



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:56 PM UTC

PDB ID : 9O7V / pdb\_00009o7v  
Title : Crystal Structure of the RIb:C Heterodimer of PKA  
Authors : Wu, J.; Ilouz, R.; Taylor, S.S.  
Deposited on : 2025-04-15  
Resolution : 3.70 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

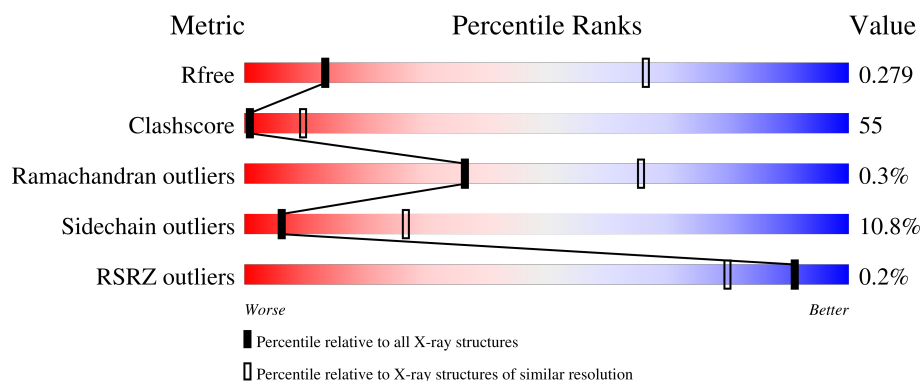
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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  $\geq 3$ , 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	350	
2	B	381	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4902 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	P	S	0	0	0
			2731	1771	454	496	2	8			

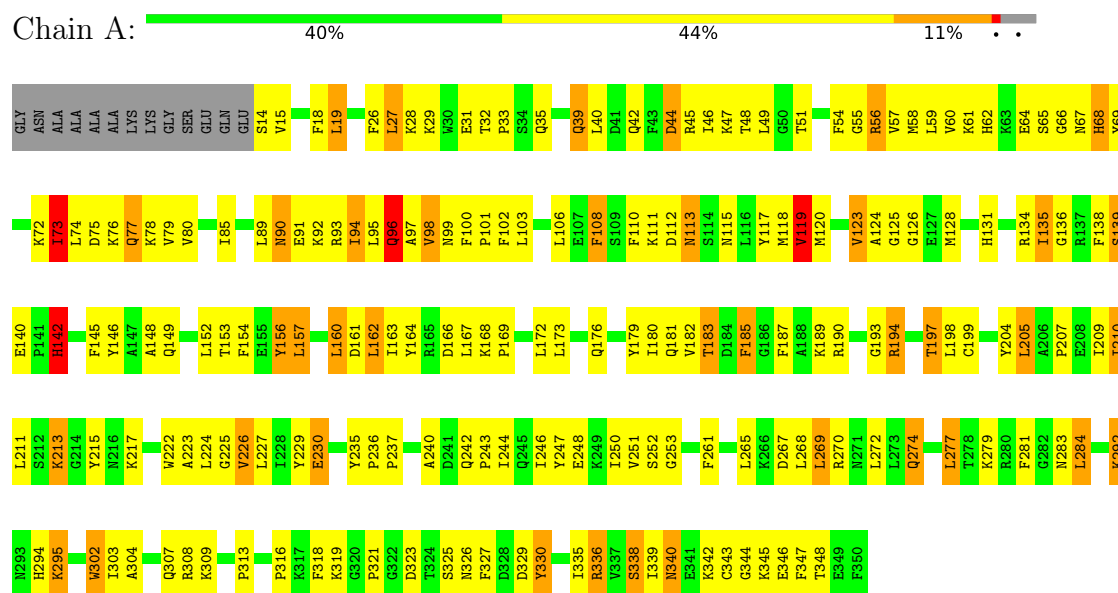
- Molecule 2 is a protein called cAMP-dependent protein kinase type I-beta regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	276	Total	C	N	O	S	0	0	0
			2171	1373	375	417	6			

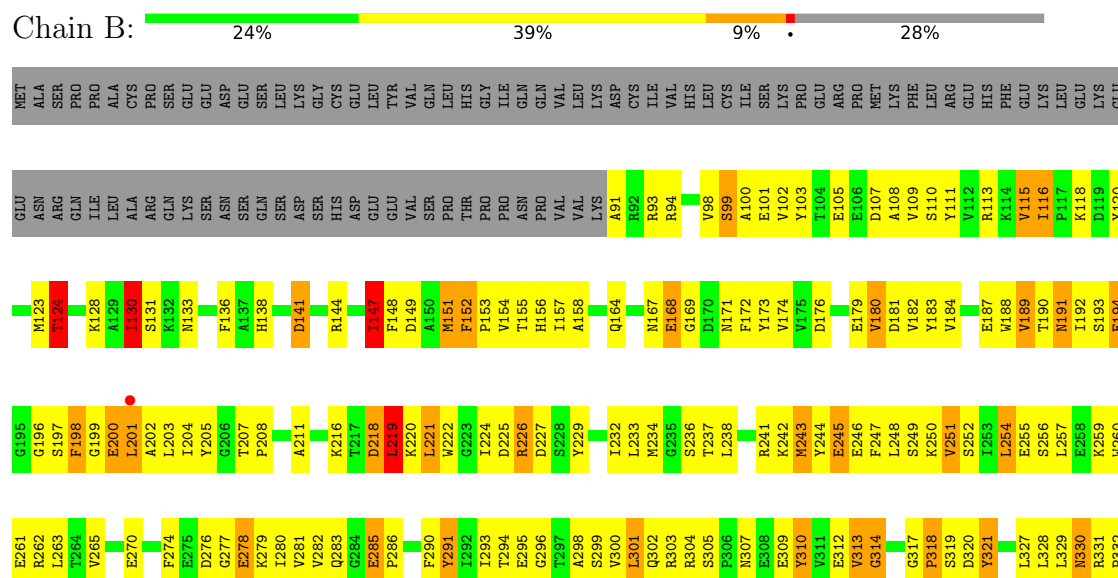
### 3 Residue-property plots

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: cAMP-dependent protein kinase catalytic subunit alpha



#### • Molecule 2: cAMP-dependent protein kinase type I-beta regulatory subunit



R333	T336	V337	V338	A339	P342	L348	D349	R350	P351	R352	F353	E354	R355	V356	L357	C358	P359	C360	S361	C362	I363	L364	K365	R366	ASN	ILE	GLN	ARG	TYR	ASN	SER	PHE	ILE	SER	LEU	THR	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.50Å 103.50Å 313.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.37 – 3.70 46.37 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.37-3.70) 99.0 (46.37-3.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.40 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, $R_{free}$	0.231 , 0.293 0.219 , 0.279	Depositor DCC
$R_{free}$ test set	539 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.3	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, SEP

