



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 PM UTC

PDB ID : 1O17 / pdb_00001o17
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

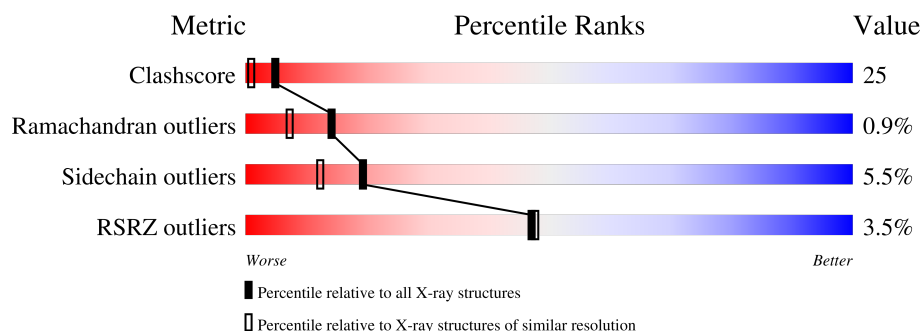
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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 $\leq 5\%$. 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	3% 64% 29% 5% •
1	B	345	6% 57% 35% 6% •
1	C	345	3% 63% 30% 6% •
1	D	345	3% 60% 35% •

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.

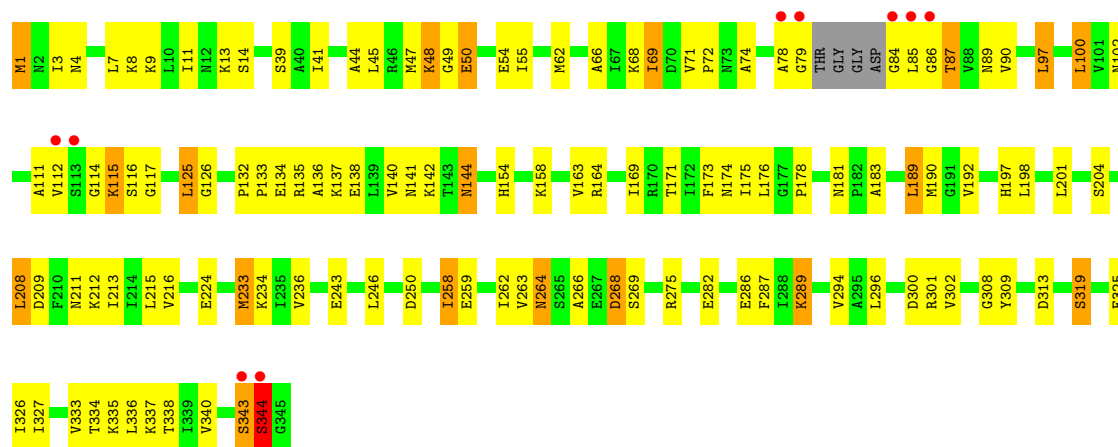
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE.

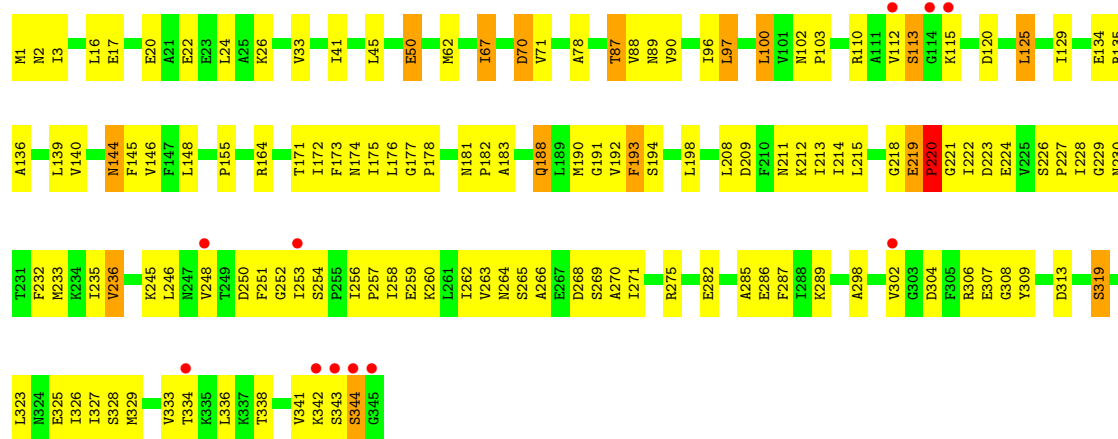
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2611	1675	440	489	7			
1	B	340	Total	C	N	O	S	0	0	0
			2619	1679	441	492	7			
1	C	341	Total	C	N	O	S	0	0	0
			2621	1680	442	492	7			
1	D	345	Total	C	N	O	S	0	0	0
			2644	1692	446	499	7			

