



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:02 am GMT

PDB ID : 1O17  
Title : ANTHRANILATE PHOSPHORIBOSYL-TRANSFERASE (TRPD)  
Authors : Mayans, O.; Ivens, A.; Kirschner, K.; Wilmanns, M.  
Deposited on : 2002-10-29  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

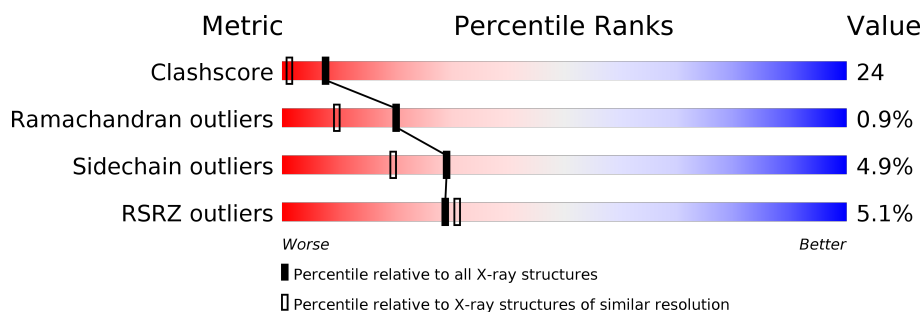
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	345	<div> <div>4%</div> <div>66%</div> <div>28%</div> <div>• •</div> </div>
1	B	345	<div> <div>7%</div> <div>59%</div> <div>35%</div> <div>• •</div> </div>
1	C	345	<div> <div>3%</div> <div>65%</div> <div>31%</div> <div>• •</div> </div>
1	D	345	<div> <div>6%</div> <div>62%</div> <div>35%</div> <div>•</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11430 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 ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2611	1675	440	489	7			
1	B	340	Total	C	N	O	S	0	0	0
			2619	1679	441	492	7			
1	C	341	Total	C	N	O	S	0	0	0
			2621	1680	442	492	7			
1	D	345	Total	C	N	O	S	0	0	0
			2644	1692	446	499	7			

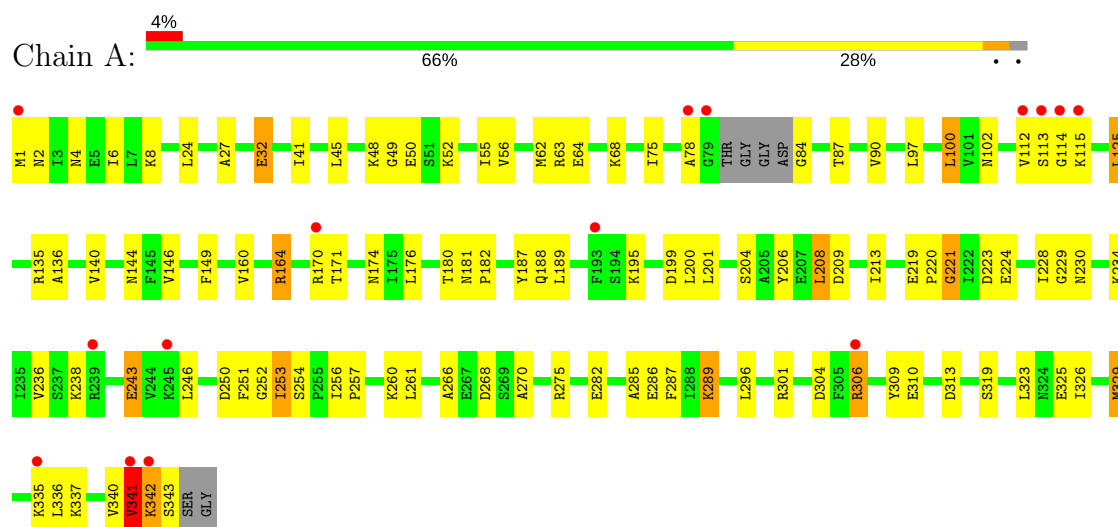
- Molecule 2 is water.

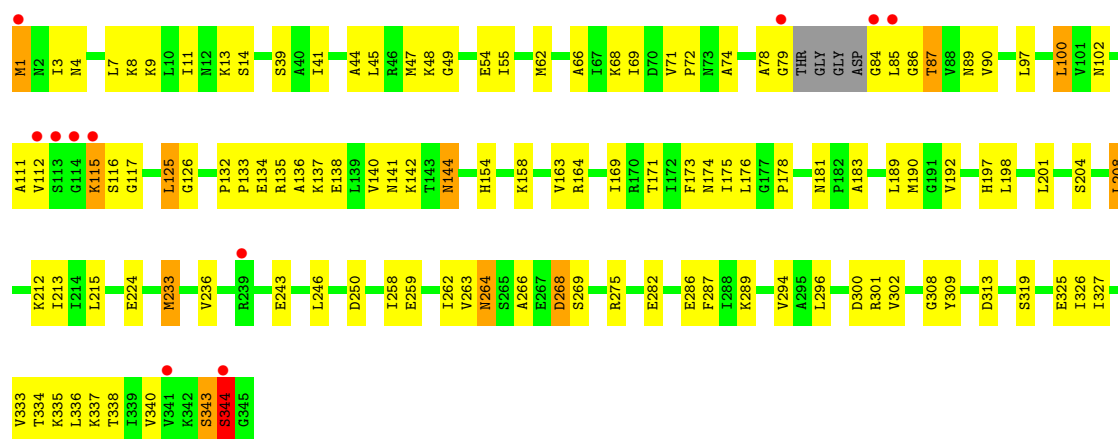
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	258	Total	O	0	0
			258	258		
2	B	218	Total	O	0	0
			218	218		
2	C	250	Total	O	0	0
			250	250		
2	D	209	Total	O	0	0
			209	209		

### 3 Residue-property plots [i](#)

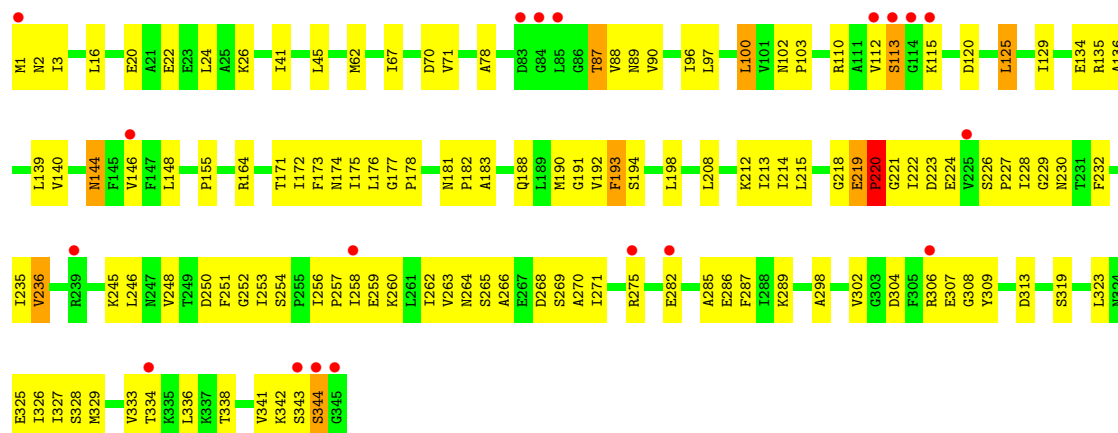
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

#### • Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE





● Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.34Å 65.85Å 116.44Å 90.00° 107.56° 90.00°	Depositor
Resolution (Å)	18.00 – 2.05 17.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.7 (18.00-2.05) 92.7 (17.99-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.05Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.260 0.216 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.38	0/2647	0.69	4/3575 (0.1%)
1	B	0.34	0/2655	0.62	0/3586
1	C	0.37	0/2657	0.64	2/3588 (0.1%)
1	D	0.35	0/2681	0.76	4/3622 (0.1%)
All	All	0.36	0/10640	0.68	10/14371 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLU	C-N-CD	-21.06	74.26	120.60
1	D	219	GLU	C-N-CA	11.28	169.38	122.00
1	D	342	LYS	C-N-CA	-7.02	104.14	121.70
1	C	344	SER	CB-CA-C	6.99	123.37	110.10
1	A	341	VAL	C-N-CA	6.36	137.60	121.70
1	D	220	PRO	CA-N-CD	-5.90	103.25	111.50
1	A	342	LYS	CA-C-N	-5.73	104.58	117.20
1	A	341	VAL	CB-CA-C	5.68	122.19	111.40
1	C	343	SER	CA-C-N	-5.04	106.11	117.20
1	A	112	VAL	N-CA-C	-5.02	97.45	111.00

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	2611	0	2730	107	0
1	B	2619	0	2734	164	0
1	C	2621	0	2738	117	0
1	D	2644	0	2756	139	0
2	A	258	0	0	43	0
2	B	218	0	0	33	0
2	C	250	0	0	34	0
2	D	209	0	0	25	1
All	All	11430	0	10958	522	1

