



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:55 PM UTC

PDB ID : 1IRX / pdb_00001irx
Title : Crystal structure of class I lysyl-tRNA synthetase
Authors : Nureki, O.; Terada, T.; Ishitani, R.; Ambrogelly, A.; Ibba, M.; Soll, D.;
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-10-25
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

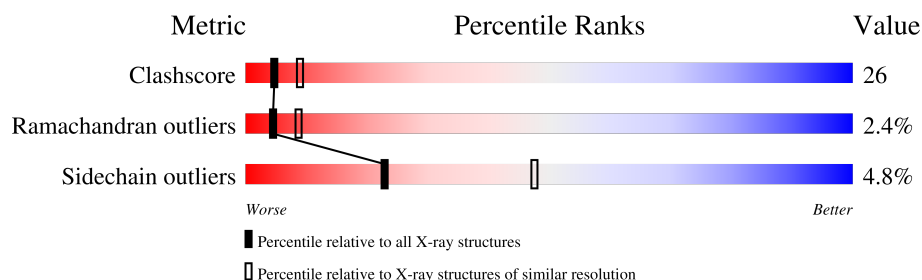
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 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	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 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 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:

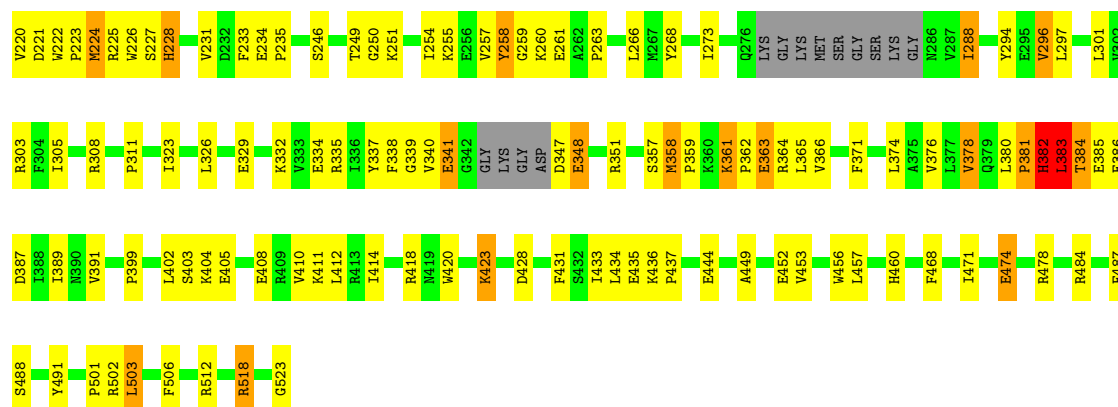
Chain	Residue	Modelled	Actual	Comment	Reference
A	124	LEU	PHE	conflict	UNP O57963
A	331	GLU	ASP	conflict	UNP O57963
B	124	LEU	PHE	conflict	UNP O57963
B	331	GLU	ASP	conflict	UNP O57963

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



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	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 ²)	53.0	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: 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	0.47	1/4361 (0.0%)	0.93	14/5886 (0.2%)
1	B	0.44	0/4369	0.92	14/5897 (0.2%)
All	All	0.45	1/8730 (0.0%)	0.93	28/11783 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	PRO	CA-C	5.13	1.54	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	LEU	N-CA-C	8.89	120.66	110.97
1	A	229	PHE	N-CA-C	-7.43	99.81	110.59
1	B	128	SER	N-CA-C	-7.32	102.69	111.69
1	A	218	TRP	N-CA-C	7.23	120.07	111.33
1	B	246	SER	N-CA-C	6.95	118.86	111.28
1	B	503	LEU	N-CA-C	6.91	119.44	111.02
1	B	140	ILE	N-CA-C	-6.88	103.60	110.62
1	A	423	LYS	N-CA-C	6.17	121.46	113.88
1	B	80	GLN	N-CA-C	6.15	117.67	110.97
1	B	217	ARG	N-CA-C	-6.14	101.19	110.28
1	A	190	ASP	CB-CA-C	-6.12	108.25	117.07
1	A	190	ASP	CA-C-O	6.09	121.47	117.94
1	A	163	GLN	N-CA-C	-6.04	102.46	110.07
1	A	164	PRO	N-CA-C	6.02	116.25	110.47
1	B	37	GLY	N-CA-C	-5.96	105.28	112.49
1	B	423	LYS	N-CA-C	5.93	121.03	113.55
1	B	437	PRO	N-CA-C	5.89	117.88	110.70
1	A	35	HIS	N-CA-C	5.87	119.04	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	THR	N-CA-C	-5.52	102.58	110.59
1	B	383	LEU	N-CA-C	5.50	122.51	110.80
1	B	371	PHE	N-CA-C	5.43	117.63	111.11
1	B	288	ILE	N-CA-C	5.39	116.35	108.58
1	A	380	LEU	CA-C-N	5.26	125.07	119.28
1	A	380	LEU	C-N-CA	5.26	125.07	119.28
1	B	72	ARG	N-CA-C	5.24	117.07	111.36