- 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		



● Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.34Å 65.85Å 116.44Å 90.00° 107.56° 90.00°	Depositor
Resolution (Å)	18.00 – 2.05 18.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.7 (18.00-2.05) 92.6 (18.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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	0.50	2/2647 (0.1%)	1.06	16/3575 (0.4%)
1	B	0.42	0/2655	0.97	9/3586 (0.3%)
1	C	0.47	0/2657	0.95	12/3588 (0.3%)
1	D	0.45	0/2681	1.39	14/3622 (0.4%)
All	All	0.46	2/10640 (0.0%)	1.11	51/14371 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	VAL	C-N	6.89	1.43	1.33
1	A	342	LYS	N-CA	6.03	1.53	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLU	CA-C-N	39.63	169.38	119.84
1	D	219	GLU	C-N-CA	39.63	169.38	119.84
1	A	112	VAL	N-CA-C	-15.06	97.45	111.45
1	D	342	LYS	CA-C-N	-13.92	104.14	122.79
1	D	342	LYS	C-N-CA	-13.92	104.14	122.79
1	D	219	GLU	C-N-CD	-12.38	74.26	125.00
1	B	334	THR	N-CA-C	-10.23	100.80	113.28
1	A	341	VAL	CA-C-N	8.41	137.60	121.54
1	A	341	VAL	C-N-CA	8.41	137.60	121.54
1	A	116	SER	N-CA-C	-7.92	103.11	114.12
1	B	275	ARG	N-CA-C	-7.51	103.18	111.36
1	A	211	ASN	N-CA-C	-7.42	102.34	111.40
1	D	67	ILE	N-CA-C	-6.91	99.77	108.89
1	D	319	SER	N-CA-C	6.91	118.89	111.36
1	C	319	SER	N-CA-C	6.89	118.87	111.36
1	A	341	VAL	CB-CA-C	6.64	122.19	111.29
1	B	211	ASN	N-CA-C	-6.62	103.55	111.69
1	B	69	ILE	N-CA-C	-6.57	99.03	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ILE	N-CA-C	-6.55	99.16	108.65
1	C	344	SER	CB-CA-C	6.51	123.37	110.42
1	D	220	PRO	CA-N-CD	-6.25	103.25	112.00
1	C	343	SER	O-C-N	6.07	129.81	122.35
1	C	343	SER	CA-C-N	6.05	133.10	121.54
1	C	343	SER	C-N-CA	6.05	133.10	121.54
1	A	110	ARG	N-CA-C	-6.04	102.40	110.55
1	A	181	ASN	CA-C-N	6.01	125.69	119.56
1	A	181	ASN	C-N-CA	6.01	125.69	119.56
1	B	209	ASP	N-CA-C	5.98	119.89	111.52
1	B	342	LYS	N-CA-C	-5.94	104.88	111.71
1	D	209	ASP	N-CA-C	5.77	119.60	111.52
1	A	209	ASP	N-CA-C	5.71	119.28	111.39
1	B	189	LEU	N-CA-C	-5.69	99.25	108.52
1	A	17	GLU	N-CA-C	-5.66	103.23	110.53
1	C	209	ASP	N-CA-C	5.63	119.16	111.39
1	B	289	LYS	N-CA-C	5.61	117.47	111.36
1	C	289	LYS	N-CA-C	5.60	117.46	111.36
1	D	188	GLN	N-CA-C	5.59	117.02	108.52
1	C	258	ILE	N-CA-C	5.50	116.89	110.62
1	C	211	ASN	N-CA-C	-5.43	104.21	112.04
1	C	48	LYS	N-CA-C	-5.42	105.45	111.36
1	D	33	VAL	N-CA-C	5.41	113.79	107.89
1	A	115	LYS	N-CA-C	5.33	118.48	111.28
1	C	69	ILE	N-CA-C	-5.28	100.25	108.86
1	A	226	SER	N-CA-C	5.24	117.21	109.50
1	D	70	ASP	N-CA-C	5.21	117.11	108.20
1	C	189	LEU	N-CA-C	-5.14	100.14	108.52
1	D	211	ASN	N-CA-C	-5.10	104.70	112.04
1	A	342	LYS	CA-C-O	5.03	127.70	120.51
1	D	17	GLU	N-CA-C	-5.02	103.78	110.55
1	B	333	VAL	N-CA-C	5.01	111.57	106.21
1	A	233	MET	N-CA-C	5.00	117.28	109.52