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 (522) 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:91:SER:HB2	2:B:537:HOH:O	1.22	1.34
1:D:134:GLU:HG2	2:D:551:HOH:O	1.35	1.24
1:B:306:ARG:HD3	2:B:556:HOH:O	1.37	1.23
1:C:1:MET:HB3	2:C:546:HOH:O	1.36	1.21
1:D:70:ASP:HA	2:D:538:HOH:O	1.36	1.20
1:B:116:SER:HB2	2:B:563:HOH:O	1.41	1.17
1:D:275:ARG:NE	1:D:343:SER:OG	1.82	1.12
1:B:215:LEU:HD13	2:B:391:HOH:O	1.48	1.12
1:D:343:SER:O	1:D:344:SER:O	1.70	1.09
1:B:86:GLY:HA3	1:B:262:ILE:HG23	1.37	1.07
1:D:282:GLU:HG2	2:D:535:HOH:O	1.55	1.07
1:A:48:LYS:HE3	2:A:574:HOH:O	1.55	1.05
1:B:339:ILE:HA	1:B:342:LYS:HD2	1.36	1.03
1:A:286:GLU:HG3	2:A:594:HOH:O	1.56	1.03
1:C:112:VAL:HA	2:C:593:HOH:O	1.60	1.01
1:A:342:LYS:HE2	2:A:555:HOH:O	1.59	0.99
1:D:257:PRO:HB2	1:D:260:LYS:HD3	1.43	0.99
1:C:62:MET:HE1	1:C:176:LEU:HD13	1.44	0.98
1:D:220:PRO:HD2	1:D:221:GLY:H	1.28	0.98
1:C:171:THR:H	1:C:174:ASN:HD22	1.12	0.97
1:B:339:ILE:HA	1:B:342:LYS:CD	1.95	0.97
1:A:221:GLY:C	2:A:572:HOH:O	2.02	0.96
1:A:261:LEU:HB3	2:A:595:HOH:O	1.65	0.96
1:A:337:LYS:O	1:A:341:VAL:HG23	1.65	0.96
1:A:282:GLU:O	1:A:286:GLU:HG2	1.67	0.95
1:D:22:GLU:HB3	2:D:553:HOH:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLU:HG2	2:C:592:HOH:O	1.66	0.95
1:B:171:THR:H	1:B:174:ASN:HD22	1.12	0.94
1:C:340:VAL:O	1:C:344:SER:O	1.85	0.94
1:B:343:SER:HA	2:B:511:HOH:O	1.67	0.93
1:C:87:THR:HG21	1:C:224:GLU:OE2	1.69	0.92
1:A:221:GLY:CA	2:A:572:HOH:O	2.16	0.92
1:A:206:TYR:CZ	2:A:593:HOH:O	2.22	0.91
1:A:335:LYS:HD3	2:A:600:HOH:O	1.70	0.91
1:D:71:VAL:HA	2:D:491:HOH:O	1.73	0.89
1:A:64:GLU:HB3	2:A:569:HOH:O	1.72	0.88
1:C:102:ASN:HD22	1:C:301:ARG:HH12	1.22	0.87
1:A:87:THR:HB	2:A:595:HOH:O	1.75	0.87
1:D:171:THR:H	1:D:174:ASN:HD22	1.22	0.87
1:D:22:GLU:CB	2:D:553:HOH:O	2.22	0.85
1:B:190:MET:HB3	1:B:215:LEU:HD12	1.59	0.85
1:A:171:THR:H	1:A:174:ASN:HD22	1.22	0.85
1:D:268:ASP:CB	2:D:554:HOH:O	2.24	0.84
1:B:115:LYS:HB3	1:B:266:ALA:HB2	1.59	0.84
1:A:195:LYS:CE	2:A:535:HOH:O	2.24	0.84
1:D:327:ILE:HD12	1:D:336:LEU:HD22	1.60	0.83
1:B:253:ILE:HD11	1:B:309:TYR:CZ	2.14	0.83
1:C:262:ILE:CD1	2:C:579:HOH:O	2.26	0.83
1:D:26:LYS:HG2	2:D:544:HOH:O	1.79	0.82
1:C:62:MET:HE1	1:C:176:LEU:CD1	2.10	0.82
1:D:253:ILE:HD11	1:D:309:TYR:CE1	2.15	0.82
1:B:139:LEU:O	1:B:143:THR:HG22	1.79	0.81
1:A:195:LYS:HE3	2:A:535:HOH:O	1.80	0.81
1:D:62:MET:HE1	1:D:176:LEU:HD13	1.62	0.81
1:C:286:GLU:HG3	2:C:418:HOH:O	1.80	0.80
1:B:67:ILE:HD11	1:B:133:PRO:HD3	1.62	0.80
1:A:115:LYS:HB3	1:A:266:ALA:HB2	1.62	0.80
1:B:253:ILE:HD11	1:B:309:TYR:CE1	2.16	0.80
1:C:112:VAL:CA	2:C:593:HOH:O	2.24	0.80
1:D:275:ARG:HG3	1:D:343:SER:CB	2.13	0.79
1:B:164:ARG:NE	2:B:561:HOH:O	2.16	0.79
1:A:97:LEU:HD22	1:A:319:SER:OG	1.82	0.79
1:C:243:GLU:CG	2:C:592:HOH:O	2.24	0.79
1:B:24:LEU:HD11	1:B:41:ILE:HD13	1.65	0.78
1:A:257:PRO:HG2	1:A:260:LYS:HD3	1.64	0.78
1:B:343:SER:O	2:B:555:HOH:O	2.00	0.78
1:B:97:LEU:HD22	1:B:319:SER:OG	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:NZ	2:B:558:HOH:O	2.16	0.77
1:B:190:MET:SD	1:B:215:LEU:HD11	2.24	0.77
1:B:340:VAL:O	1:B:343:SER:HB2	1.85	0.77
1:B:275:ARG:HH12	1:B:280:LYS:HB3	1.50	0.76
1:B:263:VAL:HG13	1:B:268:ASP:OD2	1.86	0.76
1:B:253:ILE:HG22	1:B:254:SER:H	1.49	0.76
1:B:274:VAL:HB	1:B:342:LYS:HD3	1.67	0.76
1:C:89:ASN:HA	2:C:580:HOH:O	1.85	0.76
1:A:310:GLU:HG2	2:A:548:HOH:O	1.86	0.76
1:A:24:LEU:HD11	1:A:41:ILE:HD13	1.67	0.75
1:D:275:ARG:CZ	1:D:343:SER:OG	2.34	0.75
1:D:282:GLU:O	1:D:286:GLU:HG3	1.86	0.75
1:B:275:ARG:HB3	1:B:275:ARG:HH11	1.52	0.75
1:A:114:GLY:HA3	2:A:524:HOH:O	1.87	0.74
1:A:342:LYS:CE	2:A:555:HOH:O	2.24	0.74
1:C:302:VAL:HG11	1:C:308:GLY:HA2	1.69	0.74
1:D:112:VAL:HA	2:D:549:HOH:O	1.86	0.74
1:C:171:THR:H	1:C:174:ASN:ND2	1.85	0.74
1:A:84:GLY:HA3	2:A:451:HOH:O	1.88	0.74
1:B:300:ASP:HB3	2:B:562:HOH:O	1.86	0.74
1:C:62:MET:CE	1:C:176:LEU:HD13	2.16	0.73
1:C:1:MET:CE	1:C:3:ILE:HD13	2.18	0.73
1:C:115:LYS:HB3	1:C:266:ALA:HB2	1.68	0.73
1:C:282:GLU:O	1:C:286:GLU:HG2	1.88	0.73
1:B:171:THR:H	1:B:174:ASN:ND2	1.85	0.73
1:B:274:VAL:HB	1:B:342:LYS:CD	2.19	0.73
1:B:274:VAL:HG11	1:B:342:LYS:NZ	2.04	0.73
1:D:343:SER:O	1:D:344:SER:C	2.27	0.73
1:A:102:ASN:HD22	1:A:301:ARG:NH2	1.86	0.72
1:D:219:GLU:H	1:D:226:SER:HB2	1.53	0.72
1:B:3:ILE:HD13	1:B:37:LEU:HD13	1.72	0.72
1:D:220:PRO:CD	1:D:221:GLY:H	2.01	0.72
1:C:175:ILE:HG22	2:C:585:HOH:O	1.89	0.72
1:A:62:MET:CE	1:A:180:THR:HG21	2.20	0.71
1:D:1:MET:HE1	1:D:3:ILE:HD13	1.71	0.71
1:A:4:ASN:HB3	2:A:424:HOH:O	1.89	0.71
1:D:253:ILE:HG22	1:D:254:SER:N	2.06	0.71
1:B:292:THR:HG22	1:B:296:LEU:HD22	1.72	0.70
1:A:125:LEU:HD13	1:A:270:ALA:HB1	1.73	0.70
1:A:115:LYS:HD2	2:A:376:HOH:O	1.90	0.70
1:B:125:LEU:HD13	1:B:270:ALA:HB1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ALA:O	1:B:274:VAL:HG23	1.91	0.70
1:B:2:ASN:HB3	1:B:5:GLU:HG3	1.73	0.70
1:A:164:ARG:HD2	2:A:358:HOH:O	1.92	0.69
1:D:253:ILE:HG22	1:D:254:SER:H	1.58	0.69
1:C:97:LEU:HD22	1:C:319:SER:OG	1.93	0.69
1:C:243:GLU:HB3	2:C:592:HOH:O	1.93	0.69
1:C:134:GLU:CG	2:C:560:HOH:O	2.40	0.68
1:A:171:THR:H	1:A:174:ASN:ND2	1.91	0.68
1:C:112:VAL:C	2:C:593:HOH:O	2.30	0.68
1:C:134:GLU:HG2	2:C:560:HOH:O	1.94	0.68
1:C:289:LYS:HD3	1:C:313:ASP:HA	1.74	0.67
1:D:115:LYS:HG2	1:D:266:ALA:HB2	1.75	0.67
1:D:220:PRO:HD2	1:D:221:GLY:N	2.06	0.67
1:B:338:THR:C	1:B:342:LYS:HE3	2.15	0.67
1:D:220:PRO:HG2	1:D:222:ILE:HG13	1.77	0.67
1:C:132:PRO:HB2	2:C:560:HOH:O	1.95	0.66
1:B:164:ARG:CD	2:B:561:HOH:O	2.44	0.66
1:C:71:VAL:N	1:C:72:PRO:HD3	2.10	0.66
1:B:62:MET:HE1	1:B:176:LEU:CD1	2.25	0.66
1:B:336:LEU:O	1:B:340:VAL:HG23	1.95	0.66
1:B:336:LEU:HA	1:B:339:ILE:HG22	1.77	0.66
