Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 02:23 PM EDT

PDB ID	:	1EX5
Title	:	FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM RABBIT MUSCLE
Authors	:	Maurady, A.; Sygusch, J.
Deposited on	:	2000-04-25
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

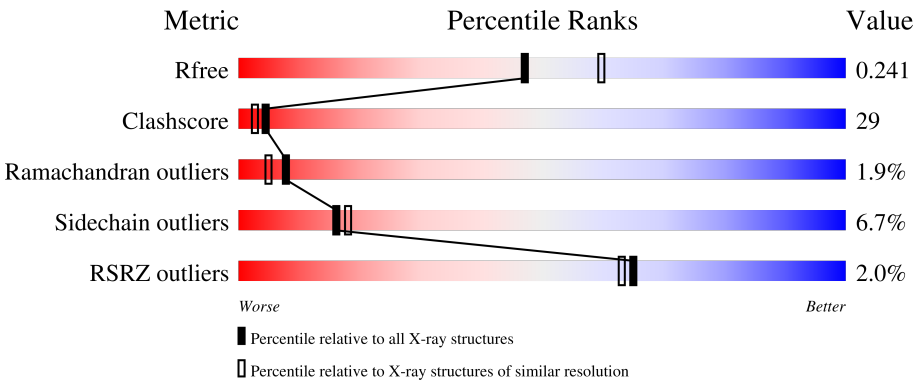
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	363	3% 55% 41% •
1	B	363	2% 52% 45% •
1	C	363	2% 55% 42% •
1	D	363	% 54% 43% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17144 atoms, of which 2628 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 FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	363	3547	1812	673	512	539	11	0	15	0
1	B	363	3507	1794	661	505	535	12	0	11	0
1	C	363	3428	1751	646	494	526	11	0	3	0
1	D	363	3444	1759	648	496	530	11	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ALA	GLU	engineered mutation	UNP P00883
B	187	ALA	GLU	engineered mutation	UNP P00883
C	187	ALA	GLU	engineered mutation	UNP P00883
D	187	ALA	GLU	engineered mutation	UNP P00883

- Molecule 2 is water.

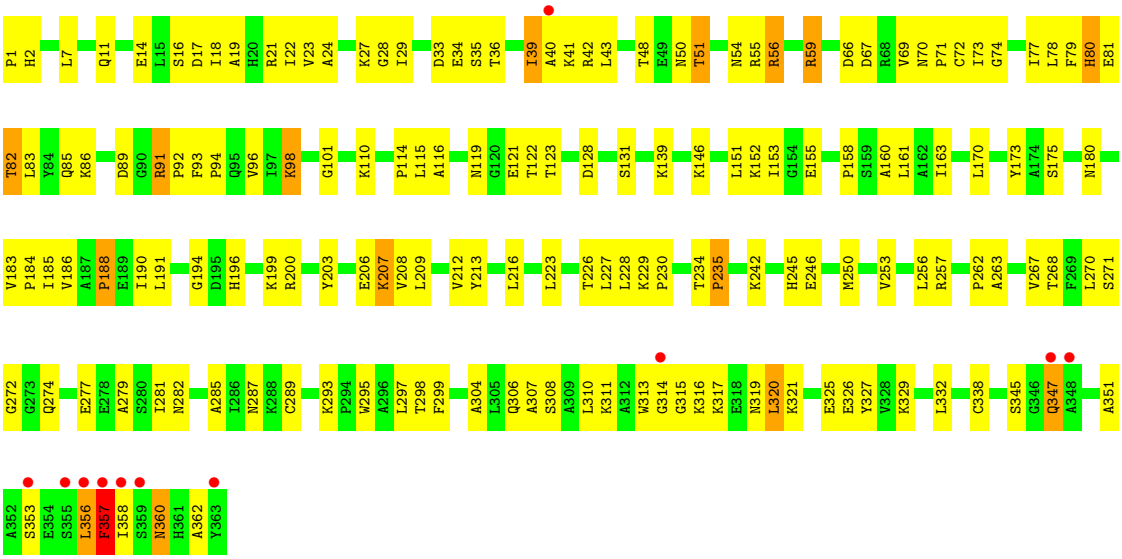
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	750	750	750	0	0
2	B	700	700	700	0	0
2	C	888	888	888	0	0
2	D	880	880	880	0	0

3 Residue-property plots (i)

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 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.

