



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:26 PM GMT

PDB ID : 1IRX  
Title : Crystal structure of class I lysyl-tRNA synthetase  
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Deposited on : 2001-10-25  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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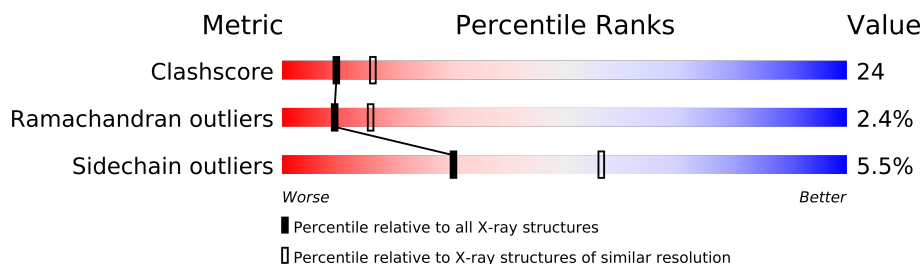
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8754 atoms, of which 0 are hydrogen and 0 are deuterium.

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 lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4247	2738	733	764	12			
1	B	508	Total	C	N	O	S	0	0	0
			4255	2742	734	767	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	LEU	PHE	CONFLICT	UNP O57963
A	331	GLU	ASP	CONFLICT	UNP O57963
B	124	LEU	PHE	CONFLICT	UNP O57963
B	331	GLU	ASP	CONFLICT	UNP O57963

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	102	Total	O	0	0
			102	102		

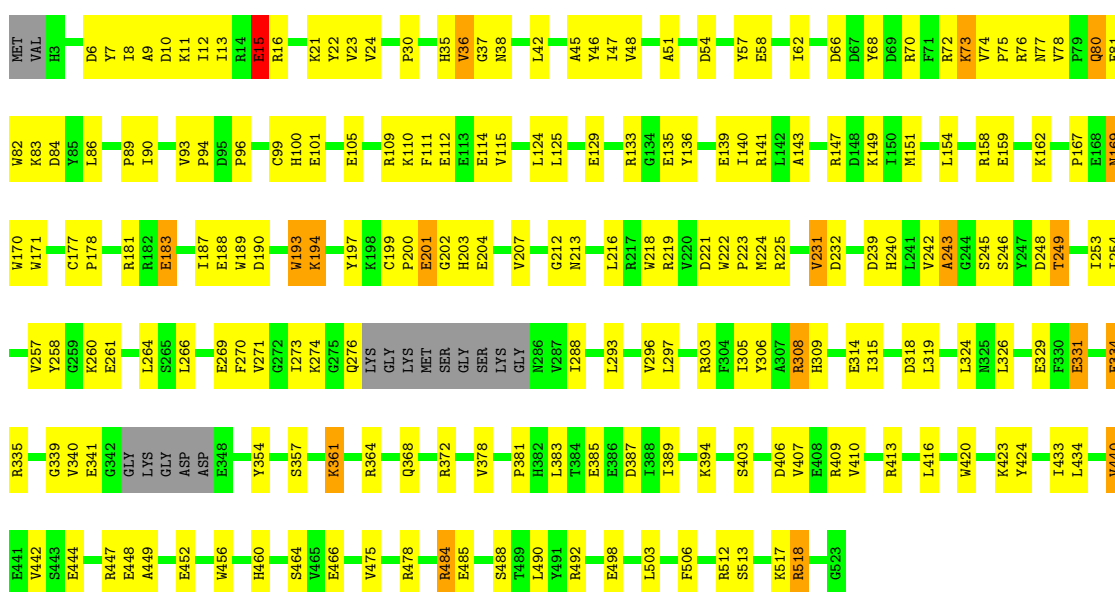
### 3 Residue-property plots

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.

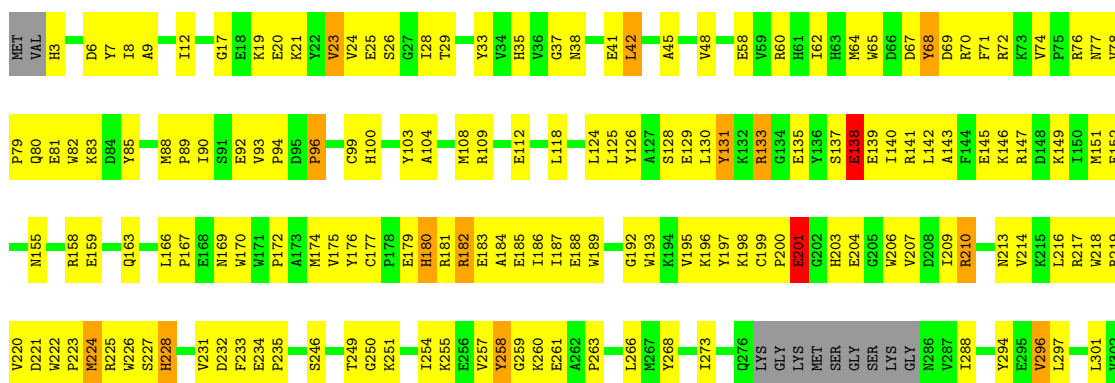
#### • Molecule 1: lysyl-tRNA synthetase