1:B:338:THR:O	1:B:342:LYS:HG3	1.95	0.66
1:C:4:ASN:O	1:C:8:LYS:HG2	1.94	0.66
1:D:97:LEU:HD22	1:D:319:SER:OG	1.95	0.66
1:D:302:VAL:CG1	1:D:307:GLU:HB3	2.25	0.66
1:A:268:ASP:HB3	2:A:459:HOH:O	1.96	0.66
1:D:175:ILE:HG23	2:D:548:HOH:O	1.96	0.65
1:A:49:GLY:O	2:A:574:HOH:O	2.15	0.65
1:D:263:VAL:HG12	1:D:265:SER:H	1.62	0.65
1:B:55:ILE:HD11	1:B:200:LEU:HD21	1.78	0.65
1:B:271:ILE:O	1:B:275:ARG:HG3	1.96	0.65
1:B:168:GLY:C	2:B:535:HOH:O	2.35	0.64
1:C:275:ARG:HG3	1:C:343:SER:HB3	1.80	0.64
1:D:136:ALA:O	1:D:140:VAL:HG23	1.97	0.64
1:C:85:LEU:HA	2:C:395:HOH:O	1.98	0.64
1:D:275:ARG:HG3	1:D:343:SER:HB3	1.79	0.64
1:A:221:GLY:HA2	2:A:572:HOH:O	1.87	0.64
1:B:300:ASP:CB	2:B:562:HOH:O	2.43	0.64
1:A:63:ARG:O	1:A:68:LYS:HE2	1.98	0.64
1:A:238:LYS:HG2	2:A:428:HOH:O	1.96	0.64
1:B:274:VAL:CG1	1:B:342:LYS:HD3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:MET:CE	1:D:176:LEU:HD13	2.27	0.64
1:D:289:LYS:HE2	1:D:313:ASP:HA	1.80	0.63
1:B:274:VAL:HG11	1:B:342:LYS:HZ2	1.63	0.63
1:D:302:VAL:HG13	1:D:307:GLU:HB3	1.81	0.63
1:D:285:ALA:O	1:D:289:LYS:HG2	1.98	0.63
1:D:263:VAL:HG13	1:D:268:ASP:HB2	1.80	0.63
1:A:204:SER:O	1:A:208:LEU:HD22	1.98	0.62
1:B:78:ALA:HA	2:B:473:HOH:O	1.99	0.62
1:D:268:ASP:HB3	2:D:554:HOH:O	1.93	0.62
1:A:213:ILE:HG23	1:A:236:VAL:HB	1.80	0.62
1:A:325:GLU:HG3	1:A:326:ILE:N	2.15	0.62
1:B:3:ILE:HD11	1:B:37:LEU:HB3	1.81	0.62
1:A:64:GLU:CB	2:A:569:HOH:O	2.37	0.61
1:B:29:ILE:HG22	1:B:156:ALA:HB1	1.81	0.61
1:D:334:THR:O	1:D:338:THR:HG23	1.99	0.61
1:D:341:VAL:HG12	1:D:341:VAL:O	2.00	0.61
1:A:62:MET:HE2	1:A:180:THR:HG21	1.82	0.61
1:A:340:VAL:O	1:A:342:LYS:N	2.34	0.61
1:B:274:VAL:CB	1:B:342:LYS:HD3	2.29	0.61
1:C:175:ILE:CG2	2:C:585:HOH:O	2.47	0.61
1:B:324:ASN:CA	1:B:335:LYS:HZ2	2.13	0.61
1:B:274:VAL:HG21	1:B:342:LYS:HE2	1.81	0.61
1:C:134:GLU:CD	2:C:560:HOH:O	2.38	0.61
1:C:233:MET:HE1	1:C:294:VAL:HG11	1.83	0.61
1:C:327:ILE:HD12	1:C:336:LEU:HD22	1.83	0.60
1:D:220:PRO:CD	1:D:221:GLY:N	2.63	0.60
1:D:22:GLU:CG	2:D:553:HOH:O	2.44	0.60
1:C:333:VAL:HG12	1:C:337:LYS:HE3	1.83	0.60
1:A:62:MET:HE3	1:A:180:THR:HG21	1.82	0.60
1:B:339:ILE:CA	1:B:342:LYS:HD2	2.23	0.60
1:C:181:ASN:HD21	1:C:183:ALA:HB3	1.64	0.60
1:B:313:ASP:HB2	2:B:551:HOH:O	2.00	0.60
1:C:68:LYS:HE3	2:C:519:HOH:O	2.00	0.60
1:A:285:ALA:O	1:A:289:LYS:HG3	2.00	0.60
1:D:268:ASP:CG	2:D:554:HOH:O	2.37	0.60
1:D:97:LEU:O	1:D:100:LEU:HB2	2.02	0.60
1:A:341:VAL:C	1:A:343:SER:H	2.05	0.60
1:B:339:ILE:N	1:B:342:LYS:HE3	2.17	0.60
1:B:160:VAL:O	1:B:160:VAL:HG22	2.01	0.60
1:A:336:LEU:O	1:A:340:VAL:HG23	2.02	0.59
1:D:263:VAL:HG13	1:D:268:ASP:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ARG:CD	1:D:343:SER:OG	2.51	0.59
1:B:181:ASN:HD21	1:B:183:ALA:HB3	1.68	0.59
1:C:138:GLU:O	1:C:142:LYS:HG2	2.03	0.59
1:B:213:ILE:HG23	1:B:236:VAL:HB	1.84	0.59
1:D:302:VAL:HG11	1:D:308:GLY:N	2.18	0.59
1:B:109:ASN:HD22	1:B:150:ALA:HB3	1.67	0.59
1:B:190:MET:HB3	1:B:215:LEU:CD1	2.30	0.59
1:A:8:LYS:HE3	2:A:424:HOH:O	2.02	0.59
1:C:141:ASN:OD1	2:C:564:HOH:O	2.15	0.59
1:D:125:LEU:HD13	1:D:270:ALA:HB1	1.85	0.59
1:C:111:ALA:HB3	1:C:116:SER:H	1.66	0.58
1:D:115:LYS:HE2	2:D:423:HOH:O	2.03	0.58
1:D:181:ASN:ND2	1:D:183:ALA:H	2.01	0.58
1:D:226:SER:O	1:D:248:VAL:HG22	2.04	0.58
1:C:173:PHE:HA	1:C:176:LEU:HD12	1.85	0.58
1:A:195:LYS:CD	2:A:535:HOH:O	2.48	0.58
1:D:134:GLU:HG2	1:D:135:ARG:H	1.69	0.58
1:D:253:ILE:HD11	1:D:309:TYR:HE1	1.68	0.58
1:A:90:VAL:HG11	1:A:287:PHE:CD2	2.38	0.58
1:A:246:LEU:HD21	1:A:251:PHE:CZ	2.39	0.58
1:B:274:VAL:CG2	1:B:342:LYS:HE2	2.34	0.58
1:D:173:PHE:HA	1:D:176:LEU:HD12	1.84	0.58
1:C:334:THR:O	1:C:338:THR:HG23	2.04	0.58
1:C:133:PRO:O	1:C:137:LYS:HG3	2.04	0.57
1:C:262:ILE:HD12	2:C:579:HOH:O	1.97	0.57
1:C:213:ILE:HG23	1:C:236:VAL:HB	1.87	0.57
1:B:282:GLU:O	1:B:286:GLU:HG3	2.05	0.57
1:B:1:MET:HB2	2:B:554:HOH:O	2.03	0.57
1:D:134:GLU:HG2	1:D:135:ARG:N	2.20	0.57
1:C:333:VAL:HG23	2:C:400:HOH:O	2.05	0.57
1:C:1:MET:HE3	1:C:3:ILE:HD13	1.87	0.56
1:A:257:PRO:CG	1:A:260:LYS:HD3	2.33	0.56
1:B:109:ASN:ND2	1:B:150:ALA:HB3	2.21	0.56
1:D:62:MET:HE1	1:D:176:LEU:CD1	2.35	0.56
1:B:164:ARG:HD2	2:B:350:HOH:O	2.04	0.56
1:D:24:LEU:HD11	1:D:41:ILE:HD13	1.86	0.56
1:D:263:VAL:HG13	2:D:554:HOH:O	2.06	0.56
1:A:50:GLU:H	1:A:50:GLU:CD	2.08	0.55
1:B:339:ILE:HA	1:B:342:LYS:CE	2.36	0.55
1:C:8:LYS:HB3	2:C:467:HOH:O	2.06	0.55
1:A:64:GLU:CG	2:A:569:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:HD3	2:B:559:HOH:O	2.07	0.55
1:B:233:MET:CG	1:B:244:VAL:HB	2.36	0.55
1:D:113:SER:HB2	2:D:506:HOH:O	2.07	0.55
1:B:125:LEU:CD1	1:B:270:ALA:HB1	2.36	0.55
1:B:71:VAL:N	1:B:72:PRO:HD3	2.22	0.55
1:D:227:PRO:HG3	1:D:287:PHE:CE1	2.42	0.55
1:B:190:MET:HE3	1:B:213:ILE:HD11	1.89	0.55
1:C:136:ALA:O	1:C:140:VAL:HG23	2.07	0.55
1:D:115:LYS:HG2	1:D:120:ASP:HB3	1.88	0.55
1:B:338:THR:HG22	1:B:342:LYS:HE3	1.88	0.55
1:B:275:ARG:NH1	1:B:280:LYS:HB3	2.21	0.55
1:C:158:LYS:HD3	2:C:528:HOH:O	2.06	0.55
1:B:178:PRO:HB2	1:B:190:MET:CE	2.37	0.54
1:D:275:ARG:NE	1:D:343:SER:HG	2.03	0.54
1:A:195:LYS:HD3	2:A:535:HOH:O	2.06	0.54
1:B:189:LEU:HD23	2:B:529:HOH:O	2.07	0.54
1:C:164:ARG:HD2	2:C:382:HOH:O	2.07	0.54
1:D:275:ARG:CG	1:D:343:SER:OG	2.56	0.54
1:A:55:ILE:HG13	1:A:200:LEU:HD21	1.88	0.54
1:A:1:MET:HE1	1:A:24:LEU:HA	1.90	0.54
1:C:1:MET:HE2	1:C:3:ILE:HD13	1.90	0.54
1:D:172:ILE:HG12	1:D:176:LEU:HD11	1.90	0.54
1:B:73:ASN:ND2	1:B:103:PRO:HG3	2.23	0.54
1:C:48:LYS:NZ	1:C:54:GLU:OE2	2.40	0.54
1:C:62:MET:HE3	1:C:176:LEU:HB3	1.90	0.54
1:B:198:LEU:HD22	1:B:234:LYS:HG2	1.90	0.54
1:C:301:ARG:HG3	1:C:301:ARG:HH21	1.73	0.54
1:D:1:MET:CE	1:D:3:ILE:HD13	2.36	0.54
1:A:62:MET:HE1	1:A:176:LEU:HB2	1.89	0.53
1:B:336:LEU:O	1:B:339:ILE:HG22	2.08	0.53