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	106	0
1	B	2619	0	2734	172	0
1	C	2621	0	2738	123	0
1	D	2644	0	2756	146	0
2	A	258	0	0	44	0
2	B	218	0	0	33	0
2	C	250	0	0	35	0
2	D	209	0	0	25	1
All	All	11430	0	10958	542	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 25.

All (542) 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:A:62:MET:HE3	1:A:180:THR:HG21	1.28	1.14
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:221:GLY:C	2:A:572:HOH:O	2.02	1.00
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: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:261:LEU:HB3	2:A:595:HOH:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:178:PRO:HB2	1:B:190:MET:HE2	1.50	0.93
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: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:A:221:GLY:CA	2:A:572:HOH:O	2.16	0.90
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:B:179:LEU:HD23	1:B:190:MET:HE1	1.56	0.84
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: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: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:C:62:MET:HE1	1:C:176:LEU:HB3	1.64	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:LEU:HD22	1:B:319:SER:OG	1.83	0.78
1:B:343:SER:O	2:B:555:HOH:O	2.00	0.78
1:D:343:SER:O	1:D:344:SER:C	2.27	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:C:62:MET:HE1	1:C:176:LEU:CB	2.15	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:62:MET:CE	1:C:176:LEU:HD13	2.16	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: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: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:C:62:MET:HE2	1:C:176:LEU:HD13	1.70	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:112:VAL:C	2:C:593:HOH:O	2.30	0.72
1:C:175:ILE:HG22	2:C:585:HOH:O	1.89	0.72
1:C:1:MET:HE3	1:C:3:ILE:HD13	1.72	0.71
1:B:338:THR:C	1:B:342:LYS:HE3	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:168:GLY:C	2:B:535:HOH:O	2.35	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:D:220:PRO:HG2	1:D:222:ILE:HG13	1.77	0.67
1:B:179:LEU:CD2	1:B:190:MET:HE1	2.25	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: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:C:134:GLU:CD	2:C:560:HOH:O	2.38	0.66
1:A:268:ASP:HB3	2:A:459:HOH:O	1.96	0.66
1:D:268:ASP:CG	2:D:554:HOH:O	2.37	0.65
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:190:MET:HE3	1:B:213:ILE:HD11	1.79	0.65
1:B:271:ILE:O	1:B:275:ARG:HG3	1.96	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:341:VAL:C	1:A:343:SER:H	2.05	0.63
1:D:62:MET:HE1	1:D:176:LEU:CB	2.28	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: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:274:VAL:HG21	1:B:342:LYS:HE2	1.81	0.61
1:C:327:ILE:HD12	1:C:336:LEU:HD22	1.83	0.60
1:D:22:GLU:CG	2:D:553:HOH:O	2.44	0.60
1:D:220:PRO:CD	1:D:221:GLY:N	2.63	0.60
1:C:333:VAL:HG12	1:C:337:LYS:HE3	1.83	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:A:50:GLU:CD	1:A:50:GLU:H	2.08	0.60
1:D:97:LEU:O	1:D:100:LEU:HB2	2.02	0.60
1:B:339:ILE:N	1:B:342:LYS:HE3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG22	1:B:160:VAL:O	2.01	0.60
1:A:336:LEU:O	1:A:340:VAL:HG23	2.02	0.59
1:B:62:MET:HE1	1:B:176:LEU:HB2	1.82	0.59
1:D:263:VAL:HG13	1:D:268:ASP:CB	2.32	0.59
1:D:275:ARG:CD	1:D:343:SER:OG	2.51	0.59
1:B:178:PRO:CB	1:B:190:MET:HE2	2.30	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:B:62:MET:HE3	1:B:180:THR:HG21	1.85	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:D:62:MET:HE1	1:D:176:LEU:HB3	1.85	0.58
1:D:102:ASN:CG	1:D:103:PRO:HD2	2.29	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:B:1:MET:HE1	1:B:6:ILE:HD12	1.86	0.58
1:D:62:MET:HE1	1:D:176:LEU:HD13	1.84	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:62:MET:HE2	1:B:176:LEU:HD13	1.86	0.57
