Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1MAS
Title	:	PURINE NUCLEOSIDE HYDROLASE
Authors	:	Degano, M.; Gopaul, D.N.; Scapin, G.; Schramm, V.L.; Sacchettini, J.C.
Deposited on	:	1995-12-18
Resolution	:	2.50 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 (i) symbol.

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

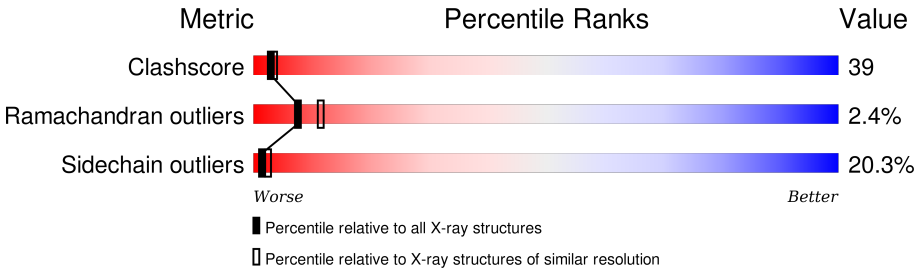
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	56% 31% 10%
1	B	314	35% 41% 14% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4693 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 INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2356	1497	401	443	15			
1	B	295	Total	C	N	O	S	0	0	0
			2262	1437	388	423	14			

- 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	34	Total	O	0	0
			34	34		

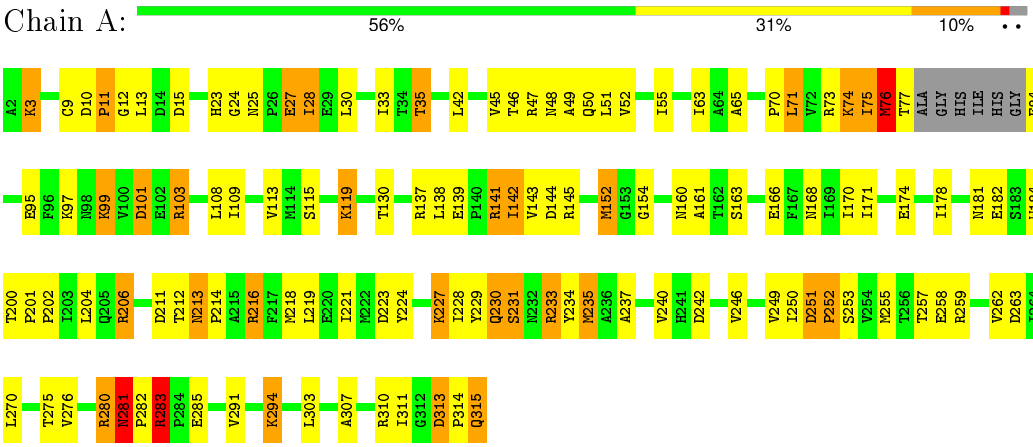
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

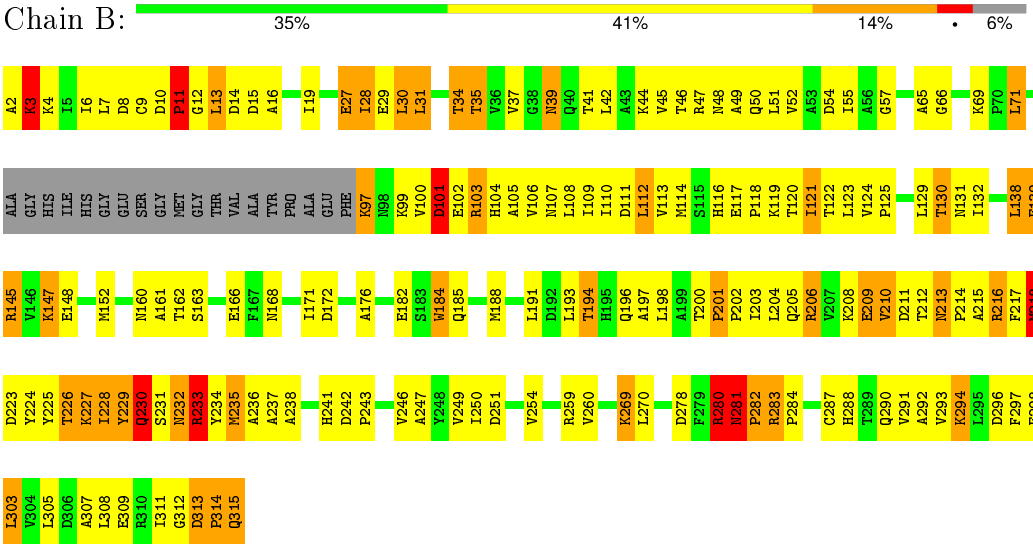
- Molecule 1: INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE

Chain A:



- Molecule 1: INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.84Å 131.53Å 90.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.50	Depositor
% Data completeness (in resolution range)	89.1 (99.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

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	0.97	1/2399 (0.0%)	1.01	10/3268 (0.3%)
1	B	0.89	7/2302 (0.3%)	1.18	22/3136 (0.7%)
All	All	0.93	8/4701 (0.2%)	1.10	32/6404 (0.5%)

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	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	GLN	C-OXT	31.97	1.84	1.23
1	B	282	PRO	CA-C	11.39	1.75	1.52
1	B	219	LEU	N-CA	11.21	1.68	1.46
1	B	283	ARG	N-CA	11.08	1.68	1.46
1	B	281	ASN	C-N	-8.74	1.17	1.34
1	B	234	TYR	N-CA	8.09	1.62	1.46
1	B	282	PRO	C-N	6.96	1.50	1.34
1	B	101	ASP	N-CA	5.84	1.58	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	281	ASN	O-C-N	-14.24	94.04	121.10
1	B	144	ASP	CA-CB-CG	10.71	136.95	113.40
1	B	234	TYR	N-CA-CB	9.65	127.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ASN	O-C-N	-8.59	104.79	121.10
1	B	282	PRO	CA-N-CD	8.32	123.34	111.70
1	A	251	ASP	C-N-CD	-8.20	102.57	120.60
1	A	12	GLY	N-CA-C	-7.87	93.44	113.10
1	B	281	ASN	CA-C-N	7.77	138.85	117.10
1	B	233	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	280	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	B	283	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	3	LYS	N-CA-C	7.20	130.43	111.00
1	B	230	GLN	CB-CA-C	-6.92	96.57	110.40
1	B	282	PRO	O-C-N	-6.84	111.76	122.70
1	A	283	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	310	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	280	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	B	222	MET	CG-SD-CE	6.22	110.16	100.20
