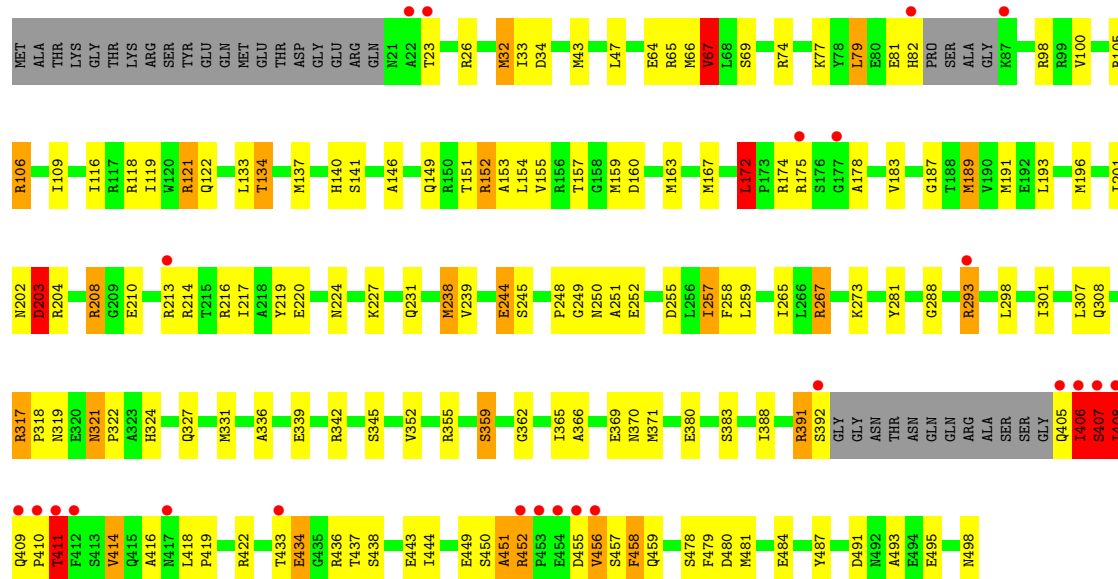


• Molecule 1: NUCLEOCAPSID PROTEIN





● 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 – 2.69 143.12 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (143.12-2.69) 99.4 (143.12-2.69)	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 (5.03%)	wwPDB-VP
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 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
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
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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	1.00	1/3734 (0.0%)	1.09	8/5022 (0.2%)
1	B	1.10	4/3768 (0.1%)	1.16	19/5070 (0.4%)
1	C	1.08	2/3740 (0.1%)	1.18	17/5030 (0.3%)
All	All	1.06	7/11242 (0.1%)	1.15	44/15122 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	SER	CA-C	6.01	1.60	1.52
1	C	411	THR	N-CA	5.44	1.50	1.46
1	C	140	HIS	CG-ND1	-5.33	1.32	1.38
1	A	454	GLU	CA-C	5.33	1.56	1.52
1	B	140	HIS	CG-CD2	5.33	1.41	1.35
1	B	393	GLY	N-CA	5.09	1.53	1.45
1	B	459	GLN	N-CA	5.07	1.52	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	LEU	CA-C-N	-13.54	107.12	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	LEU	C-N-CA	-13.54	107.12	120.52
1	B	422	ARG	CA-C-N	-8.71	109.95	119.19
1	B	422	ARG	C-N-CA	-8.71	109.95	119.19
1	B	391	ARG	N-CA-C	8.38	123.15	111.92
1	A	443	GLU	N-CA-C	-7.76	100.32	110.33
1	B	67	VAL	CB-CA-C	-7.29	102.64	111.97
1	B	246	ARG	N-CA-C	-6.79	101.57	110.53
1	C	77	LYS	N-CA-C	-6.60	105.77	113.88
1	B	172	LEU	CA-C-N	-6.57	113.22	119.85
1	B	172	LEU	C-N-CA	-6.57	113.22	119.85
1	A	213	ARG	N-CA-C	-6.51	104.95	114.39
1	C	411	THR	CB-CA-C	-6.48	107.00	116.53
1	C	391	ARG	N-CA-C	6.44	124.52	110.80
1	C	67	VAL	CB-CA-C	-6.34	103.85	111.97
1	A	430	THR	N-CA-C	5.96	117.11	108.34
1	C	422	ARG	CA-C-N	-5.83	113.00	119.19
1	C	422	ARG	C-N-CA	-5.83	113.00	119.19
1	B	167	MET	CG-SD-CE	-5.71	88.34	100.90
1	B	101	ASP	CB-CA-C	-5.63	103.42	112.09
1	B	438	SER	N-CA-C	5.57	116.61	108.14
1	B	148	TYR	N-CA-C	5.55	118.29	109.24
1	C	451	ALA	N-CA-C	5.50	122.52	110.80
1	B	239	VAL	N-CA-C	-5.48	105.03	110.62
1	C	321	ASN	CA-C-O	5.46	122.84	119.29
1	B	176	SER	N-CA-C	-5.44	103.71	110.41
1	A	302	ASP	CA-C-N	-5.37	114.13	119.56
1	A	302	ASP	C-N-CA	-5.37	114.13	119.56
1	C	317	ARG	CA-C-N	-5.36	114.42	119.89
1	C	317	ARG	C-N-CA	-5.36	114.42	119.89
1	C	69	SER	N-CA-C	-5.31	105.39	111.07
1	A	183	VAL	N-CA-CB	-5.31	106.37	112.21
1	B	265	ILE	CB-CA-C	-5.29	107.21	111.71
1	C	301	ILE	N-CA-C	5.28	117.69	111.09
1	C	133	LEU	N-CA-C	-5.27	105.62	111.36
1	B	363	VAL	N-CA-C	5.26	115.88	110.36
1	C	65	ARG	N-CA-C	-5.25	105.56	111.28
1	C	265	ILE	CB-CA-C	-5.22	106.48	111.44
1	B	81	GLU	N-CA-C	-5.19	105.66	112.41
1	A	329	VAL	N-CA-C	5.12	115.34	110.53
