



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:42 pm BST

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 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) : 2.11

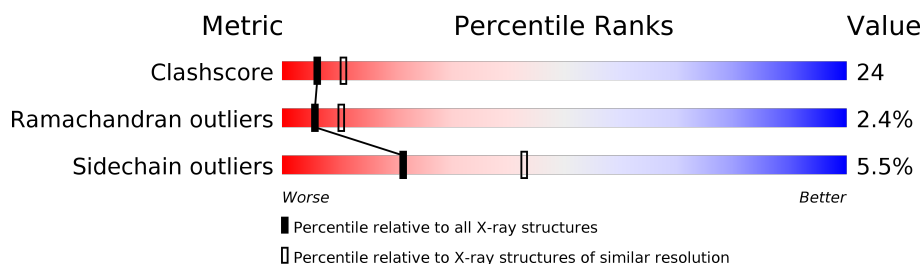
1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 ≥ 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 (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.

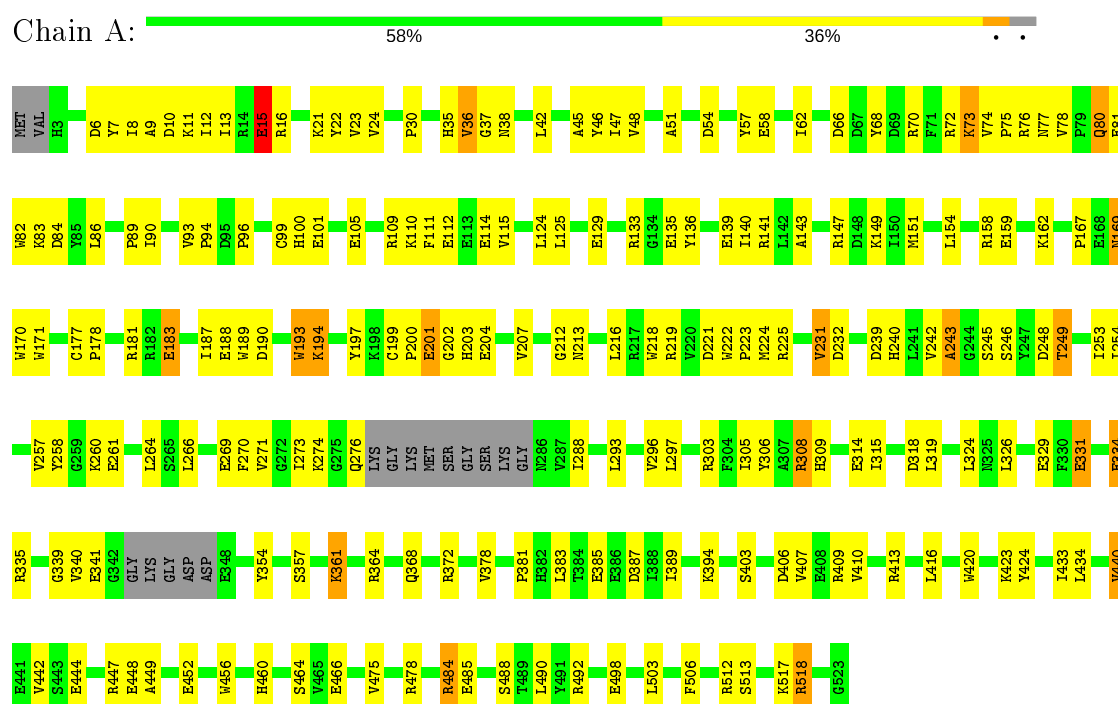
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	102	Total	O	0	0
			102	102		

