



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 08:22 AM EDT

PDB ID : 1JHZ
Title : Purine Repressor Mutant Corepressor Binding Domain Structure
Authors : Huffman, J.L.; Lu, F.; Zalkin, H.; Brennan, R.G.
Deposited on : 2001-06-28
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

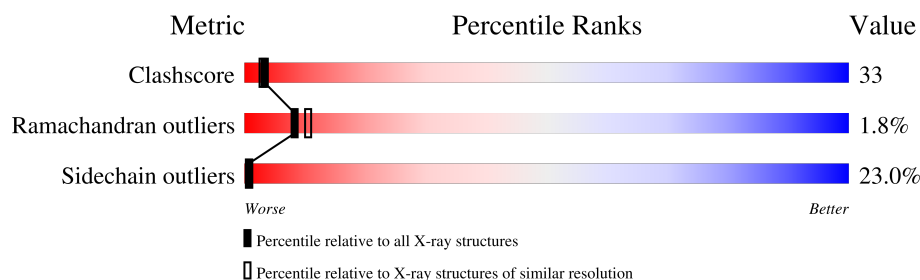
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	 51% 36% 8% .
1	B	289	 42% 39% 14% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4489 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 PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2168	1370	377	402	19			
1	B	276	Total	C	N	O	S	0	0	0
			2168	1370	377	402	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	PHE	TRP	engineered mutation	UNP P0ACP7
B	147	PHE	TRP	engineered mutation	UNP P0ACP7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

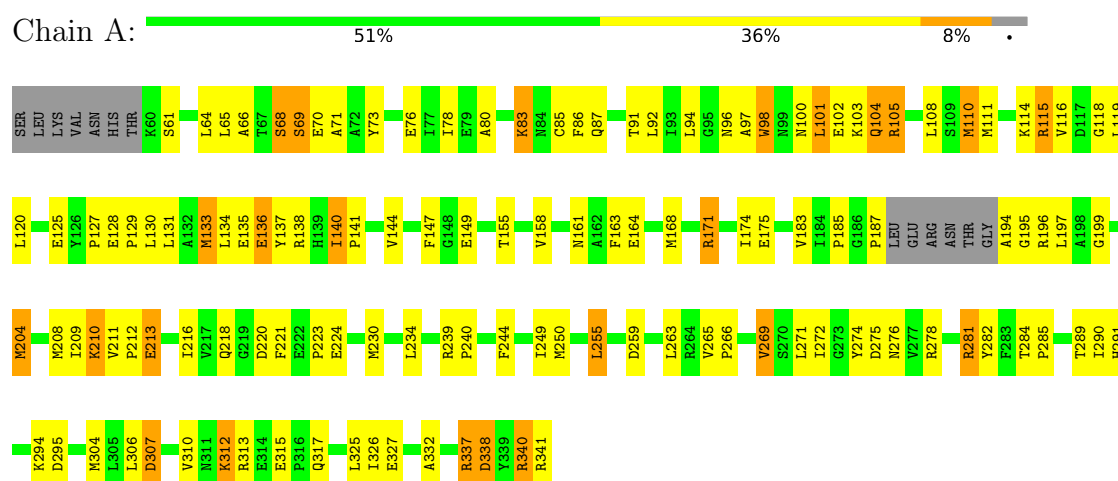
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	59	Total	O	0	0
			59	59		