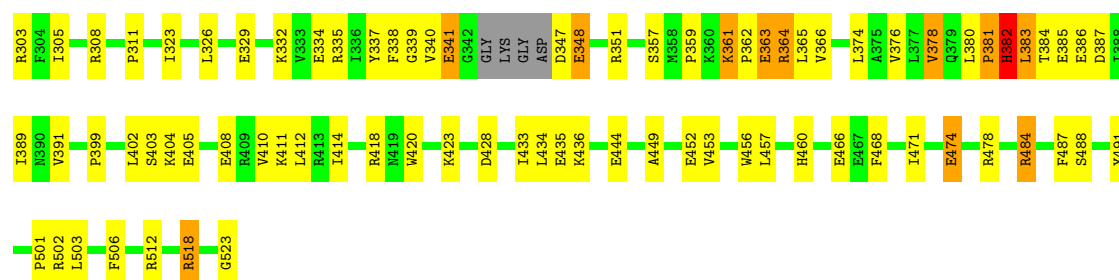
Chain A:



#### • Molecule 1: lysyl-tRNA synthetase

Chain B:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.95Å 74.77Å 156.94Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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: ZN

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	0.40	0/4361	0.60	0/5886
1	B	0.38	0/4369	0.59	0/5897
All	All	0.39	0/8730	0.59	0/11783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4247	0	4181	173	0
1	B	4255	0	4187	239	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	146	0	0	8	0
3	B	102	0	0	10	0
All	All	8754	0	8368	412	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (412) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:361:LYS:HD2	1:A:361:LYS:H	1.21	1.01
1:B:361:LYS:H	1:B:361:LYS:HE3	1.22	1.01
1:A:218:TRP:HZ3	1:A:246:SER:HG	0.99	0.98
1:B:209:ILE:HB	1:B:210:ARG:HH21	1.24	0.97
1:B:89:PRO:HB2	1:B:92:GLU:HG2	1.51	0.93
1:B:435:GLU:O	1:B:436:LYS:HD2	1.72	0.88
1:B:363:GLU:HG2	1:B:364:ARG:HE	1.39	0.88
1:A:35:HIS:HD2	1:A:37:GLY:H	1.20	0.87
1:A:187:ILE:HG22	1:A:188:GLU:HG3	1.58	0.86
1:A:242:VAL:HG23	1:A:245:SER:HB2	1.59	0.85
1:A:70:ARG:HD3	1:A:183:GLU:OE2	1.78	0.84
1:B:218:TRP:HA	1:B:221:ASP:HB3	1.61	0.83
1:A:361:LYS:HD2	1:A:361:LYS:N	1.96	0.81
1:B:124:LEU:O	1:B:125:LEU:HD23	1.80	0.80
1:A:199:CYS:HB3	1:A:203:HIS:HB3	1.63	0.80
1:A:394:LYS:HD2	3:A:657:HOH:O	1.81	0.80
1:A:305:ILE:HD11	1:A:326:LEU:HD21	1.64	0.80
1:B:361:LYS:H	1:B:361:LYS:CE	1.94	0.80
1:B:70:ARG:HH21	1:B:72:ARG:HH11	1.26	0.79
1:B:434:LEU:O	1:B:518:ARG:NH2	2.15	0.79
1:B:209:ILE:HB	1:B:210:ARG:NH2	1.98	0.79
1:B:140:ILE:HG12	1:B:216:LEU:HD11	1.64	0.78
1:B:35:HIS:H	1:B:38:ASN:HD22	1.29	0.78
1:A:331:GLU:CD	1:A:413:ARG:HH12	1.88	0.77
1:B:224:MET:HG3	1:B:225:ARG:H	1.50	0.77
1:B:224:MET:HG3	1:B:225:ARG:N	2.01	0.74
1:A:329:GLU:HB3	3:A:693:HOH:O	1.87	0.74
1:A:203:HIS:CD2	1:A:204:GLU:H	2.06	0.73
1:A:72:ARG:O	1:A:86:LEU:HD22	1.87	0.73
1:B:26:SER:HB2	1:B:41:GLU:HG2	1.71	0.73
1:A:296:VAL:CG2	1:A:420:TRP:HB2	2.18	0.72
1:B:147:ARG:HG3	1:B:172:PRO:HD3	1.72	0.71
1:B:70:ARG:HH21	1:B:72:ARG:NH1	1.89	0.71
1:A:488:SER:O	1:A:492:ARG:HG3	1.91	0.70
1:A:35:HIS:HD2	1:A:37:GLY:N	1.88	0.70
1:B:340:VAL:O	1:B:340:VAL:HG12	1.90	0.70
1:A:136:TYR:O	1:A:140:ILE:HG13	1.91	0.70
1:B:23:VAL:HG13	1:B:231:VAL:HA	1.74	0.69
1:A:296:VAL:HG21	1:A:420:TRP:HB2	1.74	0.69
1:B:70:ARG:HD3	1:B:183:GLU:CD	2.12	0.69
1:B:93:VAL:HG23	1:B:103:TYR:HB3	1.74	0.69
1:A:190:ASP:OD2	1:A:194:LYS:HB2	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:HIS:CD2	1:A:37:GLY:H	2.09	0.69
1:B:410:VAL:O	1:B:414:ILE:HG13	1.93	0.69
1:A:364:ARG:HH11	1:A:364:ARG:HG3	1.58	0.68
1:B:227:SER:HB2	1:B:260:LYS:HG3	1.73	0.68
1:B:35:HIS:N	1:B:38:ASN:HD22	1.91	0.68
1:A:274:LYS:HD2	1:A:318:ASP:HB2	1.76	0.67
1:B:518:ARG:HD3	1:B:523:GLY:O	1.93	0.67
1:A:35:HIS:H	1:A:38:ASN:HD22	1.41	0.67
1:B:137:SER:HB3	3:B:674:HOH:O	1.93	0.67
1:B:74:VAL:O	1:B:74:VAL:HG23	1.95	0.67
1:A:383:LEU:HD22	1:A:387:ASP:HB3	1.75	0.66
1:B:82:TRP:CZ3	1:B:94:PRO:HG2	2.30	0.66
1:A:147:ARG:HD2	1:A:171:TRP:CZ3	2.30	0.66
1:A:82:TRP:CH2	1:A:94:PRO:HB2	2.31	0.66