3 Residue-property plots

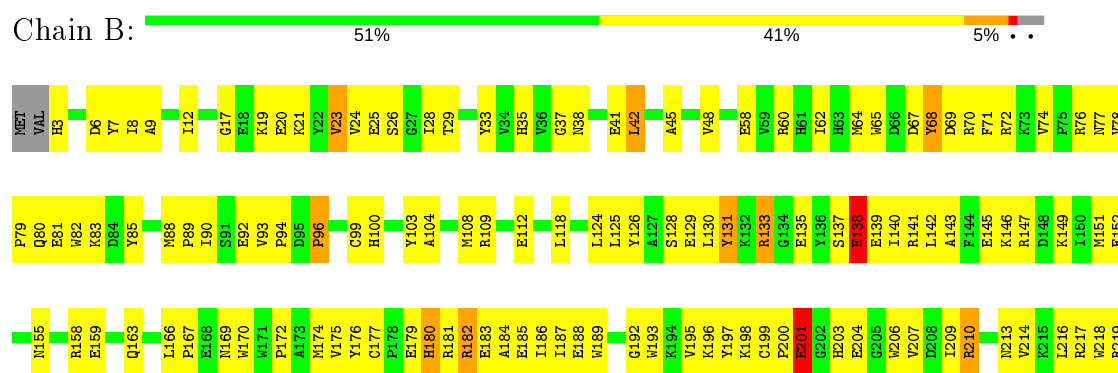
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



- Molecule 1: lysyl-tRNA synthetase



V220	R303	I389	P501
D221	F304	R390	R502
W222	I305	V391	L503
P223			
M224	R308	P399	F506
R225			
W226	P311	L402	R512
S227	I323	S403	R518
H228		R404	
		E405	G523
V231	L326	E408	
D232	E329	R409	
F233		V410	
E234	K332	R411	
P235	V333	L412	
	E334	R413	
S246	R335	I414	
T249	I336	R418	
G250	Y337	R419	
K251	F338	W420	
	G339		
I254	V340	K423	
K255	E341		
E256	G342	D428	
V257	GLY		
Y258	LYS	I433	
G259	GLY	L434	
K260	ASP	E435	
E261	D347	K436	
A262	E348		
P263		E444	
	R351	A449	
L266	S357		
M267	M358	E452	
Y268	P359	V453	
	K360		
I273		W456	
	K361	L457	
Q276	P362		
LYS	E363	H460	
GLY	R364		
GLY	L365	E466	
LYS	V366	E467	
MET		F468	
SER			
SER	L374	I471	
GLY	A375		
LYS	V376	E474	
GLY	I377	R478	
V286	V378	R484	
V287	Q379		
I288	L380	F487	
	P381	S488	
Y294	H382	Y491	
E295	L383		
V296	T384		
L297	E385		
	E386		
L301	D387		
V302	I388		

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

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 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	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

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 24.