1	B	210	GLU	N-CA-C	-5.10	105.63	111.14
1	B	473	SER	N-CA-C	5.10	118.40	108.21
1	B	353	VAL	N-CA-CB	-5.08	104.10	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLU	N-CA-C	-5.01	100.73	108.90

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

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	146	0
1	B	3703	0	3661	103	0
1	C	3677	0	3637	141	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
All	All	11113	0	10928	385	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 18.

All (385) 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:A:157:THR:HG21	1:A:159:MET:HE2	1.27	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:C	1:A:370:ASN:CA	2.19	1.13
1:C:208:ARG:HG2	1:C:208:ARG:HH11	0.98	1.13
1:C:324:HIS:CD2	1:C:359:SER:H	1.67	1.12
1:A:167:MET:HE1	1:A:187:GLY:HA3	1.26	1.11
1:B:78:TYR:HA	1:B:137:MET:CE	1.80	1.10
1:C:189:MET:HA	1:C:189:MET:HE2	1.31	1.07
1:A:369:GLU:O	1:A:370:ASN:CA	2.01	1.06
1:A:167:MET:CE	1:A:187:GLY:HA3	1.85	1.06
1:A:196:MET:HE1	1:A:219:TYR:HB2	1.31	1.06
1:A:167:MET:HE1	1:A:187:GLY:CA	1.86	1.04
1:C:267:ARG:HG3	1:C:267:ARG:HH11	1.17	1.04
1:C:160:ASP:N	1:C:163:MET:HE2	1.74	1.02
1:B:78:TYR:HA	1:B:137:MET:HE2	1.07	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:B:78:TYR:CA	1:B:137:MET:HE2	1.95	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:HG3	1:C:121:ARG:HH11	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:A:154:LEU:HD23	1:A:159:MET:HE3	1.51	0.93
1:C:167:MET:CE	1:C:187:GLY:HA3	1.99	0.93
1:B:196:MET:HE1	1:B:219:TYR:HB2	1.50	0.93
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:C:317:ARG:HD3	1:C:369:GLU:OE1	1.73	0.88
1:C:208:ARG:HG2	1:C:208:ARG:NH1	1.78	0.88
1:B:167:MET:HE1	1:B:187:GLY:HA3	1.55	0.88
1:A:192:GLU:HB3	1:A:222:MET:HE3	1.57	0.87
1:C:160:ASP:H	1:C:163:MET:HE2	1.31	0.87
1:A:157:THR:HG22	1:A:159:MET:HG3	1.55	0.87
1:B:454:GLU:HG2	1:B:455:ASP:N	1.89	0.86
1:A:167:MET:HE1	1:A:187:GLY:C	2.01	0.85
1:C:43:MET:HE1	1:C:119:ILE:HD12	1.59	0.84
1:C:238:MET:CE	1:C:444:ILE:HD12	2.08	0.84
1:B:174:ARG:H	1:B:174:ARG:HD3	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:C	1:B:321:ASN:HD22	1.87	0.83
1:B:408:ILE:C	1:B:409:GLN:HG2	2.04	0.82
1:C:267:ARG:HG3	1:C:267:ARG:NH1	1.87	0.82
1:C:238:MET:HE1	1:C:444:ILE:HD12	1.61	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:C:167:MET:HE2	1:C:187:GLY:HA3	1.62	0.81
1:C:160:ASP:N	1:C:163:MET:CE	2.39	0.80
1:A:115:GLU:OE2	1:A:118:ARG:NH1	2.14	0.80
1:C:189:MET:HA	1:C:189:MET:CE	2.11	0.80
1:A:159:MET:HE1	1:A:191:MET:HB2	1.62	0.80
1:C:159:MET:HB3	1:C:163:MET:HE3	1.63	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:167:MET:CE	1:B:187:GLY:HA3	2.13	0.78
1:B:430:THR:HG23	1:B:431:GLY:H	1.49	0.77