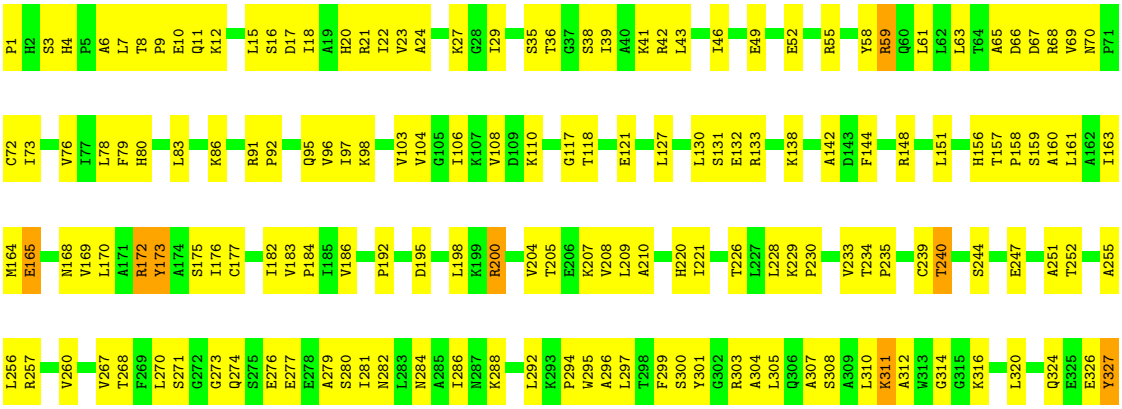
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

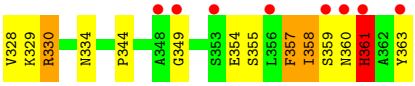
Chain A:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

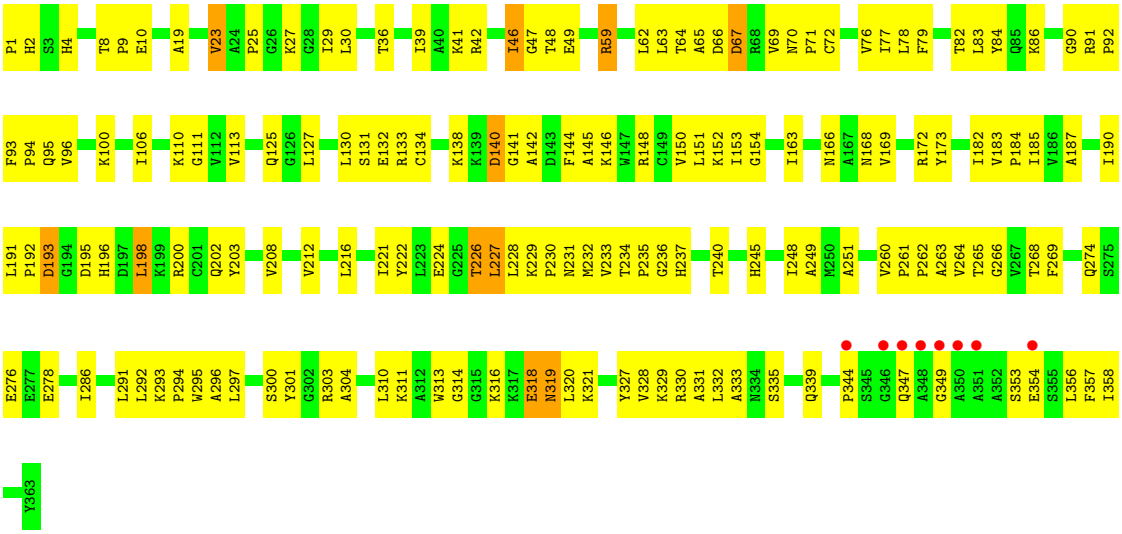
Chain B:





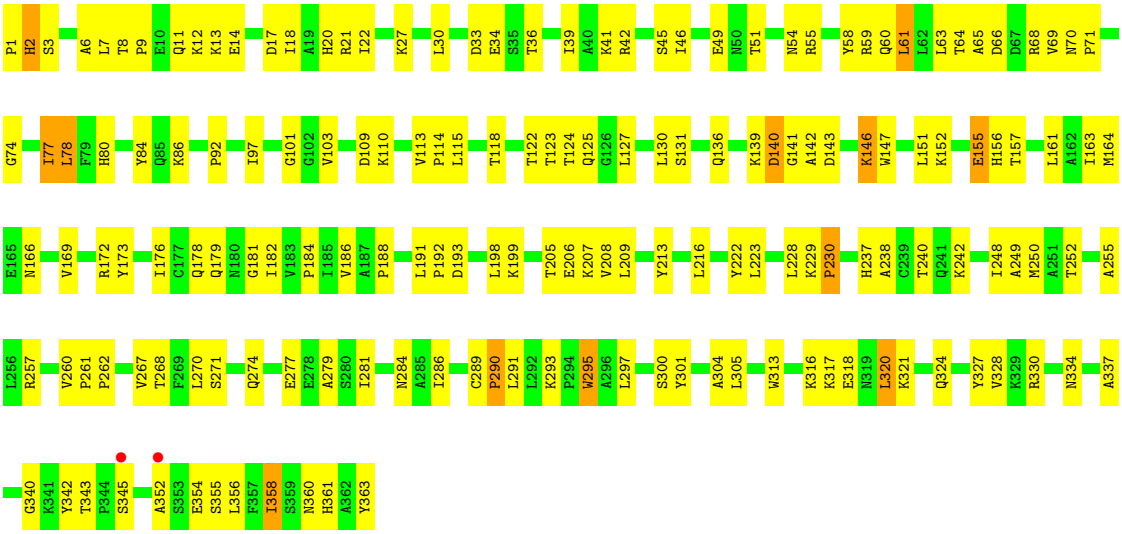
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain C:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	165.97Å 58.36Å 86.95Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	9.00 – 2.20 32.34 – 2.15	Depositor EDS
% Data completeness (in resolution range)	8.0 (9.00-2.20) 58.6 (32.34-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 2.16Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.179 , 0.229 0.178 , 0.241	Depositor DCC
R_{free} test set	4641 reflections (8.19%)	wwPDB-VP
Wilson B-factor (Å^2)	2.4	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 156.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	0.216 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	17144	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/2930	0.64	2/3967 (0.1%)
1	B	0.34	0/2903	0.65	2/3933 (0.1%)
1	C	0.34	0/2838	0.59	0/3846
1	D	0.34	0/2851	0.64	1/3863 (0.0%)
All	All	0.34	0/11522	0.63	5/15609 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2	HIS	N-CA-C	-8.08	89.18	111.00
1	A	360	ASN	N-CA-C	-7.35	91.15	111.00
1	B	360	ASN	N-CA-C	5.54	125.96	111.00
1	B	361	HIS	N-CA-C	5.45	125.72	111.00
1	A	357	PHE	N-CA-C	5.29	125.28	111.00

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	2874	673	2916	168	0
1	B	2846	661	2879	177	0
1	C	2782	646	2802	159	0
1	D	2796	648	2823	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	750	0	0	61	0
2	B	700	0	0	85	0
2	C	888	0	0	64	0
2	D	880	0	0	77	0
All	All	14516	2628	11420	652	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 29.