1:B:210:ARG:HA	3:B:674:HOH:O	1.94	0.66
1:A:218:TRP:HZ3	1:A:246:SER:OG	1.74	0.65
1:B:484:ARG:HH11	1:B:484:ARG:HG2	1.62	0.65
1:B:149:LYS:O	1:B:152:GLU:HG2	1.95	0.65
1:A:72:ARG:HB2	1:A:73:LYS:HD2	1.79	0.64
1:A:484:ARG:HG3	1:A:485:GLU:N	2.11	0.64
1:B:58:GLU:HG2	3:B:617:HOH:O	1.98	0.64
1:B:192:GLY:O	1:B:193:TRP:HB2	1.96	0.64
1:B:209:ILE:CB	1:B:210:ARG:HH21	2.05	0.64
1:B:89:PRO:HG3	1:B:176:TYR:CE1	2.33	0.63
1:B:209:ILE:HA	1:B:214:VAL:HG11	1.80	0.63
1:B:109:ARG:HD3	1:B:112:GLU:OE1	1.98	0.63
1:B:138:GLU:H	1:B:138:GLU:CD	2.02	0.63
1:A:258:TYR:O	1:A:260:LYS:HG2	1.98	0.63
1:A:200:PRO:O	1:A:201:GLU:HB2	1.98	0.63
1:B:147:ARG:HD2	1:B:170:TRP:O	1.99	0.63
1:B:79:PRO:HB2	1:B:82:TRP:CD1	2.34	0.63
1:A:243:ALA:O	1:A:248:ASP:OD1	2.16	0.63
1:A:219:ARG:HD2	1:A:249:THR:HG21	1.81	0.62
1:B:222:TRP:HB3	1:B:223:PRO:HD3	1.80	0.62
1:B:70:ARG:HD3	1:B:183:GLU:OE1	1.99	0.62
1:B:219:ARG:NH1	1:B:249:THR:HG21	2.15	0.62
1:A:464:SER:OG	1:A:466:GLU:HG2	2.00	0.62
1:A:340:VAL:HG12	1:A:340:VAL:O	1.99	0.62
1:B:226:TRP:HA	1:B:231:VAL:HG12	1.82	0.62
1:B:90:ILE:HG22	1:B:104:ALA:HB2	1.82	0.62
1:B:361:LYS:N	1:B:361:LYS:HE3	2.05	0.62
1:B:35:HIS:CD2	1:B:37:GLY:H	2.19	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:24:VAL:HG12	1:B:45:ALA:HB1	1.83	0.61
1:A:100:HIS:CD2	1:A:109:ARG:HG3	2.36	0.61
1:A:334:GLU:HG3	1:A:354:TYR:CE1	2.36	0.60
1:A:216:LEU:O	1:A:221:ASP:HB2	2.00	0.60
1:B:217:ARG:HA	1:B:217:ARG:HH11	1.65	0.60
1:A:169:ASN:ND2	1:A:169:ASN:H	1.99	0.60
1:A:9:ALA:O	1:A:13:ILE:HG12	2.02	0.60
1:B:6:ASP:O	1:B:9:ALA:HB3	2.02	0.60
1:B:209:ILE:HG23	1:B:214:VAL:HG11	1.83	0.60
1:A:288:ILE:N	1:A:288:ILE:HD12	2.17	0.60
1:A:110:LYS:O	1:A:114:GLU:HG3	2.02	0.59
1:B:109:ARG:HA	1:B:112:GLU:OE1	2.03	0.59
1:A:303:ARG:HD2	1:A:357:SER:O	2.02	0.59
1:B:108:MET:O	1:B:112:GLU:HG3	2.03	0.58
1:A:512:ARG:HH11	1:A:512:ARG:HG2	1.68	0.58
1:A:89:PRO:O	1:A:93:VAL:HG23	2.03	0.58
1:A:169:ASN:HD22	1:A:169:ASN:H	1.50	0.58
1:A:361:LYS:CD	1:A:361:LYS:H	1.93	0.58
1:A:444:GLU:O	1:A:448:GLU:HG3	2.03	0.58
1:B:67:ASP:OD2	1:B:126:TYR:HB3	2.04	0.58
1:A:82:TRP:HH2	1:A:94:PRO:C	2.07	0.58
1:A:8:ILE:O	1:A:12:ILE:HG13	2.04	0.58
1:A:361:LYS:HB3	1:A:361:LYS:NZ	2.20	0.57
1:B:21:LYS:HE2	1:B:60:ARG:HB2	1.86	0.57
1:A:181:ARG:HH12	1:A:213:ASN:ND2	2.02	0.57
1:A:213:ASN:HD22	1:A:213:ASN:N	2.01	0.57
1:A:154:LEU:O	1:A:158:ARG:HG3	2.05	0.57
1:B:435:GLU:C	1:B:436:LYS:HD2	2.23	0.57
1:B:3:HIS:N	3:B:660:HOH:O	2.37	0.56
1:B:423:LYS:HB2	3:B:680:HOH:O	2.05	0.56
1:B:79:PRO:HD2	1:B:96:PRO:HB3	1.86	0.56
1:B:146:LYS:CE	1:B:149:LYS:HG3	2.36	0.55
1:A:331:GLU:HB3	1:A:335:ARG:HH12	1.71	0.55
1:A:112:GLU:OE2	1:A:124:LEU:HD13	2.06	0.55
1:B:231:VAL:O	1:B:263:PRO:HB3	2.06	0.55
1:B:93:VAL:CG2	1:B:103:TYR:HB3	2.37	0.55
1:B:340:VAL:O	1:B:341:GLU:HB2	2.07	0.55
1:A:219:ARG:CD	1:A:249:THR:HG21	2.35	0.55
1:A:73:LYS:H	1:A:73:LYS:HD2	1.72	0.55
1:B:100:HIS:NE2	1:B:109:ARG:HG3	2.22	0.55
1:A:219:ARG:HH11	1:A:249:THR:HG21	1.72	0.55
1:A:24:VAL:HG12	1:A:45:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:GLU:HG2	1:B:364:ARG:NE	2.16	0.55
1:B:141:ARG:HG3	1:B:141:ARG:HH11	1.72	0.55
1:A:169:ASN:HD22	1:A:169:ASN:N	2.05	0.54
1:B:363:GLU:CG	1:B:364:ARG:HE	2.16	0.54