1	A	511	ASP	N-CA-C	-5.19	102.36	110.10
1	A	103	TYR	N-CA-C	-5.16	105.57	111.14
1	A	16	ARG	N-CA-C	-5.13	103.76	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4247	0	4181	185	0
1	B	4255	0	4187	249	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	434	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 26.

All (434) 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:361:LYS:H	1:A:361:LYS:HD2	1.21	1.01
1:B:361:LYS:HE3	1:B:361:LYS:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:331:GLU:CD	1:A:413:ARG:HH12	1.88	0.81
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: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:B:70:ARG:HD3	1:B:183:GLU:CD	2.12	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:HG12	1:B:340:VAL:O	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:A:190:ASP:OD2	1:A:194:LYS:HB2	1.92	0.69
1:B:93:VAL:HG23	1:B:103:TYR:HB3	1.74	0.69
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:HG3	1:A:364:ARG:HH11	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:GLU:H	1:B:138:GLU:CD	2.02	0.67
1:B:74:VAL:HG23	1:B:74:VAL:O	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:64:MET:HE3	1:B:65:TRP:N	2.11	0.65
1:B:484:ARG:HG2	1:B:484:ARG:HH11	1.62	0.65
1:B:149:LYS:O	1:B:152:GLU:HG2	1.95	0.65
1:B:64:MET:HE3	1:B:65:TRP:H	1.61	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: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:A:243:ALA:O	1:A:248:ASP:OD1	2.16	0.63
1:B:79:PRO:HB2	1:B:82:TRP:CD1	2.34	0.63
1:B:147:ARG:HD2	1:B:170:TRP:O	1.99	0.63
1:A:219:ARG:HD2	1:A:249:THR:HG21	1.81	0.62
1:A:82:TRP:HH2	1:A:94:PRO:C	2.07	0.62
1:B:222:TRP:HB3	1:B:223:PRO:HD3	1.80	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:90:ILE:HG22	1:B:104:ALA:HB2	1.82	0.62
1:B:226:TRP:HA	1:B:231:VAL:HG12	1.82	0.62
1:B:361:LYS:HE3	1:B:361:LYS:N	2.05	0.62
1:B:435:GLU:C	1:B:436:LYS:HD2	2.23	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HD3	1:B:183:GLU:OE1	1.99	0.61
1:B:35:HIS:CD2	1:B:37:GLY:H	2.19	0.61
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: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:A:288:ILE:HD12	1:A:288:ILE:N	2.17	0.60
1:B:209:ILE:HG23	1:B:214:VAL:HG11	1.83	0.60
1:A:169:ASN:ND2	1:A:169:ASN:H	1.99	0.59
1:A:110:LYS:O	1:A:114:GLU:HG3	2.02	0.59
1:A:303:ARG:HD2	1:A:357:SER:O	2.02	0.59
1:B:109:ARG:HA	1:B:112:GLU:OE1	2.03	0.59
1:B:308:ARG:HH12	1:B:329:GLU:CD	2.11	0.58
1:A:89:PRO:O	1:A:93:VAL:HG23	2.03	0.58