All (652) 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:D:27:LYS:HE2	1:D:74:GLY:HA2	1.36	1.07
1:A:91:ARG:HD2	1:A:96:VAL:HG22	1.47	0.97
1:B:207:LYS:HD3	1:C:1:PRO:HG2	1.49	0.94
1:A:203:TYR:HE2	1:D:1:PRO:HB3	1.36	0.90
1:C:187:ALA:HB2	1:C:229:LYS:HB3	1.55	0.88
1:A:36:THR:HG23	1:A:55:ARG:HH12	1.37	0.88
1:A:311[B]:LYS:HG3	1:A:353:SER:HB2	1.57	0.85
1:D:65:ALA:HB1	1:D:69:VAL:HG21	1.59	0.85
1:A:36:THR:HG23	1:A:55:ARG:NH1	1.92	0.85
1:A:282:ASN:HA	2:A:1423:HOH:O	1.78	0.82
1:B:118:THR:HB	1:B:121:GLU:HG3	1.60	0.82
1:C:42:ARG:HB3	1:C:310:LEU:HD21	1.61	0.82
1:D:206:GLU:HA	2:D:6525:HOH:O	1.80	0.81
1:A:311[A]:LYS:HG3	1:A:353:SER:HB2	1.62	0.80
1:C:191:LEU:HD21	2:C:4961:HOH:O	1.82	0.79
1:A:209:LEU:HD21	2:A:1440:HOH:O	1.83	0.78
1:D:268:THR:HB	1:D:300:SER:HB2	1.66	0.78
1:B:46:ILE:HG21	1:B:314:GLY:HA2	1.65	0.78
1:C:316:LYS:HA	2:C:4857:HOH:O	1.84	0.77
1:B:274:GLN:HG2	2:B:3542:HOH:O	1.86	0.76
1:B:158:PRO:HG3	2:B:3515:HOH:O	1.86	0.76
1:B:156:HIS:HA	2:C:5039:HOH:O	1.86	0.75
1:D:27:LYS:HE2	1:D:74:GLY:CA	2.15	0.75
1:D:164:MET:HG2	2:D:6857:HOH:O	1.87	0.75
1:A:306:GLN:HG3	2:A:1999:HOH:O	1.87	0.75
1:A:93:PHE:HA	1:A:96:VAL:HG23	1.67	0.74
1:A:175:SER:HB3	2:A:1627:HOH:O	1.87	0.74
1:C:221:ILE:HG21	2:C:4729:HOH:O	1.86	0.74
1:A:27:LYS:O	1:A:298:THR:HG21	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:HH22	1:B:292:LEU:HB3	1.54	0.73
1:C:86:LYS:HE2	1:C:92:PRO:HG3	1.69	0.73
1:D:161:LEU:HB3	2:D:6542:HOH:O	1.88	0.73
1:D:127:LEU:HB3	2:D:6387:HOH:O	1.89	0.72
1:D:6:ALA:HB3	2:D:7116:HOH:O	1.88	0.72
1:A:184:PRO:HG2	1:A:226:THR:HG22	1.71	0.72
1:B:68:ARG:HH11	1:B:328:VAL:HG11	1.53	0.72
1:B:284:ASN:O	1:B:288:LYS:HG2	1.89	0.72
1:C:354:GLU:HG3	2:C:4710:HOH:O	1.90	0.71
1:C:47:GLY:HA2	2:C:5116:HOH:O	1.91	0.71
1:C:172:ARG:NH1	1:D:123:THR:HG21	2.04	0.71
1:C:198:LEU:HG	2:C:4918:HOH:O	1.91	0.71
1:C:67:ASP:HB2	2:C:5228:HOH:O	1.88	0.71
1:B:312:ALA:HA	2:B:3869:HOH:O	1.90	0.71
1:C:46:ILE:HB	1:C:314:GLY:HA2	1.73	0.70
1:B:357:PHE:HD1	1:B:357:PHE:H	1.38	0.70
1:B:96:VAL:HG21	2:B:3462:HOH:O	1.92	0.70
1:A:199:LYS:HE3	2:A:6933:HOH:O	1.89	0.70
1:C:172:ARG:HH11	1:D:123:THR:HG21	1.57	0.70
1:D:118:THR:HG23	2:D:6920:HOH:O	1.92	0.70
1:D:242:LYS:HG3	1:D:358:ILE:HG21	1.74	0.70
1:B:108[B]:VAL:HG11	2:B:3589:HOH:O	1.90	0.70
1:A:152:LYS:HG2	1:A:191:LEU:HD12	1.73	0.69
1:A:229:LYS:NZ	1:A:270:LEU:HD21	2.06	0.69
1:A:80:HIS:HB2	2:A:2009:HOH:O	1.91	0.69
1:D:27:LYS:CE	1:D:74:GLY:HA2	2.18	0.69
1:D:228[B]:LEU:HG	1:D:230[B]:PRO:HD3	1.74	0.69
1:A:188:PRO:HB2	2:A:1427:HOH:O	1.92	0.69