1:C:167:MET:HE1	1:C:187:GLY:HA3	1.65	0.76
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:213:ARG:HA	1:A:216:ARG:HB3	1.67	0.76
1:C:159:MET:HB3	1:C:163:MET:HE1	1.68	0.75
1:C:317:ARG:NH2	1:C:362:GLY:O	2.18	0.75
1:B:324:HIS:CD2	1:B:359:SER:H	2.05	0.75
1:B:324:HIS:HD2	1:B:359:SER:H	1.31	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:HA	1:C:434:GLU:OE1	1.87	0.74
1:A:308:GLN:HE22	1:A:383:SER:H	1.32	0.73
1:A:321:ASN:C	1:A:321:ASN:HD22	1.95	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:HH11	1:C:267:ARG:CG	2.00	0.72
1:A:157:THR:CG2	1:A:159:MET:HE2	2.15	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:B:167:MET:HE1	1:B:187:GLY:CA	2.19	0.72
1:A:235:GLN:O	1:A:239:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:405:GLN:O	1:C:406:ILE:O	2.07	0.71
1:C:159:MET:HE1	1:C:191:MET:CA	2.21	0.71
1:A:171:THR:HG22	3:A:2005:HOH:O	1.89	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:A:144:ASN:HB2	1:A:171:THR:HG21	1.73	0.69
1:B:321:ASN:HD22	1:B:322:PRO:N	1.90	0.69
1:A:141:SER:HB2	1:A:172:LEU:HD13	1.74	0.68
1:A:152:ARG:HB3	1:A:495:GLU:CD	2.19	0.68
1:A:192:GLU:HB3	1:A:222:MET:CE	2.24	0.68
1:C:355:ARG:CD	1:C:493:ALA:HB2	2.16	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:196:MET:CE	1:A:219:TYR:HB2	2.16	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: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:196:MET:HE1	1:C:219:TYR:HB2	1.77	0.65
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:A:21:ASN:N	1:A:23:THR:HG1	1.94	0.65
1:A:43:MET:HE1	1:A:119:ILE:CD1	2.26	0.65
1:B:174:ARG:H	1:B:174:ARG:CD	2.05	0.65
1:B:166:LEU:C	1:B:167:MET:HE2	2.23	0.64
1:A:432:ASN:C	1:A:434:GLU:H	2.04	0.64
1:A:43:MET:HE1	1:A:119:ILE:HD12	1.78	0.64
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:A:43:MET:HE3	1:A:119:ILE:HG21	1.79	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:232:THR:OG1	1:A:235:GLN:HG2	1.98	0.63
1:C:331:MET:HE1	1:C:487:TYR:CE1	2.34	0.63
1:C:167:MET:HE1	1:C:187:GLY:CA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:430:THR:O	1:A:432:ASN:N	2.28	0.61
1:C:160:ASP:H	1:C:163:MET:HE1	1.63	0.61
1:A:361:ARG:HD2	1:B:481:MET:HE3	1.83	0.60
1:C:216:ARG:O	1:C:220:GLU:HG3	2.01	0.60
1:C:331:MET:HG3	1:C:336:ALA:HB3	1.83	0.60
1:A:154:LEU:HD23	1:A:159:MET:CE	2.29	0.60
1:A:189:MET:CE	1:A:189:MET:HA	2.32	0.60
1:A:144:ASN:CB	1:A:171:THR:HG21	2.31	0.60
1:A:157:THR:CG2	1:A:157:THR:O	2.50	0.60
1:B:26:ARG:NH1	1:B:295:GLY:HA3	2.17	0.59
1:C:159:MET:CB	1:C:163:MET:HE1	2.31	0.59
1:C:308:GLN:HE22	1:C:383:SER:H	1.47	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:B:355:ARG:NH1	1:B:491:ASP:OD2	2.32	0.59
1:A:272:HIS:HD2	1:A:339:GLU:OE2	1.84	0.59