1:A:512:ARG:HH11	1:A:512:ARG:HG2	1.68	0.58
1:B:108:MET:O	1:B:112:GLU:HG3	2.03	0.58
1:A:169:ASN:H	1:A:169:ASN:HD22	1.50	0.58
1:A:361:LYS:H	1:A:361:LYS:CD	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:8:ILE:O	1:A:12:ILE:HG13	2.04	0.58
1:A:361:LYS:NZ	1:A:361:LYS:HB3	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:154:LEU:O	1:A:158:ARG:HG3	2.05	0.57
1:A:213:ASN:N	1:A:213:ASN:HD22	2.01	0.57
1:B:129:GLU:C	1:B:131:TYR:H	2.12	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:A:42:LEU:HD23	1:A:42:LEU:C	2.31	0.56
1:B:137:SER:C	1:B:139:GLU:H	2.13	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:112:GLU:OE2	1:A:124:LEU:HD13	2.06	0.55
1:A:331:GLU:HB3	1:A:335:ARG:HH12	1.71	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:A:219:ARG:CD	1:A:249:THR:HG21	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:O	1:B:341:GLU:HB2	2.07	0.55
1:A:73:LYS:HD2	1:A:73:LYS:H	1.72	0.55
1:A:24:VAL:HG12	1:A:45:ALA:HB1	1.89	0.55
1:A:219:ARG:HH11	1:A:249:THR:HG21	1.72	0.55
1:B:100:HIS:NE2	1:B:109:ARG:HG3	2.22	0.55
1:B:141:ARG:HG3	1:B:141:ARG:HH11	1.72	0.55
1:B:151:MET:HE3	1:B:170:TRP:HB3	1.88	0.55
1:B:363:GLU:HG2	1:B:364:ARG:NE	2.16	0.55
1:A:82:TRP:CH2	1:A:94:PRO:C	2.84	0.54
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: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:133:ARG:HH11	1:B:133:ARG:HB3	1.73	0.53
1:B:135:GLU:HG2	1:B:228:HIS:CE1	2.43	0.53
1:B:220:VAL:C	1:B:223:PRO:HD2	2.33	0.53
1:B:452:GLU:CD	1:B:478:ARG:HH22	2.17	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:A:339:GLY:C	1:A:341:GLU:H	2.15	0.53
1:A:30:PRO:HG2	1:A:90:ILE:HD12	1.90	0.53
1:B:376:VAL:HG21	1:B:501:PRO:HB3	1.91	0.53
1:B:457:LEU:O	1:B:512:ARG:NH1	2.42	0.53
1:B:303:ARG:HH12	1:B:358:MET:HE2	1.73	0.53
1:B:80:GLN:HG3	1:B:81:GLU:H	1.74	0.52
1:B:104:ALA:O	1:B:108:MET:HG3	2.09	0.52
1:B:224:MET:CE	1:B:228:HIS:HB2	2.38	0.52
1:A:73:LYS:HD2	1:A:73:LYS:N	2.23	0.52
1:B:25:GLU:HG2	1:B:26:SER:N	2.25	0.52
1:B:35:HIS:HB2	1:B:288:ILE:O	2.10	0.52
1:A:490:LEU:HD13	1:A:503:LEU:HD21	1.92	0.52
1:B:90:ILE:HG23	1:B:103:TYR:HD2	1.74	0.52
1:B:364:ARG:H	1:B:364:ARG:HD2	1.74	0.52
1:B:382:HIS:ND1	1:B:382:HIS:N	2.58	0.52
1:B:185:GLU:H	1:B:185:GLU:CD	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:VAL:C	1:B:259:GLY:H	2.19	0.51
1:A:254:ILE:HG12	1:A:260:LYS:HB2	1.92	0.51
1:B:135:GLU:HG2	1:B:228:HIS:HE1	1.76	0.51
1:A:447:ARG:HG3	3:A:647:HOH:O	2.09	0.51
1:B:181:ARG:O	1:B:182:ARG:O	2.28	0.51
