



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:29 AM UTC

PDB ID : 2A4M / pdb_00002a4m
Title : Structure of Trprs II bound to ATP
Authors : Buddha, M.R.; Crane, B.R.
Deposited on : 2005-06-29
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

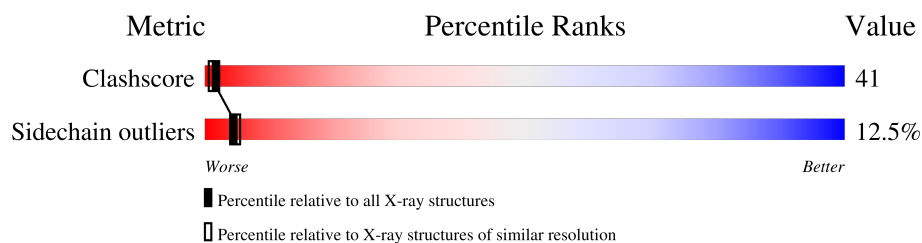
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

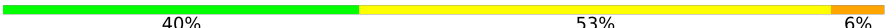
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	331	
1	B	331	
1	C	331	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRP	C	500	-	-	X	-

2 Entry composition [i](#)

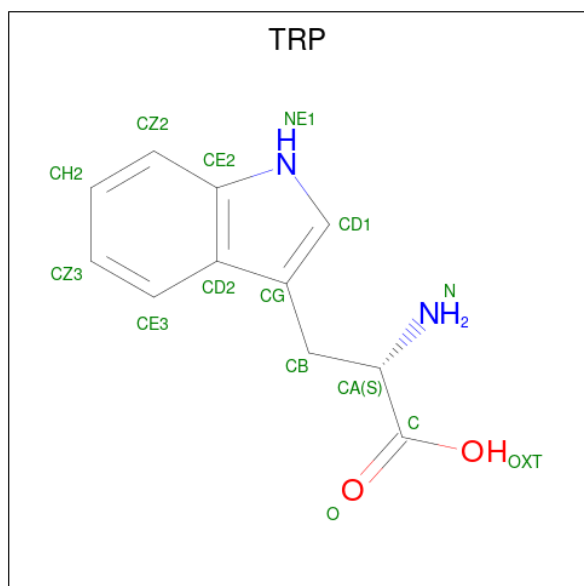
There are 3 unique types of molecules in this entry. The entry contains 8788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophanyl-tRNA synthetase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	2	0	0
			2544	1599	468	471	6			
1	B	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2527	1591	462	468	6			

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is water.

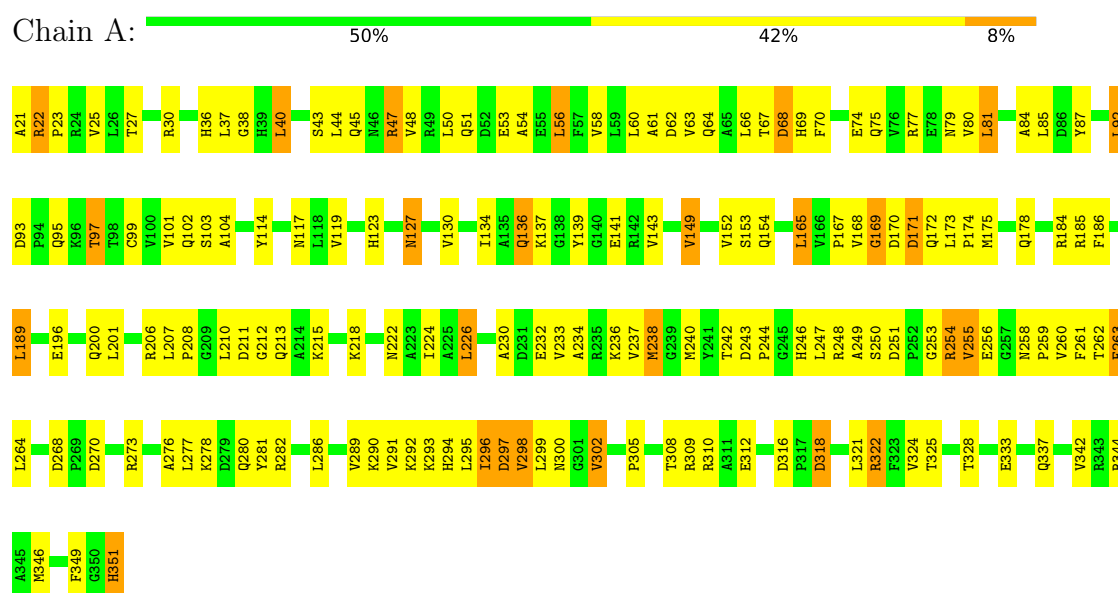
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total 382	O 382	0	0
3	B	395	Total 395	O 395	0	0
3	C	414	Total 414	O 414	0	0

3 Residue-property plots

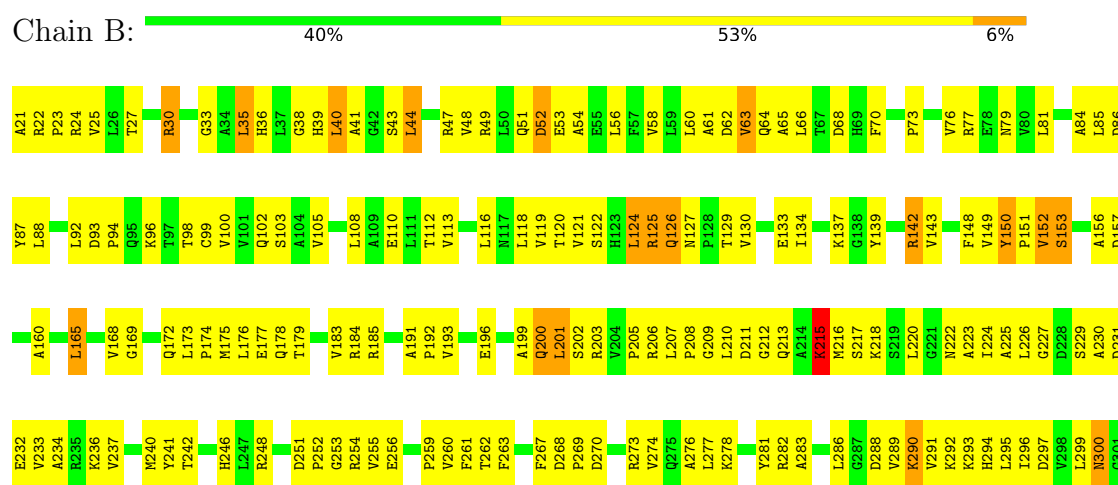
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

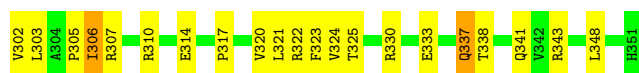
Note EDS was not executed.

• Molecule 1: Tryptophanyl-tRNA synthetase II



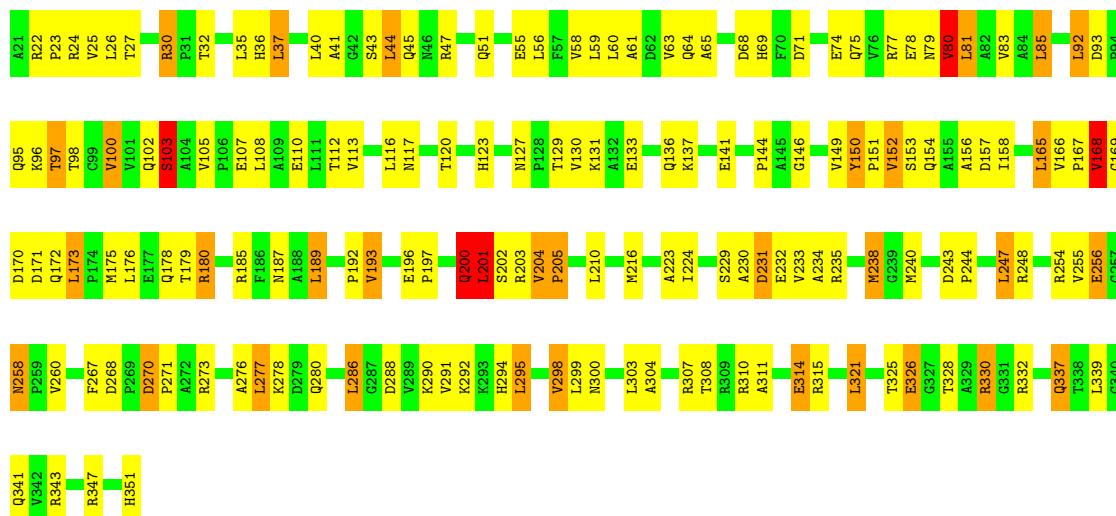
• Molecule 1: Tryptophanyl-tRNA synthetase II