1	B	145	ARG	NE-CZ-NH2	6.19	123.40	120.30
1	A	76	MET	CG-SD-CE	6.16	110.05	100.20
1	A	86	GLY	N-CA-C	-6.06	97.95	113.10
1	B	233	ARG	C-N-CA	-5.86	107.06	121.70
1	B	76	MET	N-CA-C	5.84	126.76	111.00
1	B	218	MET	C-N-CA	-5.78	107.25	121.70
1	B	281	ASN	C-N-CA	-5.71	98.04	122.00
1	B	10	ASP	C-N-CD	-5.69	108.08	120.60
1	A	281	ASN	CA-C-N	5.66	132.94	117.10
1	B	139	GLU	C-N-CD	-5.30	108.95	120.60
1	B	282	PRO	N-CD-CG	-5.28	95.28	103.20
1	B	219	LEU	N-CA-CB	-5.24	99.92	110.40
1	A	85	SER	N-CA-C	5.22	125.10	111.00
1	B	11	PRO	O-C-N	5.12	131.91	123.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	218	MET	Peptide
1	B	281	ASN	Mainchain,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	2356	0	2395	126	0
1	B	2262	0	2312	246	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	39	0	0	4	0
3	B	34	0	0	1	0
All	All	4693	0	4707	365	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 39.

All (365) 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:B:283:ARG:N	1:B:283:ARG:CA	1.68	1.56
1:B:219:LEU:CA	1:B:219:LEU:N	1.68	1.54
1:B:282:PRO:C	1:B:282:PRO:CA	1.75	1.51
1:B:226:THR:CG2	1:B:230:GLN:HE22	1.29	1.44
1:B:226:THR:HG23	1:B:230:GLN:NE2	1.23	1.42
1:A:315:GLN:OXT	1:A:315:GLN:C	1.84	1.16
1:A:11:PRO:HD2	1:A:45:VAL:HG13	1.28	1.16
1:B:11:PRO:HD2	1:B:45:VAL:HG13	1.24	1.15
1:A:315:GLN:OXT	1:A:315:GLN:HB3	1.47	1.13
1:A:269:LYS:HE2	1:A:270:LEU:HD21	1.24	1.10
1:B:185:GLN:NE2	1:B:259:ARG:HH22	1.52	1.07
1:B:185:GLN:HE22	1:B:259:ARG:NH2	1.51	1.06
1:B:13:LEU:HD12	1:B:225:TYR:HB2	1.05	1.03
1:A:35:THR:HG22	1:A:65:ALA:HA	1.38	1.02
1:B:223:ASP:HA	1:B:226:THR:HB	1.41	1.00
1:A:315:GLN:OXT	1:A:315:GLN:CB	2.09	1.00
1:B:212:THR:HB	1:B:214:PRO:HD2	1.44	0.99
1:A:28:ILE:HD11	1:A:250:ILE:HG12	1.41	0.96
1:B:75:ILE:H	1:B:75:ILE:HD13	1.31	0.95
1:B:269:LYS:HE3	1:B:270:LEU:HG	1.49	0.93
1:B:13:LEU:CD1	1:B:225:TYR:HB2	1.98	0.93
1:A:315:GLN:OXT	1:A:315:GLN:CA	2.20	0.90
1:A:28:ILE:CD1	1:A:250:ILE:HG12	2.01	0.90
1:B:13:LEU:HD12	1:B:225:TYR:CB	1.99	0.88
1:B:75:ILE:HG12	1:B:76:MET:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HE2	1:A:270:LEU:CD2	2.04	0.86
1:B:218:MET:C	1:B:219:LEU:CA	2.43	0.85
1:B:11:PRO:HD2	1:B:45:VAL:CG1	2.07	0.84
1:B:201:PRO:HG2	1:B:202:PRO:HD3	1.62	0.81
1:A:75:ILE:HD13	1:A:76:MET:H	1.45	0.81
1:B:223:ASP:CA	1:B:226:THR:HB	2.10	0.81
1:B:294:LYS:NZ	1:B:294:LYS:HB2	1.93	0.80
1:A:11:PRO:CD	1:A:45:VAL:HG13	2.11	0.80
1:B:219:LEU:CB	1:B:219:LEU:N	2.46	0.78
1:A:224:TYR:O	1:A:228:ILE:HD13	1.83	0.78
1:B:11:PRO:HA	1:B:15:ASP:HB2	1.65	0.78
1:A:230:GLN:HG2	1:A:235:MET:CB	2.14	0.78
1:A:35:THR:HG21	1:A:46:THR:OG1	1.82	0.78
1:A:101:ASP:OD2	1:A:103:ARG:HG3	1.86	0.76