1:A:112:GLU:CD	1:A:124:LEU:HD13	2.35	0.51
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:28:ILE:HG22	1:B:29:THR:N	2.26	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: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:A:269:GLU:HG3	1:A:270:PHE:N	2.27	0.50
1:B:67:ASP:OD1	1:B:128:SER:N	2.45	0.50
1:B:139:GLU:HB3	1:B:258:TYR:HE2	1.76	0.50
1:A:76:ARG:O	1:A:77:ASN:HB2	2.10	0.50
1:A:177:CYS:O	1:A:181:ARG:N	2.39	0.50
1:B:24:VAL:CG1	1:B:45:ALA:HB1	2.41	0.50
1:B:484:ARG:HG2	1:B:484:ARG:NH1	2.26	0.50
1:A:218:TRP:CH2	1:A:246:SER:HB3	2.47	0.50
1:A:513:SER:O	1:A:517:LYS:HG3	2.10	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: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:268:TYR:HA	1:B:311:PRO:O	2.11	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: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:B:143:ALA:O	1:B:172:PRO:HG3	2.12	0.49
1:A:456:TRP:O	1:A:460:HIS:HD2	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:HG2	1:A:512:ARG:NH1	2.27	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:A:36:VAL:CG2	1:A:293:LEU:HD11	2.42	0.49
1:B:129:GLU:O	1:B:131:TYR:N	2.42	0.49
1:B:138:GLU:CD	1:B:138:GLU:N	2.70	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:385:GLU:CD	1:B:411:LYS:HG2	2.38	0.49
1:B:80:GLN:HG3	1:B:81:GLU:N	2.28	0.48
1:A:7:TYR:O	1:A:10:ASP:N	2.46	0.48
1:A:129:GLU:O	1:A:133:ARG:HG3	2.13	0.48
1:A:269:GLU:HG3	1:A:314:GLU:HB3	1.95	0.48
1:A:273:ILE:HD13	1:A:319:LEU:HD12	1.94	0.48
1:A:212:GLY:C	1:A:213:ASN:HD22	2.22	0.48
1:A:36:VAL:HG21	1:A:293:LEU:HD11	1.96	0.48
1:B:41:GLU:HB2	1:B:268:TYR:OH	2.13	0.48
1:B:131:TYR:OH	1:B:216:LEU:HD13	2.13	0.48
1:B:219:ARG:HH12	1:B:249:THR:HG21	1.78	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:35:HIS:ND1	1:B:38:ASN:ND2	2.62	0.48
1:B:137:SER:O	1:B:139:GLU:N	2.47	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:O	1:B:340:VAL:CG1	2.61	0.47
1:A:406:ASP:O	1:A:410:VAL:HG23	2.14	0.47
1:A:51:ALA:O	1:A:54:ASP:HB2	2.14	0.47
1:A:147:ARG:NE	1:A:151:MET:HE2	2.29	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:334:GLU:HG3	1:A:354:TYR:CZ	2.50	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:35:HIS:H	1:A:38:ASN:ND2	2.10	0.47
1:A:331:GLU:HG3	1:A:368:GLN:CD	2.40	0.47
1:A:12:ILE:HG12	1:A:264:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:CYS:SG	1:A:200:PRO:HD2	2.54	0.47
1:A:308:ARG:NH1	1:A:308:ARG:HG3	2.29	0.47
1:B:42:LEU:C	1:B:42:LEU:HD12	2.39	0.47