1:B:308:ARG:HH12	1:B:329:GLU:CD	2.11	0.54
1:B:303:ARG:HD2	1:B:357:SER:O	2.08	0.54
1:A:385:GLU:O	1:A:389:ILE:HG13	2.07	0.54
1:B:82:TRP:CH2	1:B:94:PRO:HG2	2.43	0.54
1:B:20:GLU:OE2	1:B:20:GLU:HA	2.07	0.54
1:B:60:ARG:O	1:B:60:ARG:HG3	2.09	0.53
1:B:135:GLU:HG2	1:B:228:HIS:CE1	2.43	0.53
1:B:133:ARG:HH11	1:B:133:ARG:HB3	1.73	0.53
1:B:158:ARG:HE	1:B:166:LEU:CD2	2.22	0.53
1:B:85:TYR:O	1:B:88:MET:HG2	2.09	0.53
1:B:146:LYS:HE3	1:B:149:LYS:HG3	1.90	0.53
1:B:376:VAL:HG21	1:B:501:PRO:HB3	1.91	0.53
1:A:30:PRO:HG2	1:A:90:ILE:HD12	1.90	0.53
1:B:457:LEU:O	1:B:512:ARG:NH1	2.42	0.53
1:B:218:TRP:HH2	1:B:246:SER:HG	1.55	0.53
1:B:224:MET:CE	1:B:228:HIS:HB2	2.38	0.52
1:B:104:ALA:O	1:B:108:MET:HG3	2.09	0.52
1:B:80:GLN:HG3	1:B:81:GLU:H	1.74	0.52
1:B:129:GLU:C	1:B:131:TYR:H	2.12	0.52
1:B:35:HIS:HB2	1:B:288:ILE:O	2.10	0.52
1:A:73:LYS:N	1:A:73:LYS:HD2	2.23	0.52
1:B:25:GLU:HG2	1:B:26:SER:N	2.25	0.52
1:A:490:LEU:HD13	1:A:503:LEU:HD21	1.92	0.52
1:B:137:SER:C	1:B:139:GLU:H	2.13	0.52
1:A:42:LEU:HD23	1:A:42:LEU:C	2.31	0.52
1:B:364:ARG:HD2	1:B:364:ARG:H	1.74	0.52
1:B:90:ILE:HG23	1:B:103:TYR:HD2	1.74	0.52
1:B:382:HIS:ND1	1:B:382:HIS:N	2.58	0.52
1:A:147:ARG:HG2	1:A:151:MET:HE2	1.92	0.52
1:B:187:ILE:HG23	1:B:188:GLU:HG2	1.92	0.52
1:B:201:GLU:OE1	1:B:203:HIS:HB2	2.10	0.51
1:B:78:VAL:HG13	1:B:96:PRO:HG2	1.92	0.51
1:A:101:GLU:HB2	1:A:105:GLU:OE2	2.11	0.51
1:A:403:SER:O	1:A:407:VAL:HG23	2.10	0.51
1:B:135:GLU:HG2	1:B:228:HIS:HE1	1.76	0.51
1:A:254:ILE:HG12	1:A:260:LYS:HB2	1.92	0.51
1:B:181:ARG:O	1:B:182:ARG:O	2.28	0.51
1:A:447:ARG:HG3	3:A:647:HOH:O	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:TRP:CZ3	1:A:246:SER:HB3	2.45	0.51
1:B:206:TRP:O	1:B:207:VAL:HG13	2.11	0.51
1:B:65:TRP:HE1	1:B:124:LEU:HD22	1.74	0.51
1:B:223:PRO:HG3	1:B:250:GLY:CA	2.41	0.51
1:B:28:ILE:HG22	1:B:29:THR:N	2.26	0.51
1:B:484:ARG:O	1:B:488:SER:HB2	2.11	0.50
1:A:218:TRP:CZ3	1:A:246:SER:OG	2.57	0.50
1:B:334:GLU:HG2	1:B:365:LEU:HD13	1.94	0.50
1:B:133:ARG:HH11	1:B:133:ARG:CB	2.24	0.50
1:B:139:GLU:HB3	1:B:258:TYR:HE2	1.76	0.50
1:B:67:ASP:OD1	1:B:128:SER:N	2.45	0.50
1:A:269:GLU:HG3	1:A:270:PHE:N	2.27	0.50
1:B:484:ARG:HG2	1:B:484:ARG:NH1	2.26	0.50
1:B:24:VAL:CG1	1:B:45:ALA:HB1	2.41	0.50
1:A:177:CYS:O	1:A:181:ARG:N	2.39	0.50
1:A:76:ARG:O	1:A:77:ASN:HB2	2.10	0.50
1:A:218:TRP:CH2	1:A:246:SER:HB3	2.47	0.50
1:A:82:TRP:CH2	1:A:94:PRO:C	2.84	0.50
1:B:255:LYS:CE	1:B:261:GLU:HA	2.42	0.50
1:B:456:TRP:O	1:B:460:HIS:HD2	1.95	0.50
1:A:513:SER:O	1:A:517:LYS:HG3	2.10	0.50
1:B:268:TYR:HA	1:B:311:PRO:O	2.11	0.50
1:A:293:LEU:HB3	1:A:297:LEU:HD12	1.93	0.50
1:A:452:GLU:OE2	1:A:478:ARG:NH2	2.36	0.50
1:B:35:HIS:H	1:B:38:ASN:ND2	2.03	0.49
1:B:404:LYS:NZ	3:B:694:HOH:O	2.45	0.49
1:B:33:TYR:HA	3:B:675:HOH:O	2.12	0.49
1:B:433:ILE:HD11	1:B:506:PHE:CZ	2.47	0.49
1:B:143:ALA:O	1:B:172:PRO:HG3	2.12	0.49
1:B:71:PHE:CZ	1:B:74:VAL:HG12	2.48	0.49
1:B:78:VAL:HG13	1:B:79:PRO:HD2	1.93	0.49
1:B:141:ARG:NH1	1:B:189:TRP:HZ2	2.10	0.49
1:A:512:ARG:NH1	1:A:512:ARG:HG2	2.27	0.49
1:A:456:TRP:O	1:A:460:HIS:HD2	1.96	0.49
1:B:474:GLU:OE1	1:B:478:ARG:HB2	2.13	0.49
1:A:218:TRP:CZ3	1:A:246:SER:CB	2.95	0.49