• Molecule 1: Tryptophanyl-tRNA synthetase II

Chain C: 50% 39% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.58Å 58.57Å 85.15Å 90.00° 96.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	71.5 (30.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8788	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.46	0/2591	1.00	15/3519 (0.4%)
1	B	0.40	0/2558	0.98	7/3478 (0.2%)
1	C	0.54	0/2574	1.05	15/3499 (0.4%)
All	All	0.47	0/7723	1.01	37/10496 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	LYS	N-CA-C	9.59	121.31	108.07
1	C	201	LEU	N-CA-C	8.16	122.07	110.23
1	B	43	SER	N-CA-C	7.63	120.71	111.40
1	A	212	GLY	N-CA-C	-7.43	104.30	115.00
1	C	44	LEU	CB-CA-C	6.42	121.05	110.90
1	A	169	GLY	N-CA-C	-6.26	104.53	112.54
1	B	44	LEU	N-CA-C	6.03	118.63	111.33
1	A	56	LEU	N-CA-C	5.82	118.21	108.96
1	A	61	ALA	CA-C-N	5.74	128.28	120.54
1	A	61	ALA	C-N-CA	5.74	128.28	120.54
1	A	255	VAL	N-CA-C	5.72	115.91	110.53
1	A	298	VAL	N-CA-C	-5.68	103.99	111.09
1	C	169	GLY	N-CA-C	-5.65	101.78	112.51
1	C	141	GLU	N-CA-C	-5.62	106.59	113.50
1	C	200	GLN	N-CA-C	-5.62	95.36	107.49
1	B	100	VAL	N-CA-C	5.61	115.96	108.11
1	C	103	SER	CB-CA-C	-5.50	101.33	110.68
1	C	173	LEU	CA-C-N	-5.50	113.36	119.19
1	C	173	LEU	C-N-CA	-5.50	113.36	119.19
1	C	270	ASP	CA-C-N	5.46	125.13	119.56
1	C	270	ASP	C-N-CA	5.46	125.13	119.56
1	B	30	ARG	N-CA-C	-5.41	101.42	109.42
1	C	168	VAL	N-CA-C	5.38	115.45	108.35
1	A	127	ASN	CA-C-N	5.32	124.95	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASN	C-N-CA	5.32	124.95	119.05
1	A	79	ASN	N-CA-C	5.31	119.63	113.20
1	A	153	SER	N-CA-C	-5.29	105.59	111.36
1	C	80	VAL	N-CA-C	-5.28	105.46	110.42
1	A	268	ASP	CA-C-N	5.27	124.78	119.19
1	A	268	ASP	C-N-CA	5.27	124.78	119.19
1	C	240	MET	N-CA-C	5.25	118.04	110.28
1	C	179	THR	N-CA-C	-5.22	105.50	111.14
1	A	324	VAL	N-CA-C	5.15	115.37	110.53
1	C	61	ALA	N-CA-C	5.14	117.46	108.52
1	B	153	SER	N-CA-C	-5.13	105.76	112.23
1	A	210	LEU	N-CA-C	-5.09	105.92	111.82
1	B	337	GLN	N-CA-C	-5.08	105.65	111.14