1:B:340:VAL:C	1:B:343:SER:HB2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:VAL:HG23	2:C:400:HOH:O	2.05	0.57
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: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: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
1:B:238:LYS:HD3	2:B:559:HOH:O	2.07	0.55
1:D:1:MET:CE	1:D:3:ILE:HD13	2.36	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:C:84:GLY:C	1:C:86:GLY:H	2.14	0.55
1:D:227:PRO:HG3	1:D:287:PHE:CE1	2.42	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:D:275:ARG:NE	1:D:343:SER:HG	2.03	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:B:336:LEU:C	1:B:339:ILE:HG22	2.32	0.55
1:C:78:ALA:O	1:C:79:GLY:C	2.49	0.55
1:C:158:LYS:HD3	2:C:528:HOH:O	2.06	0.55
1:C:233:MET:HE1	1:C:294:VAL:CG2	2.37	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: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: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: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:B:336:LEU:CA	1:B:339:ILE:HG22	2.38	0.53
1:C:90:VAL:HG11	1:C:287:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:ASP:HB3	1:B:188:GLN:HG2	1.90	0.53
1:B:239:ARG:NH2	1:B:242:GLU:HB2	2.22	0.53
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:A:250:ASP:C	1:A:252:GLY:H	2.15	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:D:246:LEU:HD11	1:D:250:ASP:HB2	1.91	0.53
1:B:67:ILE:O	1:B:67:ILE:HG12	2.09	0.52
1:B:324:ASN:N	1:B:335:LYS:HZ2	2.07	0.52
1:D:134:GLU:CG	2:D:551:HOH:O	2.17	0.52
1:D:302:VAL:HG13	1:D:307:GLU:CD	2.35	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:C:62:MET:HE1	1:C:176:LEU:HD13	1.91	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:1:MET:HE3	1:D:2:ASN:N	2.24	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:C:216:VAL:CG1	1:C:233:MET:HE2	2.40	0.52
1:D:135:ARG:NH2	1:D:329:MET:O	2.43	0.52
1:C:233:MET:HE1	1:C:294:VAL:HG21	1.91	0.51
1:C:300:ASP:HB3	2:C:595:HOH:O	2.10	0.51
1:B:115:LYS:NZ	2:B:558:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HE1	1:B:176:LEU:CB	2.41	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:259:GLU:CD	1:D:259:GLU:H	2.19	0.50
1:A:200:LEU:C	1:A:200:LEU:HD23	2.36	0.50
1:C:84:GLY:C	1:C:86:GLY:N	2.68	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:B:274:VAL:HB	1:B:342:LYS:HE2	1.91	0.50
1:D:171:THR:H	1:D:174:ASN:ND2	2.01	0.50
1:D:1:MET:HE3	1:D:1:MET:C	2.37	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:C:243:GLU:CB	2:C:592:HOH:O	2.46	0.50
1:D:1:MET:HE1	1:D:3:ILE:HD13	1.93	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:A:1:MET:HE3	2:A:468:HOH:O	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:76:ASP:HB3	1:B:188:GLN:CG	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:C:41:ILE:O	1:C:45:LEU:HB2	2.13	0.49
1:C:134:GLU:HG2	1:C:135:ARG:N	2.28	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:O	1:D:341:VAL:CG1	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:D:1:MET:HG3	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:C:79:GLY:HA2	2:C:469:HOH:O	2.14	0.47
1:C:275:ARG:CG	1:C:343:SER:HB3	2.44	0.47
1:A:256:ILE:HD12	1:A:256:ILE:N	2.29	0.47
1:B:90:VAL:HG11	1:B:287:PHE:CD2	2.50	0.47
1:B:116:SER:CB	2:B:563:HOH:O	2.25	0.47
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: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:233:MET:HG3	1:B:244:VAL:HB	1.96	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:N	1:D:260:LYS:HD2	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:125:LEU:HB3	1:B:327:ILE:HD11	1.96	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: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:71:VAL:N	1:C:72:PRO:CD	2.76	0.46
1:C:246:LEU:HD11	1:C:250:ASP:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HD2	1:A:260:LYS:N	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:B:181:ASN:ND2	1:B:183:ALA:H	2.14	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