1:B:129:GLU:O	1:B:131:TYR:N	2.42	0.49
1:A:36:VAL:CG2	1:A:293:LEU:HD11	2.42	0.49
1:B:100:HIS:CD2	1:B:109:ARG:HG3	2.47	0.49
1:B:255:LYS:HE2	1:B:261:GLU:HA	1.94	0.49
1:B:220:VAL:C	1:B:223:PRO:HD2	2.33	0.49
1:B:452:GLU:CD	1:B:478:ARG:HH22	2.17	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:GLN:HG3	1:B:81:GLU:N	2.28	0.48
1:A:269:GLU:HG3	1:A:314:GLU:HB3	1.95	0.48
1:A:129:GLU:O	1:A:133:ARG:HG3	2.13	0.48
1:A:7:TYR:O	1:A:10:ASP:N	2.46	0.48
1:A:273:ILE:HD13	1:A:319:LEU:HD12	1.94	0.48
1:A:339:GLY:C	1:A:341:GLU:H	2.15	0.48
1:B:131:TYR:OH	1:B:216:LEU:HD13	2.13	0.48
1:B:41:GLU:HB2	1:B:268:TYR:OH	2.13	0.48
1:A:36:VAL:HG21	1:A:293:LEU:HD11	1.96	0.48
1:B:219:ARG:HH12	1:B:249:THR:HG21	1.78	0.48
1:B:137:SER:O	1:B:139:GLU:N	2.47	0.48
1:B:35:HIS:ND1	1:B:38:ASN:ND2	2.62	0.48
1:A:409:ARG:HH21	1:A:413:ARG:NH2	2.12	0.48
1:A:423:LYS:HE3	1:A:424:TYR:CZ	2.49	0.48
1:B:175:VAL:HA	1:B:213:ASN:O	2.13	0.48
1:B:82:TRP:HZ3	1:B:94:PRO:O	1.96	0.48
1:B:334:GLU:O	1:B:338:PHE:HD1	1.97	0.48
1:B:41:GLU:HB2	1:B:268:TYR:CZ	2.49	0.48
1:B:64:MET:HG2	1:B:225:ARG:NH1	2.29	0.48
1:B:209:ILE:HA	1:B:214:VAL:CG1	2.43	0.47
1:B:340:VAL:CG1	1:B:340:VAL:O	2.61	0.47
1:A:112:GLU:CD	1:A:124:LEU:HD13	2.35	0.47
1:A:406:ASP:O	1:A:410:VAL:HG23	2.14	0.47
1:A:202:GLY:O	1:A:203:HIS:HB2	2.14	0.47
1:B:151:MET:O	1:B:155:ASN:ND2	2.46	0.47
1:A:51:ALA:O	1:A:54:ASP:HB2	2.14	0.47
1:A:335:ARG:HD3	3:A:692:HOH:O	2.13	0.47
1:B:223:PRO:O	1:B:226:TRP:HB2	2.13	0.47
1:A:334:GLU:HG3	1:A:354:TYR:CZ	2.50	0.47
1:A:35:HIS:H	1:A:38:ASN:ND2	2.10	0.47
1:A:199:CYS:SG	1:A:200:PRO:HD2	2.54	0.47
1:A:12:ILE:HG12	1:A:264:LEU:HD12	1.96	0.47
1:B:387:ASP:O	1:B:391:VAL:HG23	2.15	0.47
1:B:305:ILE:HD11	1:B:326:LEU:HD21	1.97	0.47
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.29	0.47
1:B:308:ARG:NH2	1:B:329:GLU:OE1	2.48	0.47
1:B:378:VAL:HG11	1:B:418:ARG:HA	1.97	0.47
1:B:214:VAL:O	1:B:214:VAL:HG13	2.14	0.47
1:A:133:ARG:NH2	1:A:135:GLU:OE2	2.44	0.46
1:B:257:VAL:C	1:B:259:GLY:H	2.19	0.46
1:B:380:LEU:HD21	1:B:506:PHE:HE1	1.80	0.46
1:A:16:ARG:HD2	1:A:232:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:LEU:O	1:B:378:VAL:HB	2.15	0.46
1:B:42:LEU:HD12	1:B:42:LEU:O	2.15	0.46
1:A:253:ILE:O	1:A:257:VAL:HB	2.16	0.46
1:B:35:HIS:O	1:B:38:ASN:HB2	2.16	0.46
1:B:82:TRP:CZ3	1:B:94:PRO:O	2.69	0.46
1:B:158:ARG:O	1:B:163:GLN:HG2	2.16	0.46
1:A:222:TRP:HB3	1:A:223:PRO:CD	2.46	0.46
1:B:297:LEU:HD22	1:B:301:LEU:HD23	1.97	0.46
1:A:269:GLU:HG3	1:A:270:PHE:H	1.80	0.46
1:A:193:TRP:O	1:A:194:LYS:O	2.34	0.46
1:B:382:HIS:CG	1:B:383:LEU:H	2.34	0.46
1:A:364:ARG:HG3	1:A:364:ARG:NH1	2.28	0.46
1:B:28:ILE:HG22	1:B:29:THR:H	1.80	0.46
1:A:433:ILE:HD11	1:A:506:PHE:CZ	2.51	0.46
1:A:394:LYS:NZ	3:A:646:HOH:O	2.39	0.45
1:B:179:GLU:O	1:B:180:HIS:HB2	2.15	0.45
1:A:218:TRP:HZ3	1:A:246:SER:CB	2.29	0.45
1:B:140:ILE:HG12	1:B:216:LEU:CD1	2.41	0.45
1:B:384:THR:HG23	1:B:387:ASP:OD2	2.16	0.45
1:B:186:ILE:HG23	1:B:196:LYS:O	2.16	0.45
1:B:189:TRP:CD1	1:B:195:VAL:HG12	2.51	0.45
1:B:23:VAL:HG12	3:B:625:HOH:O	2.17	0.45
1:B:502:ARG:HG3	1:B:502:ARG:HH11	1.81	0.45
1:B:357:SER:O	1:B:359:PRO:HD3	2.16	0.45
1:A:420:TRP:CD1	1:A:424:TYR:HB2	2.52	0.45