3 Residue-property plots [i](#)

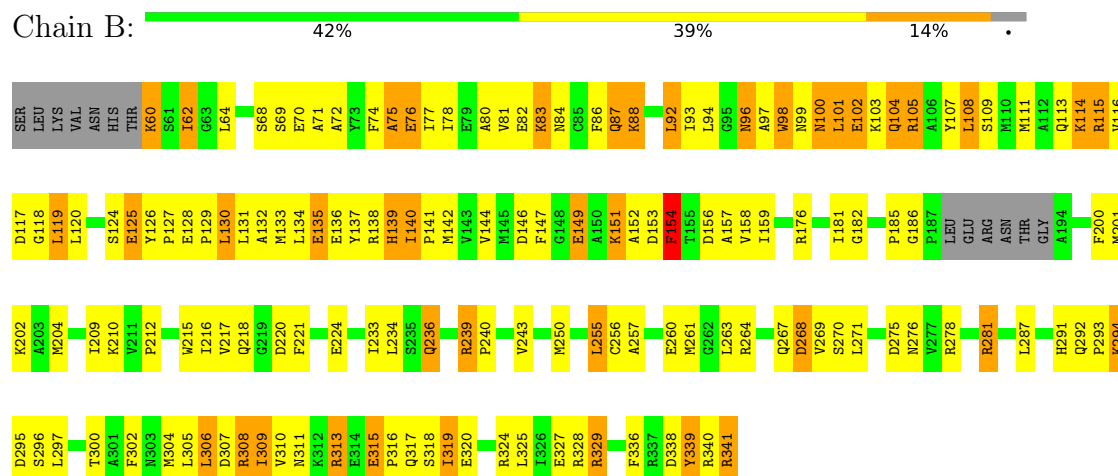
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR



• Molecule 1: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.02Å 126.13Å 61.84Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4489	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.55	0/2212	0.65	1/2984 (0.0%)
1	B	0.51	0/2212	0.63	1/2984 (0.0%)
All	All	0.53	0/4424	0.64	2/5968 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLY	C-N-CD	-6.39	106.55	120.60
1	A	195	GLY	N-CA-C	-5.09	100.38	113.10

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	2168	0	2141	112	0
1	B	2168	0	2141	171	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	91	0	0	7	0
3	B	59	0	0	8	0
All	All	4489	0	4282	281	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 33.