1:B:194:THR:HB	1:B:241:HIS:HD2	1.49	0.76
1:B:235:MET:HE3	1:B:238:ALA:HA	1.67	0.75
1:A:139:GLU:OE2	1:A:141:ARG:HB2	1.86	0.75
1:B:307:ALA:O	1:B:311:ILE:HG23	1.89	0.73
1:B:212:THR:CB	1:B:214:PRO:HD2	2.18	0.72
1:B:200:THR:HB	1:B:201:PRO:HD2	1.71	0.72
1:B:212:THR:O	1:B:216:ARG:HG2	1.88	0.72
1:B:296:ASP:OD2	1:B:299:LYS:HB2	1.89	0.71
1:B:35:THR:HG22	1:B:65:ALA:HA	1.71	0.71
1:B:219:LEU:N	1:B:219:LEU:C	2.44	0.71
1:A:202:PRO:O	1:A:206:ARG:HG2	1.91	0.71
1:A:227:LYS:O	1:A:231:SER:HB2	1.91	0.71
1:B:13:LEU:HG	1:B:221:ILE:HG23	1.72	0.70
1:A:230:GLN:HG2	1:A:235:MET:HB3	1.73	0.70
1:B:48:ASN:O	1:B:52:VAL:HG23	1.91	0.70
1:A:11:PRO:HA	1:A:15:ASP:HB2	1.73	0.70
1:B:110:ILE:HD13	1:B:139:GLU:HB3	1.73	0.70
1:B:282:PRO:C	1:B:282:PRO:CB	2.59	0.69
1:B:235:MET:CE	1:B:238:ALA:HA	2.22	0.69
1:B:105:ALA:O	1:B:109:ILE:HG13	1.93	0.69
1:B:219:LEU:O	1:B:222:MET:HB2	1.94	0.68
1:B:55:ILE:HD13	1:B:55:ILE:N	2.09	0.68
1:B:75:ILE:HG12	1:B:76:MET:N	2.08	0.68
1:A:115:SER:OG	3:A:918:HOH:O	2.12	0.68
1:B:9:CYS:HB2	1:B:15:ASP:OD2	1.94	0.67
1:A:74:LYS:HD3	1:A:76:MET:CE	2.24	0.67
1:A:75:ILE:H	1:A:75:ILE:CD1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:O	1:B:219:LEU:N	2.26	0.67
1:B:226:THR:HG22	1:B:227:LYS:N	2.09	0.67
1:B:74:LYS:HG2	1:B:76:MET:SD	2.34	0.67
1:A:48:ASN:O	1:A:52:VAL:HG23	1.95	0.67
1:B:35:THR:HG21	1:B:46:THR:OG1	1.95	0.67
1:A:281:ASN:HB3	1:A:282:PRO:HD3	1.75	0.67
1:A:235:MET:HG2	1:A:237:ALA:O	1.94	0.66
1:A:35:THR:HG23	1:A:42:LEU:CD1	2.25	0.66
1:A:307:ALA:O	1:A:311:ILE:HG12	1.94	0.66
1:B:118:PRO:O	1:B:120:THR:HG23	1.95	0.66
1:A:103:ARG:HE	1:A:108:LEU:HD13	1.61	0.66
1:B:160:ASN:OD1	1:B:161:ALA:N	2.28	0.66
1:B:216:ARG:HH11	1:B:216:ARG:HG3	1.61	0.66
1:B:121:ILE:O	1:B:147:LYS:HB3	1.96	0.65
1:B:281:ASN:ND2	1:B:281:ASN:O	2.29	0.65
1:A:269:LYS:HG2	1:A:270:LEU:HD23	1.79	0.65
1:A:251:ASP:OD1	1:A:252:PRO:HD2	1.96	0.65
1:B:228:ILE:O	1:B:231:SER:HB2	1.97	0.65
1:B:101:ASP:OD1	1:B:103:ARG:HD2	1.96	0.65
1:B:201:PRO:CG	1:B:202:PRO:HD3	2.25	0.65
1:B:219:LEU:HA	1:B:222:MET:HB2	1.79	0.65
1:B:11:PRO:CD	1:B:45:VAL:HG13	2.16	0.65
1:A:75:ILE:N	1:A:75:ILE:HD13	2.12	0.64
1:A:75:ILE:H	1:A:75:ILE:HD13	1.63	0.64
1:A:230:GLN:HG2	1:A:235:MET:HB2	1.80	0.64
1:A:119:LYS:N	1:A:145:ARG:O	2.28	0.64
1:B:214:PRO:HG2	1:B:311:ILE:CD1	2.28	0.63
1:B:51:LEU:CD1	1:B:55:ILE:HD11	2.29	0.63
1:A:283:ARG:HG3	1:A:283:ARG:NH1	2.13	0.62
1:A:74:LYS:HD3	1:A:76:MET:SD	2.40	0.62
1:B:229:TYR:C	1:B:231:SER:H	2.03	0.62
1:B:227:LYS:HA	1:B:230:GLN:OE1	2.00	0.61
1:B:224:TYR:CE1	1:B:228:ILE:HD11	2.36	0.61
1:A:185:GLN:HE22	1:A:259:ARG:HH22	1.47	0.61
1:B:31:LEU:HD23	1:B:31:LEU:N	2.16	0.60
1:B:34:THR:CG2	1:B:105:ALA:HB1	2.31	0.60
1:B:259:ARG:HG2	1:B:290:GLN:HB3	1.83	0.60
3:A:911:HOH:O	1:B:269:LYS:NZ	2.31	0.60