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:191:GLY:C	1:D:223:ASP:HB2	2.41	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:HE2	1:B:52:LYS:HB3	1.85	0.45
1:C:66:ALA:HB2	1:C:154:HIS:CE1	2.52	0.45
1:C:259:GLU:H	1:C:259:GLU:CD	2.23	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:D:263:VAL:HG12	1:D:264:ASN:N	2.30	0.45
1:A:87:THR:CB	2:A:595:HOH:O	2.49	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:B:47:MET:SD	1:C:44:ALA:HA	2.57	0.45
1:C:190:MET:HE2	1:C:201:LEU:HD13	1.98	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:86:GLY:O	1:C:263:VAL:N	2.38	0.44
1:C:192:VAL:HG13	1:C:197:HIS:HB3	1.98	0.44
1:D:50:GLU:H	1:D:50:GLU:CD	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:62:MET:CE	1:A:180:THR:HG21	2.20	0.44
1:B:334:THR:O	1:B:337:LYS:HB3	2.18	0.44
1:A:250:ASP:C	1:A:252:GLY:N	2.74	0.44
1:C:13:LYS:HD2	2:C:562:HOH:O	2.18	0.44
1:A:27:ALA:O	1:A:32:GLU:HG3	2.17	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:B:62:MET:HE2	1:B:176:LEU:CD1	2.47	0.43
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
1:C:62:MET:HE1	1:C:176:LEU:CD1	2.47	0.43
1:C:215:LEU:N	1:C:215:LEU:HD12	2.33	0.43
1:D:148:LEU:HD13	1:D:182:PRO:HB2	1.99	0.43
1:C:114:GLY:O	1:C:115:LYS:C	2.61	0.43
1:C:144:ASN:HD22	1:C:144:ASN:HA	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:D:233:MET:HE3	1:D:233:MET:HB2	1.86	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:HD12	1:D:215:LEU:N	2.34	0.43
1:A:115:LYS:HA	1:A:115:LYS:HD3	1.79	0.43
1:B:50:GLU:H	1:B:50:GLU:CD	2.26	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: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: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:HD22	1:D:144:ASN:HA	1.61	0.43
1:D:222:ILE:HG22	1:D:223:ASP:N	2.33	0.43
1:A:47:MET:HE2	1:A:47:MET:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:216:VAL:HG11	1:C:233:MET:HE2	2.00	0.43
1:B:259:GLU:CD	1:B:259:GLU:H	2.26	0.42
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:2:ASN:HA	2:D:537:HOH:O	2.20	0.42
1:D:192:VAL:HG12	1:D:193:PHE:N	2.33	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:C:212:LYS:NZ	2:C:591:HOH:O	2.49	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
1:D:302:VAL:HG13	1:D:307:GLU:CB	2.50	0.42
1:A:160:VAL:O	1:A:160:VAL:HG12	2.20	0.42
1:B:11:ILE:C	1:B:13:LYS:H	2.27	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:1:MET:HB3	2:A:468:HOH:O	2.20	0.42
1:A:170:ARG:NH2	2:A:575:HOH:O	2.52	0.42
1:B:275:ARG:HH12	1:B:280:LYS:CB	2.27	0.42
1:D:145:PHE:C	1:D:145:PHE:CD2	2.97	0.42
1:A:2:ASN:O	1:A:6:ILE:HG12	2.20	0.42
1:A:209:ASP:OD1	1:A:238:LYS:NZ	2.53	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:B:70:ASP:OD1	1:B:70:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:THR:HG21	1:D:224:GLU:OE1	2.21	0.41
1:D:228:ILE:CG2	1:D:258:ILE:HG12	2.51	0.41
1:C:50:GLU:CD	1:C:50:GLU:H	2.28	0.41
1:C:111:ALA:HB2	1:C:117:GLY:N	2.36	0.41
1:C:134:GLU:HG2	1:C:135:ARG:H	1.86	0.41
1:C:3:ILE:H	1:C:3:ILE:HG12	1.67	0.41
1:C:71:VAL:HG12	1:C:74:ALA:HB2	2.03	0.41
1:D:62:MET:HE1	1:D:176:LEU:CD1	2.50	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:D:62:MET:HE2	1:D:176:LEU:HD13	2.01	0.40
1:A:339:ILE:O	1:A:343:SER:C	2.64	0.40
1:B:3:ILE:HD12	1:B:33:VAL:HG13	2.03	0.40
1:B:337:LYS:O	1:B:341:VAL:HG23	2.21	0.40
1:D:96:ILE:HD13	1:D:323:LEU:HD13	2.02	0.40
1:D:246:LEU:CD1	1:D:250:ASP:HB2	2.51	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
1:D:22:GLU:O	1:D:26:LYS:HG3	2.20	0.40
1:D:113:SER:CB	2:D:506:HOH:O	2.66	0.40
1:B:302:VAL:HG11	1:B:308:GLY:HA2	2.03	0.40
1:C:234:LYS:NZ	2:C:592:HOH:O	2.49	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%)	10	4
1	B	336/345 (97%)	321 (96%)	13 (4%)	2 (1%)	21	13
1	C	337/345 (98%)	323 (96%)	12 (4%)	2 (1%)	21	13
1	D	343/345 (99%)	331 (96%)	8 (2%)	4 (1%)	10	4
All	All	1351/1380 (98%)	1296 (96%)	43 (3%)	12 (1%)	14	7