All (412) 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: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:CE	1:B:361:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD2	1:A:194:LYS:HB2	1.92	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: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:484:ARG:HG3	1:A:485:GLU:N	2.11	0.64
1:A:72:ARG:HB2	1:A:73:LYS:HD2	1.79	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:B:138:GLU:H	1:B:138:GLU:CD	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:169:ASN:H	1:A:169:ASN:ND2	1.99	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:N	1:A:288:ILE:HD12	2.17	0.60
1:B:209:ILE:HG23	1:B:214:VAL:HG11	1.83	0.60
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:A:512:ARG:HG2	1:A:512:ARG:HH11	1.68	0.58
1:A:89:PRO:O	1:A:93:VAL:HG23	2.03	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: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:154:LEU:O	1:A:158:ARG:HG3	2.05	0.57
1:A:213:ASN:HD22	1:A:213:ASN:N	2.01	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: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
1:B:340:VAL:O	1:B:341:GLU:HB2	2.07	0.55
1:A:73:LYS:H	1:A:73:LYS:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:100:HIS:NE2	1:B:109:ARG:HG3	2.22	0.55
1:B:141:ARG:HH11	1:B:141:ARG:HG3	1.72	0.55
1:B:363:GLU:HG2	1:B:364:ARG:NE	2.16	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:20:GLU:OE2	1:B:20:GLU:HA	2.07	0.54
1:B:82:TRP:CH2	1:B:94:PRO:HG2	2.43	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:158:ARG:HE	1:B:166:LEU:CD2	2.22	0.53
1:B:146:LYS:HE3	1:B:149:LYS:HG3	1.90	0.53
1:B:85:TYR:O	1:B:88:MET:HG2	2.09	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:218:TRP:HH2	1:B:246:SER:HG	1.55	0.53
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: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: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: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:A:42:LEU:HD23	1:A:42:LEU:C	2.31	0.52
1:B:137:SER:C	1:B:139:GLU:H	2.13	0.52
1:B:90:ILE:HG23	1:B:103:TYR:HD2	1.74	0.52
1:B:364:ARG:HD2	1:B:364:ARG:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:269:GLU:HG3	1:A:270:PHE:N	2.27	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: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: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: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: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: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: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:A:456:TRP:O	1:A:460:HIS:HD2	1.96	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:O	1:B:131:TYR:N	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
1:B:80:GLN:HG3	1:B:81:GLU:N	2.28	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:7:TYR:O	1:A:10:ASP:N	2.46	0.48
1:A:339:GLY:C	1:A:341:GLU:H	2.15	0.48
1:A:36:VAL:HG21	1:A:293:LEU:HD11	1.96	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: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: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:35:HIS:ND1	1:B:38:ASN:ND2	2.62	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:A:51:ALA:O	1:A:54:ASP: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:199:CYS:SG	1:A:200:PRO:HD2	2.54	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:A:12:ILE:HG12	1:A:264:LEU:HD12	1.96	0.47
1:A:308:ARG:NH1	1:A:308:ARG:HG3	2.29	0.47
1:B:308:ARG:NH2	1:B:329:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:222:TRP:HB3	1:A:223:PRO:CD	2.46	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: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: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:NH1	1:A:364:ARG:HG3	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
1:A:361:LYS:HB3	1:A:361:LYS:HZ2	1.82	0.45
1:A:440:VAL:O	1:A:442:VAL:HG23	2.17	0.45
1:B:130:LEU:HD23	1:B:133:ARG:HH12	1.81	0.45
1:B:89:PRO:HD2	1:B:92:GLU:HG3	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:23:VAL:HG12	1:A:231:VAL:HA	2.00	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:B:93:VAL:HG23	1:B:103:TYR:CB	2.44	0.44
1:A:66:ASP:OD1	1:A:225:ARG:NH2	2.50	0.44
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:213:ASN:N	1:A:213:ASN:ND2	2.66	0.44
1:A:35:HIS:N	1:A:38:ASN:HD22	2.12	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:A:308:ARG:HH11	1:A:308:ARG:HG3	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: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:A:456:TRP:O	1:A:460:HIS:CD2	2.72	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:B:42:LEU:C	1:B:42:LEU:HD12	2.39	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:138:GLU:CD	1:B:138:GLU:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:364:ARG:CG	1:A:364:ARG:HH11	2.29	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: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:180:HIS:ND1	1:B:180:HIS:O	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: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:7:TYR:HD2	1:B:8:ILE:HD12	1.85	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: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:A:197:TYR:CE2	1:A:207:VAL:HG23	2.55	0.42
1:A:21:LYS:HA	1:A:58:GLU:O	2.19	0.42
1:A:331:GLU:HG3	1:A:368:GLN:NE2	2.35	0.42
1:A:80:GLN:OE1	1:A:81:GLU:N	2.53	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:105:GLU:O	1:A:109:ARG:HG2	2.20	0.41
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: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:B:444:GLU:CD	1:B:444:GLU:H	2.23	0.41
1:A:147:ARG:HD2	1:A:171:TRP:CE3	2.54	0.41
1:A:139:GLU:HB3	1:A:224:MET:HG2	2.02	0.41
1:B:158:ARG:HA	1:B:163:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:364:ARG:NH1	1:A:364:ARG:CG	2.84	0.41
1:B:224:MET:HE2	1:B:225:ARG:HA	2.02	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:B:366:VAL:HG21	1:B:405:GLU:OE1	2.21	0.41
1:B:74:VAL:O	1:B:74:VAL:CG2	2.66	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: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: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: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: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:B:85:TYR:CD2	1:B:94:PRO:HD2	2.56	0.41
1:A:11:LYS:O	1:A:15:GLU:HB2	2.21	0.40
1:A:42:LEU:O	1:A:42:LEU:HD23	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: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:133:ARG:NH1	1:B:133:ARG:HB3	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:B:68:TYR:HA	1:B:68:TYR:HD1	1.74	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:OE1	1:B:138:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	501/523 (96%)	457 (91%)	37 (7%)	7 (1%)	11	22
1	B	502/523 (96%)	443 (88%)	42 (8%)	17 (3%)	3	5
All	All	1003/1046 (96%)	900 (90%)	79 (8%)	24 (2%)	6	10

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

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Mol	Chain	Res	Type
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%)	25	48
1	B	452/462 (98%)	424 (94%)	28 (6%)	18	37
All	All	903/924 (98%)	853 (94%)	50 (6%)	21	43

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.