1:A:178:PRO:HG3	1:A:213:ASN:OD1	2.17	0.45
1:A:361:LYS:HB3	1:A:361:LYS:HZ2	1.82	0.45
1:B:89:PRO:HD2	1:B:92:GLU:HG3	1.99	0.45
1:B:130:LEU:HD23	1:B:133:ARG:HH12	1.81	0.45
1:A:440:VAL:O	1:A:442:VAL:HG23	2.17	0.45
1:A:331:GLU:HB3	1:A:335:ARG:NH1	2.32	0.45
1:B:418:ARG:HG2	1:B:418:ARG:HH11	1.82	0.45
1:B:147:ARG:O	1:B:151:MET:HG3	2.17	0.44
1:B:70:ARG:NH2	1:B:72:ARG:HD2	2.33	0.44
1:A:324:LEU:HD22	1:A:372:ARG:HA	2.00	0.44
1:B:158:ARG:HA	1:B:163:GLN:HE21	1.82	0.44
1:B:408:GLU:OE1	1:B:408:GLU:HA	2.18	0.44
1:B:137:SER:HB2	1:B:210:ARG:HD3	1.99	0.44
1:B:93:VAL:HG23	1:B:103:TYR:CB	2.44	0.44
1:B:381:PRO:HG2	1:B:382:HIS:ND1	2.32	0.44
1:A:23:VAL:HG12	1:A:231:VAL:HA	2.00	0.44
1:A:66:ASP:OD1	1:A:225:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:385:GLU:CD	1:B:411:LYS:HG2	2.38	0.44
1:A:167:PRO:HG2	1:A:170:TRP:HB2	1.99	0.44
1:A:449:ALA:HB1	1:A:475:VAL:HG12	2.00	0.44
1:A:35:HIS:N	1:A:38:ASN:HD22	2.12	0.44
1:A:213:ASN:ND2	1:A:213:ASN:N	2.66	0.44
1:A:434:LEU:O	1:A:518:ARG:NH2	2.40	0.44
1:A:212:GLY:C	1:A:213:ASN:HD22	2.22	0.44
1:B:177:CYS:O	1:B:181:ARG:N	2.44	0.44
1:B:435:GLU:HB2	3:B:653:HOH:O	2.18	0.43
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.83	0.43
1:B:449:ALA:O	1:B:453:VAL:HG23	2.18	0.43
1:B:332:LYS:HA	1:B:335:ARG:NH1	2.32	0.43
1:B:444:GLU:HG3	3:B:664:HOH:O	2.18	0.43
1:B:399:PRO:HG2	1:B:402:LEU:HD23	2.00	0.43
1:A:423:LYS:NZ	3:A:639:HOH:O	2.50	0.43
1:B:48:VAL:HG21	1:B:233:PHE:CE2	2.53	0.43
1:A:276:GLN:HE22	1:A:288:ILE:HD11	1.83	0.43
1:B:433:ILE:HD11	1:B:506:PHE:HZ	1.84	0.43
1:A:383:LEU:CD2	1:A:387:ASP:HB3	2.46	0.43
1:B:199:CYS:O	1:B:201:GLU:N	2.51	0.43
1:B:487:PHE:O	1:B:491:TYR:CD1	2.71	0.43
1:A:200:PRO:O	1:A:201:GLU:CB	2.65	0.43
1:B:224:MET:CG	1:B:225:ARG:N	2.78	0.43
1:B:23:VAL:CG1	1:B:231:VAL:HA	2.47	0.43
1:A:456:TRP:O	1:A:460:HIS:CD2	2.72	0.43
1:B:42:LEU:C	1:B:42:LEU:HD12	2.39	0.43
1:B:138:GLU:CD	1:B:138:GLU:N	2.70	0.43
1:A:6:ASP:O	1:A:9:ALA:HB3	2.18	0.43
1:B:118:LEU:HG	1:B:294:TYR:OH	2.18	0.43
1:B:25:GLU:O	1:B:234:GLU:HG3	2.19	0.43
1:B:296:VAL:CG1	1:B:323:ILE:CD1	2.97	0.43
1:A:62:ILE:HG23	1:A:125:LEU:HD12	2.01	0.42
1:A:239:ASP:OD1	1:A:240:HIS:CD2	2.72	0.42
1:A:203:HIS:CD2	1:A:204:GLU:N	2.83	0.42
1:B:456:TRP:CE2	1:B:471:ILE:CD1	3.02	0.42
1:A:331:GLU:HG3	1:A:368:GLN:CD	2.40	0.42
1:B:223:PRO:HG3	1:B:250:GLY:HA2	2.01	0.42
1:A:364:ARG:CG	1:A:364:ARG:HH11	2.29	0.42
1:B:254:ILE:HD13	1:B:261:GLU:O	2.19	0.42
1:B:251:LYS:O	1:B:254:ILE:HG22	2.19	0.42
1:B:169:ASN:O	1:B:169:ASN:OD1	2.37	0.42
1:B:223:PRO:HG3	1:B:250:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:TRP:CZ2	1:A:96:PRO:HA	2.54	0.42
1:B:180:HIS:ND1	1:B:180:HIS:O	2.50	0.42
1:B:296:VAL:HG22	1:B:420:TRP:HB2	2.01	0.42
1:B:174:MET:O	1:B:214:VAL:HA	2.19	0.42
1:B:8:ILE:O	1:B:12:ILE:HG13	2.19	0.42
1:B:7:TYR:HD2	1:B:8:ILE:HD12	1.85	0.42
1:B:60:ARG:NE	1:B:62:ILE:HG12	2.34	0.42
1:B:80:GLN:O	1:B:83:LYS:HE3	2.19	0.42
1:A:36:VAL:HG22	1:A:306:TYR:OH	2.20	0.42
1:B:337:TYR:HE2	1:B:362:PRO:HB2	1.85	0.42
1:A:203:HIS:CG	1:A:204:GLU:N	2.87	0.42
1:B:170:TRP:CH2	1:B:172:PRO:HA	2.54	0.42
1:A:309:HIS:ND1	1:A:315:ILE:HG12	2.35	0.42
1:A:110:LYS:HA	1:A:110:LYS:HD2	1.89	0.42
1:A:47:ILE:CG2	1:A:48:VAL:N	2.83	0.42