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	2544	0	2568	190	0
1	B	2511	0	2507	241	0
1	C	2527	0	2539	199	0
2	C	15	0	9	7	0
3	A	382	0	0	12	0
3	B	395	0	0	6	0
3	C	414	0	0	11	0
All	All	8788	0	7623	620	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 41.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG21	1:B:341:GLN:HB3	1.20	1.14
1:C:120:THR:HG23	1:C:123:HIS:H	1.13	1.08
1:B:207:LEU:HD23	1:B:216:MET:HE1	1.36	1.08
1:A:240:MET:HE3	1:A:260:VAL:HG12	1.31	1.07
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.21	1.06
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.16	1.05
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.11	1.05
1:B:226:LEU:HB3	1:B:306:ILE:HD11	1.39	1.03
1:C:204:VAL:HG12	1:C:205:PRO:HD2	1.41	1.02
1:C:77:ARG:O	1:C:80:VAL:HG12	1.64	0.97
1:A:51:GLN:HE22	1:A:93:ASP:H	1.06	0.97
1:A:51:GLN:HE21	1:A:97:THR:HG22	1.27	0.96
1:C:180:ARG:HD3	1:C:197:PRO:O	1.66	0.95
1:C:26:LEU:HD23	1:C:158:ILE:HD13	1.48	0.93
1:A:255:VAL:HG21	1:A:278:LYS:HG3	1.51	0.93
1:C:166:VAL:HG21	1:C:176:LEU:HD23	1.49	0.92
1:A:322:ARG:HG2	1:A:322:ARG:HH21	1.35	0.91
1:C:51:GLN:HE22	1:C:93:ASP:H	1.19	0.91
1:B:226:LEU:HD12	1:B:226:LEU:H	1.38	0.89
1:C:216:MET:HE3	1:C:224:ILE:H	1.39	0.88
1:C:254:ARG:HD3	1:C:256:GLU:HG2	1.56	0.88
1:C:180:ARG:HH11	1:C:180:ARG:CG	1.86	0.86
1:B:52:ASP:HB3	1:B:96:LYS:NZ	1.91	0.85
1:A:51:GLN:HE22	1:A:93:ASP:N	1.75	0.85
1:C:108:LEU:O	1:C:112:THR:HG23	1.76	0.84
1:A:68:ASP:HB3	1:A:69:HIS:HD2	1.42	0.84
1:B:108:LEU:O	1:B:112:THR:HG23	1.77	0.84
1:B:230:ALA:HB1	1:B:300:ASN:HD21	1.40	0.84
1:C:337:GLN:HA	1:C:337:GLN:NE2	1.87	0.84
1:A:189:LEU:HD21	1:C:71:ASP:HA	1.59	0.84
1:A:295:LEU:O	1:A:298:VAL:HG12	1.75	0.84
1:B:73:PRO:O	1:B:76:VAL:HG12	1.76	0.84
1:C:255:VAL:HG21	1:C:278:LYS:HG2	1.59	0.84
1:A:254:ARG:HD3	1:A:256:GLU:HG2	1.60	0.83
1:B:168:VAL:CG2	1:B:172:GLN:HB2	2.08	0.82
1:A:68:ASP:OD1	1:A:137:LYS:HE2	1.80	0.82
1:A:184:ARG:HE	1:A:196:GLU:CD	1.88	0.81
1:B:218:LYS:HE2	1:B:218:LYS:HA	1.62	0.81
1:B:127:ASN:HB3	1:B:130:VAL:HG12	1.62	0.81
1:B:36:HIS:HD2	1:B:38:GLY:H	1.28	0.80
1:C:35:LEU:HD23	1:C:44:LEU:HD11	1.63	0.79
1:A:43:SER:O	1:A:47:ARG:HD2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:HD2	1:A:38:GLY:H	1.27	0.79
1:B:116:LEU:HD21	1:B:149:VAL:HG11	1.65	0.79
1:A:247:LEU:HB2	1:A:248:ARG:HH21	1.47	0.78
1:C:36:HIS:HB2	1:C:216:MET:HE2	1.64	0.78
1:C:136:GLN:NE2	1:C:137:LYS:HD2	1.99	0.78
1:B:30:ARG:HD2	1:B:65:ALA:HA	1.65	0.78
1:B:30:ARG:HH22	1:B:68:ASP:HB3	1.48	0.77
1:B:33:GLY:HA2	1:B:79:ASN:ND2	1.99	0.77
1:B:333:GLU:O	1:B:337:GLN:HG2	1.84	0.77
1:C:120:THR:CG2	1:C:123:HIS:H	1.93	0.77
1:C:234:ALA:O	1:C:238:MET:HG2	1.85	0.77
1:C:168:VAL:HG22	1:C:172:GLN:HB2	1.67	0.76
1:B:259:PRO:HA	1:B:262:THR:CG2	2.15	0.76
1:C:92:LEU:HG	1:C:97:THR:HG21	1.67	0.76
1:A:50:LEU:HD11	1:A:56:LEU:HD13	1.68	0.75
1:A:277:LEU:HD12	1:A:286:LEU:HD11	1.68	0.75
1:A:22:ARG:CB	1:A:23:PRO:HD3	2.17	0.75
1:B:193:VAL:HG21	1:B:341:GLN:CB	2.09	0.75
1:A:22:ARG:HB2	1:A:23:PRO:HD3	1.68	0.74
1:A:47:ARG:HA	1:A:50:LEU:HG	1.68	0.74
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.53	0.74
1:C:127:ASN:HB3	1:C:130:VAL:HG22	1.70	0.74
1:C:180:ARG:HG3	1:C:180:ARG:NH1	1.92	0.74
1:A:280:GLN:HB2	1:A:286:LEU:HD12	1.70	0.74
1:B:133:GLU:O	1:B:137:LYS:HG3	1.86	0.74
1:B:226:LEU:HB3	1:B:306:ILE:CD1	2.17	0.74
1:A:51:GLN:NE2	1:A:93:ASP:H	1.84	0.73
1:B:176:LEU:HD13	1:B:176:LEU:O	1.87	0.73
1:C:56:LEU:HD11	1:C:58:VAL:HG13	1.68	0.73
1:C:56:LEU:HD12	1:C:97:THR:HB	1.69	0.73
1:B:52:ASP:HB3	1:B:96:LYS:HZ1	1.54	0.73
1:B:149:VAL:HG13	1:B:152:VAL:HG13	1.70	0.73
1:B:121:VAL:O	1:B:125:ARG:HB2	1.89	0.73
1:C:216:MET:CE	1:C:224:ILE:H	2.02	0.73
1:A:168:VAL:HG23	1:A:172:GLN:HB2	1.71	0.73
1:B:134:ILE:HG23	1:B:139:TYR:HB2	1.71	0.72
1:B:169:GLY:H	1:B:172:GLN:HG3	1.55	0.72
1:C:216:MET:HE3	1:C:224:ILE:N	2.05	0.72
1:C:171:ASP:HB2	1:C:172:GLN:NE2	2.05	0.71
1:C:260:VAL:HG13	1:C:295:LEU:HD12	1.71	0.71
1:A:40:LEU:HD23	1:A:226:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.72	0.71
1:A:51:GLN:HE21	1:A:97:THR:CG2	2.01	0.71
1:C:276:ALA:O	1:C:280:GLN:HG3	1.91	0.70
1:B:168:VAL:HG23	1:B:172:GLN:CB	2.12	0.70
1:C:22:ARG:HB2	1:C:23:PRO:HD3	1.73	0.70
1:B:274:VAL:HG12	1:B:278:LYS:HE3	1.72	0.70
1:A:22:ARG:HH21	1:A:53:GLU:HG3	1.57	0.70
1:C:30:ARG:HG2	3:C:1939:HOH:O	1.89	0.70
1:C:120:THR:HG23	1:C:123:HIS:N	1.98	0.70
1:C:171:ASP:HB2	1:C:172:GLN:HE22	1.56	0.70
1:C:175:MET:SD	1:C:175:MET:C	2.75	0.69
1:C:56:LEU:CD1	1:C:58:VAL:HG13	2.23	0.69
1:C:22:ARG:HB2	1:C:23:PRO:CD	2.23	0.69
1:C:233:VAL:HG21	1:C:307:ARG:HH21	1.58	0.69
1:A:36:HIS:HD2	1:A:38:GLY:N	1.91	0.68
1:A:101:VAL:HG13	1:A:104:ALA:HB3	1.74	0.68
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.76	0.68
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.74	0.68
1:A:305:PRO:HB2	1:A:309:ARG:NH2	2.09	0.68
1:A:40:LEU:O	1:A:45:GLN:HG2	1.93	0.68
1:A:127:ASN:HB3	1:A:130:VAL:CG1	2.23	0.68
1:B:21:ALA:HB3	1:B:53:GLU:O	1.93	0.68
1:A:232:GLU:O	1:A:236:LYS:HG2	1.94	0.67
1:B:259:PRO:HA	1:B:262:THR:HG22	1.74	0.67
1:B:160:ALA:HA	1:B:338:THR:HG21	1.76	0.67
1:C:36:HIS:CG	1:C:216:MET:HE2	2.29	0.67
1:B:229:SER:OG	1:B:232:GLU:HB2	1.94	0.67
1:C:176:LEU:C	1:C:176:LEU:HD13	2.20	0.67
1:A:25:VAL:HG22	1:A:165:LEU:HB3	1.77	0.67
1:C:201:LEU:HD23	1:C:202:SER:H	1.60	0.67
1:B:130:VAL:O	1:B:134:ILE:HG13	1.95	0.66
1:B:232:GLU:O	1:B:236:LYS:HB2	1.96	0.66
1:C:204:VAL:HG12	1:C:205:PRO:CD	2.23	0.66
1:B:35:LEU:HD12	1:B:226:LEU:HD13	1.77	0.66
1:B:321:LEU:O	1:B:325:THR:HG23	1.96	0.66
1:C:158:ILE:HD11	2:C:500:TRP:HH2	1.61	0.66
1:A:101:VAL:HG12	1:A:328:THR:OG1	1.96	0.66
1:A:342:VAL:HG12	1:A:346:MET:HE2	1.77	0.66
1:B:208:PRO:HG3	1:B:262:THR:HG23	1.78	0.66
1:C:36:HIS:HB2	1:C:216:MET:CE	2.26	0.66
1:C:79:ASN:O	1:C:83:VAL:HG22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:VAL:HG23	1:C:166:VAL:O	1.95	0.65
1:A:68:ASP:HB3	1:A:69:HIS:CD2	2.30	0.65
1:B:288:ASP:HA	1:B:291:VAL:HG12	1.79	0.65
1:A:184:ARG:HG2	1:A:184:ARG:HH21	1.61	0.65
1:C:295:LEU:O	1:C:298:VAL:HG13	1.97	0.65
1:A:273:ARG:NH2	1:A:294:HIS:NE2	2.45	0.65
1:B:35:LEU:HD11	1:B:86:ASP:HB3	1.79	0.65
1:B:119:VAL:HG21	1:B:178:GLN:OE1	1.96	0.65
1:B:149:VAL:HG12	1:B:149:VAL:O	1.95	0.65
1:C:254:ARG:CD	1:C:256:GLU:HG2	2.27	0.65
1:A:211:ASP:OD1	1:A:222:ASN:HB3	1.96	0.64
1:A:349:PHE:CD2	1:C:80:VAL:HG11	2.32	0.64
1:B:317:PRO:O	1:B:320:VAL:HG12	1.97	0.64
1:B:36:HIS:HD2	1:B:38:GLY:N	1.96	0.64
1:B:168:VAL:HG11	1:B:199:ALA:HB1	1.79	0.64
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.28	0.64
1:A:22:ARG:HH21	1:A:53:GLU:CG	2.10	0.64
1:A:22:ARG:H	1:A:54:ALA:HA	1.61	0.64
1:B:52:ASP:HB3	1:B:96:LYS:HZ3	1.62	0.64
1:B:230:ALA:CB	1:B:300:ASN:HD21	2.11	0.64
1:B:110:GLU:O	1:B:113:VAL:HG12	1.98	0.64
1:B:229:SER:O	1:B:233:VAL:HG23	1.97	0.64
1:C:290:LYS:HE2	1:C:290:LYS:HA	1.80	0.63
1:A:173:LEU:N	1:A:174:PRO:HD2	2.13	0.63
1:C:120:THR:HG21	3:C:1438:HOH:O	1.98	0.63
1:B:296:ILE:O	1:B:300:ASN:HB2	1.99	0.63