1:D:164:ARG:HD2	2:D:352:HOH:O	2.07	0.53
1:D:262:ILE:HD12	2:D:547:HOH:O	2.06	0.53
1:A:62:MET:HE1	1:A:176:LEU:CB	2.38	0.53
1:B:336:LEU:CA	1:B:339:ILE:HG22	2.38	0.53
1:D:102:ASN:CG	1:D:103:PRO:HD2	2.29	0.53
1:C:90:VAL:HG11	1:C:287:PHE:CD2	2.43	0.53
1:D:229:GLY:O	1:D:248:VAL:HG23	2.08	0.53
1:B:25:ALA:O	1:B:29:ILE:HG13	2.07	0.53
1:B:2:ASN:HB3	1:B:5:GLU:CG	2.38	0.53
1:B:239:ARG:NH2	1:B:242:GLU:HB2	2.22	0.53
1:B:76:ASP:HB3	1:B:188:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LYS:HE3	1:D:235:ILE:CG2	2.38	0.53
1:A:223:ASP:O	1:A:224:GLU:HG3	2.09	0.53
1:D:16:LEU:HD22	1:D:20:GLU:OE2	2.08	0.53
1:D:275:ARG:HG3	1:D:343:SER:OG	2.08	0.53
1:B:135:ARG:NH2	1:B:330:ASN:HA	2.24	0.53
1:B:62:MET:HE1	1:B:176:LEU:HD13	1.90	0.53
1:D:246:LEU:HD11	1:D:250:ASP:HB2	1.91	0.53
1:B:324:ASN:HA	1:B:335:LYS:HZ2	1.74	0.53
1:B:62:MET:HE1	1:B:176:LEU:HD12	1.90	0.52
1:B:67:ILE:O	1:B:67:ILE:HG12	2.09	0.52
1:B:340:VAL:C	1:B:343:SER:HB2	2.28	0.52
1:D:134:GLU:CG	2:D:551:HOH:O	2.17	0.52
1:B:4:ASN:O	1:B:8:LYS:HG3	2.08	0.52
1:B:336:LEU:HA	1:B:339:ILE:CG2	2.40	0.52
1:D:125:LEU:O	1:D:327:ILE:HD13	2.08	0.52
1:B:247:ASN:HD22	1:B:249:THR:H	1.56	0.52
1:D:140:VAL:HG22	1:D:146:VAL:HB	1.91	0.52
1:A:189:LEU:HD23	2:A:481:HOH:O	2.10	0.52
1:C:48:LYS:HE3	1:C:49:GLY:O	2.09	0.52
1:D:175:ILE:CG2	2:D:548:HOH:O	2.57	0.52
1:B:274:VAL:HB	1:B:342:LYS:CE	2.39	0.52
1:D:222:ILE:HG22	1:D:224:GLU:N	2.25	0.52
1:D:135:ARG:NH2	1:D:329:MET:O	2.43	0.52
1:C:300:ASP:HB3	2:C:595:HOH:O	2.10	0.51
1:A:254:SER:HA	2:A:549:HOH:O	2.10	0.51
1:B:274:VAL:CB	1:B:342:LYS:HE2	2.41	0.51
1:A:251:PHE:O	1:A:306:ARG:NH2	2.44	0.51
1:A:114:GLY:CA	2:A:524:HOH:O	2.49	0.51
1:A:256:ILE:HD12	1:A:256:ILE:H	1.75	0.51
1:B:253:ILE:HG22	1:B:254:SER:N	2.21	0.51
1:C:69:ILE:HD11	1:C:183:ALA:HB2	1.93	0.51
1:D:328:SER:HB3	1:D:333:VAL:HG11	1.93	0.51
1:C:84:GLY:C	1:C:86:GLY:H	2.14	0.51
1:B:253:ILE:HG22	2:B:543:HOH:O	2.10	0.51
1:B:321:ASP:O	1:B:325:GLU:HG2	2.10	0.51
1:C:85:LEU:O	2:C:579:HOH:O	2.19	0.50
1:D:214:ILE:HD12	1:D:298:ALA:HB2	1.92	0.50
1:D:228:ILE:HG21	1:D:258:ILE:HG12	1.92	0.50
1:B:220:PRO:HA	2:B:419:HOH:O	2.11	0.50
1:C:78:ALA:O	1:C:79:GLY:C	2.49	0.50
1:B:274:VAL:HB	1:B:342:LYS:HE2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:THR:H	1:D:174:ASN:ND2	2.01	0.50
1:A:206:TYR:CE1	2:A:593:HOH:O	2.58	0.50
1:A:337:LYS:HE3	2:A:561:HOH:O	2.11	0.50
1:B:336:LEU:C	1:B:339:ILE:HG22	2.32	0.50
1:C:243:GLU:CB	2:C:592:HOH:O	2.46	0.50
1:A:114:GLY:HA2	2:A:480:HOH:O	2.11	0.49
1:A:289:LYS:HE2	1:A:313:ASP:OD2	2.12	0.49
1:B:338:THR:HG22	1:B:342:LYS:CE	2.43	0.49
1:B:171:THR:N	1:B:174:ASN:HD22	1.95	0.49
1:B:11:ILE:CD1	1:C:169:ILE:HD13	2.43	0.49
1:B:219:GLU:HG3	1:B:230:ASN:O	2.13	0.49
1:B:322:LYS:O	1:B:326:ILE:HG13	2.11	0.49
1:B:324:ASN:HB2	1:B:335:LYS:NZ	2.27	0.49
1:B:76:ASP:HB3	1:B:188:GLN:CG	2.43	0.49
1:C:134:GLU:HG2	1:C:135:ARG:N	2.28	0.49
1:C:41:ILE:O	1:C:45:LEU:HB2	2.13	0.49
1:D:110:ARG:NH2	1:D:129:ILE:HD11	2.28	0.49
1:A:243:GLU:HG3	2:A:578:HOH:O	2.12	0.49
1:C:192:VAL:HG13	1:C:197:HIS:CB	2.43	0.49
1:D:181:ASN:HD21	1:D:183:ALA:HB3	1.77	0.49
1:A:63:ARG:NH2	2:A:560:HOH:O	2.46	0.48
1:C:336:LEU:O	1:C:340:VAL:HG23	2.13	0.48
1:C:246:LEU:HD12	1:C:250:ASP:OD2	2.13	0.48
1:D:341:VAL:CG1	1:D:341:VAL:O	2.61	0.48
1:A:250:ASP:C	1:A:252:GLY:H	2.15	0.48
1:A:253:ILE:HD11	1:A:309:TYR:CE1	2.47	0.48
1:B:137:LYS:O	1:B:141:ASN:ND2	2.46	0.48
1:B:272:LYS:HG3	2:B:560:HOH:O	2.13	0.48
1:D:115:LYS:HG2	1:D:266:ALA:CB	2.43	0.48
1:B:272:LYS:CE	2:B:560:HOH:O	2.61	0.48
1:C:264:ASN:ND2	1:C:268:ASP:OD2	2.47	0.48
1:D:1:MET:HG3	1:D:1:MET:O	2.12	0.48
1:B:1:MET:O	1:B:1:MET:HG3	2.14	0.48
1:C:7:LEU:O	1:C:11:ILE:HG12	2.13	0.48
1:A:286:GLU:CG	2:A:594:HOH:O	2.32	0.48
1:B:178:PRO:HB2	1:B:190:MET:HE2	1.95	0.47
1:C:275:ARG:CG	1:C:343:SER:HB3	2.44	0.47
1:C:79:GLY:HA2	2:C:469:HOH:O	2.14	0.47
1:A:256:ILE:HD12	1:A:256:ILE:N	2.29	0.47
1:B:116:SER:CB	2:B:563:HOH:O	2.25	0.47
1:B:90:VAL:HG11	1:B:287:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:CG1	1:C:287:PHE:CD2	2.96	0.47
1:D:230:ASN:HA	1:D:246:LEU:O	2.14	0.47
1:D:246:LEU:HD21	1:D:251:PHE:CZ	2.50	0.47
1:B:198:LEU:HD22	1:B:234:LYS:CG	2.44	0.47
1:C:112:VAL:HG12	1:C:112:VAL:O	2.14	0.47
1:B:3:ILE:HG13	1:B:41:ILE:HD11	1.97	0.47
1:D:177:GLY:HA3	2:D:460:HOH:O	2.14	0.47
1:B:233:MET:HG3	1:B:244:VAL:HB	1.96	0.47
1:D:263:VAL:HG12	1:D:264:ASN:N	2.30	0.47
1:D:302:VAL:HG13	1:D:307:GLU:CD	2.35	0.47
1:A:200:LEU:HD23	1:A:201:LEU:N	2.29	0.47
1:B:83:ASP:N	1:B:193:PHE:CE2	2.82	0.47
1:B:272:LYS:HE3	2:B:560:HOH:O	2.14	0.47
1:B:138:GLU:O	1:B:142:LYS:HG3	2.14	0.47
1:B:263:VAL:HG12	1:B:264:ASN:N	2.29	0.47
1:D:178:PRO:HB2	1:D:188:GLN:NE2	2.30	0.47
1:D:260:LYS:HD2	1:D:260:LYS:N	2.30	0.47
1:A:219:GLU:HG3	1:A:230:ASN:O	2.15	0.47
1:D:232:PHE:CE2	1:D:245:LYS:HE3	2.50	0.47
1:D:325:GLU:HG3	1:D:326:ILE:N	2.29	0.47
1:B:213:ILE:CG2	1:B:236:VAL:HB	2.44	0.47
1:B:272:LYS:CG	2:B:560:HOH:O	2.63	0.47
1:B:125:LEU:HB3	1:B:327:ILE:HD11	1.96	0.47
1:C:181:ASN:ND2	1:C:183:ALA:HB3	2.30	0.46
1:D:253:ILE:CG2	1:D:254:SER:N	2.76	0.46
1:B:275:ARG:HB3	1:B:275:ARG:NH1	2.26	0.46
1:C:246:LEU:HD11	1:C:250:ASP:HB2	1.98	0.46
1:C:71:VAL:N	1:C:72:PRO:CD	2.76	0.46
1:B:2:ASN:HB3	1:B:5:GLU:OE2	2.16	0.46
1:D:115:LYS:CG	1:D:120:ASP:HB3	2.45	0.46
1:A:135:ARG:NH2	1:A:329:MET:O	2.48	0.46
1:A:188:GLN:HG3	1:A:189:LEU:N	2.30	0.46
1:A:260:LYS:N	1:A:260:LYS:HD2	2.30	0.46
1:B:5:GLU:HG2	2:B:533:HOH:O	2.16	0.46
1:D:252:GLY:HA2	1:D:306:ARG:NH2	2.30	0.46
1:A:200:LEU:HD23	1:A:200:LEU:C	2.36	0.46
1:D:259:GLU:H	1:D:259:GLU:CD	2.19	0.46
1:B:181:ASN:ND2	1:B:183:ALA:H	2.14	0.46
1:C:212:LYS:NZ	2:C:591:HOH:O	2.49	0.46