1:B:273:ILE:CD1	1:B:288:ILE:HG12	2.50	0.42
1:A:331:GLU:HG3	1:A:368:GLN:NE2	2.35	0.42
1:B:234:GLU:HA	1:B:235:PRO:HD3	1.94	0.42
1:B:457:LEU:HD21	1:B:468:PHE:CE1	2.55	0.42
1:B:384:THR:OG1	1:B:386:GLU:HB3	2.20	0.42
1:A:197:TYR:CE2	1:A:207:VAL:HG23	2.55	0.42
1:A:80:GLN:OE1	1:A:81:GLU:N	2.53	0.42
1:A:21:LYS:HA	1:A:58:GLU:O	2.19	0.42
1:B:223:PRO:CG	1:B:250:GLY:HA2	2.50	0.42
1:A:105:GLU:O	1:A:109:ARG:HG2	2.20	0.41
1:B:203:HIS:CD2	1:B:204:GLU:N	2.88	0.41
1:B:366:VAL:HG21	1:B:405:GLU:CD	2.41	0.41
1:A:36:VAL:HG13	1:A:271:VAL:CG1	2.50	0.41
1:B:444:GLU:CD	1:B:444:GLU:H	2.23	0.41
1:A:22:TYR:HE1	1:A:57:TYR:CD2	2.38	0.41
1:B:288:ILE:HD12	1:B:288:ILE:N	2.35	0.41
1:A:147:ARG:HD2	1:A:171:TRP:CE3	2.54	0.41
1:B:189:TRP:HD1	1:B:195:VAL:HG12	1.82	0.41
1:B:158:ARG:HA	1:B:163:GLN:HG2	2.02	0.41
1:B:197:TYR:HE2	1:B:207:VAL:HG13	1.84	0.41
1:A:139:GLU:HB3	1:A:224:MET:HG2	2.02	0.41
1:B:518:ARG:NH1	1:B:523:GLY:OXT	2.53	0.41
1:B:82:TRP:CZ3	1:B:96:PRO:HG3	2.55	0.41
1:B:141:ARG:HH11	1:B:189:TRP:HZ2	1.67	0.41
1:B:351:ARG:HB2	1:B:351:ARG:NH1	2.36	0.41
1:B:224:MET:HE2	1:B:225:ARG:HA	2.02	0.41
1:A:364:ARG:CG	1:A:364:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:VAL:O	1:B:74:VAL:CG2	2.66	0.41
1:B:366:VAL:HG21	1:B:405:GLU:OE1	2.21	0.41
1:A:76:ARG:C	1:A:78:VAL:H	2.23	0.41
1:A:74:VAL:HG21	1:A:83:LYS:HD3	2.01	0.41
1:A:484:ARG:NH1	1:A:485:GLU:HA	2.36	0.41
1:B:17:GLY:O	1:B:19:LYS:HG3	2.21	0.41
1:A:335:ARG:NE	1:A:341:GLU:OE1	2.52	0.41
1:A:140:ILE:O	1:A:143:ALA:HB3	2.20	0.41
1:A:189:TRP:CG	1:A:190:ASP:N	2.89	0.41
1:A:111:PHE:O	1:A:115:VAL:HG23	2.20	0.41
1:A:141:ARG:HD2	3:A:742:HOH:O	2.20	0.41
1:A:331:GLU:HG2	1:A:368:GLN:HB3	2.03	0.41
1:B:85:TYR:CD2	1:B:94:PRO:HD2	2.56	0.41
1:A:181:ARG:HH12	1:A:213:ASN:HD21	1.66	0.41
1:B:198:LYS:HG3	1:B:203:HIS:O	2.20	0.41
1:B:385:GLU:O	1:B:389:ILE:HG13	2.21	0.41
1:A:159:GLU:O	1:A:162:LYS:HD2	2.21	0.41
1:A:42:LEU:O	1:A:42:LEU:HD23	2.21	0.40
1:A:11:LYS:O	1:A:15:GLU:HB2	2.21	0.40
1:B:347:ASP:O	1:B:348:GLU:HB2	2.20	0.40
1:A:218:TRP:HA	1:A:221:ASP:HB3	2.04	0.40
1:A:381:PRO:C	1:A:383:LEU:H	2.24	0.40
1:B:166:LEU:HA	1:B:167:PRO:HD3	1.92	0.40
1:B:142:LEU:HA	1:B:145:GLU:HG2	2.03	0.40
1:B:133:ARG:NH1	1:B:133:ARG:HB3	2.37	0.40
1:B:365:LEU:HD12	1:B:366:VAL:H	1.86	0.40
1:B:175:VAL:HG22	1:B:184:ALA:O	2.22	0.40
1:B:297:LEU:HD22	1:B:301:LEU:CD2	2.51	0.40
1:B:68:TYR:HA	1:B:68:TYR:HD1	1.74	0.40
1:B:361:LYS:HA	1:B:362:PRO:HD3	1.84	0.40
1:A:413:ARG:HA	1:A:416:LEU:HD12	2.04	0.40
1:B:138:GLU:OE1	1:B:138:GLU:N	2.54	0.40
1:B:141:ARG:NH1	1:B:189:TRP:CZ2	2.89	0.40
1:A:498:GLU:HG2	3:A:701:HOH:O	2.21	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	501/523 (96%)	457 (91%)	37 (7%)	7 (1%)	16	32
1	B	502/523 (96%)	443 (88%)	42 (8%)	17 (3%)	6	8
All	All	1003/1046 (96%)	900 (90%)	79 (8%)	24 (2%)	9	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	LYS
1	A	243	ALA
1	B	77	ASN
1	B	138	GLU
1	B	180	HIS
1	B	363	GLU
1	B	382	HIS
1	A	193	TRP
1	A	201	GLU
1	B	182	ARG
1	B	201	GLU
1	B	348	GLU
1	B	383	LEU
1	B	200	PRO
1	B	228	HIS
1	B	339	GLY
1	B	341	GLU
1	B	381	PRO
1	A	75	PRO
1	B	258	TYR
1	B	403	SER
1	A	15	GLU
1	B	96	PRO
1	A	231	VAL