1:A:322:ARG:HG2	1:A:322:ARG:NH2	2.11	0.62
1:B:207:LEU:HD12	1:B:208:PRO:HD2	1.81	0.62
1:C:258:ASN:C	1:C:258:ASN:HD22	2.07	0.62
1:C:110:GLU:O	1:C:113:VAL:HG12	1.99	0.62
1:C:36:HIS:CB	1:C:216:MET:HE2	2.29	0.62
1:A:30:ARG:HH22	1:A:68:ASP:HB2	1.65	0.62
1:B:108:LEU:HD13	1:B:157:ASP:OD1	2.00	0.62
1:B:30:ARG:NH2	1:B:68:ASP:HB3	2.14	0.62
1:B:105:VAL:HG13	1:B:108:LEU:HG	1.82	0.62
1:B:149:VAL:HG13	1:B:152:VAL:CG1	2.29	0.62
1:A:248:ARG:HD3	1:A:248:ARG:N	2.14	0.61
1:B:201:LEU:HD22	1:B:202:SER:H	1.64	0.61
1:B:208:PRO:HG3	1:B:262:THR:CG2	2.30	0.61
1:B:173:LEU:O	1:B:177:GLU:HB2	1.99	0.61
1:C:180:ARG:HD2	1:C:196:GLU:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:O	1:A:302:VAL:HG12	2.00	0.61
1:B:127:ASN:HB3	1:B:130:VAL:CG1	2.30	0.61
1:B:172:GLN:C	1:B:174:PRO:HD2	2.25	0.61
1:C:60:LEU:HD22	1:C:83:VAL:CG2	2.30	0.61
1:B:220:LEU:C	1:B:222:ASN:H	2.07	0.61
1:C:154:GLN:CD	2:C:500:TRP:OXT	2.43	0.61
1:B:215:LYS:HB2	1:B:215:LYS:NZ	2.16	0.61
1:B:226:LEU:HD12	1:B:226:LEU:N	2.14	0.61
1:C:32:THR:HG22	1:C:32:THR:O	2.00	0.61
1:C:294:HIS:O	1:C:298:VAL:HG12	2.00	0.61
1:A:47:ARG:HH11	1:A:47:ARG:HG2	1.64	0.60
1:B:23:PRO:O	1:B:54:ALA:HB1	2.01	0.60
1:C:37:LEU:HD13	3:C:2057:HOH:O	2.00	0.60
1:A:22:ARG:CG	1:A:23:PRO:HD3	2.31	0.60
1:B:41:ALA:CB	1:B:207:LEU:HD22	2.31	0.60
1:B:173:LEU:N	1:B:174:PRO:HD2	2.16	0.60
1:C:41:ALA:HB2	1:C:267:PHE:CZ	2.35	0.60
1:B:63:VAL:HG13	1:B:102:GLN:CD	2.25	0.60
1:C:56:LEU:HD11	1:C:58:VAL:CG1	2.30	0.60
1:A:114:TYR:CD1	1:A:346:MET:HE1	2.36	0.60
1:C:105:VAL:HG13	1:C:108:LEU:HG	1.82	0.60
1:A:77:ARG:NH2	1:C:351:HIS:O	2.33	0.60
1:C:268:ASP:OD1	1:C:294:HIS:HE1	1.84	0.60
1:A:62:ASP:O	1:A:66:LEU:HD23	2.02	0.60
1:B:253:GLY:O	1:B:282:ARG:HA	2.00	0.60
1:B:303:LEU:O	1:B:306:ILE:HG23	2.02	0.60
1:A:114:TYR:CE1	1:A:346:MET:HE1	2.37	0.60
1:A:44:LEU:O	1:A:48:VAL:HG23	2.02	0.59
1:B:139:TYR:O	1:B:142:ARG:HG3	2.02	0.59
1:B:295:LEU:O	1:B:299:LEU:HG	2.02	0.59
1:C:203:ARG:C	1:C:204:VAL:HG23	2.27	0.59
1:A:44:LEU:HA	1:A:47:ARG:CD	2.31	0.59
1:C:120:THR:HG22	1:C:123:HIS:HB2	1.83	0.59
1:C:107:GLU:OE2	1:C:332:ARG:NH1	2.35	0.59
1:B:201:LEU:CD2	1:B:202:SER:H	2.16	0.59
1:C:230:ALA:HB1	1:C:300:ASN:HD21	1.68	0.59
1:A:316:ASP:OD1	1:A:318:ASP:OD2	2.21	0.59
1:B:288:ASP:O	1:B:291:VAL:HG12	2.01	0.59
1:A:64:GLN:NE2	1:A:154:GLN:HG3	2.18	0.58
1:A:237:VAL:HG13	1:A:240:MET:HE1	1.85	0.58
2:C:500:TRP:OXT	2:C:500:TRP:CG	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:VAL:HG13	1:B:292:LYS:N	2.16	0.58
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.17	0.58
1:B:36:HIS:CD2	1:B:38:GLY:H	2.17	0.58
1:B:142:ARG:O	1:B:142:ARG:HD3	2.03	0.58
1:C:175:MET:HB2	3:C:1000:HOH:O	2.02	0.58
1:C:116:LEU:CD2	1:C:152:VAL:HG21	2.33	0.58
1:B:125:ARG:HH21	1:B:125:ARG:HG3	1.68	0.58
1:A:264:LEU:HG	1:A:295:LEU:HD12	1.86	0.57
1:B:220:LEU:C	1:B:222:ASN:N	2.59	0.57
1:A:244:PRO:C	1:A:246:HIS:H	2.12	0.57
1:C:201:LEU:HD23	1:C:202:SER:N	2.19	0.57
1:C:98:THR:HG21	1:C:330:ARG:HG2	1.86	0.57
1:B:112:THR:HG22	1:B:156:ALA:CB	2.34	0.57
1:C:255:VAL:HG21	1:C:278:LYS:CG	2.34	0.57
1:B:274:VAL:O	1:B:278:LYS:HG3	2.04	0.57
1:C:116:LEU:HD23	1:C:152:VAL:HG21	1.85	0.57
1:B:112:THR:O	1:B:116:LEU:HG	2.03	0.57
1:B:36:HIS:H	1:B:39:HIS:HD2	1.52	0.57
1:B:27:THR:O	1:B:58:VAL:HA	2.04	0.57
1:B:193:VAL:O	1:B:193:VAL:HG22	2.04	0.56
1:A:22:ARG:HB2	1:A:23:PRO:CD	2.35	0.56
1:A:63:VAL:H	1:A:102:GLN:HE21	1.53	0.56
1:B:179:THR:O	1:B:183:VAL:HG23	2.04	0.56
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.18	0.56
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.33	0.56
1:B:60:LEU:O	1:B:62:ASP:N	2.38	0.56
1:A:64:GLN:H	1:A:102:GLN:HE22	1.54	0.56
1:C:295:LEU:HA	1:C:298:VAL:CG1	2.36	0.56
1:A:238:MET:HE1	1:A:289:VAL:HG13	1.88	0.56
1:C:315:ARG:HB2	3:C:1506:HOH:O	2.06	0.56
1:A:248:ARG:HD3	1:A:248:ARG:H	1.71	0.56
3:A:1267:HOH:O	1:C:103:SER:HB3	2.06	0.56
1:A:321:LEU:O	1:A:325:THR:HG23	2.06	0.56
1:A:40:LEU:CD2	1:A:226:LEU:HD21	2.36	0.56
1:B:35:LEU:HD12	1:B:226:LEU:CD1	2.36	0.56
1:B:36:HIS:HA	1:B:225:ALA:HA	1.86	0.56
1:B:293:LYS:HZ2	1:B:296:ILE:HD11	1.69	0.56
1:B:168:VAL:HG22	1:B:169:GLY:N	2.21	0.55
1:B:241:TYR:O	1:B:259:PRO:HD2	2.06	0.55
1:B:254:ARG:HD3	1:B:256:GLU:HB2	1.88	0.55
1:A:175:MET:SD	1:A:175:MET:C	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HA	1:A:262:THR:CG2	2.37	0.55
1:B:40:LEU:HD13	1:B:267:PHE:HE2	1.71	0.55
1:A:292:LYS:O	1:A:296:ILE:HG23	2.07	0.55
1:A:342:VAL:CG1	1:A:346:MET:HE2	2.36	0.55
1:B:98:THR:OG1	1:B:330:ARG:NH1	2.39	0.55
1:B:149:VAL:O	1:B:149:VAL:CG1	2.54	0.55
1:B:269:PRO:HD2	1:B:273:ARG:NH1	2.22	0.55
1:A:93:ASP:O	1:A:97:THR:HG23	2.07	0.54
1:A:137:LYS:HE3	3:A:1401:HOH:O	2.07	0.54
1:C:40:LEU:O	1:C:45:GLN:HG3	2.07	0.54
1:A:322:ARG:HH21	1:A:322:ARG:CG	2.11	0.54
1:B:207:LEU:CD1	1:B:208:PRO:HD2	2.37	0.54
1:C:64:GLN:OE1	1:C:154:GLN:HG3	2.06	0.54
1:B:52:ASP:OD2	1:B:52:ASP:N	2.36	0.54
1:C:24:ARG:HD3	1:C:55:GLU:OE2	2.08	0.54
1:A:58:VAL:HG23	1:A:99:CYS:HA	1.89	0.54
1:B:242:THR:HG23	1:B:292:LYS:CE	2.37	0.54
1:B:255:VAL:HG13	1:B:261:PHE:HB3	1.90	0.54
1:C:216:MET:HE3	1:C:223:ALA:HB1	1.89	0.54
1:B:129:THR:O	1:B:133:GLU:HG3	2.08	0.54
1:B:201:LEU:HD22	1:B:202:SER:N	2.23	0.54
1:C:133:GLU:O	1:C:137:LYS:HD3	2.07	0.54
1:B:175:MET:SD	1:B:175:MET:C	2.91	0.54
1:B:226:LEU:HD23	1:B:306:ILE:CD1	2.37	0.54
1:B:254:ARG:HH11	1:B:256:GLU:HB2	1.73	0.54
1:A:50:LEU:HD12	1:A:50:LEU:C	2.33	0.54
1:B:259:PRO:O	1:B:263:PHE:HB2	2.08	0.54
1:C:254:ARG:HD2	1:C:256:GLU:O	2.08	0.54
1:A:58:VAL:HG23	1:A:58:VAL:O	2.07	0.54
1:A:237:VAL:HG13	1:A:240:MET:CE	2.38	0.54
1:B:289:VAL:O	1:B:293:LYS:HB2	2.08	0.53
1:A:21:ALA:HB1	1:A:54:ALA:C	2.32	0.53
1:B:299:LEU:O	1:B:303:LEU:HD13	2.08	0.53
1:A:22:ARG:NH2	1:A:53:GLU:HG3	2.24	0.53
1:B:215:LYS:HB2	1:B:215:LYS:HZ3	1.73	0.53
1:C:154:GLN:OE1	2:C:500:TRP:OXT	2.26	0.53
1:B:116:LEU:HD23	1:B:152:VAL:HG21	1.91	0.53
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.71	0.53
1:B:119:VAL:HG22	1:B:120:THR:N	2.24	0.53
1:C:256:GLU:H	1:C:256:GLU:CD	2.15	0.53
1:A:318:ASP:HA	3:A:2065:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD22	1:A:44:LEU:HD12	1.90	0.53
1:A:233:VAL:O	1:A:237:VAL:HG23	2.09	0.53
1:C:60:LEU:HD22	1:C:83:VAL:HG23	1.91	0.53
1:C:286:LEU:HD12	1:C:291:VAL:HG23	1.91	0.53
1:A:189:LEU:CD2	1:C:71:ASP:HA	2.35	0.52
1:A:206:ARG:NH1	1:A:215:LYS:HE2	2.24	0.52
1:A:62:ASP:OD1	1:A:103:SER:OG	2.28	0.52
1:B:47:ARG:O	1:B:51:GLN:HB2	2.09	0.52
1:C:51:GLN:HE22	1:C:93:ASP:N	1.98	0.52
1:B:61:ALA:HB1	1:B:64:GLN:HB3	1.91	0.52
1:B:254:ARG:HH11	1:B:256:GLU:CB	2.22	0.52
1:C:180:ARG:CG	1:C:180:ARG:NH1	2.56	0.52
1:A:27:THR:OG1	1:A:47:ARG:NH1	2.43	0.52
1:C:180:ARG:HD2	1:C:196:GLU:HG3	1.91	0.52
1:A:168:VAL:HG22	1:A:169:GLY:O	2.10	0.52
1:B:293:LYS:NZ	1:B:296:ILE:HD11	2.23	0.52
1:B:149:VAL:CG1	1:B:152:VAL:HG13	2.40	0.52
1:B:202:SER:OG	1:B:205:PRO:HB3	2.09	0.52
1:C:339:LEU:O	1:C:343:ARG:HG3	2.10	0.52
1:A:248:ARG:NE	1:A:251:ASP:OD2	2.43	0.51