1:A:337:LYS:O	1:A:341:VAL:CG2	2.52	0.45
1:B:313:ASP:O	1:B:316:ILE:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLY:C	1:C:86:GLY:N	2.68	0.45
1:B:274:VAL:CB	1:B:342:LYS:CE	2.93	0.45
1:C:262:ILE:HD13	2:C:579:HOH:O	2.05	0.45
1:D:302:VAL:HG12	1:D:304:ASP:H	1.81	0.45
1:A:136:ALA:O	1:A:140:VAL:HG23	2.17	0.45
1:C:181:ASN:ND2	1:C:183:ALA:H	2.14	0.45
1:D:258:ILE:O	1:D:262:ILE:HG13	2.16	0.45
1:C:333:VAL:CG1	1:C:337:LYS:HE3	2.46	0.45
1:D:250:ASP:O	1:D:306:ARG:HG3	2.17	0.45
1:B:52:LYS:HB3	1:B:52:LYS:HE2	1.85	0.45
1:C:66:ALA:HB2	1:C:154:HIS:CE1	2.52	0.45
1:D:192:VAL:HG12	1:D:194:SER:H	1.81	0.45
1:C:190:MET:O	1:C:215:LEU:HA	2.17	0.45
1:D:90:VAL:HG12	1:D:224:GLU:OE2	2.16	0.45
1:A:164:ARG:HG3	2:A:368:HOH:O	2.16	0.45
1:A:181:ASN:HA	1:A:182:PRO:HD3	1.82	0.45
1:A:87:THR:CB	2:A:595:HOH:O	2.49	0.45
1:B:47:MET:SD	1:C:44:ALA:HA	2.57	0.45
1:B:36:ILE:HG23	1:C:39:SER:HB2	1.99	0.45
1:B:88:VAL:HG13	1:B:90:VAL:HG13	1.99	0.45
1:B:3:ILE:HG23	1:B:4:ASN:N	2.32	0.44
1:B:111:ALA:HB2	1:B:117:GLY:N	2.31	0.44
1:D:253:ILE:CG2	1:D:254:SER:H	2.29	0.44
1:D:271:ILE:HG23	1:D:343:SER:HB2	1.97	0.44
1:A:75:ILE:HA	1:A:187:TYR:O	2.17	0.44
1:B:67:ILE:HD11	1:B:133:PRO:CD	2.39	0.44
1:C:192:VAL:HG13	1:C:197:HIS:HB3	1.98	0.44
1:C:86:GLY:O	1:C:263:VAL:N	2.38	0.44
1:A:140:VAL:HG22	1:A:146:VAL:CG1	2.48	0.44
1:B:110:ARG:HD2	2:B:538:HOH:O	2.17	0.44
1:C:9:LYS:HG2	1:C:14:SER:HB2	1.99	0.44
1:D:191:GLY:HA3	1:D:223:ASP:O	2.18	0.44
1:D:218:GLY:N	1:D:222:ILE:O	2.48	0.44
1:A:52:LYS:O	1:A:56:VAL:HG23	2.17	0.44
1:B:334:THR:O	1:B:337:LYS:HB3	2.18	0.44
1:C:13:LYS:HD2	2:C:562:HOH:O	2.18	0.44
1:A:125:LEU:HG	1:A:323:LEU:HD21	2.00	0.44
1:A:228:ILE:HG13	1:A:229:GLY:N	2.31	0.44
1:A:27:ALA:O	1:A:32:GLU:HG3	2.17	0.44
1:C:97:LEU:O	1:C:100:LEU:HB2	2.18	0.43
1:A:102:ASN:HD22	1:A:301:ARG:HH22	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD12	1:C:215:LEU:N	2.33	0.43
1:D:148:LEU:HD13	1:D:182:PRO:HB2	1.99	0.43
1:C:144:ASN:HA	1:C:144:ASN:HD22	1.60	0.43
1:B:6:ILE:HG21	1:B:24:LEU:HD22	1.99	0.43
1:B:44:ALA:HA	1:C:47:MET:SD	2.58	0.43
1:B:249:THR:HG22	2:B:456:HOH:O	2.18	0.43
1:C:163:VAL:HG23	2:C:366:HOH:O	2.19	0.43
1:D:178:PRO:HB2	1:D:188:GLN:HE22	1.83	0.43
1:D:215:LEU:N	1:D:215:LEU:HD12	2.34	0.43
1:A:115:LYS:HD3	1:A:115:LYS:HA	1.79	0.43
1:B:191:GLY:HA3	1:B:223:ASP:O	2.19	0.43
1:C:126:GLY:HA2	1:C:335:LYS:HD3	2.00	0.43
1:C:190:MET:HE1	1:C:201:LEU:HD13	1.99	0.43
1:A:220:PRO:HD3	1:A:228:ILE:HD13	1.99	0.43
1:B:215:LEU:HB2	2:B:391:HOH:O	2.18	0.43
1:C:62:MET:CE	1:C:176:LEU:HB3	2.48	0.43
1:D:67:ILE:HD13	1:D:155:PRO:CD	2.48	0.43
1:A:282:GLU:HG2	2:A:469:HOH:O	2.18	0.43
1:A:341:VAL:N	2:A:590:HOH:O	2.52	0.43
1:B:10:LEU:HD22	1:B:45:LEU:HD13	2.01	0.43
1:B:11:ILE:HD11	1:C:169:ILE:HD13	2.00	0.43
1:D:144:ASN:HA	1:D:144:ASN:HD22	1.61	0.43
1:D:222:ILE:HG22	1:D:223:ASP:N	2.33	0.43
1:A:170:ARG:HH11	1:A:174:ASN:HB3	1.84	0.43
1:C:78:ALA:CB	1:C:178:PRO:HB3	2.49	0.43
1:D:213:ILE:HG23	1:D:236:VAL:HG13	2.01	0.43
1:A:275:ARG:HH22	1:A:342:LYS:HE2	1.84	0.43
1:D:190:MET:O	1:D:215:LEU:HA	2.19	0.42
1:D:87:THR:CG2	1:D:88:VAL:N	2.82	0.42
1:B:160:VAL:O	1:B:160:VAL:CG2	2.67	0.42
1:C:325:GLU:HG3	1:C:326:ILE:N	2.33	0.42
1:A:220:PRO:HD3	1:A:228:ILE:CD1	2.49	0.42
1:C:111:ALA:CB	1:C:116:SER:H	2.30	0.42
1:D:192:VAL:HG12	1:D:193:PHE:N	2.33	0.42
1:D:2:ASN:HA	2:D:537:HOH:O	2.20	0.42
1:A:199:ASP:HA	1:A:234:LYS:NZ	2.35	0.42
1:C:125:LEU:O	1:C:327:ILE:HD13	2.19	0.42
1:B:336:LEU:HG	2:B:441:HOH:O	2.19	0.42
1:B:339:ILE:HB	1:B:342:LYS:NZ	2.35	0.42
1:B:135:ARG:O	1:B:139:LEU:HG	2.19	0.42
1:D:256:ILE:HA	1:D:257:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:VAL:HG13	1:D:307:GLU:CB	2.50	0.42
1:A:160:VAL:HG12	1:A:160:VAL:O	2.20	0.42
1:B:235:ILE:HB	1:B:242:GLU:HB3	2.01	0.42
1:B:333:VAL:CG1	1:B:336:LEU:HG	2.50	0.42
1:D:78:ALA:O	1:D:190:MET:HA	2.20	0.42
1:A:170:ARG:NH2	2:A:575:HOH:O	2.52	0.42
1:A:1:MET:HB3	2:A:468:HOH:O	2.20	0.42
1:B:275:ARG:HH12	1:B:280:LYS:CB	2.27	0.42
1:A:209:ASP:OD1	1:A:238:LYS:NZ	2.53	0.42
1:A:2:ASN:O	1:A:6:ILE:HG12	2.20	0.42
1:B:268:ASP:HB2	2:B:417:HOH:O	2.20	0.42
1:D:263:VAL:CG1	1:D:264:ASN:N	2.82	0.42
1:B:271:ILE:HD11	1:B:341:VAL:HG11	2.01	0.41
1:D:67:ILE:HD13	1:D:155:PRO:HD2	2.02	0.41
1:C:1:MET:CB	2:C:546:HOH:O	2.19	0.41
1:C:286:GLU:OE1	1:C:309:TYR:OH	2.38	0.41
1:D:70:ASP:CA	2:D:538:HOH:O	2.20	0.41
1:A:97:LEU:O	1:A:100:LEU:HB2	2.20	0.41
1:C:204:SER:O	1:C:208:LEU:HD22	2.21	0.41
1:C:102:ASN:HD22	1:C:301:ARG:NH1	2.04	0.41
1:B:339:ILE:CA	1:B:342:LYS:CE	2.98	0.41
1:D:139:LEU:HD22	2:D:353:HOH:O	2.19	0.41
1:D:228:ILE:CG2	1:D:258:ILE:HG12	2.51	0.41
1:D:87:THR:HG21	1:D:224:GLU:OE1	2.21	0.41
1:C:134:GLU:HG2	1:C:135:ARG:H	1.86	0.41
1:C:111:ALA:HB2	1:C:117:GLY:N	2.36	0.41
1:D:191:GLY:C	1:D:223:ASP:HB2	2.41	0.41
1:C:259:GLU:CD	1:C:259:GLU:H	2.23	0.41
1:C:3:ILE:HG12	1:C:3:ILE:H	1.67	0.41
1:C:71:VAL:HG12	1:C:74:ALA:HB2	2.03	0.41
1:A:102:ASN:ND2	1:A:301:ARG:NH2	2.63	0.40
1:C:112:VAL:HB	2:C:394:HOH:O	2.21	0.40
1:B:337:LYS:O	1:B:341:VAL:HG23	2.21	0.40
1:B:3:ILE:HD12	1:B:33:VAL:HG13	2.03	0.40
1:D:1:MET:HE3	1:D:2:ASN:N	2.37	0.40
1:D:246:LEU:CD1	1:D:250:ASP:HB2	2.51	0.40
1:D:96:ILE:HD13	1:D:323:LEU:HD13	2.02	0.40
1:B:164:ARG:CD	2:B:350:HOH:O	2.65	0.40
1:B:164:ARG:HG3	2:B:561:HOH:O	2.21	0.40
1:B:332:ASP:OD1	1:B:333:VAL:N	2.55	0.40
1:C:55:ILE:HD13	1:C:201:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:SER:CB	2:D:506:HOH:O	2.66	0.40
1:D:22:GLU:O	1:D:26:LYS:HG3	2.20	0.40
1:B:302:VAL:HG11	1:B:308:GLY:HA2	2.03	0.40
1:A:250:ASP:C	1:A:252:GLY:N	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:525:HOH:O	2:D:525:HOH:O[2_656]	1.89	0.31