1:B:305:ILE:HD11	1:B:326:LEU:HD21	1.97	0.47
1:B:387:ASP:O	1:B:391:VAL:HG23	2.15	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:HG13	1:B:214:VAL:O	2.14	0.47
1:A:133:ARG:NH2	1:A:135:GLU:OE2	2.44	0.46
1:B:366:VAL:HG21	1:B:405:GLU:CD	2.41	0.46
1:A:16:ARG:HD2	1:A:232:ASP:OD2	2.15	0.46
1:B:380:LEU:HD21	1:B:506:PHE:HE1	1.80	0.46
1:B:42:LEU:HD12	1:B:42:LEU:O	2.15	0.46
1:B:374:LEU:O	1:B:378:VAL:HB	2.15	0.46
1:B:444:GLU:CD	1:B:444:GLU:H	2.23	0.46
1:A:253:ILE:O	1:A:257:VAL:HB	2.16	0.46
1:A:222:TRP:HB3	1:A:223:PRO:CD	2.46	0.46
1:A:446:VAL:HG12	1:A:450:MET:HE2	1.98	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: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:76:ARG:C	1:A:78:VAL:H	2.23	0.46
1:A:364:ARG:HG3	1:A:364:ARG:NH1	2.28	0.46
1:A:433:ILE:HD11	1:A:506:PHE:CZ	2.51	0.46
1:B:28:ILE:HG22	1:B:29:THR:H	1.80	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:186:ILE:HG23	1:B:196:LYS:O	2.16	0.45
1:B:384:THR:HG23	1:B:387:ASP:OD2	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:178:PRO:HG3	1:A:213:ASN:OD1	2.17	0.45
1:A:420:TRP:CD1	1:A:424:TYR:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB1	1:A:108:MET:HE2	1.99	0.45
1:A:361:LYS:HB3	1:A:361:LYS:HZ2	1.82	0.45
1:A:381:PRO:C	1:A:383:LEU:H	2.24	0.45
1:A:440:VAL:O	1:A:442:VAL:HG23	2.17	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:331:GLU:HB3	1:A:335:ARG:NH1	2.32	0.45
1:B:129:GLU:C	1:B:131:TYR:N	2.75	0.45
1:A:181:ARG:HH12	1:A:213:ASN:CG	2.25	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:A:64:MET:HE1	1:A:130:LEU:HD11	1.98	0.44
1:A:324:LEU:HD22	1:A:372:ARG:HA	2.00	0.44
1:B:70:ARG:NH2	1:B:72:ARG:HD2	2.33	0.44
1:B:95:ASP:C	1:B:97:TRP:H	2.25	0.44
1:B:158:ARG:HA	1:B:163:GLN:HE21	1.82	0.44
1:B:408:GLU:HA	1:B:408:GLU:OE1	2.18	0.44
1:A:23:VAL:HG12	1:A:231:VAL:HA	2.00	0.44
1:B:93:VAL:HG23	1:B:103:TYR:CB	2.44	0.44
1:B:137:SER:HB2	1:B:210:ARG:HD3	1.99	0.44
1:B:381:PRO:HG2	1:B:382:HIS:ND1	2.32	0.44
1:A:66:ASP:OD1	1:A:225:ARG:NH2	2.50	0.44
1:A:80:GLN:C	1:A:82:TRP:H	2.24	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:B:177:CYS:O	1:B:181:ARG:N	2.44	0.44
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.83	0.43
1:B:332:LYS:HA	1:B:335:ARG:NH1	2.32	0.43
1:B:435:GLU:HB2	3:B:653:HOH:O	2.18	0.43
1:B:449:ALA:O	1:B:453:VAL:HG23	2.18	0.43
1:B:399:PRO:HG2	1:B:402:LEU:HD23	2.00	0.43
1:B:444:GLU:HG3	3:B:664:HOH:O	2.18	0.43
1:A:230:GLY:O	1:A:231:VAL:C	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:456:TRP:O	1:A:460:HIS:CD2	2.72	0.43