1:C:159:MET:HE1	1:C:191:MET:HA	1.82	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:A:321:ASN:ND2	1:A:321:ASN:C	2.60	0.59
1:A:245:SER:OG	1:A:246:ARG:N	2.34	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:43:MET:HE2	1:C:119:ILE:HG21	1.86	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:43:MET:HE1	1:C:119:ILE:CD1	2.33	0.57
1:B:321:ASN:C	1:B:321:ASN:ND2	2.58	0.57
1:A:43:MET:HE2	1:A:43:MET:HA	1.87	0.57
1:C:238:MET:HE3	1:C:444:ILE:CD1	2.34	0.57
1:A:331:MET:HE1	1:A:487:TYR:CD1	2.40	0.57
1:B:196:MET:HE2	1:B:219:TYR:HD1	1.70	0.57
1:B:78:TYR:HD1	1:B:137:MET:HE3	1.70	0.56
1:A:166:LEU:C	1:A:167:MET:HE2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:452:ARG:NH2	1:C:456:VAL:HG23	2.21	0.56
1:C:452:ARG:HH22	1:C:456:VAL:HG23	1.70	0.56
1:A:157:THR:CG2	1:A:159:MET:HG3	2.31	0.56
1:C:324:HIS:CD2	1:C:359:SER:N	2.52	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:56:LEU:HD21	1:A:315:LEU:HG	1.88	0.56
1:A:321:ASN:HD22	1:A:322:PRO:N	2.04	0.56
1:B:459:GLN:HG3	1:B:459:GLN:O	2.06	0.55
1:A:22:ALA:HA	1:A:25:ILE:HB	1.87	0.55
1:B:261:ARG:HD3	1:B:430:THR:HG22	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:C:159:MET:HE1	1:C:191:MET:CB	2.36	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:C:160:ASP:CA	1:C:163:MET:HE2	2.37	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:244:GLU:O	1:C:245:SER:C	2.50	0.53
1:C:153:ALA:O	1:C:157:THR:HG23	2.09	0.53
1:C:392:SER:C	1:C:408:ILE:HD13	2.33	0.53
1:C:43:MET:CE	1:C:119:ILE:HD12	2.36	0.53
1:A:77:LYS:HA	1:A:175:ARG:O	2.08	0.53
1:B:196:MET:HE1	1:B:219:TYR:CB	2.31	0.53
1:B:238:MET:O	1:B:242:VAL:HG23	2.09	0.53
1:A:432:ASN:C	1:A:434:GLU:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ARG:O	1:A:445:ILE:HG13	2.08	0.52
1:C:324:HIS:HD2	1:C:359:SER:HB2	1.73	0.52
1:A:177:GLY:O	1:A:178:ALA:C	2.53	0.52
1:C:433:THR:HG23	1:C:434:GLU:HB2	1.91	0.52
1:B:196:MET:CE	1:B:219:TYR:HB2	2.32	0.52
1:B:430:THR:HG23	1:B:431:GLY:N	2.23	0.52
1:C:213:ARG:HH21	1:C:214:ARG:HH12	1.57	0.52
1:C:273:LYS:HE2	1:C:405:GLN:CA	2.39	0.52
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:A:442:THR:C	1:A:443:GLU:O	2.48	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:B:361:ARG:HD2	1:C:481:MET:HE3	1.93	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:A:297:SER:OG	1:A:299:VAL:HG22	2.12	0.50
1:B:331:MET:HE1	1:B:487:TYR:CE1	2.47	0.50
1:C:324:HIS:CD2	1:C:359:SER:HB2	2.47	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:A:168:GLN:HG3	1:A:338:PHE:CD1	2.47	0.49
1:B:166:LEU:HB3	1:B:187:GLY:H	1.77	0.49
1:B:291:PHE:O	1:B:295:GLY:N	2.45	0.49
1:A:368:ASN:HD22	1:A:368:ASN:N	1.92	0.49
1:B:353:VAL:HG13	1:B:357:LYS:HB2	1.94	0.49
1:C:118:ARG:HH12	1:C:122:GLN:HE22	1.60	0.49
1:C:355:ARG:HD2	1:C:491:ASP:OD1	2.11	0.49
1:A:207:TRP:CZ3	1:A:216:ARG:HD2	2.47	0.49