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/345 (97%)	321 (96%)	10 (3%)	4 (1%)	15	6
1	B	336/345 (97%)	321 (96%)	13 (4%)	2 (1%)	28	17
1	C	337/345 (98%)	323 (96%)	12 (4%)	2 (1%)	28	17
1	D	343/345 (99%)	331 (96%)	8 (2%)	4 (1%)	15	6
All	All	1351/1380 (98%)	1296 (96%)	43 (3%)	12 (1%)	20	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	220	PRO
1	D	344	SER
1	A	113	SER
1	C	115	LYS
1	D	113	SER
1	C	344	SER

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Mol	Chain	Res	Type
1	D	89	ASN
1	A	78	ALA
1	B	78	ALA
1	A	221	GLY
1	B	87	THR
1	A	341	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	286/289 (99%)	271 (95%)	15 (5%)	27	17
1	B	287/289 (99%)	270 (94%)	17 (6%)	23	13
1	C	287/289 (99%)	273 (95%)	14 (5%)	29	20
1	D	289/289 (100%)	279 (96%)	10 (4%)	41	33
All	All	1149/1156 (99%)	1093 (95%)	56 (5%)	29	20

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	45	LEU
1	A	100	LEU
1	A	125	LEU
1	A	144	ASN
1	A	149	PHE
1	A	164	ARG
1	A	208	LEU
1	A	243	GLU
1	A	253	ILE
1	A	289	LYS
1	A	296	LEU
1	A	304	ASP
1	A	306	ARG
1	A	329	MET