All (281) 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:105:ARG:HB2	1:B:105:ARG:HH11	1.19	1.07
1:B:80:ALA:HA	1:B:83:LYS:HE3	1.41	1.02
1:B:119:LEU:HB2	1:B:140:ILE:HD11	1.45	0.96
1:A:185:PRO:HD2	1:A:218:GLN:HA	1.49	0.95
1:A:97:ALA:HB1	1:A:104:GLN:HG2	1.47	0.94
1:A:80:ALA:HA	1:A:83:LYS:NZ	1.84	0.92
1:B:308:ARG:HH22	1:B:316:PRO:HA	1.36	0.90
1:B:313:ARG:HH11	1:B:313:ARG:HB3	1.36	0.90
1:B:115:ARG:HH11	1:B:115:ARG:HB3	1.38	0.89
1:B:140:ILE:HD12	1:B:141:PRO:HD2	1.55	0.87
1:A:80:ALA:HA	1:A:83:LYS:HZ3	1.40	0.83
1:B:340:ARG:HG3	1:B:340:ARG:HH11	1.45	0.82
1:B:313:ARG:HB3	1:B:313:ARG:NH1	1.95	0.81
1:B:101:LEU:CD1	1:B:105:ARG:HH12	1.93	0.80
1:B:115:ARG:HB3	1:B:115:ARG:NH1	1.96	0.79
1:A:304:MET:HG2	1:A:313:ARG:NH2	1.98	0.79
1:B:76:GLU:HB2	1:B:294:LYS:HZ3	1.47	0.78
1:B:151:LYS:HD3	1:B:153:ASP:OD2	1.83	0.78
1:B:105:ARG:HH11	1:B:105:ARG:CB	1.96	0.78
1:B:118:GLY:HA2	1:B:141:PRO:HG2	1.67	0.76
1:A:230:MET:HG3	1:A:234:LEU:HD12	1.66	0.75
1:A:68:SER:HB3	1:A:71:ALA:HB2	1.68	0.75
1:A:337:ARG:HG3	1:A:338:ASP:N	2.01	0.75
1:A:76:GLU:OE1	1:A:294:LYS:HE2	1.86	0.74
1:B:132:ALA:O	1:B:135:GLU:HB2	1.88	0.73
1:A:340:ARG:HD2	1:A:341:ARG:H	1.53	0.73
1:B:71:ALA:O	1:B:75:ALA:HB2	1.88	0.73
1:B:62:ILE:HG13	1:B:118:GLY:O	1.89	0.72
1:A:266:PRO:HA	1:A:269:VAL:O	1.89	0.72
1:A:304:MET:HG2	1:A:313:ARG:HH22	1.55	0.72
1:A:340:ARG:CD	1:A:341:ARG:H	2.03	0.72
1:A:140:ILE:HD12	1:A:141:PRO:HD2	1.71	0.70
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.57	0.70
1:B:159:ILE:HB	1:B:320:GLU:HG3	1.73	0.70
1:B:340:ARG:HG3	1:B:340:ARG:NH1	2.06	0.70
1:A:187:PRO:HD2	1:A:221:PHE:CE2	2.27	0.70
1:B:62:ILE:HD11	1:B:118:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD13	1:B:105:ARG:HH12	1.56	0.70
1:A:115:ARG:HB3	1:A:115:ARG:HH11	1.57	0.69
1:B:305:LEU:O	1:B:309:ILE:HG22	1.92	0.69
1:A:223:PRO:HD3	1:A:249:ILE:CG2	2.22	0.69
1:B:80:ALA:O	1:B:83:LYS:HG3	1.92	0.69
1:B:102:GLU:O	1:B:105:ARG:HB3	1.93	0.69
1:B:119:LEU:HB3	1:B:142:MET:HB3	1.76	0.68
1:B:128:GLU:N	1:B:129:PRO:HD2	2.08	0.68
1:B:239:ARG:HD2	3:B:409:HOH:O	1.92	0.68
1:B:264:ARG:HB2	1:B:268:ASP:OD1	1.93	0.68
1:B:137:TYR:HA	1:B:139:HIS:NE2	2.09	0.67
1:A:271:LEU:HD12	1:A:272:ILE:N	2.09	0.67
1:B:130:LEU:O	1:B:134:LEU:HG	1.95	0.67
1:A:110:MET:CE	1:A:114:LYS:HG3	2.25	0.67
1:B:126:TYR:N	1:B:127:PRO:HD3	2.10	0.67
1:B:119:LEU:O	1:B:142:MET:HA	1.95	0.66
1:A:100:ASN:O	1:A:104:GLN:HG3	1.96	0.66
1:B:308:ARG:HG3	1:B:313:ARG:O	1.96	0.66
1:B:267:GLN:NE2	1:B:267:GLN:H	1.94	0.65
1:B:125:GLU:HB3	1:B:127:PRO:HD3	1.77	0.65