1:A:167:MET:HE2	1:A:167:MET:HA	1.95	0.48
1:A:193:LEU:HD21	1:A:222:MET:HB3	1.94	0.48
1:A:311:GLN:NE2	1:A:313:TYR:OH	2.42	0.48
1:A:465:GLU:HG2	1:A:475:ILE:HD11	1.95	0.48
1:C:293:ARG:HA	1:C:293:ARG:HD3	1.54	0.48
1:C:189:MET:CE	1:C:189:MET:CA	2.90	0.48
1:A:128:ASP:O	1:A:129:ALA:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:MET:CA	1:C:163:MET:HE1	2.43	0.48
1:A:276:LEU:HB3	1:A:277:PRO:HD2	1.95	0.48
1:C:134:THR:O	1:C:137:MET:HB3	2.14	0.47
1:B:495:GLU:HB2	1:B:498:ASN:HD22	1.78	0.47
1:C:23:THR:HA	1:C:26:ARG:HB2	1.97	0.47
1:A:149:GLN:HE21	1:A:151:THR:HB	1.80	0.47
1:B:26:ARG:NH1	1:B:294:GLU:O	2.47	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:169:GLY:C	1:A:171:THR:H	2.23	0.47
1:C:238:MET:HG2	1:C:259:LEU:HD11	1.97	0.47
1:B:78:TYR:HD1	1:B:137:MET:CE	2.28	0.46
1:B:452:ARG:HB3	1:B:455:ASP:H	1.80	0.46
1:B:454:GLU:O	1:B:455:ASP:HB2	2.16	0.46
1:C:47:LEU:HD21	1:C:109:ILE:HD13	1.96	0.46
1:C:317:ARG:O	1:C:318:PRO:C	2.58	0.46
1:C:324:HIS:HD2	1:C:359:SER:CB	2.28	0.46
1:A:226:LEU:HD22	1:A:230:PHE:CE2	2.51	0.46
1:C:159:MET:HE1	1:C:191:MET:HB2	1.96	0.46
1:C:208:ARG:NH1	1:C:208:ARG:CG	2.60	0.46
1:A:159:MET:HE1	1:A:191:MET:CB	2.40	0.46
1:C:146:ALA:C	1:C:355:ARG:HH21	2.24	0.46
1:B:226:LEU:HD22	1:B:230:PHE:CE2	2.51	0.46
1:A:479:PHE:HB2	1:A:481:MET:HE2	1.98	0.46
1:B:290:ASP:OD1	1:B:293:ARG:HB3	2.16	0.46
1:A:43:MET:CE	1:A:119:ILE:HG21	2.44	0.45
1:A:167:MET:O	1:A:170:SER:HB3	2.16	0.45
1:A:454:GLU:O	1:A:455:ASP:CB	2.56	0.45
1:B:452:ARG:HA	1:B:453:PRO:HD2	1.87	0.45
1:B:244:GLU:O	1:B:245:SER:C	2.58	0.45
1:B:249:GLY:O	1:B:250:ASN:C	2.60	0.45
1:C:231:GLN:HG3	1:C:457:SER:OG	2.17	0.45
1:B:327:GLN:HE21	1:B:331:MET:HE1	1.82	0.45
1:C:79:LEU:HD22	1:C:79:LEU:HA	1.58	0.45
1:A:166:LEU:O	1:A:167:MET:HE2	2.17	0.45
1:A:236:ARG:HG2	1:A:236:ARG:HH11	1.82	0.45
1:C:43:MET:CE	1:C:119:ILE:CD1	2.93	0.45
1:A:291:PHE:O	1:A:295:GLY:N	2.43	0.45
1:B:213:ARG:NH1	1:B:246:ARG:HH22	2.14	0.45
1:C:116:ILE:HD13	1:C:116:ILE:HA	1.77	0.45
1:B:167:MET:HE2	1:B:187:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLU:O	1:C:67:VAL:HG23	2.17	0.45
1:C:437:THR:O	1:C:438:SER:CB	2.55	0.45
1:A:102:GLY:O	1:A:103:LYS:HE2	2.18	0.44
1:A:244:GLU:C	1:A:245:SER:O	2.57	0.44
1:A:316:ILE:N	1:A:375:GLU:O	2.43	0.44
1:A:387:ALA:HA	1:A:462:GLY:O	2.18	0.44
1:A:189:MET:HA	1:A:189:MET:HE2	1.99	0.44
1:A:177:GLY:O	1:A:179:ALA:N	2.49	0.44
1:A:236:ARG:HG2	1:A:236:ARG:NH1	2.31	0.44
1:B:234:ALA:HB1	1:B:444:ILE:HG13	1.98	0.44
1:C:443:GLU:OE1	1:C:443:GLU:HA	2.17	0.44
1:C:456:VAL:CG1	1:C:457:SER:N	2.80	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:A:241:GLN:NE2	1:A:440:MET:HG3	2.33	0.44
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:388:ILE:HG21	1:A:409:GLN:HG3	2.01	0.43