1:B:106:VAL:O	1:B:110:ILE:HG13	2.02	0.60
1:B:219:LEU:N	1:B:220:GLU:N	2.49	0.60
1:B:223:ASP:HA	1:B:226:THR:CB	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASN:HA	1:B:216:ARG:HG3	1.84	0.59
1:A:281:ASN:HB3	1:A:282:PRO:CD	2.32	0.59
1:A:11:PRO:HG2	1:A:49:ALA:HB2	1.83	0.59
1:B:129:LEU:HD12	1:B:176:ALA:HA	1.84	0.59
1:B:219:LEU:O	1:B:222:MET:N	2.36	0.59
1:B:11:PRO:HA	1:B:15:ASP:CB	2.33	0.58
1:A:265:GLU:OE1	1:B:270:LEU:HB2	2.03	0.58
1:B:102:GLU:HG3	1:B:102:GLU:O	2.02	0.58
1:B:214:PRO:HG2	1:B:311:ILE:HD12	1.86	0.58
1:B:227:LYS:O	1:B:230:GLN:N	2.36	0.58
1:B:188:MET:CE	1:B:291:VAL:HG12	2.34	0.58
1:A:47:ARG:HA	1:A:50:GLN:HE21	1.67	0.58
1:B:121:ILE:HG22	1:B:122:THR:N	2.18	0.58
1:B:259:ARG:NH2	1:B:287:CYS:O	2.31	0.58
1:B:223:ASP:O	1:B:226:THR:HB	2.04	0.58
1:B:51:LEU:O	1:B:55:ILE:HG12	2.04	0.58
1:A:24:GLY:CA	1:A:311:ILE:HD11	2.34	0.58
1:A:218:MET:O	1:A:221:ILE:HG12	2.04	0.57
1:B:308:LEU:O	1:B:311:ILE:HG12	2.05	0.57
1:B:194:THR:HB	1:B:241:HIS:CD2	2.34	0.57
1:B:51:LEU:HD12	1:B:55:ILE:HD11	1.86	0.57
1:B:303:LEU:HD23	1:B:303:LEU:N	2.19	0.57
1:B:235:MET:O	1:B:236:ALA:C	2.43	0.56
1:B:110:ILE:HD13	1:B:139:GLU:CB	2.33	0.56
1:B:246:VAL:O	1:B:249:VAL:HB	2.05	0.56
1:A:280:ARG:NH1	1:B:162:THR:HA	2.20	0.56
1:B:111:ASP:O	1:B:112:LEU:C	2.41	0.56
1:B:74:LYS:HB3	1:B:76:MET:HB2	1.87	0.56
1:B:213:ASN:HA	1:B:216:ARG:NH1	2.20	0.56
1:B:4:LYS:HE3	1:B:29:GLU:OE1	2.06	0.56
1:B:4:LYS:HD3	1:B:31:LEU:HD21	1.88	0.56
1:B:34:THR:HG22	1:B:105:ALA:CB	2.36	0.56
1:A:73:ARG:NE	1:A:174:GLU:OE2	2.37	0.56
1:A:35:THR:HG23	1:A:42:LEU:HD12	1.87	0.55
1:B:223:ASP:O	1:B:224:TYR:C	2.44	0.55
1:A:35:THR:CG2	1:A:65:ALA:HA	2.26	0.55
1:A:199:ALA:HB1	1:A:204:LEU:HD21	1.89	0.55
1:B:226:THR:CG2	1:B:230:GLN:NE2	2.12	0.55
1:B:226:THR:C	1:B:230:GLN:NE2	2.61	0.54
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.32	0.54
1:B:124:VAL:HG12	1:B:124:VAL:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HA	1:A:50:GLN:NE2	2.22	0.54
1:B:50:GLN:OE1	1:B:100:VAL:HG23	2.07	0.54
1:B:108:LEU:O	1:B:108:LEU:HD12	2.07	0.54
1:A:283:ARG:HH11	1:A:283:ARG:CG	2.19	0.54
1:B:269:LYS:HE3	1:B:270:LEU:CG	2.31	0.54
1:B:229:TYR:C	1:B:231:SER:N	2.62	0.54
1:A:233:ARG:HD2	1:A:234:TYR:N	2.23	0.53
1:A:3:LYS:HB2	1:A:27:GLU:O	2.08	0.53
1:B:168:ASN:O	1:B:171:ILE:HG22	2.08	0.53
1:B:216:ARG:HG3	1:B:216:ARG:NH1	2.23	0.53
1:A:185:GLN:NE2	1:A:259:ARG:HH22	2.05	0.53
1:B:130:THR:HB	1:B:172:ASP:OD2	2.09	0.53
1:B:303:LEU:HD23	1:B:303:LEU:H	1.74	0.53
1:B:229:TYR:O	1:B:231:SER:N	2.41	0.53
1:B:201:PRO:CB	1:B:202:PRO:HD3	2.39	0.52
1:B:215:ALA:O	1:B:218:MET:HB3	2.08	0.52
1:A:35:THR:HG23	1:A:42:LEU:HD11	1.91	0.52
1:A:230:GLN:CG	1:A:235:MET:HB3	2.38	0.52
1:B:223:ASP:O	1:B:226:THR:N	2.42	0.52
1:A:229:TYR:C	1:A:231:SER:H	2.12	0.52