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	0/2779	1.38	37/3755 (1.0%)
2	B	0.79	0/2210	1.50	40/2990 (1.3%)
All	All	0.77	0/4989	1.44	77/6745 (1.1%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLU	CA-C-N	-12.47	105.21	119.05
1	A	140	GLU	C-N-CA	-12.47	105.21	119.05
2	B	133	ASN	N-CA-C	-10.31	90.44	108.69
2	B	285	GLU	CA-C-N	-10.18	110.34	120.31
2	B	285	GLU	C-N-CA	-10.18	110.34	120.31
2	B	304	ARG	N-CA-C	-10.00	100.49	112.89
2	B	152	PHE	CA-C-N	9.84	130.62	119.99
2	B	152	PHE	C-N-CA	9.84	130.62	119.99
1	A	77	GLN	N-CA-C	9.49	122.83	111.82
2	B	198	PHE	N-CA-C	8.81	122.27	108.79
1	A	89	LEU	N-CA-C	8.73	120.80	111.28
1	A	94	ILE	N-CA-C	8.35	120.10	111.00
2	B	243	MET	N-CA-C	8.11	119.74	111.07
2	B	270	GLU	CA-C-N	8.11	127.86	119.76
2	B	270	GLU	C-N-CA	8.11	127.86	119.76
2	B	321	TYR	N-CA-C	7.94	122.41	109.94
1	A	242	GLN	CA-C-N	7.58	127.96	119.32
1	A	242	GLN	C-N-CA	7.58	127.96	119.32
2	B	105	GLU	N-CA-C	7.57	119.53	111.28
1	A	73	ILE	N-CA-C	7.55	119.01	107.99
2	B	244	TYR	N-CA-C	7.35	119.29	111.28
2	B	124	THR	N-CA-C	-7.32	103.24	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	N-CA-C	-7.16	99.86	110.46
1	A	330	TYR	N-CA-C	-7.13	98.59	109.85
1	A	236	PRO	CA-C-N	7.12	126.74	119.19
1	A	236	PRO	C-N-CA	7.12	126.74	119.19
2	B	296	GLY	N-CA-C	-6.87	104.60	112.29
1	A	142	HIS	N-CA-CB	6.86	121.78	110.39
2	B	358	GLY	CA-C-N	6.83	128.23	120.85
2	B	358	GLY	C-N-CA	6.83	128.23	120.85
1	A	108	PHE	N-CA-C	6.75	119.43	109.24
2	B	115	VAL	N-CA-C	6.58	117.51	107.77
2	B	254	LEU	N-CA-C	6.58	121.01	112.92
2	B	116	ILE	CA-C-N	6.56	126.78	119.90
2	B	116	ILE	C-N-CA	6.56	126.78	119.90
1	A	156	TYR	N-CA-C	6.48	118.04	110.97
1	A	136	GLY	N-CA-C	6.48	121.37	113.79
1	A	161	ASP	N-CA-C	6.44	120.53	111.52
2	B	232	ILE	N-CA-C	6.39	116.56	110.42
2	B	168	GLU	CA-C-N	-6.32	115.55	121.62
2	B	168	GLU	C-N-CA	-6.32	115.55	121.62
2	B	314	GLY	N-CA-C	-6.17	102.09	111.10
1	A	26	PHE	N-CA-C	6.02	117.51	111.07
1	A	269	LEU	N-CA-C	6.00	117.89	111.36
2	B	330	ASN	N-CA-C	5.99	119.42	107.62
2	B	348	LEU	N-CA-C	-5.98	99.96	109.23
1	A	113	ASN	N-CA-C	5.96	117.78	111.28
1	A	185	PHE	N-CA-C	5.90	119.54	112.93
1	A	281	PHE	N-CA-C	5.89	118.77	110.23
2	B	147	ILE	N-CA-CB	5.86	119.37	110.58
1	A	222	TRP	N-CA-C	-5.78	104.89	111.07
2	B	236	SER	N-CA-C	5.76	117.23	111.07
2	B	219	LEU	N-CA-C	5.75	117.22	108.07
2	B	218	ASP	N-CA-C	-5.59	103.25	110.19
2	B	169	GLY	CA-C-O	5.56	125.26	120.76
2	B	317	GLY	N-CA-C	-5.50	101.13	112.34
1	A	119	VAL	N-CA-C	5.47	115.66	107.51
1	A	194	ARG	N-CA-C	-5.42	101.04	109.72
2	B	151	MET	N-CA-C	5.36	118.00	110.23
1	A	224	LEU	N-CA-C	5.35	117.11	111.28
1	A	340	ASN	N-CA-C	5.33	118.92	109.96
2	B	277	GLY	N-CA-C	-5.32	107.45	115.32
2	B	141	ASP	N-CA-C	5.27	117.02	111.28
1	A	277	LEU	N-CA-C	5.26	118.95	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	VAL	N-CA-C	-5.25	105.27	110.62
1	A	96	GLN	N-CA-CB	5.21	118.24	110.22
1	A	210	ILE	N-CA-C	-5.21	105.31	110.62
2	B	227	ASP	N-CA-C	5.17	116.92	111.28
1	A	274	GLN	CA-C-N	5.17	128.78	120.30
1	A	274	GLN	C-N-CA	5.17	128.78	120.30
1	A	19	LEU	N-CA-C	-5.13	105.81	111.71
2	B	226	ARG	CA-CB-CG	5.10	124.29	114.10
2	B	285	GLU	N-CA-C	-5.09	102.87	110.20
1	A	302	TRP	N-CA-C	5.03	117.42	111.33
1	A	193	GLY	N-CA-C	5.02	116.72	110.29
1	A	295	LYS	N-CA-C	5.01	117.40	111.33
2	B	130	ILE	N-CA-C	-5.01	107.06	113.22

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2731	0	2654	295	0
2	B	2171	0	2148	256	0
All	All	4902	0	4802	532	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 55.