1:B:140:ILE:O	1:B:140:ILE:HG13	1.94	0.65
1:B:243:VAL:HB	1:B:271:LEU:HD12	1.78	0.65
1:A:110:MET:HE3	1:A:114:LYS:HG3	1.79	0.65
1:A:100:ASN:OD1	1:A:102:GLU:HB2	1.97	0.65
1:A:110:MET:HG3	1:A:111:MET:N	2.11	0.64
1:A:135:GLU:O	1:A:138:ARG:HG3	1.97	0.64
1:B:101:LEU:O	1:B:101:LEU:HD22	1.97	0.64
1:A:315:GLU:HA	3:A:482:HOH:O	1.97	0.64
1:A:171:ARG:HD3	3:A:455:HOH:O	1.97	0.63
1:B:315:GLU:HG3	3:B:435:HOH:O	1.97	0.63
1:B:126:TYR:HB3	1:B:131:LEU:CD1	2.29	0.63
1:B:304:MET:SD	1:B:317:GLN:HB2	2.38	0.63
1:B:80:ALA:CA	1:B:83:LYS:HE3	2.22	0.63
1:B:306:LEU:HD13	1:B:306:LEU:N	2.14	0.63
1:B:233:ILE:O	1:B:236:GLN:HG3	1.98	0.62
1:A:174:ILE:HD11	1:A:204:MET:CE	2.30	0.62
1:A:194:ALA:HB3	1:A:196:ARG:HG2	1.82	0.62
1:B:308:ARG:NH2	1:B:316:PRO:HA	2.12	0.62
1:B:115:ARG:HH11	1:B:115:ARG:CB	2.10	0.61
1:B:76:GLU:HB2	1:B:294:LYS:NZ	2.14	0.61
1:A:271:LEU:HD12	1:A:272:ILE:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:OH	1:B:224:GLU:HG3	2.00	0.61
1:A:239:ARG:HB2	1:A:240:PRO:HD2	1.82	0.61
1:A:168:MET:HE3	1:A:325:LEU:HB2	1.81	0.61
1:B:139:HIS:H	1:B:139:HIS:CD2	2.18	0.61
1:A:80:ALA:HA	1:A:83:LYS:HZ1	1.64	0.60
1:A:194:ALA:N	1:A:197:LEU:HB3	2.17	0.60
1:B:204:MET:HE1	1:B:209:ILE:HG21	1.83	0.60
1:B:302:PHE:CZ	1:B:306:LEU:HD21	2.37	0.60
1:B:306:LEU:O	1:B:309:ILE:HG23	2.01	0.60
1:B:313:ARG:HD2	3:B:435:HOH:O	2.00	0.60
1:A:168:MET:HE1	1:A:325:LEU:N	2.17	0.60
1:A:291:HIS:HB2	1:A:326:ILE:HD12	1.83	0.60
1:B:105:ARG:HD3	1:B:133:MET:SD	2.42	0.60
1:A:168:MET:HE2	1:A:290:ILE:HD12	1.85	0.59
1:B:77:ILE:O	1:B:81:VAL:HG23	2.02	0.59
1:B:135:GLU:O	1:B:138:ARG:HB2	2.03	0.58
1:A:149:GLU:CD	1:A:149:GLU:H	2.07	0.58
1:B:101:LEU:HD11	1:B:105:ARG:HH12	1.66	0.58
1:B:153:ASP:O	1:B:154:PHE:HB3	2.03	0.58
1:B:329:ARG:NH1	1:B:329:ARG:HG3	2.17	0.58
1:A:83:LYS:NZ	1:A:83:LYS:HB3	2.15	0.58
1:A:161:ASN:HB3	1:A:164:GLU:HG2	1.84	0.57
1:B:119:LEU:O	1:B:305:LEU:HD11	2.05	0.57
1:B:159:ILE:CG2	1:B:320:GLU:HG3	2.35	0.57
1:B:100:ASN:ND2	1:B:103:LYS:HB2	2.19	0.57
1:B:147:PHE:CD2	1:B:158:VAL:HG11	2.39	0.57
1:B:310:VAL:HG13	1:B:311:ASN:N	2.20	0.57
1:A:144:VAL:CG2	1:A:155:THR:HG22	2.35	0.57
1:B:126:TYR:HB3	1:B:131:LEU:HD13	1.86	0.57
1:B:256:CYS:O	1:B:260:GLU:HG3	2.04	0.57
1:A:211:VAL:HG22	1:A:216:ILE:HD11	1.87	0.57
1:A:135:GLU:HA	1:A:138:ARG:CG	2.35	0.56
1:A:213:GLU:HA	1:A:213:GLU:OE2	2.05	0.56
1:B:307:ASP:OD1	1:B:313:ARG:HB2	2.06	0.56
1:B:107:TYR:O	1:B:111:MET:HG3	2.05	0.56
1:B:147:PHE:HA	1:B:158:VAL:HG13	1.88	0.56
1:B:149:GLU:O	1:B:149:GLU:HG3	2.07	0.55