1:C:77:ILE:HD11	2:C:4860:HOH:O	1.93	0.69
1:C:329:LYS:HA	2:C:5242:HOH:O	1.92	0.69
1:A:253:VAL:HA	1:A:256:LEU:HD12	1.75	0.68
1:B:228[B]:LEU:HG	1:B:230[B]:PRO:HD3	1.76	0.68
1:C:349:GLY:HA3	2:C:4384:HOH:O	1.91	0.68
1:D:30:LEU:HD22	1:D:327:TYR:OH	1.93	0.68
1:B:255:ALA:HB3	2:B:3513:HOH:O	1.94	0.68
1:C:327:TYR:HB2	2:C:4526:HOH:O	1.94	0.68
1:A:161:LEU:HD12	2:A:2022:HOH:O	1.94	0.68
1:A:262:PRO:HB2	2:D:1997:HOH:O	1.93	0.68
1:B:83:LEU:HA	2:B:3369:HOH:O	1.94	0.68
1:C:39:ILE:HD11	1:C:59:ARG:CZ	2.24	0.68
1:B:108[A]:VAL:HG11	2:B:3589:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228[A]:LEU:HG	1:D:230[A]:PRO:HD3	1.75	0.68
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.76	0.67
1:B:257:ARG:HB3	2:B:5188:HOH:O	1.92	0.67
1:B:132:GLU:HG2	2:B:3527:HOH:O	1.94	0.67
1:B:252:THR:HG22	2:B:3823:HOH:O	1.94	0.67
1:C:78:LEU:HD11	1:C:83:LEU:HD13	1.77	0.67
1:D:277:GLU:O	1:D:281:ILE:HG12	1.95	0.66
1:A:253:VAL:O	1:A:257:ARG:HG3	1.95	0.66
1:C:10:GLU:HB3	2:C:4409:HOH:O	1.95	0.66
1:D:179:GLN:HG3	2:D:4515:HOH:O	1.96	0.66
1:A:22:ILE:HB	2:A:1702:HOH:O	1.96	0.66
1:B:7:LEU:HD11	2:B:3592:HOH:O	1.95	0.65
1:A:229:LYS:NZ	1:A:229:LYS:HB3	2.11	0.65
1:B:35:SER:HA	1:B:79:PHE:CE2	2.31	0.65
1:C:316:LYS:HB2	1:C:319:ASN:OD1	1.96	0.65
1:A:190:ILE:HD11	1:A:208:VAL:HG21	1.78	0.65
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.78	0.65
1:D:252:THR:HA	2:D:7143:HOH:O	1.96	0.65
1:B:200:ARG:HH22	1:C:2:HIS:HA	1.61	0.65
1:D:68:ARG:HH11	1:D:328:VAL:HG11	1.62	0.65
1:A:7:LEU:CD2	1:A:11:GLN:HB3	2.27	0.64
1:B:308:SER:HA	1:B:311:LYS:HE3	1.78	0.64
1:A:308:SER:HB2	2:A:1654:HOH:O	1.96	0.64
1:A:146[B]:LYS:NZ	1:A:229:LYS:HE3	2.12	0.64
1:C:293:LYS:HD2	1:C:297:LEU:HD11	1.79	0.64
1:D:192:PRO:HB3	2:D:6862:HOH:O	1.98	0.64
1:B:169:VAL:HG12	2:B:3872:HOH:O	1.97	0.64
1:C:110:LYS:HA	2:C:4584:HOH:O	1.96	0.64
1:C:332:LEU:HD12	2:C:5242:HOH:O	1.97	0.64
1:A:16:SER:HB2	2:A:1695:HOH:O	1.97	0.64
1:A:83:LEU:HD13	2:A:1991:HOH:O	1.98	0.64
1:B:257:ARG:O	1:C:262:PRO:HD2	1.97	0.64
1:B:49:GLU:HG2	2:B:3702:HOH:O	1.97	0.64
1:A:277:GLU:O	1:A:281:ILE:HG13	1.98	0.64
1:C:190:ILE:HG12	2:C:4583:HOH:O	1.97	0.64
1:B:195:ASP:HB2	2:B:3767:HOH:O	1.97	0.64
1:A:298:THR:HG22	1:A:299:PHE:H	1.62	0.63
1:A:326:GLU:HG3	2:A:1654:HOH:O	1.97	0.63
1:C:318:GLU:HB3	2:C:4888:HOH:O	1.99	0.63
1:B:17:ASP:O	1:B:21:ARG:HG3	1.99	0.63
1:B:92:PRO:HD3	2:B:3995:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLY:HA3	2:A:1996:HOH:O	1.97	0.63
1:D:192:PRO:HG2	2:D:6708:HOH:O	1.97	0.63