All (532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLN:HG3	1:A:342:LYS:NZ	1.63	1.12
1:A:93:ARG:HA	1:A:96:GLN:HE22	1.02	1.12
2:B:188:TRP:CH2	2:B:191:ASN:HB3	1.84	1.10
2:B:188:TRP:HH2	2:B:191:ASN:HB3	1.11	1.10
1:A:77:GLN:CG	1:A:342:LYS:HD3	1.80	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB3	1:A:78:LYS:HG2	1.26	1.09
1:A:39:GLN:HE22	1:A:42:GLN:CD	1.61	1.07
1:A:77:GLN:HG2	1:A:342:LYS:HD3	1.08	1.07
1:A:75:ASP:H	1:A:78:LYS:HE2	1.20	1.06
2:B:359:PRO:O	2:B:363:ILE:HD13	1.55	1.06
2:B:144:ARG:HB2	2:B:148:PHE:HE2	1.22	1.04
1:A:39:GLN:NE2	1:A:42:GLN:HG3	1.74	1.03
1:A:93:ARG:CA	1:A:96:GLN:HE22	1.72	1.02
1:A:142:HIS:HB3	1:A:313:PRO:HG2	1.37	1.02
1:A:124:ALA:O	1:A:326:ASN:ND2	1.91	1.01
2:B:241:ARG:O	2:B:245:GLU:OE2	1.79	1.01
1:A:243:PRO:O	1:A:246:ILE:HG13	1.61	1.00
1:A:45:ARG:NH1	1:A:335:ILE:HG22	1.78	0.98
1:A:93:ARG:HA	1:A:96:GLN:NE2	1.80	0.97
1:A:210:ILE:HD11	1:A:251:VAL:HG23	1.46	0.94
1:A:73:ILE:HD11	1:A:115:ASN:ND2	1.85	0.92
2:B:280:ILE:HD12	2:B:281:VAL:HG13	1.49	0.92
2:B:293:ILE:HG22	2:B:320:ASP:O	1.69	0.92
1:A:48:THR:HG21	1:A:56:ARG:HH21	1.34	0.92
2:B:233:LEU:O	2:B:237:THR:HG23	1.69	0.91
1:A:142:HIS:CB	1:A:313:PRO:HG2	2.01	0.91
1:A:75:ASP:N	1:A:78:LYS:HE2	1.87	0.90
2:B:301:LEU:C	2:B:301:LEU:HD12	1.98	0.90
2:B:219:LEU:HD22	2:B:221:LEU:HD23	1.55	0.88
1:A:39:GLN:HE22	1:A:42:GLN:CG	1.86	0.88
2:B:101:GLU:CD	2:B:102:VAL:H	1.82	0.87
1:A:138:PHE:HB3	1:A:142:HIS:CE1	2.10	0.87
2:B:278:GLU:HA	2:B:278:GLU:OE1	1.75	0.87
1:A:77:GLN:HG3	1:A:342:LYS:HZ3	1.35	0.86
1:A:80:VAL:HA	1:A:85:ILE:HD11	1.54	0.86
1:A:75:ASP:HB3	1:A:78:LYS:CG	2.05	0.86
1:A:77:GLN:HG3	1:A:342:LYS:HZ2	1.40	0.86
1:A:246:ILE:HD11	1:A:247:TYR:CE1	2.11	0.86
1:A:54:PHE:CD1	1:A:74:LEU:HD21	2.11	0.85
1:A:75:ASP:H	1:A:78:LYS:CE	1.89	0.85
1:A:148:ALA:O	1:A:152:LEU:HD12	1.75	0.85
1:A:169:PRO:HG2	1:A:230:GLU:OE2	1.75	0.85
1:A:28:LYS:HG3	1:A:29:LYS:N	1.88	0.85
1:A:73:ILE:HD11	1:A:115:ASN:HD22	1.39	0.85
2:B:349:ASP:OD2	2:B:351:PRO:HG2	1.76	0.85
1:A:154:PHE:HA	1:A:157:LEU:CD1	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:HD1	1:A:74:LEU:CD2	1.89	0.84
2:B:188:TRP:HH2	2:B:191:ASN:CB	1.90	0.84
1:A:176:GLN:HA	1:A:318:PHE:HE2	1.42	0.84
1:A:45:ARG:NH1	1:A:335:ILE:CG2	2.41	0.83
2:B:203:LEU:O	2:B:226:ARG:HB2	1.78	0.82
2:B:301:LEU:HD13	2:B:310:TYR:HB2	1.62	0.82
1:A:48:THR:HG21	1:A:56:ARG:NH2	1.93	0.82
1:A:54:PHE:CD1	1:A:74:LEU:CD2	2.63	0.82
1:A:194:ARG:NH2	1:A:213:LYS:O	2.14	0.81
2:B:245:GLU:CD	2:B:245:GLU:H	1.87	0.81
1:A:142:HIS:HB3	1:A:313:PRO:CG	2.10	0.81
2:B:144:ARG:O	2:B:148:PHE:HD2	1.62	0.81
2:B:329:LEU:CD1	2:B:331:ARG:HG3	2.11	0.80
1:A:51:THR:OG1	2:B:94:ARG:NH2	2.13	0.80
1:A:211:LEU:HD22	2:B:138:HIS:CD2	2.16	0.80
2:B:219:LEU:HD22	2:B:221:LEU:CD2	2.11	0.80
2:B:290:PHE:HB2	2:B:327:LEU:HG	1.63	0.80
1:A:75:ASP:CB	1:A:78:LYS:HE2	2.12	0.80
1:A:176:GLN:HG2	1:A:318:PHE:CE2	2.17	0.80
2:B:144:ARG:O	2:B:148:PHE:CD2	2.34	0.79
2:B:118:LYS:HB2	2:B:123:MET:HE3	1.63	0.79
1:A:96:GLN:OE1	1:A:96:GLN:N	2.14	0.79
2:B:280:ILE:CD1	2:B:281:VAL:HG13	2.12	0.79
2:B:164:GLN:HB3	2:B:167:ASN:OD1	1.83	0.79
2:B:281:VAL:HG22	2:B:337:VAL:HG22	1.64	0.79
1:A:39:GLN:NE2	1:A:42:GLN:CG	2.42	0.78
1:A:45:ARG:HH12	1:A:335:ILE:HG22	1.46	0.78
1:A:176:GLN:HA	1:A:318:PHE:CE2	2.17	0.78
1:A:54:PHE:O	1:A:78:LYS:HD2	1.83	0.78
1:A:77:GLN:HG2	1:A:342:LYS:CD	2.03	0.78
1:A:79:VAL:HG12	1:A:85:ILE:HD13	1.65	0.77
2:B:282:VAL:HA	2:B:336:THR:HG23	1.66	0.77
1:A:73:ILE:CD1	1:A:115:ASN:HD22	1.98	0.77
2:B:183:TYR:CE1	2:B:188:TRP:HE3	2.02	0.76
1:A:274:GLN:HE22	1:A:279:LYS:HB3	1.50	0.76
2:B:144:ARG:HB2	2:B:148:PHE:CE2	2.14	0.75
2:B:200:GLU:CD	2:B:200:GLU:H	1.94	0.75
2:B:194:GLU:N	2:B:194:GLU:OE1	2.19	0.75
2:B:128:LYS:O	2:B:131:SER:HB3	1.87	0.75
1:A:210:ILE:HD11	1:A:251:VAL:CG2	2.15	0.75
1:A:45:ARG:HH12	1:A:335:ILE:CG2	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:234:MET:HE1	1.67	0.75
1:A:47:LYS:NZ	1:A:329:ASP:HB3	2.01	0.74
2:B:171:ASN:HD22	2:B:225:ASP:HA	1.52	0.74
1:A:145:PHE:CE2	1:A:313:PRO:HD3	2.22	0.74
2:B:280:ILE:HD12	2:B:281:VAL:H	1.52	0.74
2:B:310:TYR:N	2:B:310:TYR:CD2	2.53	0.74
1:A:189:LYS:NZ	1:A:197:TPO:O3P	2.21	0.74
1:A:103:LEU:HA	1:A:182:VAL:HG12	1.70	0.73
1:A:77:GLN:OE1	1:A:343:CYS:SG	2.46	0.73
1:A:316:PRO:HG2	1:A:318:PHE:CZ	2.23	0.73
2:B:280:ILE:HD12	2:B:281:VAL:N	2.03	0.73
2:B:245:GLU:HB2	2:B:262:ARG:HD3	1.68	0.73
2:B:293:ILE:HG23	2:B:318:PRO:HA	1.70	0.73
1:A:47:LYS:HZ1	1:A:329:ASP:HB3	1.53	0.73
2:B:101:GLU:CD	2:B:102:VAL:N	2.45	0.73
2:B:281:VAL:HG22	2:B:337:VAL:CG2	2.19	0.73
1:A:54:PHE:CE1	1:A:74:LEU:HD21	2.24	0.72
1:A:54:PHE:O	1:A:78:LYS:CD	2.37	0.72
1:A:338:SEP:O2P	1:A:340:ASN:ND2	2.23	0.72
1:A:32:THR:HG23	1:A:32:THR:O	1.89	0.72
2:B:245:GLU:CD	2:B:245:GLU:N	2.46	0.72
1:A:319:LYS:O	1:A:323:ASP:CG	2.33	0.72
1:A:54:PHE:HD1	1:A:74:LEU:HD23	1.55	0.72
1:A:59:LEU:HD23	1:A:60:VAL:N	2.05	0.71
2:B:245:GLU:N	2:B:245:GLU:OE1	2.21	0.71
1:A:213:LYS:NZ	2:B:237:THR:HG22	2.05	0.71
2:B:203:LEU:HD21	2:B:224:ILE:HG23	1.73	0.71
1:A:108:PHE:HB2	1:A:119:VAL:HG13	1.70	0.71
1:A:77:GLN:CG	1:A:342:LYS:CD	2.64	0.71
2:B:282:VAL:HB	2:B:285:GLU:HG2	1.71	0.71
2:B:302:GLN:C	2:B:310:TYR:HB3	2.14	0.71
1:A:209:ILE:HG12	1:A:215:TYR:CD2	2.26	0.71
2:B:295:GLU:HB2	2:B:344:LYS:HB2	1.73	0.71
1:A:154:PHE:HA	1:A:157:LEU:HD11	1.73	0.70
2:B:259:LYS:O	2:B:263:LEU:HD13	1.91	0.70
1:A:246:ILE:HD11	1:A:247:TYR:CD1	2.25	0.70
2:B:251:VAL:HG23	2:B:321:TYR:CD2	2.26	0.70
2:B:301:LEU:C	2:B:301:LEU:CD1	2.64	0.70
2:B:301:LEU:HD12	2:B:301:LEU:O	1.92	0.70
2:B:361:SER:O	2:B:365:LYS:HD3	1.91	0.70
2:B:303:ARG:CB	2:B:310:TYR:CD1	2.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB3	1:A:78:LYS:HE2	1.74	0.69
2:B:247:PHE:CE1	2:B:319:SER:HA	2.27	0.69
2:B:329:LEU:C	2:B:329:LEU:HD12	2.17	0.69
1:A:100:PHE:HB3	1:A:103:LEU:HD21	1.75	0.69