1:B:212:PRO:HD2	1:B:215:TRP:CE3	2.42	0.55
1:B:267:GLN:H	1:B:267:GLN:CD	2.10	0.55
1:A:211:VAL:CG2	1:A:216:ILE:HD11	2.37	0.55
1:B:100:ASN:HD22	1:B:103:LYS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HB2	1:B:105:ARG:NH1	2.04	0.55
1:B:120:LEU:HD12	1:B:305:LEU:HD22	1.88	0.55
1:B:340:ARG:HG2	3:B:446:HOH:O	2.05	0.55
1:B:234:LEU:CB	1:B:261:MET:HE1	2.37	0.55
1:B:220:ASP:O	1:B:221:PHE:HB2	2.07	0.54
1:B:329:ARG:HG3	1:B:329:ARG:HH11	1.72	0.54
1:B:159:ILE:CB	1:B:320:GLU:HG3	2.36	0.54
1:B:146:ASP:HB3	1:B:157:ALA:HA	1.90	0.54
1:B:152:ALA:HA	3:B:431:HOH:O	2.08	0.54
1:B:255:LEU:HD13	1:B:271:LEU:HD22	1.89	0.54
1:B:185:PRO:HD2	1:B:218:GLN:HA	1.91	0.53
1:A:83:LYS:HZ3	1:A:83:LYS:HB3	1.74	0.53
1:A:307:ASP:O	1:A:312:LYS:HB2	2.09	0.52
1:B:100:ASN:ND2	1:B:103:LYS:H	2.08	0.52
1:B:276:ASN:HD22	1:B:291:HIS:CD2	2.28	0.52
1:A:102:GLU:HG2	3:A:452:HOH:O	2.10	0.52
1:A:249:ILE:HB	3:A:404:HOH:O	2.09	0.52
1:A:259:ASP:HB3	3:A:446:HOH:O	2.09	0.52
1:A:97:ALA:CB	1:A:104:GLN:HG2	2.30	0.52
1:A:340:ARG:O	1:A:341:ARG:HB2	2.09	0.52
1:B:158:VAL:HG23	1:B:319:ILE:O	2.08	0.52
1:A:66:ALA:O	1:A:96:ASN:HA	2.10	0.52
1:B:147:PHE:HA	1:B:158:VAL:CG1	2.40	0.52
1:B:64:LEU:HD21	1:B:78:ILE:HG23	1.91	0.52
1:B:80:ALA:HA	1:B:83:LYS:HG2	1.92	0.52
1:A:337:ARG:O	1:A:338:ASP:HB2	2.10	0.51
1:A:105:ARG:HB2	1:A:133:MET:SD	2.50	0.51
1:B:159:ILE:N	1:B:159:ILE:HD12	2.25	0.51
1:B:119:LEU:CB	1:B:140:ILE:HD11	2.29	0.51
1:A:65:LEU:HD11	1:A:97:ALA:HB2	1.92	0.51
1:B:329:ARG:HH11	1:B:329:ARG:CG	2.22	0.51
1:A:101:LEU:HD13	1:A:133:MET:CE	2.41	0.51
1:A:220:ASP:O	1:A:221:PHE:HB2	2.11	0.51
1:A:310:VAL:O	1:A:310:VAL:HG23	2.10	0.50
1:A:101:LEU:HD13	1:A:133:MET:HE1	1.93	0.50
1:B:264:ARG:HB3	1:B:267:GLN:HE21	1.75	0.50
1:A:196:ARG:NH1	1:A:274:TYR:CD1	2.80	0.50
1:B:100:ASN:O	1:B:104:GLN:HG3	2.11	0.50
1:B:119:LEU:HB3	1:B:142:MET:CB	2.40	0.50
1:B:119:LEU:N	1:B:140:ILE:HD11	2.27	0.50
1:B:185:PRO:HD2	1:B:217:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD12	1:A:141:PRO:CD	2.39	0.49
1:B:201:MET:HE2	1:B:201:MET:N	2.27	0.49
1:A:105:ARG:HH11	1:A:105:ARG:CG	2.23	0.49
1:A:168:MET:CE	1:A:325:LEU:HB2	2.43	0.49
1:A:340:ARG:CG	1:A:341:ARG:H	2.24	0.49
1:B:313:ARG:HB3	3:B:435:HOH:O	2.12	0.49
1:B:239:ARG:HB2	1:B:240:PRO:HD2	1.95	0.48
1:B:257:ALA:O	1:B:261:MET:HG3	2.13	0.48
1:A:101:LEU:O	1:A:105:ARG:HB3	2.14	0.48
1:A:291:HIS:HB2	1:A:326:ILE:CD1	2.42	0.48
1:B:200:PHE:HD2	1:B:201:MET:CE	2.26	0.48
1:B:130:LEU:HD22	1:B:134:LEU:HD21	1.95	0.48
1:B:341:ARG:HD2	1:B:341:ARG:HA	1.57	0.48