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	67	ILE
1	B	69	ILE
1	B	70	ASP
1	B	100	LEU
1	B	125	LEU
1	B	142	LYS
1	B	144	ASN
1	B	188	GLN
1	B	198	LEU
1	B	215	LEU
1	B	220	PRO
1	B	239	ARG
1	B	260	LYS
1	B	275	ARG
1	B	296	LEU
1	B	343	SER
1	C	1	MET
1	C	87	THR
1	C	100	LEU
1	C	125	LEU
1	C	144	ASN
1	C	189	LEU
1	C	198	LEU
1	C	208	LEU
1	C	233	MET
1	C	258	ILE
1	C	264	ASN
1	C	268	ASP
1	C	269	SER
1	C	296	LEU
1	D	45	LEU
1	D	87	THR
1	D	100	LEU
1	D	125	LEU
1	D	144	ASN
1	D	193	PHE
1	D	198	LEU
1	D	208	LEU
1	D	236	VAL
1	D	269	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	102	ASN
1	A	144	ASN
1	A	162	ASN
1	A	174	ASN
1	A	247	ASN
1	B	141	ASN
1	B	144	ASN
1	B	174	ASN
1	B	181	ASN
1	B	247	ASN
1	C	102	ASN
1	C	141	ASN
1	C	144	ASN
1	C	151	GLN
1	C	162	ASN
1	C	174	ASN
1	C	181	ASN
1	C	197	HIS
1	C	264	ASN
1	D	144	ASN
1	D	151	GLN
1	D	162	ASN
1	D	174	ASN
1	D	181	ASN
1	D	247	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	339/345 (98%)	0.12	15 (4%) 35 38	19, 32, 53, 65	0
1	B	340/345 (98%)	0.38	25 (7%) 15 17	20, 36, 63, 77	0
1	C	341/345 (98%)	0.13	11 (3%) 48 53	19, 30, 48, 67	0
1	D	345/345 (100%)	0.30	19 (5%) 26 28	20, 34, 61, 81	0
All	All	1365/1380 (98%)	0.23	70 (5%) 29 31	19, 33, 57, 81	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	VAL	11.7
1	D	112	VAL	9.1
1	C	79	GLY	7.8
1	B	112	VAL	7.6
1	B	84	GLY	6.8
1	C	84	GLY	6.7
1	B	114	GLY	5.8
1	B	78	ALA	5.7
1	A	193	PHE	5.5
1	D	115	LYS	5.5
1	D	114	GLY	5.1
1	D	345	GLY	5.0
1	D	113	SER	4.5
1	D	344	SER	4.5
1	A	79	GLY	4.3
1	B	113	SER	4.2
1	D	83	ASP	4.1
1	B	239	ARG	3.9
1	B	115	LYS	3.9
1	C	85	LEU	3.9
1	B	79	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.8
1	A	114	GLY	3.7
1	B	1	MET	3.7
1	D	306	ARG	3.6
1	D	343	SER	3.6
1	A	78	ALA	3.6
1	C	239	ARG	3.5
1	D	1	MET	3.5
1	C	114	GLY	3.5
1	A	239	ARG	3.4
1	A	112	VAL	3.4
1	C	115	LYS	3.3
1	B	340	VAL	3.3
1	D	334	THR	3.2
1	D	85	LEU	3.1
1	B	264	ASN	3.1
1	A	341	VAL	3.0
1	D	84	GLY	3.0
1	C	344	SER	3.0
1	D	239	ARG	2.9
1	A	1	MET	2.8
1	D	275	ARG	2.8
1	B	83	ASP	2.7
1	B	343	SER	2.7
1	A	113	SER	2.7
1	A	115	LYS	2.7
1	D	225	VAL	2.7
1	A	245	LYS	2.6
1	A	170	ARG	2.6
1	D	258	ILE	2.6
1	A	306	ARG	2.5
1	B	339	ILE	2.5
1	B	19	ASN	2.5
1	B	334	THR	2.4
1	B	116	SER	2.4
1	C	113	SER	2.4
1	B	342	LYS	2.4
1	B	332	ASP	2.4
1	B	111	ALA	2.3
1	C	341	VAL	2.3
1	B	337	LYS	2.2
1	D	146	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	342	LYS	2.1
1	B	5	GLU	2.1
1	D	282	GLU	2.1
1	B	336	LEU	2.1
1	B	85	LEU	2.1
1	B	142	LYS	2.0
1	A	335	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.