2:B:156:HIS:HB2	2:B:219:LEU:HD11	1.75	0.69
2:B:286:PRO:HA	2:B:332:PRO:HA	1.75	0.68
1:A:29:LYS:HD3	1:A:96:GLN:O	1.94	0.68
2:B:168:GLU:OE1	2:B:168:GLU:HA	1.95	0.67
1:A:39:GLN:HE21	1:A:42:GLN:HG3	1.52	0.67
1:A:246:ILE:CD1	1:A:247:TYR:CD1	2.77	0.67
1:A:59:LEU:HD23	1:A:59:LEU:C	2.20	0.67
2:B:276:ASP:HB2	2:B:342:PRO:HD3	1.76	0.67
2:B:329:LEU:HD13	2:B:331:ARG:HG3	1.76	0.67
1:A:194:ARG:HD2	2:B:241:ARG:NH1	2.10	0.66
2:B:301:LEU:HD11	2:B:310:TYR:CG	2.30	0.66
1:A:110:PHE:CE1	1:A:117:TYR:HB2	2.30	0.66
2:B:303:ARG:CA	2:B:310:TYR:HB3	2.26	0.66
2:B:130:ILE:HD12	2:B:130:ILE:C	2.19	0.66
1:A:267:ASP:HA	1:A:270:ARG:NH2	2.11	0.66
2:B:202:ALA:O	2:B:226:ARG:HB3	1.96	0.66
2:B:188:TRP:CZ2	2:B:191:ASN:HB3	2.31	0.65
1:A:62:HIS:CE1	1:A:65:SER:H	2.13	0.65
2:B:183:TYR:HE1	2:B:188:TRP:HE3	1.44	0.65
2:B:303:ARG:HA	2:B:310:TYR:HB3	1.77	0.65
1:A:44:ASP:O	1:A:44:ASP:OD1	2.14	0.65
2:B:279:LYS:HB2	2:B:338:VAL:HG23	1.78	0.65
1:A:44:ASP:OD1	1:A:61:LYS:HB3	1.96	0.65
2:B:193:SER:HB2	2:B:194:GLU:OE1	1.97	0.65
2:B:242:LYS:C	2:B:245:GLU:OE2	2.39	0.65
2:B:282:VAL:HB	2:B:285:GLU:CG	2.27	0.65
1:A:344:GLY:O	1:A:348:THR:HG23	1.98	0.64
1:A:29:LYS:HB2	1:A:97:ALA:HA	1.78	0.64
1:A:103:LEU:HD12	1:A:103:LEU:O	1.97	0.64
1:A:274:GLN:NE2	1:A:279:LYS:CB	2.61	0.64
2:B:363:ILE:HA	2:B:366:ARG:HH21	1.63	0.64
2:B:200:GLU:OE1	2:B:200:GLU:N	2.27	0.63
2:B:147:ILE:HD12	2:B:147:ILE:C	2.23	0.63
2:B:293:ILE:HD11	2:B:343:LEU:HD11	1.78	0.63
2:B:181:ASP:HB3	2:B:188:TRP:HZ3	1.61	0.63
2:B:219:LEU:HD12	2:B:219:LEU:N	2.14	0.63
2:B:254:LEU:O	2:B:257:LEU:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:SER:OG	2:B:307:ASN:OD1	2.16	0.63
2:B:247:PHE:CD1	2:B:319:SER:HA	2.33	0.63
2:B:184:VAL:O	2:B:187:GLU:OE1	2.17	0.62
1:A:145:PHE:CD2	1:A:313:PRO:HD3	2.33	0.62
1:A:207:PRO:O	1:A:210:ILE:HG12	1.99	0.62
2:B:243:MET:HG3	2:B:247:PHE:CE2	2.34	0.62
2:B:328:LEU:HD11	2:B:329:LEU:HD23	1.81	0.62
1:A:75:ASP:CA	1:A:78:LYS:HE2	2.29	0.62
2:B:118:LYS:HB2	2:B:123:MET:CE	2.30	0.62
1:A:61:LYS:HD2	1:A:67:ASN:O	1.98	0.62
2:B:130:ILE:HD13	2:B:136:PHE:CB	2.29	0.62
2:B:180:VAL:HG12	2:B:192:ILE:HG23	1.82	0.62
2:B:298:ALA:HB1	2:B:338:VAL:O	1.99	0.61
2:B:301:LEU:CD1	2:B:310:TYR:CG	2.83	0.61
1:A:117:TYR:OH	1:A:335:ILE:HD11	2.00	0.61
1:A:77:GLN:CG	1:A:342:LYS:NZ	2.54	0.61
1:A:123:VAL:HG13	1:A:123:VAL:O	1.99	0.61
2:B:248:LEU:HD13	2:B:265:VAL:HG13	1.81	0.61
2:B:245:GLU:OE1	2:B:246:GLU:N	2.31	0.61
2:B:254:LEU:O	2:B:257:LEU:CB	2.48	0.61
2:B:303:ARG:N	2:B:310:TYR:HB3	2.14	0.60
1:A:106:LEU:HD13	1:A:120:MET:HG2	1.84	0.60
2:B:359:PRO:HG2	2:B:362:GLU:HG2	1.82	0.60
1:A:76:LYS:O	1:A:80:VAL:HG23	2.02	0.60
2:B:174:VAL:O	2:B:221:LEU:HB2	2.01	0.60
1:A:166:ASP:OD1	1:A:168:LYS:HE2	2.01	0.59
1:A:198:LEU:HD22	2:B:205:TYR:HD2	1.65	0.59
2:B:98:VAL:HG12	2:B:99:SER:N	2.17	0.59
2:B:310:TYR:H	2:B:310:TYR:HD2	1.50	0.59
2:B:354:GLU:HA	2:B:358:GLY:O	2.02	0.59
1:A:44:ASP:CG	1:A:61:LYS:HB3	2.28	0.59
1:A:61:LYS:HE3	1:A:66:GLY:O	2.01	0.59
1:A:62:HIS:CE1	1:A:64:GLU:HB2	2.37	0.59
2:B:274:PHE:CZ	2:B:280:ILE:HG21	2.36	0.59
1:A:92:LYS:HD3	1:A:92:LYS:C	2.27	0.59
1:A:44:ASP:OD1	1:A:44:ASP:C	2.45	0.59
2:B:242:LYS:O	2:B:245:GLU:CD	2.45	0.59
2:B:243:MET:O	2:B:247:PHE:CD2	2.56	0.59
2:B:301:LEU:HD11	2:B:310:TYR:CD1	2.38	0.59
1:A:176:GLN:HG2	1:A:318:PHE:HE2	1.65	0.59
2:B:130:ILE:HD13	2:B:136:PHE:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HZ1	2:B:237:THR:HG22	1.67	0.59
1:A:225:GLY:HA2	1:A:272:LEU:HD23	1.84	0.59
1:A:75:ASP:CB	1:A:78:LYS:HG2	2.18	0.58
2:B:301:LEU:HA	2:B:312:GLU:HA	1.84	0.58
1:A:54:PHE:O	1:A:78:LYS:CE	2.50	0.58
2:B:299:SER:OG	2:B:338:VAL:HG12	2.02	0.58
2:B:329:LEU:HD12	2:B:330:ASN:N	2.19	0.58
1:A:225:GLY:CA	1:A:272:LEU:HD23	2.34	0.58
2:B:290:PHE:CB	2:B:327:LEU:HG	2.31	0.58
1:A:226:VAL:HG23	1:A:237:PRO:HD2	1.85	0.58
1:A:57:VAL:HG22	1:A:72:LYS:HG3	1.84	0.58
2:B:290:PHE:HB3	2:B:327:LEU:HD21	1.86	0.58
1:A:230:GLU:HA	1:A:235:TYR:O	2.04	0.58
1:A:246:ILE:HD12	1:A:247:TYR:N	2.18	0.58
2:B:243:MET:HG3	2:B:247:PHE:HE2	1.68	0.58
2:B:293:ILE:CD1	2:B:343:LEU:HD11	2.34	0.58
1:A:345:LYS:HA	1:A:348:THR:HG23	1.85	0.58
2:B:327:LEU:O	2:B:350:ARG:HG3	2.03	0.58
1:A:94:ILE:O	1:A:98:VAL:HG12	2.03	0.58
1:A:176:GLN:HG2	1:A:318:PHE:CD2	2.39	0.58
2:B:182:VAL:HB	2:B:190:THR:O	2.04	0.57
2:B:278:GLU:H	2:B:339:ALA:HB3	1.69	0.57
1:A:274:GLN:NE2	1:A:279:LYS:HB3	2.16	0.57
2:B:120:TYR:O	2:B:124:THR:HG23	2.04	0.57
2:B:283:GLN:OE1	2:B:333:ARG:O	2.22	0.57
2:B:328:LEU:CD1	2:B:329:LEU:HD23	2.35	0.56
1:A:123:VAL:O	1:A:123:VAL:CG1	2.53	0.56
2:B:251:VAL:HG11	2:B:254:LEU:HD12	1.87	0.56
2:B:260:TRP:CE3	2:B:261:GLU:HG3	2.41	0.56
2:B:302:GLN:O	2:B:310:TYR:HB3	2.04	0.56
1:A:176:GLN:CG	1:A:318:PHE:CE2	2.88	0.56
1:A:28:LYS:CG	1:A:29:LYS:N	2.63	0.56
1:A:157:LEU:O	1:A:160:LEU:HD12	2.05	0.56
1:A:284:LEU:N	1:A:284:LEU:HD13	2.21	0.56
1:A:128:MET:HE2	1:A:169:PRO:HA	1.88	0.56
2:B:191:ASN:OD1	2:B:191:ASN:C	2.49	0.56
2:B:313:VAL:CG1	2:B:314:GLY:N	2.68	0.56
1:A:244:ILE:O	1:A:248:GLU:HG3	2.06	0.55
1:A:75:ASP:HB3	1:A:78:LYS:CE	2.37	0.55
1:A:98:VAL:CG2	1:A:99:ASN:N	2.69	0.55
1:A:56:ARG:H	1:A:73:ILE:HG23	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HD11	1:A:138:PHE:CE1	2.42	0.55
2:B:173:TYR:HB3	2:B:221:LEU:HD13	1.89	0.55
1:A:213:LYS:NZ	2:B:237:THR:CG2	2.70	0.55
2:B:283:GLN:OE1	2:B:283:GLN:HA	2.05	0.55
1:A:80:VAL:HG21	1:A:343:CYS:SG	2.46	0.55
1:A:213:LYS:HG3	2:B:237:THR:HG21	1.87	0.55
2:B:188:TRP:CH2	2:B:191:ASN:CB	2.73	0.55
1:A:100:PHE:H	1:A:103:LEU:HD11	1.73	0.54
2:B:157:ILE:HG22	2:B:158:ALA:N	2.22	0.54
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.21	0.54
2:B:181:ASP:CB	2:B:188:TRP:HZ3	2.19	0.54
2:B:184:VAL:HG22	2:B:211:ALA:HB2	1.89	0.54
1:A:57:VAL:HG22	1:A:72:LYS:CG	2.36	0.54
1:A:126:GLY:HA2	1:A:327:PHE:CE1	2.43	0.54
1:A:128:MET:CE	1:A:169:PRO:HA	2.37	0.54