1:B:23:VAL:CG1	1:B:231:VAL:HA	2.47	0.43
1:B:224:MET:CG	1:B:225:ARG:N	2.78	0.43
1:A:6:ASP:O	1:A:9:ALA:HB3	2.18	0.43
1:A:339:GLY:C	1:A:341:GLU:N	2.77	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:A:366:VAL:O	1:A:367:ALA:C	2.62	0.42
1:B:456:TRP:CE2	1:B:471:ILE:CD1	3.02	0.42
1:A:364:ARG:HH11	1:A:364:ARG:CG	2.29	0.42
1:B:27:GLY:C	1:B:28:ILE:HG13	2.43	0.42
1:B:169:ASN:OD1	1:B:169:ASN:O	2.37	0.42
1:B:223:PRO:HG3	1:B:250:GLY:HA2	2.01	0.42
1:B:251:LYS:O	1:B:254:ILE:HG22	2.19	0.42
1:B:254:ILE:HD13	1:B:261:GLU:O	2.19	0.42
1:A:82:TRP:CZ2	1:A:96:PRO:HA	2.54	0.42
1:B:137:SER:C	1:B:139:GLU:N	2.78	0.42
1:B:180:HIS:O	1:B:180:HIS:ND1	2.50	0.42
1:B:223:PRO:HG3	1:B:250:GLY:HA3	2.01	0.42
1:B:296:VAL:HG22	1:B:420:TRP:HB2	2.01	0.42
1:B:7:TYR:HD2	1:B:8:ILE:HD12	1.85	0.42
1:B:8:ILE:O	1:B:12:ILE:HG13	2.19	0.42
1:B:174:MET:O	1:B:214:VAL:HA	2.19	0.42
1:B:224:MET:HE2	1:B:225:ARG:HA	2.01	0.42
1:A:36:VAL:HG22	1:A:306:TYR:OH	2.20	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:203:HIS:CG	1:A:204:GLU:N	2.87	0.42
1:A:309:HIS:ND1	1:A:315:ILE:HG12	2.35	0.42
1:B:170:TRP:CH2	1:B:172:PRO:HA	2.54	0.42
1:B:337:TYR:HE2	1:B:362:PRO:HB2	1.85	0.42
1:A:47:ILE:CG2	1:A:48:VAL:N	2.83	0.42
1:A:110:LYS:HA	1:A:110:LYS:HD2	1.89	0.42
1:A:21:LYS:HA	1:A:58:GLU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:OE1	1:A:81:GLU:N	2.53	0.42
1:A:197:TYR:CE2	1:A:207:VAL:HG23	2.55	0.42
1:A:331:GLU:HG3	1:A:368:GLN:NE2	2.35	0.42
1:B:61:HIS:CD2	1:B:61:HIS:C	2.98	0.42
1:B:234:GLU:HA	1:B:235:PRO:HD3	1.94	0.42
1:B:273:ILE:CD1	1:B:288:ILE:HG12	2.50	0.42
1:B:384:THR:OG1	1:B:386:GLU:HB3	2.20	0.42
1:B:457:LEU:HD21	1:B:468:PHE:CE1	2.55	0.42
1:B:223:PRO:CG	1:B:250:GLY:HA2	2.50	0.42
1:A:22:TYR:HE1	1:A:57:TYR:CD2	2.38	0.41
1:A:36:VAL:HG13	1:A:271:VAL:CG1	2.50	0.41
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:A:139:GLU:HB3	1:A:224:MET:HG2	2.02	0.41
1:A:147:ARG:HD2	1:A:171:TRP:CE3	2.54	0.41
1:B:158:ARG:HA	1:B:163:GLN:HG2	2.02	0.41
1:B:189:TRP:HD1	1:B:195:VAL:HG12	1.82	0.41
1:B:197:TYR:HE2	1:B:207:VAL:HG13	1.84	0.41
1:B:288:ILE:HD12	1:B:288:ILE:N	2.35	0.41
1:B:82:TRP:CZ3	1:B:96:PRO:HG3	2.55	0.41
1:B:518:ARG:NH1	1:B:523:GLY:OXT	2.53	0.41
1:B:141:ARG:HH11	1:B:189:TRP:HZ2	1.67	0.41
1:B:351:ARG:NH1	1:B:351:ARG:HB2	2.36	0.41
1:A:147:ARG:HG2	1:A:151:MET:HE2	2.03	0.41
1:A:364:ARG:NH1	1:A:364:ARG:CG	2.84	0.41
1:A:74:VAL:HG21	1:A:83:LYS:HD3	2.01	0.41