1:B:28:ILE:HD13	1:B:250:ILE:HG12	1.90	0.52
1:B:302:GLY:O	1:B:303:LEU:C	2.48	0.52
1:B:193:LEU:HD13	1:B:193:LEU:C	2.30	0.52
1:B:214:PRO:HB2	1:B:311:ILE:HD11	1.91	0.52
1:A:314:PRO:O	1:A:315:GLN:CB	2.57	0.52
1:A:160:ASN:OD1	1:A:161:ALA:N	2.42	0.52
1:A:263:ASP:HB3	1:B:270:LEU:HD11	1.91	0.52
1:A:139:GLU:HG3	1:A:142:ILE:HG23	1.92	0.52
1:A:23:HIS:CD2	1:A:311:ILE:HD12	2.45	0.52
1:B:251:ASP:O	1:B:254:VAL:HG12	2.10	0.51
1:B:278:ASP:OD1	1:B:280:ARG:HB2	2.11	0.51
1:B:296:ASP:O	1:B:297:PHE:C	2.48	0.51
1:B:51:LEU:HD12	1:B:55:ILE:CD1	2.40	0.51
1:B:113:VAL:HG11	1:B:142:ILE:HB	1.93	0.51
1:B:74:LYS:HE3	1:B:76:MET:SD	2.51	0.51
1:B:12:GLY:O	1:B:13:LEU:C	2.48	0.51
1:B:214:PRO:O	1:B:215:ALA:C	2.49	0.51
1:B:35:THR:CG2	1:B:42:LEU:HD11	2.41	0.51
1:A:240:VAL:HG23	1:A:240:VAL:O	2.10	0.51
1:B:227:LYS:O	1:B:228:ILE:C	2.47	0.51
1:B:191:LEU:HA	1:B:194:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HE22	1:A:259:ARG:NH2	2.09	0.51
1:B:200:THR:CB	1:B:201:PRO:HD2	2.34	0.51
1:A:283:ARG:HG3	1:A:283:ARG:HH11	1.74	0.51
1:A:198:LEU:N	1:A:198:LEU:HD23	2.26	0.51
1:A:152:MET:HG3	1:A:242:ASP:HA	1.92	0.50
1:B:294:LYS:HB2	1:B:294:LYS:HZ1	1.75	0.50
1:B:222:MET:O	1:B:226:THR:N	2.45	0.50
1:B:39:ASN:H	1:B:39:ASN:ND2	2.09	0.50
1:A:281:ASN:CB	1:A:282:PRO:HD3	2.40	0.50
1:B:131:ASN:N	3:B:959:HOH:O	2.25	0.50
1:A:109:ILE:O	1:A:113:VAL:HG23	2.11	0.50
1:A:75:ILE:N	1:A:75:ILE:CD1	2.70	0.50
1:A:206:ARG:HE	1:A:206:ARG:HA	1.75	0.50
1:B:55:ILE:H	1:B:55:ILE:HD13	1.74	0.50
1:B:119:LYS:HE3	1:B:144:ASP:O	2.11	0.50
1:B:219:LEU:CA	1:B:222:MET:HB2	2.40	0.50
1:B:206:ARG:CZ	1:B:206:ARG:HB3	2.40	0.49
1:B:230:GLN:O	1:B:233:ARG:O	2.29	0.49
1:A:33:ILE:O	1:A:63:ILE:HA	2.13	0.49
1:B:30:LEU:O	1:B:31:LEU:C	2.51	0.49
1:B:300:PHE:O	1:B:303:LEU:HB2	2.12	0.49
1:A:257:THR:HA	1:A:291:VAL:O	2.12	0.49
1:B:188:MET:HE1	1:B:291:VAL:HG12	1.93	0.49
1:B:14:ASP:O	1:B:15:ASP:C	2.50	0.49
1:B:28:ILE:CD1	1:B:250:ILE:HG12	2.43	0.49
1:A:139:GLU:HG3	1:A:139:GLU:O	2.13	0.49
1:B:34:THR:HG22	1:B:105:ALA:HB1	1.94	0.49
1:B:314:PRO:O	1:B:315:GLN:OXT	2.30	0.49
1:A:251:ASP:O	1:A:252:PRO:C	2.52	0.48
1:A:75:ILE:HD13	1:A:76:MET:N	2.23	0.48
1:A:97:LYS:O	1:A:99:LYS:HE2	2.12	0.48
1:B:298:GLU:HA	1:B:298:GLU:OE1	2.12	0.48
1:B:108:LEU:HD11	1:B:112:LEU:HD21	1.95	0.48
1:A:3:LYS:HE2	1:A:249:VAL:O	2.14	0.48
1:B:35:THR:HG22	1:B:42:LEU:HD11	1.95	0.48
1:A:212:THR:HB	1:A:214:PRO:HD2	1.95	0.48
1:B:196:GLN:NE2	1:B:293:VAL:O	2.46	0.48
1:A:35:THR:CG2	1:A:42:LEU:HD11	2.44	0.48
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.57	0.48
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.32	0.48
1:B:188:MET:HE1	1:B:291:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:O	1:B:54:ASP:HB2	2.14	0.48