1:B:276:ASN:HD22	1:B:291:HIS:HD2	1.60	0.48
1:A:290:ILE:CD1	1:A:325:LEU:HD23	2.44	0.48
1:A:118:GLY:CA	1:A:140:ILE:HD11	2.44	0.47
1:B:80:ALA:HA	1:B:83:LYS:CG	2.44	0.47
1:B:234:LEU:CD1	1:B:261:MET:HE1	2.44	0.47
1:B:76:GLU:H	1:B:294:LYS:HZ1	1.62	0.47
1:A:223:PRO:HG2	3:B:433:HOH:O	2.13	0.47
1:A:326:ILE:O	1:A:326:ILE:HG22	2.14	0.47
1:B:84:ASN:HA	1:B:87:GLN:HE21	1.79	0.47
1:A:209:ILE:C	1:A:210:LYS:HD2	2.35	0.47
1:B:98:TRP:O	1:B:99:ASN:HB2	2.14	0.47
1:B:119:LEU:CD2	1:B:120:LEU:H	2.27	0.47
1:A:281:ARG:O	1:A:281:ARG:HD3	2.14	0.47
1:B:102:GLU:HA	1:B:102:GLU:OE1	2.14	0.47
1:A:115:ARG:HH11	1:A:115:ARG:CB	2.26	0.47
1:B:339:TYR:O	1:B:340:ARG:HG2	2.15	0.47
1:A:97:ALA:O	1:A:98:TRP:HB2	2.14	0.47
1:B:126:TYR:HB3	1:B:131:LEU:HD11	1.97	0.47
1:B:158:VAL:C	1:B:159:ILE:HD12	2.34	0.47
1:B:338:ASP:O	1:B:339:TYR:HB3	2.14	0.47
1:A:128:GLU:HB2	1:A:129:PRO:HD3	1.98	0.46
1:A:265:VAL:HA	1:A:269:VAL:O	2.14	0.46
1:A:221:PHE:HA	1:A:250:MET:HG3	1.95	0.46
1:A:284:THR:HA	1:A:285:PRO:HA	1.82	0.46
1:B:68:SER:HB3	1:B:71:ALA:HB2	1.96	0.46
1:B:307:ASP:OD1	1:B:313:ARG:HG3	2.16	0.46
1:A:325:LEU:CD1	1:A:327:GLU:HG3	2.46	0.46
1:A:133:MET:HA	1:A:136:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:PHE:C	1:B:338:ASP:H	2.18	0.46
1:A:105:ARG:HD2	3:A:465:HOH:O	2.15	0.46
1:B:88:LYS:HD2	1:B:88:LYS:N	2.31	0.46
1:B:130:LEU:CD2	1:B:134:LEU:HD21	2.46	0.45
1:A:304:MET:CG	1:A:313:ARG:HH22	2.28	0.45
1:B:74:PHE:O	1:B:78:ILE:HD12	2.15	0.45
1:B:158:VAL:HG21	1:B:297:LEU:HD11	1.97	0.45
1:B:310:VAL:CG1	1:B:311:ASN:N	2.79	0.45
1:B:62:ILE:CD1	1:B:118:GLY:HA3	2.43	0.45
1:B:261:MET:CE	1:B:263:LEU:HD12	2.46	0.45
1:B:159:ILE:N	1:B:159:ILE:CD1	2.80	0.45
1:A:340:ARG:CG	1:A:341:ARG:N	2.79	0.45
1:B:308:ARG:HH22	1:B:316:PRO:CA	2.19	0.45
1:A:86:PHE:CG	1:B:96:ASN:HB3	2.52	0.45
1:B:102:GLU:HG3	3:B:442:HOH:O	2.17	0.45
1:B:287:LEU:O	1:B:328:ARG:HD2	2.16	0.45
1:A:290:ILE:HD13	1:A:325:LEU:HD23	1.98	0.45
1:B:104:GLN:O	1:B:108:LEU:HB2	2.16	0.45
1:A:204:MET:CE	1:A:204:MET:HA	2.47	0.44
3:A:473:HOH:O	1:B:329:ARG:HG2	2.17	0.44
1:B:325:LEU:HD11	1:B:327:GLU:HG3	1.98	0.44
1:A:73:TYR:HE2	1:A:147:PHE:CE2	2.36	0.44
1:A:174:ILE:HD11	1:A:204:MET:HE3	1.99	0.44
1:A:127:PRO:HB2	1:A:129:PRO:HD2	2.00	0.44
1:B:62:ILE:HD12	1:B:117:ASP:O	2.17	0.44
1:B:86:PHE:N	1:B:86:PHE:CD1	2.84	0.44
1:A:118:GLY:HA2	1:A:140:ILE:HD11	2.00	0.44
1:A:135:GLU:HA	1:A:138:ARG:HG3	1.98	0.44
1:B:113:GLN:C	1:B:115:ARG:H	2.20	0.44
1:A:69:SER:HA	1:A:78:ILE:CD1	2.47	0.44
1:A:105:ARG:CG	1:A:105:ARG:NH1	2.80	0.44