1:C:60:LEU:CD2	1:C:83:VAL:HG23	2.40	0.51
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.94	0.51
1:A:218:LYS:HE3	3:A:1289:HOH:O	2.09	0.51
1:C:26:LEU:HD23	1:C:158:ILE:CD1	2.31	0.51
1:C:310:ARG:O	1:C:314:GLU:HG2	2.10	0.51
1:B:110:GLU:O	1:B:113:VAL:CG1	2.57	0.51
1:A:74:GLU:OE2	1:C:347:ARG:NH1	2.43	0.51
1:A:296:ILE:HD12	1:A:300:ASN:ND2	2.25	0.51
1:B:273:ARG:O	1:B:277:LEU:HD23	2.09	0.51
1:C:56:LEU:HD13	1:C:56:LEU:C	2.35	0.51
1:A:270:ASP:O	1:A:273:ARG:HB3	2.10	0.51
1:C:74:GLU:HB2	3:C:2059:HOH:O	2.09	0.51
1:B:44:LEU:O	1:B:48:VAL:HG23	2.11	0.51
1:B:299:LEU:HA	1:B:302:VAL:HG12	1.93	0.51
1:C:158:ILE:HD11	2:C:500:TRP:CH2	2.45	0.51
1:B:261:PHE:CD1	1:B:278:LYS:HG2	2.46	0.51
1:A:149:VAL:O	1:A:149:VAL:CG1	2.58	0.51
1:A:296:ILE:HG13	1:A:297:ASP:N	2.25	0.50
1:C:105:VAL:HG13	1:C:105:VAL:O	2.11	0.50
1:B:49:ARG:O	1:B:52:ASP:OD2	2.29	0.50
1:B:99:CYS:HB2	1:B:323:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:CB	1:B:306:ILE:HD11	2.27	0.50
1:A:74:GLU:OE1	1:C:347:ARG:NH1	2.44	0.50
1:A:253:GLY:O	1:A:282:ARG:HA	2.11	0.50
1:B:76:VAL:HG13	1:B:77:ARG:N	2.27	0.50
1:B:168:VAL:CG2	1:B:169:GLY:N	2.74	0.50
1:B:149:VAL:O	1:B:152:VAL:HG13	2.11	0.50
1:B:222:ASN:CG	1:B:222:ASN:O	2.54	0.50
1:B:41:ALA:HB2	1:B:207:LEU:HD22	1.94	0.49
1:A:137:LYS:HD3	1:A:139:TYR:CE2	2.48	0.49
1:B:168:VAL:HG22	1:B:169:GLY:O	2.12	0.49
1:B:121:VAL:HG13	1:B:148:PHE:CE1	2.47	0.49
1:C:170:ASP:HA	1:C:173:LEU:HD12	1.94	0.49
1:A:22:ARG:CB	1:A:23:PRO:CD	2.90	0.49
1:A:254:ARG:HH11	1:A:256:GLU:CG	2.26	0.49
1:B:98:THR:CG2	1:B:330:ARG:HD2	2.43	0.49
1:B:66:LEU:O	1:B:70:PHE:HB3	2.11	0.49
1:B:261:PHE:CE1	1:B:278:LYS:HG2	2.48	0.49
1:C:32:THR:HG23	1:C:75:GLN:NE2	2.27	0.49
1:A:43:SER:C	1:A:47:ARG:HD2	2.37	0.49
1:A:259:PRO:HA	1:A:262:THR:HG22	1.94	0.49
1:A:277:LEU:CD1	1:A:286:LEU:HD11	2.41	0.49
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.37	0.49
1:A:286:LEU:HD22	1:A:291:VAL:CG2	2.42	0.49
1:B:125:ARG:HG3	1:B:125:ARG:NH2	2.28	0.49
1:B:248:ARG:HD3	1:B:248:ARG:N	2.28	0.49
1:A:258:ASN:OD1	1:A:260:VAL:HG22	2.12	0.49
1:B:212:GLY:O	1:B:213:GLN:C	2.55	0.49
1:B:215:LYS:NZ	1:B:217:SER:OG	2.45	0.49
1:C:149:VAL:O	1:C:152:VAL:HG22	2.13	0.49
1:C:180:ARG:HD2	1:C:196:GLU:HG2	1.94	0.49
1:A:127:ASN:CB	1:A:130:VAL:HG12	2.40	0.48
1:B:220:LEU:O	1:B:222:ASN:N	2.46	0.48
1:C:231:ASP:CG	1:C:232:GLU:N	2.71	0.48
1:B:122:SER:O	1:B:126:GLN:HB2	2.13	0.48
1:B:288:ASP:CA	1:B:291:VAL:HG12	2.42	0.48
1:B:255:VAL:HG13	1:B:261:PHE:CB	2.44	0.48
1:B:291:VAL:CG1	1:B:292:LYS:N	2.75	0.48
1:B:290:LYS:HA	1:B:290:LYS:HE2	1.95	0.48
1:C:25:VAL:HG22	1:C:165:LEU:HB3	1.95	0.48
1:B:22:ARG:N	1:B:23:PRO:CD	2.77	0.48
1:A:81:LEU:HB2	3:A:1075:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG13	1:B:58:VAL:O	2.13	0.48
1:B:210:LEU:HB2	1:B:222:ASN:OD1	2.14	0.48
1:B:231:ASP:HB2	3:B:1702:HOH:O	2.13	0.48
1:B:242:THR:HG23	1:B:292:LYS:HE2	1.95	0.48
1:B:288:ASP:HA	1:B:291:VAL:CG1	2.44	0.48
1:A:51:GLN:NE2	1:A:93:ASP:N	2.51	0.48
1:A:119:VAL:HG23	3:A:1011:HOH:O	2.14	0.48
1:B:218:LYS:HA	1:B:218:LYS:CE	2.40	0.48
1:A:23:PRO:O	1:A:54:ALA:HB1	2.14	0.48
1:B:177:GLU:HG3	3:B:2105:HOH:O	2.13	0.48
1:B:256:GLU:CD	1:B:256:GLU:H	2.22	0.48
1:B:294:HIS:HA	1:B:297:ASP:OD2	2.13	0.48
1:B:314:GLU:HA	3:B:2012:HOH:O	2.14	0.48
1:C:110:GLU:O	1:C:113:VAL:CG1	2.61	0.48
1:B:215:LYS:HZ3	1:B:215:LYS:CB	2.26	0.48
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.96	0.47
1:A:351:HIS:N	1:A:351:HIS:CD2	2.81	0.47
1:C:80:VAL:HG13	1:C:81:LEU:H	1.78	0.47
1:C:120:THR:CG2	1:C:123:HIS:HB2	2.44	0.47
1:A:322:ARG:NH2	1:A:322:ARG:CG	2.72	0.47
1:C:32:THR:O	1:C:32:THR:CG2	2.63	0.47
1:C:165:LEU:HD22	1:C:200:GLN:HB2	1.95	0.47
1:C:193:VAL:HG11	1:C:341:GLN:HB3	1.96	0.47
1:C:216:MET:HE3	1:C:223:ALA:CA	2.44	0.47
1:A:211:ASP:HB3	1:A:213:GLN:HG3	1.96	0.47
1:B:112:THR:HG22	1:B:156:ALA:HB3	1.96	0.47
1:B:241:TYR:O	1:B:241:TYR:CD1	2.67	0.47
1:B:63:VAL:CG1	1:B:102:GLN:HG2	2.44	0.47
1:B:84:ALA:O	1:B:87:TYR:HB2	2.15	0.47
1:B:281:TYR:C	1:B:283:ALA:H	2.21	0.47
1:C:64:GLN:H	1:C:102:GLN:HE22	1.62	0.47
1:C:127:ASN:OD1	1:C:129:THR:CG2	2.62	0.47
1:A:255:VAL:CG2	1:A:278:LYS:HG3	2.33	0.47
1:B:269:PRO:HG2	1:B:270:ASP:H	1.80	0.47
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.26	0.47
1:A:296:ILE:HG21	3:A:1058:HOH:O	2.14	0.47
1:B:88:LEU:HD21	1:B:323:PHE:CD1	2.49	0.47
1:C:58:VAL:O	1:C:58:VAL:HG23	2.14	0.47
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.30	0.47
1:C:127:ASN:OD1	1:C:129:THR:HG22	2.15	0.47
1:C:229:SER:O	1:C:233:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CD2	1:A:38:GLY:H	2.18	0.47
1:A:292:LYS:O	1:A:296:ILE:CG2	2.62	0.47
1:B:24:ARG:CB	3:B:1811:HOH:O	2.61	0.47
1:B:120:THR:O	1:B:124:LEU:HB2	2.15	0.47
1:B:129:THR:HG22	1:B:133:GLU:OE1	2.15	0.47
1:B:216:MET:HG3	1:B:223:ALA:HA	1.96	0.47
1:C:77:ARG:O	1:C:80:VAL:CG1	2.50	0.47
1:C:175:MET:SD	1:C:175:MET:O	2.73	0.47
1:C:321:LEU:O	1:C:325:THR:HG23	2.15	0.47
1:A:66:LEU:HD12	1:A:70:PHE:HA	1.96	0.47
1:A:243:ASP:OD1	1:A:244:PRO:O	2.34	0.46
1:C:326:GLU:HG2	3:C:1724:HOH:O	2.15	0.46
1:A:175:MET:HB2	3:A:1149:HOH:O	2.15	0.46
1:A:206:ARG:CZ	1:A:215:LYS:HE2	2.45	0.46
1:A:273:ARG:O	1:A:277:LEU:HD22	2.15	0.46
1:C:81:LEU:HB2	3:C:1064:HOH:O	2.15	0.46
1:B:35:LEU:CD1	1:B:86:ASP:HB3	2.46	0.46
1:A:74:GLU:CD	1:C:347:ARG:NH1	2.74	0.46
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.80	0.46
1:A:230:ALA:O	1:A:233:VAL:HG12	2.15	0.46
1:A:295:LEU:O	1:A:295:LEU:HD23	2.15	0.46
1:B:116:LEU:HD21	1:B:149:VAL:CG1	2.41	0.46
1:B:184:ARG:HD2	1:B:196:GLU:OE1	2.16	0.46
1:C:166:VAL:CG2	1:C:176:LEU:HD23	2.33	0.46
1:B:23:PRO:HG2	1:B:54:ALA:HB2	1.96	0.46
1:A:211:ASP:OD1	1:A:213:GLN:NE2	2.49	0.46
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.51	0.46
1:C:25:VAL:HG13	1:C:167:PRO:HD3	1.97	0.46
1:A:289:VAL:O	1:A:293:LYS:HG3	2.15	0.46
1:B:205:PRO:O	1:B:206:ARG:C	2.59	0.46
1:C:154:GLN:NE2	2:C:500:TRP:OXT	2.49	0.46
1:C:258:ASN:HD22	1:C:260:VAL:H	1.62	0.46
1:A:255:VAL:HG21	1:A:278:LYS:CG	2.34	0.46
1:A:277:LEU:HD22	1:A:277:LEU:H	1.81	0.46
1:B:207:LEU:CG	1:B:208:PRO:HD2	2.46	0.46
1:A:263:PHE:HB3	1:A:295:LEU:HD11	1.97	0.46
1:B:234:ALA:HA	1:B:296:ILE:CG2	2.46	0.46
1:A:149:VAL:O	1:A:149:VAL:HG13	2.17	0.45
1:B:211:ASP:C	1:B:213:GLN:H	2.24	0.45
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.98	0.45
1:A:25:VAL:HG13	1:A:167:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:VAL:HG13	1:B:295:LEU:HD22	1.99	0.45
1:C:102:GLN:HG3	1:C:108:LEU:HD12	1.97	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD2	1.82	0.45
1:A:123:HIS:HE1	3:A:1860:HOH:O	1.97	0.45
1:C:268:ASP:OD1	1:C:294:HIS:CE1	2.69	0.45
1:B:208:PRO:HG2	1:B:263:PHE:HE2	1.81	0.45
1:A:171:ASP:OD1	1:A:171:ASP:N	2.48	0.45
1:A:255:VAL:HG13	1:A:261:PHE:CD2	2.52	0.45
1:A:295:LEU:HD23	1:A:295:LEU:C	2.42	0.45
1:B:35:LEU:HG	1:B:86:ASP:OD2	2.17	0.45
1:B:208:PRO:HG2	1:B:263:PHE:CE2	2.52	0.45
1:B:254:ARG:HB2	1:B:256:GLU:OE1	2.16	0.45
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.32	0.45