2:B:189:VAL:HG13	2:B:190:THR:H	1.72	0.54
1:A:123:VAL:CG1	1:A:173:LEU:HD13	2.38	0.54
1:A:55:GLY:HA3	1:A:73:ILE:O	2.08	0.54
1:A:335:ILE:HG12	1:A:336:ARG:N	2.23	0.54
2:B:285:GLU:O	2:B:332:PRO:HA	2.08	0.53
1:A:338:SEP:P	1:A:340:ASN:HD22	2.31	0.53
2:B:172:PHE:CE1	2:B:197:SER:HB2	2.43	0.53
1:A:54:PHE:CD1	1:A:55:GLY:N	2.77	0.53
2:B:192:ILE:HD11	2:B:197:SER:N	2.24	0.53
2:B:293:ILE:HD11	2:B:343:LEU:CD1	2.37	0.53
2:B:257:LEU:CD2	2:B:262:ARG:HB2	2.39	0.53
1:A:51:THR:HG22	1:A:56:ARG:CZ	2.38	0.53
1:A:40:LEU:HD12	1:A:117:TYR:CZ	2.43	0.53
2:B:109:VAL:HG23	2:B:110:SER:N	2.23	0.53
2:B:252:SER:O	2:B:255:GLU:CD	2.52	0.53
1:A:75:ASP:HB3	1:A:78:LYS:CD	2.39	0.53
1:A:100:PHE:HB3	1:A:103:LEU:CD2	2.39	0.53
2:B:147:ILE:HD12	2:B:147:ILE:O	2.08	0.53
1:A:95:LEU:HB3	1:A:106:LEU:HB2	1.91	0.52
1:A:135:ILE:HD11	1:A:138:PHE:HE1	1.74	0.52
2:B:107:ASP:O	2:B:111:TYR:HB2	2.09	0.52
1:A:91:GLU:HG2	1:A:118:MET:HE1	1.92	0.52
1:A:199:CYS:HA	2:B:98:VAL:O	2.10	0.52
2:B:171:ASN:HD21	2:B:225:ASP:HB3	1.75	0.52
1:A:92:LYS:C	1:A:92:LYS:CD	2.83	0.52
1:A:139:SER:H	1:A:142:HIS:HE1	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLY:HA2	1:A:78:LYS:NZ	2.24	0.52
1:A:102:PHE:O	1:A:181:GLN:HA	2.10	0.52
1:A:139:SER:H	1:A:142:HIS:CE1	2.28	0.52
1:A:157:LEU:O	1:A:160:LEU:CD1	2.57	0.52
2:B:245:GLU:HB2	2:B:262:ARG:CD	2.38	0.52
2:B:327:LEU:HA	2:B:350:ARG:HB2	1.91	0.52
1:A:31:GLU:C	1:A:33:PRO:HD3	2.34	0.52
1:A:39:GLN:NE2	1:A:42:GLN:CD	2.46	0.52
1:A:100:PHE:CG	1:A:101:PRO:HD2	2.45	0.52
2:B:108:ALA:HB2	2:B:234:MET:HE3	1.90	0.52
1:A:246:ILE:HD12	1:A:247:TYR:CD1	2.45	0.51
2:B:251:VAL:HG12	2:B:254:LEU:HB2	1.91	0.51
1:A:223:ALA:O	1:A:226:VAL:HG13	2.11	0.51
2:B:156:HIS:HB2	2:B:219:LEU:CD1	2.39	0.51
1:A:131:HIS:ND1	1:A:134:ARG:NH1	2.56	0.51
1:A:160:LEU:HD11	1:A:162:LEU:HB2	1.93	0.51
2:B:301:LEU:HD13	2:B:310:TYR:CB	2.37	0.51
2:B:363:ILE:O	2:B:366:ARG:HG2	2.11	0.51
1:A:274:GLN:HE22	1:A:279:LYS:CB	2.17	0.51
2:B:152:PHE:HB2	2:B:153:PRO:HD2	1.92	0.51
1:A:138:PHE:CB	1:A:142:HIS:CE1	2.88	0.51
2:B:179:GLU:HG2	2:B:180:VAL:N	2.26	0.51
1:A:93:ARG:C	1:A:96:GLN:HE22	2.19	0.51
1:A:80:VAL:CA	1:A:85:ILE:HD11	2.35	0.50
1:A:123:VAL:HG11	1:A:173:LEU:HD13	1.91	0.50
1:A:29:LYS:CB	1:A:97:ALA:HA	2.41	0.50
1:A:100:PHE:CE2	1:A:153:THR:HA	2.46	0.50
1:A:145:PHE:CD2	1:A:313:PRO:CD	2.94	0.50
2:B:113:ARG:HH12	2:B:149:ASP:CB	2.25	0.50
2:B:184:VAL:HG23	2:B:189:VAL:HG11	1.93	0.50
2:B:350:ARG:N	2:B:351:PRO:HD2	2.26	0.50
2:B:116:ILE:HD12	2:B:151:MET:O	2.12	0.50
1:A:54:PHE:CG	1:A:55:GLY:N	2.79	0.50
1:A:194:ARG:CD	2:B:241:ARG:NH1	2.74	0.50
1:A:213:LYS:HZ3	2:B:237:THR:CG2	2.25	0.50
2:B:243:MET:O	2:B:247:PHE:HD2	1.93	0.50
1:A:146:TYR:HA	1:A:149:GLN:OE1	2.11	0.50
2:B:141:ASP:HA	2:B:144:ARG:HG2	1.94	0.50
1:A:68:HIS:O	1:A:69:TYR:CD1	2.64	0.50
2:B:91:ALA:N	2:B:93:ARG:NH2	2.60	0.50
2:B:171:ASN:HD22	2:B:225:ASP:CA	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ASN:ND2	2:B:225:ASP:HA	2.22	0.50
2:B:300:VAL:HG12	2:B:314:GLY:O	2.12	0.50
1:A:149:GLN:NE2	1:A:180:ILE:H	2.09	0.50
1:A:146:TYR:CD1	1:A:180:ILE:HD11	2.47	0.49
1:A:103:LEU:HA	1:A:182:VAL:CG1	2.41	0.49
1:A:125:GLY:C	1:A:326:ASN:ND2	2.70	0.49
1:A:49:LEU:O	1:A:330:TYR:CE2	2.66	0.49
1:A:303:ILE:HG13	1:A:304:ALA:N	2.28	0.49
1:A:176:GLN:CG	1:A:318:PHE:HE2	2.23	0.49
1:A:157:LEU:HD12	1:A:157:LEU:H	1.78	0.49
1:A:292:LYS:HD3	1:A:302:TRP:CD2	2.48	0.49
2:B:303:ARG:CB	2:B:310:TYR:HD1	2.23	0.49
1:A:92:LYS:O	1:A:96:GLN:OE1	2.31	0.49
1:A:210:ILE:CD1	1:A:251:VAL:HG23	2.30	0.49
2:B:364:LEU:HD23	2:B:365:LYS:HD2	1.95	0.49
1:A:33:PRO:HB3	1:A:96:GLN:HE21	1.77	0.48
1:A:108:PHE:HB2	1:A:119:VAL:CG1	2.42	0.48
2:B:328:LEU:HB2	2:B:360:CYS:HB2	1.94	0.48
1:A:119:VAL:O	1:A:119:VAL:HG22	2.13	0.48
1:A:163:ILE:HD12	1:A:217:LYS:HA	1.95	0.48
1:A:179:TYR:CE1	1:A:308:ARG:HA	2.48	0.48
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.78	0.48
1:A:223:ALA:O	1:A:226:VAL:CG1	2.61	0.48
2:B:183:TYR:CE1	2:B:188:TRP:CE3	2.92	0.48
2:B:313:VAL:HG12	2:B:314:GLY:N	2.27	0.48
1:A:28:LYS:O	1:A:32:THR:HG22	2.13	0.48
1:A:76:LYS:NZ	1:A:112:ASP:O	2.38	0.48
2:B:229:TYR:O	2:B:233:LEU:HD13	2.13	0.48
1:A:142:HIS:HB2	1:A:313:PRO:HG2	1.92	0.48
1:A:153:THR:O	1:A:157:LEU:HD11	2.14	0.48
1:A:187:PHE:N	1:A:187:PHE:CD1	2.80	0.48
2:B:260:TRP:CZ3	2:B:261:GLU:HG3	2.49	0.48
2:B:359:PRO:HD2	2:B:363:ILE:CD1	2.44	0.48
1:A:98:VAL:HG23	1:A:156:TYR:OH	2.14	0.48
2:B:329:LEU:HD11	2:B:331:ARG:HG3	1.91	0.48
1:A:68:HIS:NE2	1:A:321:PRO:HB3	2.27	0.47
2:B:353:PHE:C	2:B:353:PHE:CD2	2.91	0.47
1:A:33:PRO:O	1:A:35:GLN:OE1	2.31	0.47
1:A:31:GLU:O	1:A:33:PRO:HD3	2.14	0.47
1:A:39:GLN:N	1:A:39:GLN:OE1	2.47	0.47
1:A:128:MET:HE1	1:A:227:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HD12	1:A:246:ILE:C	2.40	0.47
2:B:207:THR:HB	2:B:208:PRO:HD2	1.96	0.47
2:B:293:ILE:HG23	2:B:293:ILE:O	2.13	0.47
1:A:128:MET:HE3	1:A:169:PRO:HB3	1.96	0.47
2:B:118:LYS:CB	2:B:123:MET:HE3	2.38	0.47
2:B:172:PHE:HD1	2:B:198:PHE:O	1.96	0.47
1:A:110:PHE:CZ	1:A:117:TYR:HB2	2.49	0.47
2:B:179:GLU:OE1	2:B:216:LYS:HD3	2.15	0.47
2:B:274:PHE:CE1	2:B:280:ILE:HG21	2.50	0.47
1:A:162:LEU:HD12	1:A:190:ARG:HA	1.97	0.47
2:B:205:TYR:CD1	2:B:205:TYR:C	2.93	0.47
1:A:198:LEU:HD22	2:B:205:TYR:CD2	2.47	0.46
1:A:45:ARG:NH1	1:A:335:ILE:HG21	2.26	0.46
1:A:160:LEU:HD13	1:A:162:LEU:HD13	1.96	0.46
1:A:261:PHE:CD2	1:A:265:LEU:HD23	2.50	0.46
2:B:363:ILE:HA	2:B:366:ARG:NH2	2.29	0.46
1:A:14:SER:O	1:A:18:PHE:N	2.38	0.46
2:B:98:VAL:HG12	2:B:99:SER:H	1.78	0.46
2:B:130:ILE:C	2:B:130:ILE:CD1	2.88	0.46
1:A:59:LEU:C	1:A:59:LEU:CD2	2.86	0.46
1:A:153:THR:O	1:A:157:LEU:CD1	2.64	0.46
1:A:179:TYR:CZ	1:A:308:ARG:HA	2.50	0.46
2:B:157:ILE:CG2	2:B:158:ALA:N	2.78	0.46
1:A:75:ASP:CB	1:A:78:LYS:CE	2.90	0.46
1:A:211:LEU:HD22	2:B:138:HIS:CG	2.49	0.46
2:B:279:LYS:HG3	2:B:336:THR:HG22	1.98	0.46