1:B:121:ILE:HG22	1:B:122:THR:H	1.78	0.47
1:A:181:ASN:ND2	3:A:923:HOH:O	2.46	0.47
1:B:213:ASN:N	1:B:214:PRO:CD	2.77	0.47
1:B:11:PRO:CG	1:B:49:ALA:HB2	2.44	0.47
1:A:200:THR:HB	1:A:201:PRO:HD2	1.95	0.47
1:B:311:ILE:HG13	1:B:312:GLY:O	2.14	0.47
1:B:35:THR:HG23	1:B:42:LEU:HD12	1.96	0.47
1:A:201:PRO:HB2	1:A:202:PRO:CD	2.44	0.47
1:B:305:LEU:O	1:B:309:GLU:HG3	2.15	0.47
1:A:266:LEU:HB2	3:A:911:HOH:O	2.13	0.47
1:B:4:LYS:HA	1:B:29:GLU:O	2.14	0.47
1:B:31:LEU:HD23	1:B:31:LEU:H	1.79	0.47
1:B:283:ARG:N	1:B:283:ARG:CB	2.65	0.47
1:B:51:LEU:HD12	1:B:55:ILE:HG12	1.97	0.47
1:B:143:VAL:HA	1:B:184:TRP:CE3	2.50	0.47
1:A:280:ARG:NH1	1:B:162:THR:CA	2.78	0.47
1:A:9:CYS:HB2	1:A:15:ASP:OD2	2.15	0.47
1:B:35:THR:HG23	1:B:42:LEU:CD1	2.44	0.47
1:B:223:ASP:C	1:B:226:THR:HB	2.34	0.46
1:B:226:THR:HG22	1:B:227:LYS:HD3	1.96	0.46
1:A:233:ARG:HD2	1:A:234:TYR:H	1.80	0.46
1:A:201:PRO:HB2	1:A:202:PRO:HD3	1.97	0.46
1:B:51:LEU:HD12	1:B:51:LEU:C	2.35	0.46
1:B:16:ALA:O	1:B:19:ILE:HB	2.15	0.46
1:B:210:VAL:CG1	1:B:215:ALA:HB2	2.46	0.46
1:A:88:GLY:HA2	1:A:224:TYR:CE2	2.51	0.46
1:B:182:GLU:OE1	1:B:182:GLU:HA	2.11	0.46
1:B:214:PRO:HG2	1:B:311:ILE:HD11	1.96	0.46
1:B:269:LYS:CE	1:B:270:LEU:HG	2.35	0.46
1:A:70:PRO:HG2	1:A:73:ARG:O	2.15	0.46
1:B:182:GLU:HB2	1:B:184:TRP:NE1	2.31	0.46
1:B:8:ASP:HB3	1:B:125:PRO:HA	1.97	0.46
1:B:14:ASP:HB2	1:B:242:ASP:CG	2.37	0.45
1:B:76:MET:O	1:B:76:MET:HG3	2.16	0.45
1:B:269:LYS:HE2	1:B:269:LYS:HB3	1.71	0.45
1:B:225:TYR:HA	1:B:228:ILE:HD12	1.99	0.45
1:B:188:MET:HE2	1:B:291:VAL:HG12	1.98	0.45
1:B:302:GLY:O	1:B:305:LEU:N	2.49	0.45
1:A:262:VAL:HA	1:A:276:VAL:O	2.16	0.45
1:B:226:THR:O	1:B:230:GLN:CD	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG11	1:B:215:ALA:HB2	1.98	0.45
1:B:219:LEU:N	1:B:220:GLU:H	2.15	0.45
1:A:201:PRO:HD2	1:A:202:PRO:HD2	1.98	0.45
1:A:294:LYS:HE3	1:A:294:LYS:HB2	1.46	0.45
1:A:281:ASN:ND2	1:B:232:ASN:ND2	2.65	0.45
1:A:233:ARG:CD	1:A:234:TYR:N	2.79	0.45
1:B:147:LYS:CB	1:B:147:LYS:NZ	2.79	0.45
1:A:213:ASN:N	1:A:214:PRO:CD	2.80	0.45
1:B:200:THR:O	1:B:203:ILE:N	2.50	0.45
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.80	0.45
1:A:219:LEU:O	1:A:223:ASP:HB2	2.17	0.45
1:B:313:ASP:HA	1:B:314:PRO:HD2	1.80	0.44
1:B:281:ASN:C	1:B:282:PRO:C	2.76	0.44
1:B:242:ASP:N	1:B:243:PRO:CD	2.80	0.44
1:B:100:VAL:O	1:B:101:ASP:C	2.55	0.44
1:A:201:PRO:CD	1:A:202:PRO:HD2	2.47	0.44
1:B:201:PRO:HA	1:B:204:LEU:HD12	1.99	0.44
1:B:226:THR:O	1:B:230:GLN:NE2	2.51	0.44
1:A:10:ASP:HA	1:A:45:VAL:HG11	2.00	0.44
1:A:255:MET:HA	1:A:294:LYS:O	2.18	0.44
1:B:123:LEU:HD13	1:B:132:ILE:HD12	2.00	0.44
1:B:222:MET:O	1:B:226:THR:CB	2.66	0.44
1:B:301:TRP:O	1:B:302:GLY:C	2.55	0.44
1:B:219:LEU:HD23	1:B:222:MET:HG3	1.98	0.43
1:A:212:THR:O	1:A:216:ARG:HG2	2.18	0.43