1:A:434:GLU:HA	1:A:434:GLU:OE1	2.19	0.43
1:A:43:MET:HE1	1:A:119:ILE:HD13	1.97	0.43
1:A:361:ARG:CD	1:B:481:MET:HE3	2.48	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:A:137:MET:HE2	1:A:137:MET:HB3	1.85	0.43
1:C:33:ILE:HD12	1:C:281:TYR:CE1	2.54	0.43
1:C:160:ASP:O	1:C:163:MET:HB2	2.19	0.43
1:B:75:ARG:CG	1:B:75:ARG:HH11	2.32	0.43
1:A:320:GLU:HG2	1:A:360:THR:HA	2.00	0.43
1:B:68:LEU:HD22	1:B:78:TYR:HB3	2.01	0.43
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:C:257:ILE:O	1:C:258:PHE:C	2.62	0.42
1:A:390:THR:O	1:A:391:ARG:C	2.61	0.42
1:A:445:ILE:O	1:A:449:GLU:HG3	2.19	0.42
1:A:480:ASP:OD1	1:A:480:ASP:C	2.63	0.42
1:C:152:ARG:HG2	1:C:495:GLU:CD	2.44	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:C:480:ASP:OD1	1:C:480:ASP:C	2.62	0.42
1:B:418:LEU:HA	1:B:419:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:327:GLN:HE21	1:C:331:MET:HE1	1.83	0.42
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.75	0.42
1:B:496:TYR:O	1:B:498:ASN:N	2.48	0.42
1:B:480:ASP:OD1	1:B:480:ASP:C	2.62	0.42
1:C:157:THR:OG1	1:C:159:MET:HE3	2.20	0.42
1:A:308:GLN:NE2	1:A:383:SER:H	2.08	0.42
1:B:66:MET:HE3	1:B:93:GLY:HA2	2.02	0.42
1:A:186:VAL:HG11	1:A:263:ALA:HB2	2.02	0.41
1:A:334:HIS:O	1:A:335:SER:C	2.62	0.41
1:A:422:ARG:N	1:A:423:PRO:HD2	2.35	0.41
1:B:38:ARG:NH1	1:B:123:ALA:O	2.52	0.41
1:B:171:THR:HG22	1:B:496:TYR:CE2	2.54	0.41
1:C:267:ARG:NH1	1:C:267:ARG:CG	2.66	0.41
1:A:71:PHE:CZ	1:A:117:ARG:HG2	2.55	0.41
1:B:203:ASP:CG	1:B:205:ASN:H	2.28	0.41
1:B:293:ARG:HG3	1:B:294:GLU:N	2.33	0.41
1:C:307:LEU:HD23	1:C:307:LEU:HA	1.86	0.41
1:A:422:ARG:HB3	1:A:423:PRO:CD	2.46	0.41
1:B:58:GLN:NE2	1:B:363:VAL:HG13	2.35	0.41
1:B:72:ASP:O	1:B:75:ARG:HG3	2.19	0.41
1:A:41:ILE:CD1	1:A:285:VAL:HG12	2.50	0.41
1:A:210:GLU:O	1:A:214:ARG:HG2	2.20	0.41
1:A:370:ASN:OD1	1:A:372:GLU:HB2	2.20	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:C:238:MET:HE2	1:C:238:MET:HB2	1.77	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:B:392:SER:N	1:B:408:ILE:HG21	2.36	0.41
1:A:21:ASN:N	1:A:23:THR:OG1	2.52	0.41
1:C:224:ASN:HD22	1:C:224:ASN:HA	1.72	0.41
1:A:79:LEU:CD1	1:A:79:LEU:C	2.94	0.41
1:A:211:ASN:O	1:A:214:ARG:HB2	2.21	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:B:361:ARG:HG3	1:C:481:MET:HG3	2.02	0.41
1:C:149:GLN:HG2	1:C:151:THR:HG23	2.03	0.41
1:C:202:ASN:O	1:C:203:ASP:CB	2.48	0.41
1:C:308:GLN:NE2	1:C:383:SER:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ALA:N	1:C:369:GLU:OE2	2.52	0.41
1:A:252:GLU:O	1:A:253:PHE:C	2.64	0.41
1:C:167:MET:CE	1:C:187:GLY:CA	2.84	0.41
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.91	0.40
1:B:301:ILE:HD12	1:B:386:TRP:CD2	2.56	0.40
1:C:298:LEU:H	1:C:406:ILE:CD1	2.30	0.40