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
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 [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	286/289 (99%)	270 (94%)	16 (6%)	19	12
1	B	287/289 (99%)	268 (93%)	19 (7%)	15	9
1	C	287/289 (99%)	271 (94%)	16 (6%)	19	12
1	D	289/289 (100%)	277 (96%)	12 (4%)	26	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1149/1156 (99%)	1086 (94%)	63 (6%)	19	12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	45	LEU
1	A	50	GLU
1	A	97	LEU
1	A	100	LEU
1	A	125	LEU
1	A	144	ASN
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
1	B	45	LEU
1	B	50	GLU
1	B	67	ILE
1	B	69	ILE
1	B	70	ASP
1	B	97	LEU
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	260	LYS
1	B	274	VAL
1	B	275	ARG
1	B	296	LEU
1	B	343	SER
1	C	1	MET
1	C	50	GLU

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Mol	Chain	Res	Type
1	C	87	THR
1	C	97	LEU
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	50	GLU
1	D	87	THR
1	D	97	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	102	ASN
1	A	144	ASN
1	A	159	ASN
1	A	162	ASN
1	A	174	ASN
1	A	247	ASN
1	B	19	ASN
1	B	141	ASN
1	B	144	ASN
1	B	151	GLN
1	B	174	ASN

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Mol	Chain	Res	Type
1	B	181	ASN
1	B	247	ASN
1	C	19	ASN
1	C	102	ASN
1	C	107	HIS
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	264	ASN
1	D	144	ASN
1	D	151	GLN
1	D	174	ASN
1	D	181	ASN
1	D	197	HIS
1	D	247	ASN
1	D	283	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th 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 ²)	Q<0.9
1	A	339/345 (98%)	0.01	9 (2%) 56 58	19, 32, 53, 65	0
1	B	340/345 (98%)	0.32	19 (5%) 30 30	20, 36, 63, 77	0
1	C	341/345 (98%)	-0.03	9 (2%) 57 59	19, 30, 48, 67	0
1	D	345/345 (100%)	0.16	11 (3%) 50 50	20, 34, 61, 81	0
All	All	1365/1380 (98%)	0.12	48 (3%) 47 48	19, 33, 57, 81	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	SER	6.4
1	B	84	GLY	5.7
1	C	112	VAL	5.4
1	B	78	ALA	4.9
1	C	79	GLY	4.4
1	C	85	LEU	4.0
1	B	342	LYS	3.9
1	D	112	VAL	3.9
1	B	112	VAL	3.8
1	C	344	SER	3.7
1	B	239	ARG	3.6
1	B	333	VAL	3.5
1	A	79	GLY	3.2
1	D	302	VAL	3.2
1	C	113	SER	3.1
1	C	343	SER	3.0
1	A	193	PHE	3.0
1	C	84	GLY	2.9
1	D	115	LYS	2.9
1	B	79	GLY	2.9
1	A	253	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	343	SER	2.8
1	A	341	VAL	2.8
1	B	336	LEU	2.7
1	D	343	SER	2.7
1	B	113	SER	2.6
1	B	340	VAL	2.5
1	B	115	LYS	2.5
1	B	253	ILE	2.5
1	B	199	ASP	2.5
1	C	86	GLY	2.5
1	D	345	GLY	2.4
1	A	112	VAL	2.4
1	B	335	LYS	2.4
1	D	114	GLY	2.4
1	B	85	LEU	2.3
1	D	253	ILE	2.3
1	A	342	LYS	2.3
1	C	78	ALA	2.2
1	B	341	VAL	2.2
1	D	248	VAL	2.1
1	D	334	THR	2.1
1	D	342	LYS	2.1
1	A	115	LYS	2.0
1	A	222	ILE	2.0
1	B	274	VAL	2.0
1	B	329	MET	2.0
1	B	114	GLY	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 oligosaccharides 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.