1:A:276:ASN:ND2	1:A:326:ILE:HD13	2.33	0.44
1:B:93:ILE:HD12	1:B:116:VAL:HG12	2.00	0.43
1:A:83:LYS:NZ	1:A:83:LYS:CB	2.80	0.43
1:B:105:ARG:NH1	1:B:133:MET:SD	2.91	0.43
1:B:281:ARG:O	1:B:281:ARG:HD3	2.18	0.43
1:A:128:GLU:N	1:A:129:PRO:CD	2.81	0.43
1:A:266:PRO:HG2	1:A:332:ALA:HB2	2.01	0.43
1:B:72:ALA:CB	1:B:221:PHE:HB3	2.49	0.43
1:B:126:TYR:N	1:B:127:PRO:CD	2.80	0.42
1:B:114:LYS:N	1:B:114:LYS:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.86	0.42
1:A:249:ILE:HA	1:A:249:ILE:HD13	1.81	0.42
1:B:111:MET:O	1:B:116:VAL:HG22	2.20	0.42
1:A:211:VAL:HA	1:A:212:PRO:HD2	1.89	0.42
1:A:276:ASN:HA	1:A:289:THR:HG21	2.01	0.42
1:B:76:GLU:HB3	1:B:295:ASP:OD1	2.20	0.42
1:B:97:ALA:O	1:B:98:TRP:HD1	2.03	0.42
1:B:181:ILE:HG22	1:B:182:GLY:N	2.34	0.42
1:A:144:VAL:HG21	1:A:155:THR:HG22	2.02	0.42
1:B:105:ARG:HH11	1:B:105:ARG:CG	2.31	0.41
1:B:119:LEU:HD23	1:B:120:LEU:H	1.85	0.41
1:A:111:MET:O	1:A:116:VAL:HG22	2.21	0.41
1:B:69:SER:HA	1:B:78:ILE:HD13	2.00	0.41
1:B:108:LEU:HA	1:B:108:LEU:HD13	1.79	0.41
1:B:149:GLU:CD	1:B:151:LYS:HG2	2.41	0.41
1:A:223:PRO:HD3	1:A:249:ILE:HG22	2.00	0.41
1:B:60:LYS:HB3	1:B:117:ASP:OD2	2.20	0.41
1:B:300:THR:HG21	1:B:319:ILE:CG2	2.50	0.41
1:A:110:MET:HE1	1:A:114:LYS:HG3	2.02	0.41
1:A:255:LEU:HD13	1:A:271:LEU:HD23	2.03	0.41
1:B:78:ILE:O	1:B:82:GLU:HG3	2.20	0.41
1:A:161:ASN:O	1:A:164:GLU:HG2	2.20	0.41
1:A:244:PHE:HD1	1:A:272:ILE:HG23	1.86	0.41
1:B:104:GLN:O	1:B:108:LEU:HD23	2.21	0.41
1:B:119:LEU:CD2	1:B:120:LEU:N	2.84	0.41
1:B:126:TYR:HA	1:B:130:LEU:HD12	2.03	0.41
1:B:302:PHE:CE2	1:B:306:LEU:HD21	2.55	0.41
1:B:119:LEU:HB2	1:B:140:ILE:CD1	2.34	0.40
1:B:62:ILE:HG12	1:B:305:LEU:CD2	2.51	0.40
1:B:128:GLU:N	1:B:129:PRO:CD	2.79	0.40
1:B:146:ASP:O	1:B:157:ALA:HA	2.22	0.40
1:B:201:MET:HE2	1:B:201:MET:CA	2.50	0.40
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.87	0.40
1:A:163:PHE:CE2	1:A:199:GLY:HA2	2.56	0.40
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.86	0.40
1:A:137:TYR:O	1:A:140:ILE:HG23	2.21	0.40
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.88	0.40
1:B:119:LEU:HD22	1:B:120:LEU:N	2.35	0.40
1:B:200:PHE:O	1:B:204:MET:HG2	2.22	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	272/289 (94%)	253 (93%)	16 (6%)	3 (1%)	14	20
1	B	272/289 (94%)	234 (86%)	31 (11%)	7 (3%)	5	5
All	All	544/578 (94%)	487 (90%)	47 (9%)	10 (2%)	8	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
1	B	154	PHE
1	B	275	ASP
1	A	275	ASP
1	A	340	ARG
1	B	339	TYR
1	B	296	SER
1	B	75	ALA
1	B	293	PRO
1	B	114	LYS