1:A:66:MET:HG3	1:A:93:GLY:HA2	2.03	0.40
1:C:66:MET:SD	1:C:109:ILE:HD11	2.62	0.40
1:C:459:GLN:O	1:C:459:GLN:HG3	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:B:167:MET:O	1:B:168:GLN:C	2.64	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%)	2	5
1	B	463/498 (93%)	423 (91%)	32 (7%)	8 (2%)	7	19
1	C	456/498 (92%)	419 (92%)	28 (6%)	9 (2%)	6	16
All	All	1375/1494 (92%)	1240 (90%)	100 (7%)	35 (2%)	4	11

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	PRO
1	A	455	ASP
1	B	87	LYS

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Mol	Chain	Res	Type
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
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%)	339 (87%)	52 (13%)	4	10
1	B	395/421 (94%)	349 (88%)	46 (12%)	5	13
1	C	393/421 (93%)	350 (89%)	43 (11%)	6	16
All	All	1179/1263 (93%)	1038 (88%)	141 (12%)	5	12

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	57	ILE
1	A	58	GLN
1	A	68	LEU
1	A	79	LEU
1	A	80	GLU
1	A	81	GLU
1	A	96	ILE
1	A	105	ARG
1	A	107	GLU
1	A	109	ILE
1	A	130	THR
1	A	151	THR
1	A	152	ARG
1	A	157	THR
1	A	170	SER
1	A	171	THR
1	A	172	LEU
1	A	183	VAL
1	A	189	MET
1	A	192	GLU
1	A	195	ARG
1	A	197	ILE
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	257	ILE
1	A	259	LEU
1	A	283	SER
1	A	321	ASN

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Mol	Chain	Res	Type
1	A	331	MET
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	425	ILE
1	A	430	THR
1	A	436	ARG
1	A	439	ASP
1	A	450	SER
1	A	454	GLU
1	A	456	VAL
1	A	470	LYS
1	A	498	ASN
1	B	31	LYS
1	B	67	VAL
1	B	75	ARG
1	B	79	LEU
1	B	80	GLU
1	B	82	HIS
1	B	87	LYS
1	B	91	LYS
1	B	98	ARG
1	B	103	LYS
1	B	108	LEU
1	B	115	GLU
1	B	130	THR
1	B	155	VAL
1	B	174	ARG
1	B	199	ARG
1	B	201	ILE
1	B	202	ASN
1	B	217	ILE
1	B	221	ARG
1	B	226	LEU
1	B	243	ARG
1	B	267	ARG
1	B	283	SER

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Mol	Chain	Res	Type
1	B	293	ARG
1	B	298	LEU
1	B	321	ASN
1	B	351	LYS
1	B	353	VAL
1	B	388	ILE
1	B	406	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	442	THR
1	B	454	GLU
1	B	457	SER
1	B	473	SER
1	B	474	PRO
1	B	478	SER
1	B	494	GLU
1	C	32	MET
1	C	34	ASP
1	C	67	VAL
1	C	74	ARG
1	C	79	LEU
1	C	106	ARG
1	C	121	ARG
1	C	134	THR
1	C	152	ARG
1	C	155	VAL
1	C	172	LEU
1	C	174	ARG
1	C	175	ARG
1	C	183	VAL
1	C	189	MET
1	C	193	LEU
1	C	203	ASP
1	C	208	ARG
1	C	210	GLU
1	C	217	ILE

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Mol	Chain	Res	Type
1	C	238	MET
1	C	244	GLU
1	C	250	ASN
1	C	257	ILE
1	C	267	ARG
1	C	293	ARG
1	C	319	ASN
1	C	359	SER
1	C	370	ASN
1	C	388	ILE
1	C	406	ILE
1	C	407	SER
1	C	408	ILE
1	C	409	GLN
1	C	411	THR
1	C	414	VAL
1	C	434	GLU
1	C	449	GLU
1	C	452	ARG
1	C	456	VAL
1	C	478	SER
1	C	484	GLU