1:B:232:ASN:ND2	1:B:233:ARG:HB2	2.33	0.43
1:B:219:LEU:C	1:B:222:MET:H	2.22	0.43
1:A:213:ASN:HB2	1:A:313:ASP:OD1	2.18	0.43
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.83	0.43
1:A:200:THR:HB	1:A:201:PRO:CD	2.48	0.43
1:B:66:GLY:CA	1:B:105:ALA:HB3	2.48	0.43
1:A:251:ASP:HA	1:A:252:PRO:HD3	1.45	0.43
1:A:51:LEU:O	1:A:55:ILE:HD12	2.19	0.43
1:B:46:THR:O	1:B:47:ARG:C	2.54	0.43
1:B:50:GLN:O	1:B:51:LEU:C	2.56	0.43
1:B:100:VAL:O	1:B:101:ASP:O	2.37	0.43
1:B:54:ASP:O	1:B:57:GLY:N	2.42	0.43
1:B:226:THR:HG23	1:B:230:GLN:HE22	0.38	0.43
1:B:235:MET:SD	1:B:237:ALA:O	2.77	0.43
1:B:51:LEU:HD12	1:B:55:ILE:CG1	2.48	0.43
1:B:206:ARG:HA	1:B:209:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PRO:N	1:A:202:PRO:HD2	2.33	0.43
1:B:166:GLU:CD	1:B:168:ASN:H	2.22	0.43
1:A:227:LYS:O	1:A:228:ILE:C	2.57	0.42
1:B:100:VAL:C	1:B:101:ASP:O	2.57	0.42
1:B:246:VAL:O	1:B:247:ALA:C	2.57	0.42
1:A:281:ASN:CB	1:A:282:PRO:CD	2.94	0.42
1:B:259:ARG:HH12	1:B:290:GLN:NE2	2.17	0.42
1:A:246:VAL:O	1:A:250:ILE:HG13	2.19	0.42
1:B:116:HIS:O	1:B:145:ARG:NH1	2.52	0.42
1:B:185:GLN:HE22	1:B:259:ARG:HH22	0.69	0.42
1:B:104:HIS:O	1:B:105:ALA:C	2.55	0.42
1:B:97:LYS:HB3	1:B:97:LYS:HE2	1.53	0.42
1:B:6:ILE:HG13	1:B:121:ILE:HG21	2.01	0.42
1:B:107:ASN:O	1:B:108:LEU:C	2.57	0.42
1:B:193:LEU:HG	1:B:292:ALA:HB1	2.02	0.42
1:B:160:ASN:OD1	1:B:166:GLU:HA	2.18	0.42
1:A:280:ARG:HH12	1:B:162:THR:HA	1.84	0.42
1:B:184:TRP:O	1:B:288:HIS:ND1	2.48	0.42
1:B:259:ARG:NH1	1:B:290:GLN:NE2	2.66	0.42
1:B:235:MET:HE1	1:B:238:ALA:HA	2.02	0.42
1:A:137:ARG:NH1	1:A:178:ILE:HG12	2.35	0.42
1:B:71:LEU:HA	1:B:71:LEU:HD12	1.84	0.42
1:A:269:LYS:HG2	1:A:270:LEU:CD2	2.48	0.42
1:B:280:ARG:HB2	1:B:280:ARG:HE	1.73	0.42
1:A:154:GLY:HA3	1:A:275:THR:HG21	2.01	0.42
1:A:228:ILE:H	1:A:228:ILE:CD1	2.33	0.42
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.65	0.42
1:B:37:VAL:HG13	1:B:37:VAL:O	2.20	0.42
1:B:214:PRO:CB	1:B:311:ILE:HD11	2.50	0.41
1:B:214:PRO:CB	1:B:311:ILE:CD1	2.99	0.41
1:B:233:ARG:HD2	1:B:233:ARG:HA	1.25	0.41
1:B:11:PRO:HG2	1:B:45:VAL:O	2.20	0.41
1:B:205:GLN:O	1:B:208:LYS:N	2.53	0.41
1:B:219:LEU:C	1:B:222:MET:HB2	2.40	0.41
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.81	0.41
1:B:216:ARG:O	1:B:217:PHE:C	2.59	0.41
1:A:314:PRO:O	1:A:315:GLN:HB2	2.21	0.41
1:B:34:THR:HG21	1:B:105:ALA:HB1	2.00	0.41
1:A:168:ASN:O	1:A:171:ILE:HG22	2.21	0.41
1:A:281:ASN:HD21	1:B:232:ASN:ND2	2.18	0.41
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:HB2	1:B:294:LYS:HZ2	1.79	0.41
1:B:171:ILE:HG23	1:B:172:ASP:N	2.35	0.41
1:A:218:MET:O	1:A:221:ILE:CG1	2.68	0.41
1:B:147:LYS:CB	1:B:147:LYS:HZ2	2.33	0.41
1:B:2:ALA:C	1:B:27:GLU:O	2.58	0.41
1:B:216:ARG:HG2	1:B:216:ARG:H	1.58	0.40