1:A:106:LEU:CD1	1:A:120:MET:HG2	2.45	0.46
2:B:130:ILE:O	2:B:131:SER:C	2.58	0.46
1:A:110:PHE:CE1	1:A:117:TYR:CB	2.99	0.46
2:B:249:SER:HA	2:B:262:ARG:HH21	1.79	0.46
1:A:160:LEU:HD12	1:A:160:LEU:C	2.41	0.46
1:A:187:PHE:HB3	1:A:199:CYS:SG	2.56	0.46
1:A:194:ARG:CB	2:B:241:ARG:HH12	2.29	0.46
1:A:303:ILE:HG13	1:A:304:ALA:H	1.81	0.46
2:B:357:LEU:HA	2:B:357:LEU:HD23	1.51	0.46
1:A:65:SER:CB	1:A:67:ASN:HD22	2.29	0.46
1:A:197:TPO:N	1:A:197:TPO:O2P	2.49	0.46
1:A:246:ILE:CD1	1:A:247:TYR:CE1	2.94	0.46
1:A:80:VAL:HG22	1:A:346:GLU:OE1	2.16	0.45
1:A:157:LEU:HD12	1:A:157:LEU:N	2.31	0.45
2:B:242:LYS:CA	2:B:245:GLU:OE2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LYS:HG2	2:B:337:VAL:O	2.16	0.45
2:B:305:SER:OG	2:B:307:ASN:CG	2.59	0.45
1:A:49:LEU:HD11	1:A:59:LEU:HB2	1.98	0.45
1:A:157:LEU:CD1	1:A:157:LEU:H	2.28	0.45
1:A:176:GLN:CA	1:A:318:PHE:HE2	2.20	0.45
1:A:194:ARG:HD2	2:B:241:ARG:HH12	1.81	0.45
2:B:171:ASN:ND2	2:B:225:ASP:CA	2.79	0.45
2:B:257:LEU:HD23	2:B:262:ARG:CZ	2.47	0.45
1:A:77:GLN:HG3	1:A:342:LYS:CE	2.43	0.45
1:A:80:VAL:HG22	1:A:85:ILE:HD11	1.99	0.45
1:A:172:LEU:HD22	1:A:180:ILE:HG21	1.99	0.45
1:A:32:THR:O	1:A:32:THR:CG2	2.62	0.45
1:A:44:ASP:OD2	1:A:46:ILE:HD11	2.16	0.45
2:B:181:ASP:OD2	2:B:216:LYS:HG3	2.17	0.45
2:B:274:PHE:CE1	2:B:280:ILE:CG2	3.00	0.45
1:A:91:GLU:HG3	1:A:185:PHE:HB2	1.99	0.45
2:B:109:VAL:CG2	2:B:110:SER:N	2.80	0.45
2:B:118:LYS:HE3	2:B:222:TRP:CZ3	2.52	0.45
2:B:251:VAL:HG11	2:B:254:LEU:CD1	2.47	0.45
2:B:359:PRO:O	2:B:363:ILE:CD1	2.46	0.45
1:A:240:ALA:HB3	1:A:246:ILE:HG23	1.99	0.45
2:B:201:LEU:H	2:B:201:LEU:HG	1.24	0.45
2:B:262:ARG:HA	2:B:265:VAL:HG12	1.98	0.45
1:A:112:ASP:OD2	1:A:117:TYR:HE2	2.01	0.44
2:B:183:TYR:HE1	2:B:188:TRP:CE3	2.29	0.44
1:A:54:PHE:CZ	1:A:72:LYS:HE2	2.51	0.44
2:B:172:PHE:CE1	2:B:200:GLU:HG3	2.53	0.44
1:A:229:TYR:CD1	1:A:229:TYR:C	2.95	0.44
2:B:176:ASP:HB2	2:B:222:TRP:CD1	2.52	0.44
2:B:327:LEU:O	2:B:350:ARG:CG	2.66	0.44
2:B:359:PRO:CG	2:B:362:GLU:HG2	2.48	0.44
1:A:274:GLN:NE2	1:A:279:LYS:HB2	2.33	0.44
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.58	0.44
1:A:330:TYR:HE1	2:B:94:ARG:CZ	2.30	0.44
2:B:242:LYS:O	2:B:245:GLU:OE1	2.35	0.44
2:B:243:MET:HE3	2:B:243:MET:HB2	1.70	0.44
1:A:46:ILE:HB	1:A:59:LEU:HD22	1.98	0.44
1:A:39:GLN:HE22	1:A:42:GLN:NE2	2.10	0.44
2:B:302:GLN:C	2:B:310:TYR:CB	2.89	0.44
1:A:125:GLY:CA	1:A:326:ASN:ND2	2.81	0.44
2:B:157:ILE:N	2:B:157:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:HE22	1:A:179:TYR:HA	1.83	0.43
2:B:101:GLU:HG3	2:B:102:VAL:O	2.18	0.43
2:B:130:ILE:HD12	2:B:131:SER:N	2.33	0.43
1:A:54:PHE:C	1:A:78:LYS:HD2	2.41	0.43
1:A:131:HIS:CE1	1:A:134:ARG:HH11	2.35	0.43
1:A:142:HIS:HB3	1:A:313:PRO:CB	2.47	0.43
2:B:291:TYR:N	2:B:291:TYR:CD2	2.86	0.43
1:A:39:GLN:N	1:A:39:GLN:CD	2.77	0.43
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.82	0.43
1:A:54:PHE:CD1	1:A:74:LEU:HD23	2.41	0.43
1:A:54:PHE:CE1	1:A:72:LYS:HE2	2.53	0.43
2:B:147:ILE:HG13	2:B:148:PHE:N	2.33	0.43
2:B:199:GLY:O	2:B:202:ALA:HB3	2.18	0.43
2:B:257:LEU:HD21	2:B:262:ARG:HB2	2.01	0.43
1:A:205:LEU:O	1:A:250:ILE:HD13	2.19	0.43
1:A:163:ILE:CD1	1:A:217:LYS:HA	2.48	0.43
1:A:283:ASN:C	1:A:284:LEU:HD13	2.43	0.43
2:B:262:ARG:O	2:B:265:VAL:HG12	2.18	0.43
2:B:250:LYS:HA	2:B:250:LYS:HD2	1.70	0.43
2:B:290:PHE:CE1	2:B:321:TYR:HB2	2.54	0.43
1:A:100:PHE:CD1	1:A:101:PRO:HD2	2.54	0.42
1:A:204:TYR:HA	1:A:226:VAL:HG11	2.01	0.42
2:B:109:VAL:C	2:B:111:TYR:N	2.76	0.42
2:B:278:GLU:O	2:B:339:ALA:N	2.35	0.42
1:A:102:PHE:CD2	1:A:149:GLN:HB3	2.54	0.42
1:A:113:ASN:ND2	1:A:339:ILE:O	2.52	0.42
1:A:164:TYR:CE1	1:A:185:PHE:CE1	3.07	0.42
1:A:251:VAL:O	1:A:252:SER:C	2.61	0.42
1:A:295:LYS:HE2	1:A:295:LYS:HB3	1.82	0.42
1:A:123:VAL:HG11	1:A:173:LEU:HB3	2.00	0.42
1:A:145:PHE:CE2	1:A:313:PRO:CD	2.99	0.42
1:A:51:THR:HG22	1:A:56:ARG:NH1	2.34	0.42
2:B:187:GLU:O	2:B:187:GLU:HG2	2.17	0.42
2:B:279:LYS:HA	2:B:338:VAL:HA	2.02	0.42
1:A:307:GLN:HB2	1:A:309:LYS:HG3	2.01	0.42
1:A:90:ASN:OD1	1:A:90:ASN:N	2.52	0.42
1:A:125:GLY:HA2	1:A:318:PHE:HE1	1.85	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.68	0.42
1:A:294:HIS:CE1	1:A:295:LYS:HG2	2.55	0.42
2:B:220:LYS:NZ	2:B:222:TRP:CZ2	2.87	0.42
1:A:65:SER:HB2	1:A:67:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ALA:HB1	2:B:238:LEU:HD12	2.01	0.42
2:B:301:LEU:HD13	2:B:310:TYR:CG	2.54	0.42
1:A:51:THR:HG1	2:B:94:ARG:HH22	1.52	0.42
1:A:160:LEU:CD1	1:A:162:LEU:HB2	2.49	0.42
2:B:290:PHE:CB	2:B:327:LEU:CG	2.96	0.42
1:A:111:LYS:NZ	1:A:347:PHE:O	2.46	0.41
1:A:164:TYR:HE1	1:A:185:PHE:CD1	2.38	0.41
2:B:115:VAL:HG13	2:B:149:ASP:HB3	2.01	0.41
2:B:172:PHE:CD1	2:B:200:GLU:HG3	2.55	0.41
1:A:194:ARG:HB2	2:B:241:ARG:HH12	1.84	0.41
2:B:219:LEU:N	2:B:219:LEU:CD1	2.82	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.78	0.41
2:B:100:ALA:HB2	2:B:205:TYR:HB3	2.03	0.41
2:B:109:VAL:C	2:B:111:TYR:H	2.27	0.41
2:B:310:TYR:N	2:B:310:TYR:HD2	2.04	0.41
2:B:225:ASP:O	2:B:226:ARG:C	2.64	0.41
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.82	0.41
2:B:352:ARG:HG3	2:B:355:ARG:NH2	2.36	0.41
1:A:173:LEU:HD11	1:A:183:THR:OG1	2.21	0.41
2:B:101:GLU:CG	2:B:102:VAL:N	2.82	0.41
1:A:164:TYR:CE2	1:A:166:ASP:C	2.98	0.41
1:A:167:LEU:O	1:A:204:TYR:CD2	2.73	0.41
2:B:218:ASP:O	2:B:219:LEU:HB3	2.21	0.41
1:A:95:LEU:HB2	1:A:106:LEU:HD22	2.02	0.41
1:A:251:VAL:C	1:A:253:GLY:N	2.75	0.41
1:A:40:LEU:HD12	1:A:117:TYR:CE1	2.55	0.41
2:B:220:LYS:O	2:B:221:LEU:HB3	2.20	0.41
1:A:194:ARG:CD	2:B:241:ARG:HH12	2.33	0.40
1:A:54:PHE:CZ	1:A:72:LYS:CE	3.05	0.40
2:B:184:VAL:O	2:B:187:GLU:CD	2.64	0.40
2:B:251:VAL:HA	2:B:321:TYR:CE2	2.56	0.40
2:B:192:ILE:HD11	2:B:196:GLY:HA3	2.02	0.40
1:A:60:VAL:HG22	1:A:69:TYR:O	2.21	0.40
1:A:98:VAL:HG22	1:A:99:ASN:N	2.36	0.40
2:B:290:PHE:HE1	2:B:321:TYR:HB2	1.87	0.40