1	C	498	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	122	GLN
1	A	144	ASN
1	A	149	GLN
1	A	231	GLN
1	A	272	HIS
1	A	308	GLN
1	A	311	GLN
1	A	321	ASN
1	A	324	HIS
1	A	364	GLN
1	A	368	ASN
1	B	124	ASN
1	B	125	ASN
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	272	HIS
1	B	308	GLN
1	B	321	ASN
1	B	324	HIS
1	B	409	GLN
1	B	415	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	205	ASN
1	C	224	ASN
1	C	231	GLN
1	C	250	ASN
1	C	308	GLN
1	C	324	HIS
1	C	370	ASN
1	C	409	GLN
1	C	415	GLN

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 oligosaccharides 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

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%)	-0.09	36 (7%)	19 16	24, 45, 116, 153	0
1	B	467/498 (93%)	-0.28	32 (6%)	23 20	23, 40, 99, 156	0
1	C	462/498 (92%)	-0.24	24 (5%)	33 29	24, 41, 98, 161	0
All	All	1391/1494 (93%)	-0.20	92 (6%)	24 21	23, 42, 104, 161	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	PRO	8.0
1	A	412	PHE	8.0
1	A	178	ALA	7.3
1	B	83	PRO	7.0
1	C	410	PRO	6.9
1	B	82	HIS	6.7
1	A	83	PRO	6.5
1	C	412	PHE	6.4
1	C	406	ILE	6.3
1	B	453	PRO	6.2
1	B	393	GLY	6.2
1	C	453	PRO	5.6
1	A	410	PRO	5.6
1	B	406	ILE	5.6
1	A	82	HIS	5.5
1	A	411	THR	5.5
1	B	412	PHE	5.5
1	A	414	VAL	5.4
1	B	410	PRO	5.3
1	A	23	THR	5.1
1	B	85	ALA	4.9
1	C	392	SER	4.9
1	C	452	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	411	THR	4.4
1	B	411	THR	4.3
1	C	82	HIS	4.2
1	B	392	SER	4.1
1	A	408	ILE	4.0
1	C	22	ALA	4.0
1	A	206	PHE	3.9
1	A	207	TRP	3.9
1	C	407	SER	3.8
1	A	86	GLY	3.7
1	B	433	THR	3.6
1	B	454	GLU	3.6
1	B	213	ARG	3.5
1	C	87	LYS	3.4
1	C	456	VAL	3.4
1	C	408	ILE	3.4
1	A	84	SER	3.4
1	A	179	ALA	3.4
1	B	408	ILE	3.3
1	B	214	ARG	3.3
1	C	23	THR	3.3
1	B	405	GLN	3.2
1	B	86	GLY	3.2
1	C	455	ASP	3.1
1	A	22	ALA	3.1
1	C	405	GLN	3.1
1	C	213	ARG	2.9
1	A	415	GLN	2.9
1	A	419	PRO	2.9
1	A	152	ARG	2.9
1	B	455	ASP	2.9
1	A	85	ALA	2.7
1	C	177	GLY	2.7
1	C	454	GLU	2.7
1	B	23	THR	2.7
1	B	174	ARG	2.7
1	A	434	GLU	2.6
1	B	178	ALA	2.6
1	A	217	ILE	2.6
1	C	417	ASN	2.6
1	B	407	SER	2.5
1	B	452	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	2.5
1	B	209	GLY	2.5
1	A	454	GLU	2.5
1	B	434	GLU	2.5
1	A	452	ARG	2.4
1	A	214	ARG	2.4
1	B	177	GLY	2.3
1	C	409	GLN	2.3
1	B	84	SER	2.3
1	C	433	THR	2.3
1	C	175	ARG	2.3
1	A	433	THR	2.3
1	B	498	ASN	2.2
1	A	213	ARG	2.2
1	A	413	SER	2.2
1	A	456	VAL	2.2
1	B	204	ARG	2.1
1	A	21	ASN	2.1
1	B	208	ARG	2.1
1	A	418	LEU	2.1
1	A	498	ASN	2.1
1	A	200	GLY	2.1
1	A	391	ARG	2.1
1	B	437	THR	2.1
1	A	199	ARG	2.0
1	A	204	ARG	2.0
1	C	293	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	K	A	1499	1/1	0.97	0.04	53,53,53,53	0
2	K	C	1499	1/1	0.98	0.03	49,49,49,49	0
2	K	B	1499	1/1	0.99	0.03	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.