1:B:11:PRO:HG3	1:B:49:ALA:HB2	2.02	0.40
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.84	0.40
1:A:25:ASN:CG	1:A:250:ILE:HD13	2.41	0.40
1:B:11:PRO:HG2	1:B:49:ALA:HB2	2.03	0.40
1:B:198:LEU:HD22	1:B:237:ALA:HB3	2.03	0.40
1:A:160:ASN:OD1	1:A:166:GLU:HA	2.21	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	304/314 (97%)	283 (93%)	17 (6%)	4 (1%)	15 26
1	B	291/314 (93%)	235 (81%)	46 (16%)	10 (3%)	5 6
All	All	595/628 (95%)	518 (87%)	63 (11%)	14 (2%)	7 11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	B	3	LYS
1	B	228	ILE
1	B	197	ALA
1	B	230	GLN
1	A	253	SER

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Mol	Chain	Res	Type
1	B	11	PRO
1	B	194	THR
1	B	314	PRO
1	A	230	GLN
1	B	13	LEU
1	B	101	ASP
1	A	11	PRO
1	B	201	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	256/259 (99%)	212 (83%)	44 (17%)	2 4
1	B	247/259 (95%)	189 (76%)	58 (24%)	1 1
All	All	503/518 (97%)	401 (80%)	102 (20%)	1 2

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	13	LEU
1	A	27	GLU
1	A	28	ILE
1	A	30	LEU
1	A	35	THR
1	A	71	LEU
1	A	74	LYS
1	A	75	ILE
1	A	76	MET
1	A	77	THR
1	A	84	GLU
1	A	85	SER
1	A	95	GLU
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	101	ASP
1	A	103	ARG
1	A	119	LYS
1	A	130	THR
1	A	138	LEU
1	A	141	ARG
1	A	142	ILE
1	A	143	VAL
1	A	144	ASP
1	A	152	MET
1	A	163	SER
1	A	170	ILE
1	A	182	GLU
1	A	184	TRP
1	A	206	ARG
1	A	211	ASP
1	A	213	ASN
1	A	216	ARG
1	A	227	LYS
1	A	231	SER
1	A	233	ARG
1	A	235	MET
1	A	252	PRO
1	A	258	GLU
1	A	269	LYS
1	A	283	ARG
1	A	285	GLU
1	A	294	LYS
1	A	313	ASP
1	B	3	LYS
1	B	7	LEU
1	B	27	GLU
1	B	28	ILE
1	B	30	LEU
1	B	31	LEU
1	B	34	THR
1	B	35	THR
1	B	39	ASN
1	B	41	THR
1	B	44	LYS
1	B	69	LYS
1	B	71	LEU

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Mol	Chain	Res	Type
1	B	74	LYS
1	B	75	ILE
1	B	76	MET
1	B	77	THR
1	B	97	LYS
1	B	99	LYS
1	B	101	ASP
1	B	103	ARG
1	B	112	LEU
1	B	114	MET
1	B	117	GLU
1	B	121	ILE
1	B	130	THR
1	B	138	LEU
1	B	143	VAL
1	B	144	ASP
1	B	147	LYS
1	B	148	GLU
1	B	152	MET
1	B	163	SER
1	B	184	TRP
1	B	206	ARG
1	B	209	GLU
1	B	210	VAL
1	B	211	ASP
1	B	213	ASN
1	B	216	ARG
1	B	218	MET
1	B	221	ILE
1	B	222	MET
1	B	226	THR
1	B	227	LYS
1	B	229	TYR
1	B	232	ASN
1	B	233	ARG
1	B	235	MET
1	B	260	VAL
1	B	269	LYS
1	B	280	ARG
1	B	281	ASN
1	B	284	PRO
1	B	294	LYS

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Mol	Chain	Res	Type
1	B	303	LEU
1	B	313	ASP
1	B	315	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	50	GLN
1	A	157	HIS
1	A	181	ASN
1	A	185	GLN
1	A	195	HIS
1	B	39	ASN
1	B	98	ASN
1	B	157	HIS
1	B	185	GLN
1	B	213	ASN
1	B	230	GLN
1	B	232	ASN
1	B	290	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 2 ligands modelled in this entry, 2 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.