Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:06 PM GMT

PDB ID	:	1IRX
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

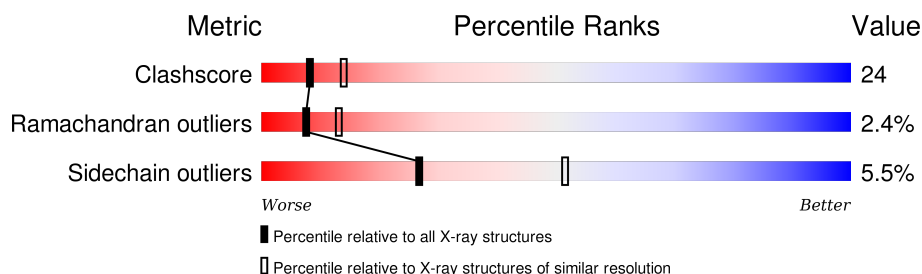|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		2.4%
Sidechain outliers		5.5%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	58% 36% · ·
1	B	523	51% 41% 5% · ·

Full wwPDB X-ray Structure Validation Report

2 Entry composition (i)

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).

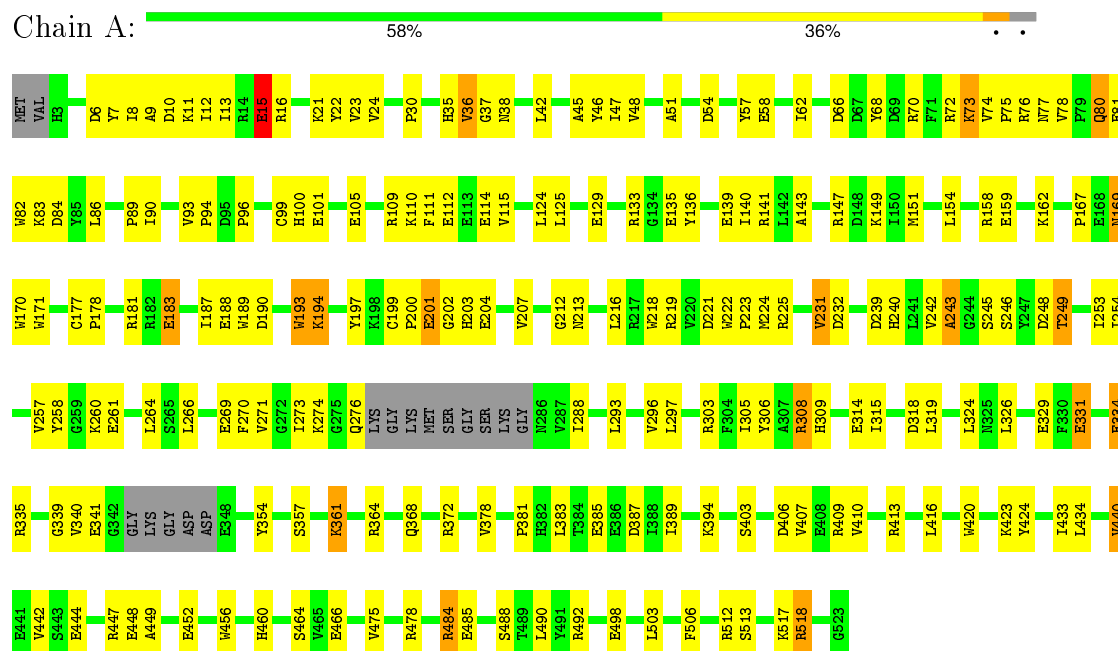| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

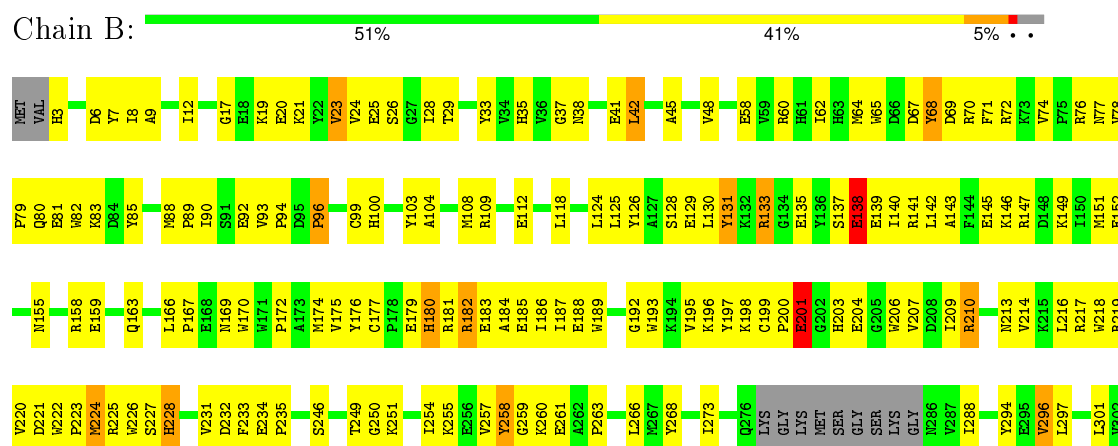| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	102	Total	O	0	0
			102	102		

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 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

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R303 F304 I305 R308 P311 I323 L326 E329 K332 V333 E334 R335 I336 Y337 F338 G339 V340 E341 G342 GLY LYS GLY ASP D347 E348 R351 S357 M358 P359 K360 K361 P362 E363 R364 L365 V366 L374 A375 V376 L377 V378 Q379 L380 P381 H382 L383 T384 E385 E386 D387 I388

I389 N390 V391 P399 L402 S403 K404 E405 E408 R409 V410 K411 L412 R413 I414 R418 N419 W420 K423 D428 I433 L434 E435 K436 E444 A449 E452 V453 W456 L457 H460 E466 E467 F468 I471 E474 R478 R484 F487 S488 Y491

P501 R502 L503 F506 R512 R518 G523

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 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	0.40	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 (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	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: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

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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: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

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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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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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: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
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

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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: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
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

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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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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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:A:498:GLU:HG2	3:A:701:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/523 (96%)	457 (91%)	37 (7%)	7 (1%)	14	28
1	B	502/523 (96%)	443 (88%)	42 (8%)	17 (3%)	5	7
All	All	1003/1046 (96%)	900 (90%)	79 (8%)	24 (2%)	7	13

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/462 (98%)	429 (95%)	22 (5%)	31	57
1	B	452/462 (98%)	424 (94%)	28 (6%)	23	45
All	All	903/924 (98%)	853 (94%)	50 (6%)	27	51

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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