There are no symmetry-related clashes.

## 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	333/350 (95%)	318 (96%)	15 (4%)	0	100	100
2	B	274/381 (72%)	258 (94%)	14 (5%)	2 (1%)	18	50
All	All	607/731 (83%)	576 (95%)	29 (5%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	GLU
2	B	318	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	282/303 (93%)	254 (90%)	28 (10%)	7	30
2	B	229/334 (69%)	202 (88%)	27 (12%)	5	23
All	All	511/637 (80%)	456 (89%)	55 (11%)	6	27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	39	GLN
1	A	44	ASP
1	A	56	ARG

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Mol	Chain	Res	Type
1	A	58	MET
1	A	68	HIS
1	A	73	ILE
1	A	90	ASN
1	A	96	GLN
1	A	98	VAL
1	A	119	VAL
1	A	123	VAL
1	A	135	ILE
1	A	142	HIS
1	A	157	LEU
1	A	160	LEU
1	A	162	LEU
1	A	183	THR
1	A	205	LEU
1	A	213	LYS
1	A	226	VAL
1	A	230	GLU
1	A	269	LEU
1	A	277	LEU
1	A	284	LEU
1	A	292	LYS
1	A	325	SER
1	A	336	ARG
2	B	99	SER
2	B	124	THR
2	B	130	ILE
2	B	147	ILE
2	B	154	VAL
2	B	155	THR
2	B	180	VAL
2	B	189	VAL
2	B	191	ASN
2	B	194	GLU
2	B	200	GLU
2	B	201	LEU
2	B	204	ILE
2	B	219	LEU
2	B	221	LEU
2	B	245	GLU
2	B	251	VAL
2	B	256	SER