1:C:85:LEU:CD1	1:C:310:ARG:CZ	2.94	0.45
1:C:254:ARG:CG	1:C:256:GLU:HG2	2.45	0.45
1:A:84:ALA:O	1:A:87:TYR:HB2	2.17	0.45
1:B:288:ASP:C	1:B:291:VAL:HG12	2.42	0.45
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.82	0.45
1:A:273:ARG:O	1:A:276:ALA:HB3	2.16	0.44
1:B:86:ASP:OD1	1:B:310:ARG:NH1	2.49	0.44
1:B:105:VAL:HG13	1:B:105:VAL:O	2.18	0.44
1:C:60:LEU:HD22	1:C:83:VAL:HG21	1.99	0.44
1:A:186:PHE:CD1	1:A:186:PHE:C	2.95	0.44
3:A:2166:HOH:O	1:B:322:ARG:HD2	2.16	0.44
1:B:324:VAL:HG23	1:B:325:THR:N	2.32	0.44
1:C:102:GLN:O	1:C:105:VAL:HG12	2.17	0.44
1:C:150:TYR:N	1:C:151:PRO:CD	2.80	0.44
1:C:168:VAL:O	1:C:202:SER:N	2.49	0.44
1:C:258:ASN:ND2	1:C:260:VAL:H	2.15	0.44
1:B:241:TYR:O	1:B:259:PRO:CD	2.66	0.44
1:C:30:ARG:HB2	1:C:65:ALA:HB2	2.00	0.44
1:C:127:ASN:O	1:C:131:LYS:HB2	2.17	0.44
1:C:304:ALA:O	1:C:308:THR:HG23	2.17	0.44
1:B:23:PRO:HG2	1:B:54:ALA:CB	2.47	0.44
1:B:40:LEU:HA	1:B:44:LEU:HB3	1.99	0.44
1:B:269:PRO:HD2	1:B:273:ARG:HH11	1.83	0.44
1:B:320:VAL:HG13	1:B:321:LEU:N	2.33	0.44
1:C:51:GLN:NE2	1:C:97:THR:CG2	2.79	0.44
1:A:211:ASP:CG	1:A:213:GLN:HE21	2.25	0.44
1:A:333:GLU:O	1:A:337:GLN:HG3	2.18	0.44
1:B:215:LYS:NZ	1:B:215:LYS:CB	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASN:CG	1:C:192:PRO:HA	2.42	0.44
1:A:44:LEU:HA	1:A:47:ARG:HD2	2.00	0.44
1:C:165:LEU:CD2	1:C:200:GLN:HB2	2.48	0.44
1:A:296:ILE:CD1	1:A:300:ASN:ND2	2.80	0.44
1:B:207:LEU:HG	1:B:208:PRO:HD2	2.00	0.44
1:C:136:GLN:NE2	1:C:137:LYS:CD	2.77	0.44
1:C:273:ARG:O	1:C:277:LEU:CD2	2.66	0.44
1:A:249:ALA:O	1:A:250:SER:C	2.61	0.44
1:A:277:LEU:O	1:A:281:TYR:HB2	2.18	0.44
1:B:237:VAL:O	1:B:240:MET:N	2.45	0.44
1:C:238:MET:HG2	1:C:238:MET:H	1.61	0.43
1:A:37:LEU:HD22	1:A:224:ILE:HB	1.99	0.43
1:A:308:THR:O	1:A:312:GLU:HG3	2.18	0.43
1:C:112:THR:HG22	1:C:153:SER:HA	2.00	0.43
1:A:173:LEU:N	1:A:174:PRO:CD	2.80	0.43
1:A:184:ARG:HG2	1:A:184:ARG:NH2	2.31	0.43
1:B:242:THR:HG21	1:B:288:ASP:HB3	2.01	0.43
1:A:60:LEU:HD13	1:A:80:VAL:HG13	1.99	0.43
1:A:233:VAL:HG13	1:A:234:ALA:N	2.33	0.43
1:B:116:LEU:CD2	1:B:149:VAL:HG11	2.42	0.43
1:B:273:ARG:O	1:B:276:ALA:HB3	2.19	0.43
1:B:215:LYS:O	1:B:222:ASN:ND2	2.50	0.43
1:A:299:LEU:HA	1:A:302:VAL:CG1	2.47	0.43
1:B:142:ARG:O	1:B:142:ARG:CD	2.66	0.43
1:B:168:VAL:HG12	1:B:200:GLN:H	1.84	0.43
1:B:252:PRO:HG3	3:B:1440:HOH:O	2.18	0.43
1:C:288:ASP:O	1:C:292:LYS:HG3	2.19	0.43
1:B:25:VAL:HA	1:B:165:LEU:O	2.18	0.43
1:B:193:VAL:CG2	1:B:341:GLN:HE21	2.31	0.43
1:C:230:ALA:HB1	1:C:300:ASN:ND2	2.31	0.43
1:B:150:TYR:N	1:B:151:PRO:CD	2.82	0.43
1:C:216:MET:HE3	1:C:223:ALA:CB	2.48	0.43
1:A:184:ARG:HH21	1:A:184:ARG:CG	2.29	0.43
1:A:208:PRO:HG3	1:A:262:THR:HG21	2.01	0.43
1:B:169:GLY:H	1:B:172:GLN:CG	2.29	0.43
1:C:100:VAL:HB	1:C:328:THR:HA	2.00	0.43
1:C:247:LEU:N	1:C:247:LEU:CD1	2.82	0.43
1:A:40:LEU:HA	1:A:44:LEU:HB2	1.99	0.43
1:A:101:VAL:HG13	1:A:101:VAL:O	2.19	0.42
1:A:244:PRO:C	1:A:246:HIS:N	2.77	0.42
1:A:310:ARG:HD3	3:A:1286:HOH:O	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HD13	1:B:143:VAL:HG21	2.01	0.42
1:B:234:ALA:HA	1:B:296:ILE:HG22	2.01	0.42
1:C:133:GLU:O	1:C:136:GLN:HG3	2.19	0.42
1:C:129:THR:O	1:C:133:GLU:HG3	2.19	0.42
1:C:80:VAL:HG13	1:C:81:LEU:N	2.34	0.42
1:C:178:GLN:HA	3:C:1087:HOH:O	2.20	0.42
1:B:41:ALA:HB1	1:B:207:LEU:HD13	2.00	0.42
1:B:216:MET:HA	1:B:222:ASN:O	2.19	0.42
1:C:35:LEU:HD23	1:C:44:LEU:CD1	2.43	0.42
1:C:243:ASP:HA	1:C:244:PRO:HD2	1.87	0.42
1:A:117:ASN:HD22	1:C:146:GLY:HA3	1.83	0.42
1:B:40:LEU:HA	1:B:44:LEU:CB	2.49	0.42
1:B:193:VAL:HG21	1:B:341:GLN:HE21	1.84	0.42
1:B:209:GLY:O	1:B:210:LEU:C	2.62	0.42
1:B:211:ASP:O	1:B:213:GLN:N	2.43	0.42
1:C:108:LEU:HD13	1:C:157:ASP:OD1	2.20	0.42
1:A:299:LEU:O	1:A:302:VAL:HG13	2.19	0.42
1:B:119:VAL:HG22	1:B:120:THR:H	1.83	0.42
1:B:226:LEU:H	1:B:226:LEU:CD1	2.16	0.42
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.95	0.42
1:A:254:ARG:HH11	1:A:256:GLU:HG2	1.85	0.42
1:B:253:GLY:O	1:B:282:ARG:CA	2.65	0.42
1:C:78:GLU:OE2	1:C:78:GLU:HA	2.20	0.42
1:C:64:GLN:HE22	2:C:500:TRP:C	2.28	0.42
1:B:213:GLN:O	1:B:215:LYS:N	2.53	0.42
1:A:64:GLN:HE22	1:A:154:GLN:CD	2.28	0.41
1:A:66:LEU:O	1:A:70:PHE:HB3	2.19	0.41
1:A:349:PHE:HE2	1:C:81:LEU:HD22	1.85	0.41
1:A:127:ASN:O	1:A:130:VAL:HG12	2.19	0.41
1:B:191:ALA:HA	1:B:192:PRO:HD3	1.89	0.41
1:B:299:LEU:C	1:B:302:VAL:HG12	2.46	0.41
1:C:112:THR:HG22	1:C:156:ALA:CB	2.50	0.41
1:B:118:LEU:HD13	1:B:185:ARG:HG3	2.02	0.41
1:C:93:ASP:HB3	1:C:96:LYS:HB2	2.02	0.41
1:A:136:GLN:HE21	1:A:136:GLN:CA	2.32	0.41
1:A:165:LEU:HD21	1:A:200:GLN:HB2	2.02	0.41
1:B:202:SER:HG	1:B:205:PRO:HB3	1.84	0.41
1:B:289:VAL:HG12	1:B:290:LYS:HE3	2.01	0.41
1:C:43:SER:O	1:C:47:ARG:HD3	2.21	0.41
1:C:59:LEU:HD12	1:C:100:VAL:HG22	2.02	0.41
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:O	1:A:233:VAL:CG1	2.68	0.41
1:A:22:ARG:HE	1:A:53:GLU:HG3	1.85	0.41
1:A:67:THR:HA	1:C:117:ASN:ND2	2.36	0.41
1:C:85:LEU:HD13	1:C:310:ARG:CZ	2.50	0.41
1:A:22:ARG:CD	1:A:23:PRO:HD3	2.51	0.41
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.33	0.41
1:A:136:GLN:HA	1:A:136:GLN:NE2	2.36	0.41
1:A:295:LEU:HD23	1:A:299:LEU:HG	2.03	0.41
1:B:105:VAL:HG13	1:B:108:LEU:CG	2.49	0.41
1:B:120:THR:C	1:B:122:SER:N	2.78	0.41
1:B:254:ARG:CD	1:B:256:GLU:HB2	2.51	0.41
1:C:299:LEU:O	1:C:303:LEU:HB2	2.20	0.41
1:B:225:ALA:C	1:B:227:GLY:H	2.29	0.41
1:C:36:HIS:ND1	1:C:216:MET:HE2	2.36	0.41
1:A:305:PRO:HB2	1:A:309:ARG:HH22	1.79	0.41
1:B:193:VAL:O	1:B:193:VAL:CG2	2.69	0.41
1:B:233:VAL:HG21	1:B:303:LEU:CD2	2.51	0.41
1:B:343:ARG:HD2	3:B:1116:HOH:O	2.21	0.41
1:C:144:PRO:HB2	3:C:1014:HOH:O	2.20	0.41
1:C:185:ARG:HH11	1:C:189:LEU:CD2	2.34	0.41
1:C:295:LEU:HD22	1:C:299:LEU:HG	2.03	0.41
1:A:22:ARG:HH21	1:A:53:GLU:HG2	1.85	0.40
1:A:247:LEU:N	1:A:247:LEU:CD1	2.83	0.40
1:B:296:ILE:HG13	1:B:297:ASP:N	2.36	0.40
1:A:93:ASP:O	1:A:97:THR:CG2	2.69	0.40
1:A:117:ASN:ND2	1:C:146:GLY:HA3	2.35	0.40
1:B:62:ASP:OD1	1:B:103:SER:HB2	2.22	0.40
1:B:105:VAL:HG13	1:B:108:LEU:CD1	2.51	0.40
1:B:173:LEU:N	1:B:174:PRO:CD	2.82	0.40
1:B:253:GLY:HA3	1:B:281:TYR:CE2	2.56	0.40
1:C:60:LEU:HD13	1:C:80:VAL:HG23	2.03	0.40
1:C:172:GLN:CD	1:C:172:GLN:N	2.79	0.40
1:A:64:GLN:H	1:A:102:GLN:NE2	2.17	0.40
1:A:286:LEU:HD22	1:A:291:VAL:HG22	2.03	0.40
1:B:303:LEU:O	1:B:307:ARG:HB2	2.22	0.40
1:C:310:ARG:O	1:C:314:GLU:CG	2.69	0.40
1:A:178:GLN:HB3	3:A:1713:HOH:O	2.22	0.40
1:A:248:ARG:N	1:A:248:ARG:CD	2.81	0.40
1:B:93:ASP:HA	1:B:94:PRO:HD3	2.00	0.40
1:B:118:LEU:HB3	1:B:185:ARG:HG2	2.03	0.40
1:B:302:VAL:O	1:B:305:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PRO:HA	1:C:200:GLN:HB3	2.02	0.40
1:C:176:LEU:C	1:C:176:LEU:CD1	2.91	0.40
1:B:321:LEU:O	1:B:324:VAL:HG22	2.21	0.40
1:C:205:PRO:HB3	3:C:1637:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	264/264 (100%)	231 (88%)	33 (12%)	4	5
1	B	256/264 (97%)	227 (89%)	29 (11%)	5	7
1	C	260/264 (98%)	224 (86%)	36 (14%)	3	4
All	All	780/792 (98%)	682 (87%)	98 (13%)	4	5