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: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:111:PHE:O	1:A:115:VAL:HG23	2.20	0.41
1:A:140:ILE:O	1:A:143:ALA:HB3	2.20	0.41
1:A:141:ARG:HD2	3:A:742:HOH:O	2.20	0.41
1:A:189:TRP:CG	1:A:190:ASP:N	2.89	0.41
1:A:335:ARG:NE	1:A:341:GLU:OE1	2.52	0.41
1:B:431:PHE:CD1	1:B:431:PHE:C	2.99	0.41
1:A:159:GLU:O	1:A:162:LYS:HD2	2.21	0.41
1:A:181:ARG:HH12	1:A:213:ASN:HD21	1.66	0.41
1:A:331:GLU:HG2	1:A:368:GLN:HB3	2.03	0.41
1:A:501:PRO:O	1:A:502:ARG:C	2.63	0.41
1:B:85:TYR:CD2	1:B:94:PRO:HD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:11:LYS:O	1:A:15:GLU:HB2	2.21	0.40
1:A:42:LEU:HD23	1:A:42:LEU:O	2.21	0.40
1:A:267:MET:SD	1:A:267:MET:C	3.04	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:7:TYR:C	1:A:9:ALA:N	2.78	0.40
1:B:142:LEU:HA	1:B:145:GLU:HG2	2.03	0.40
1:B:166:LEU:HA	1:B:167:PRO:HD3	1.92	0.40
1:B:68:TYR:HD1	1:B:68:TYR:HA	1.74	0.40
1:B:133:ARG:HB3	1:B:133:ARG:NH1	2.37	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:365:LEU:HD12	1:B:366:VAL:H	1.86	0.40
1:A:413:ARG:HA	1:A:416:LEU:HD12	2.04	0.40
1:A:498:GLU:HG2	3:A:701:HOH:O	2.21	0.40
1:B:138:GLU:N	1:B:138:GLU:OE1	2.54	0.40
1:B:141:ARG:NH1	1:B:189:TRP:CZ2	2.89	0.40
1:B:361:LYS:HA	1:B:362:PRO:HD3	1.84	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%)	9	19
1	B	502/523 (96%)	443 (88%)	42 (8%)	17 (3%)	3	4
All	All	1003/1046 (96%)	900 (90%)	79 (8%)	24 (2%)	4	9

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%)	431 (96%)	20 (4%)	25	50
1	B	452/462 (98%)	429 (95%)	23 (5%)	21	45
All	All	903/924 (98%)	860 (95%)	43 (5%)	23	47

All (43) 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	73	LYS
1	A	80	GLN
1	A	90	ILE
1	A	99	CYS
1	A	149	LYS
1	A	169	ASN
1	A	190	ASP
1	A	249	THR
1	A	261	GLU
1	A	266	LEU
1	A	308	ARG
1	A	331	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	99	CYS
1	B	133	ARG
1	B	138	GLU
1	B	142	LEU
1	B	159	GLU
1	B	201	GLU
1	B	210	ARG
1	B	224	MET
1	B	266	LEU
1	B	296	VAL
1	B	358	MET
1	B	361	LYS
1	B	378	VAL
1	B	382	HIS
1	B	412	LEU
1	B	428	ASP
1	B	474	GLU
1	B	503	LEU
1	B	518	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	397	HIS
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	276	GLN
1	B	312	ASN
1	B	460	HIS

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 oligosaccharides 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.

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 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.