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Mol	Chain	Res	Type
2	B	278	GLU
2	B	291	TYR
2	B	294	THR
2	B	301	LEU
2	B	310	TYR
2	B	313	VAL
2	B	336	THR
2	B	338	VAL
2	B	345	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	67	ASN
1	A	84	GLN
1	A	142	HIS
1	A	149	GLN
1	A	181	GLN
1	A	274	GLN
2	B	138	HIS
2	B	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	A	338	1	8,9,10	1.64	1 (12%)	7,12,14	2.34	2 (28%)
1	TPO	A	197	1	8,10,11	1.21	1 (12%)	10,14,16	2.79	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	338	1	-	2/6/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	3.57	1.61	1.50
1	A	197	TPO	CB-CA	-2.49	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	P-OG1-CB	-8.09	101.35	123.33
1	A	338	SEP	OG-CB-CA	5.51	113.51	108.14
1	A	197	TPO	O-C-CA	-2.23	119.04	124.77
1	A	338	SEP	OG-P-O1P	2.02	111.89	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	2	0
1	A	197	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/350 (95%)	-0.35	0	100   100	79, 115, 182, 194	0
2	B	276/381 (72%)	-0.33	1 (0%)	88   72	80, 122, 170, 210	0
All	All	611/731 (83%)	-0.34	1 (0%)	91   80	79, 119, 180, 210	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	201	LEU	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	338	10/11	0.63	0.10	185,191,195,201	0
1	TPO	A	197	11/12	0.96	0.09	87,102,115,115	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.