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	40	LEU
1	A	47	ARG
1	A	68	ASP
1	A	75	GLN
1	A	81	LEU
1	A	85	LEU
1	A	92	LEU

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	97	THR
1	A	136	GLN
1	A	141	GLU
1	A	149	VAL
1	A	152	VAL
1	A	165	LEU
1	A	170	ASP
1	A	171	ASP
1	A	185	ARG
1	A	189	LEU
1	A	201	LEU
1	A	226	LEU
1	A	238	MET
1	A	242	THR
1	A	254	ARG
1	A	263	PHE
1	A	290	LYS
1	A	296	ILE
1	A	297	ASP
1	A	302	VAL
1	A	318	ASP
1	A	322	ARG
1	A	344	ARG
1	A	351	HIS
1	B	35	LEU
1	B	40	LEU
1	B	52	ASP
1	B	56	LEU
1	B	63	VAL
1	B	81	LEU
1	B	85	LEU
1	B	92	LEU
1	B	124	LEU
1	B	125	ARG
1	B	126	GLN
1	B	142	ARG
1	B	150	TYR
1	B	152	VAL
1	B	153	SER
1	B	165	LEU
1	B	200	GLN

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Mol	Chain	Res	Type
1	B	201	LEU
1	B	203	ARG
1	B	215	LYS
1	B	224	ILE
1	B	246	HIS
1	B	251	ASP
1	B	268	ASP
1	B	286	LEU
1	B	290	LYS
1	B	300	ASN
1	B	306	ILE
1	B	348	LEU
1	C	30	ARG
1	C	37	LEU
1	C	80	VAL
1	C	81	LEU
1	C	85	LEU
1	C	92	LEU
1	C	97	THR
1	C	100	VAL
1	C	103	SER
1	C	150	TYR
1	C	152	VAL
1	C	165	LEU
1	C	168	VAL
1	C	180	ARG
1	C	189	LEU
1	C	193	VAL
1	C	200	GLN
1	C	201	LEU
1	C	204	VAL
1	C	205	PRO
1	C	210	LEU
1	C	231	ASP
1	C	238	MET
1	C	247	LEU
1	C	248	ARG
1	C	256	GLU
1	C	258	ASN
1	C	277	LEU
1	C	286	LEU
1	C	295	LEU