### 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	451/462 (98%)	429 (95%)	22 (5%)	35	62
1	B	452/462 (98%)	424 (94%)	28 (6%)	26	49
All	All	903/924 (98%)	853 (94%)	50 (6%)	30	56

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	36	VAL
1	A	46	TYR
1	A	68	TYR
1	A	73	LYS
1	A	80	GLN
1	A	84	ASP
1	A	99	CYS
1	A	149	LYS
1	A	169	ASN
1	A	183	GLU
1	A	249	THR
1	A	261	GLU
1	A	266	LEU
1	A	308	ARG
1	A	331	GLU
1	A	334	GLU
1	A	361	LYS
1	A	378	VAL
1	A	440	VAL
1	A	484	ARG
1	A	518	ARG
1	B	23	VAL
1	B	42	LEU
1	B	68	TYR
1	B	69	ASP
1	B	76	ARG
1	B	99	CYS
1	B	131	TYR

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	133	ARG
1	B	138	GLU
1	B	159	GLU
1	B	185	GLU
1	B	201	GLU
1	B	210	ARG
1	B	224	MET
1	B	232	ASP
1	B	266	LEU
1	B	296	VAL
1	B	361	LYS
1	B	364	ARG
1	B	378	VAL
1	B	382	HIS
1	B	412	LEU
1	B	428	ASP
1	B	466	GLU
1	B	474	GLU
1	B	484	ARG
1	B	503	LEU
1	B	518	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	38	ASN
1	A	169	ASN
1	A	203	HIS
1	A	213	ASN
1	A	276	GLN
1	A	460	HIS
1	A	469	ASN
1	B	3	HIS
1	B	38	ASN
1	B	61	HIS
1	B	163	GLN
1	B	169	ASN
1	B	203	HIS
1	B	286	ASN
1	B	460	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 4 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.

## 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.