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	226/238 (95%)	179 (79%)	47 (21%)	1	1
1	B	226/238 (95%)	169 (75%)	57 (25%)	0	0
All	All	452/476 (95%)	348 (77%)	104 (23%)	1	1

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	64	LEU
1	A	68	SER
1	A	69	SER
1	A	70	GLU
1	A	83	LYS
1	A	85	CYS
1	A	87	GLN
1	A	91	THR
1	A	92	LEU
1	A	94	LEU
1	A	98	TRP
1	A	101	LEU
1	A	103	LYS
1	A	104	GLN
1	A	105	ARG
1	A	108	LEU
1	A	110	MET
1	A	115	ARG
1	A	119	LEU
1	A	120	LEU
1	A	125	GLU
1	A	130	LEU
1	A	131	LEU
1	A	133	MET
1	A	136	GLU
1	A	140	ILE
1	A	158	VAL
1	A	171	ARG
1	A	175	GLU
1	A	183	VAL
1	A	204	MET
1	A	208	MET
1	A	210	LYS
1	A	213	GLU
1	A	224	GLU
1	A	255	LEU
1	A	263	LEU
1	A	269	VAL
1	A	278	ARG
1	A	281	ARG
1	A	295	ASP

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Mol	Chain	Res	Type
1	A	306	LEU
1	A	307	ASP
1	A	312	LYS
1	A	317	GLN
1	A	337	ARG
1	B	60	LYS
1	B	62	ILE
1	B	70	GLU
1	B	76	GLU
1	B	83	LYS
1	B	87	GLN
1	B	88	LYS
1	B	92	LEU
1	B	94	LEU
1	B	96	ASN
1	B	98	TRP
1	B	100	ASN
1	B	101	LEU
1	B	102	GLU
1	B	104	GLN
1	B	105	ARG
1	B	108	LEU
1	B	109	SER
1	B	115	ARG
1	B	119	LEU
1	B	124	SER
1	B	125	GLU
1	B	130	LEU
1	B	135	GLU
1	B	136	GLU
1	B	139	HIS
1	B	140	ILE
1	B	144	VAL
1	B	149	GLU
1	B	151	LYS
1	B	154	PHE
1	B	156	ASP
1	B	176	ARG
1	B	202	LYS
1	B	210	LYS
1	B	216	ILE
1	B	236	GLN

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Mol	Chain	Res	Type
1	B	239	ARG
1	B	250	MET
1	B	255	LEU
1	B	268	ASP
1	B	269	VAL
1	B	270	SER
1	B	278	ARG
1	B	281	ARG
1	B	292	GLN
1	B	294	LYS
1	B	306	LEU
1	B	308	ARG
1	B	309	ILE
1	B	313	ARG
1	B	315	GLU
1	B	318	SER
1	B	319	ILE
1	B	324	ARG
1	B	329	ARG
1	B	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	99	ASN
1	A	104	GLN
1	B	84	ASN
1	B	87	GLN
1	B	100	ASN
1	B	139	HIS
1	B	236	GLN
1	B	267	GLN
1	B	291	HIS
1	B	303	ASN
1	B	311	ASN

5.3.3 RNA ⓘ

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 monosaccharides 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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.