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Mol	Chain	Res	Type
1	C	298	VAL
1	C	314	GLU
1	C	321	LEU
1	C	326	GLU
1	C	330	ARG
1	C	337	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	46	ASN
1	A	51	GLN
1	A	64	GLN
1	A	69	HIS
1	A	102	GLN
1	A	117	ASN
1	A	136	GLN
1	A	200	GLN
1	A	213	GLN
1	A	351	HIS
1	B	36	HIS
1	B	39	HIS
1	B	46	ASN
1	B	69	HIS
1	B	79	ASN
1	B	172	GLN
1	B	200	GLN
1	B	280	GLN
1	B	300	ASN
1	B	341	GLN
1	C	46	ASN
1	C	51	GLN
1	C	69	HIS
1	C	75	GLN
1	C	79	ASN
1	C	95	GLN
1	C	102	GLN
1	C	117	ASN
1	C	126	GLN
1	C	154	GLN
1	C	213	GLN

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	294	HIS
1	C	300	ASN
1	C	337	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRP	C	500	-	15,16,16	0.70	0	18,22,22	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	C	500	-	-	4/8/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	TRP	CA-CB-CG-CD1
2	C	500	TRP	OXT-C-CA-CB
2	C	500	TRP	CA-CB-CG-CD2
2	C	500	TRP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	TRP	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.