1:B:299:PHE:CE1	1:B:334:ASN:HB3	2.34	0.63
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.80	0.63
1:C:286:ILE:HG22	1:C:297:LEU:HD13	1.79	0.63
1:A:196:HIS:HB2	1:A:200:ARG:HG2	1.80	0.63
1:A:250:MET:HG3	2:A:1471:HOH:O	1.98	0.62
1:B:68:ARG:NH1	1:B:328:VAL:HG11	2.13	0.62
1:C:151:LEU:HB3	2:C:4379:HOH:O	1.99	0.62
1:C:314:GLY:HA3	2:C:4542:HOH:O	1.98	0.62
1:B:97:ILE:HD13	2:B:3529:HOH:O	1.98	0.62
1:C:23:VAL:HG11	1:C:266:GLY:HA3	1.82	0.62
1:D:320:LEU:HD13	2:D:7211:HOH:O	2.00	0.61
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.82	0.61
1:A:151:LEU:HD12	1:A:158:PRO:HB3	1.82	0.61
2:A:6706:HOH:O	1:D:9:PRO:HD3	1.99	0.61
1:B:80:HIS:HB3	2:B:3780:HOH:O	2.01	0.61
1:B:228[A]:LEU:HG	1:B:230[A]:PRO:HD3	1.83	0.61
1:B:117:GLY:HA3	2:B:3564:HOH:O	1.99	0.61
1:C:148:ARG:HG2	2:C:4872:HOH:O	2.01	0.61
1:D:198:LEU:HD23	1:D:199:LYS:NZ	2.16	0.61
1:D:295:TRP:HB2	2:D:7072:HOH:O	2.01	0.61
1:B:96:VAL:HG12	2:B:4029:HOH:O	1.99	0.61
1:C:69:VAL:HG13	1:C:328:VAL:HG13	1.81	0.61
1:C:134:CYS:HB3	2:C:5025:HOH:O	2.00	0.61
1:B:22:ILE:HG21	1:B:29:ILE:HD11	1.83	0.60
1:B:165:GLU:O	1:B:169:VAL:HG23	2.01	0.60
1:C:29:ILE:HD12	1:C:268:THR:HG21	1.83	0.60
1:C:63:LEU:HD21	2:C:4414:HOH:O	2.00	0.60
1:B:204:VAL:O	1:B:208:VAL:HG23	2.01	0.60
1:C:184:PRO:HG2	1:C:226:THR:HG23	1.81	0.60
2:B:3557:HOH:O	1:C:261:PRO:HA	2.01	0.60
1:B:292:LEU:HB2	2:B:3704:HOH:O	2.02	0.60
1:B:9:PRO:HA	1:B:12:LYS:CE	2.32	0.60
1:D:209:LEU:HD22	2:D:6393:HOH:O	2.00	0.60
1:D:186:VAL:HG12	1:D:188:PRO:HD3	1.82	0.60
1:A:78:LEU:HD22	2:A:1991:HOH:O	2.02	0.60
1:B:103:VAL:HG23	1:B:144:PHE:HE2	1.67	0.59
1:A:183:VAL:HA	2:A:1690:HOH:O	2.03	0.59
2:B:3575:HOH:O	1:C:262:PRO:HG3	2.01	0.59
1:C:27:LYS:HA	1:C:72:CYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLU:HG2	2:D:6953:HOH:O	2.03	0.59
1:A:351:ALA:HB2	2:A:1491:HOH:O	2.01	0.59
1:B:18:ILE:HG12	1:B:21:ARG:HH11	1.68	0.58
1:A:277:GLU:HG2	1:A:347:GLN:HB3	1.85	0.58
1:B:170:LEU:HD13	1:B:186:VAL:HG13	1.85	0.58
1:A:92:PRO:HB2	1:A:94:PRO:HD2	1.84	0.58
1:B:163:ILE:HD11	1:C:1:PRO:HD3	1.84	0.58
1:C:111:GLY:HA3	2:C:5067:HOH:O	2.03	0.58
1:D:248:ILE:HD12	1:D:249:ALA:N	2.17	0.58
1:A:151:LEU:HD11	2:A:1582:HOH:O	2.03	0.58
1:B:234:THR:HG21	2:B:4037:HOH:O	2.02	0.58
1:B:55:ARG:HD3	2:B:3423:HOH:O	2.03	0.58
1:B:61:LEU:HD13	1:B:320:LEU:HD12	1.85	0.58
1:D:255:ALA:HB3	2:D:7143:HOH:O	2.03	0.58
1:A:203:TYR:CE2	1:D:1:PRO:HB3	2.28	0.58
1:C:36:THR:HG21	2:C:4552:HOH:O	2.02	0.58
1:D:286:ILE:HD11	2:D:6451:HOH:O	2.04	0.58
1:A:351:ALA:HA	2:A:1499:HOH:O	2.04	0.58
1:C:92:PRO:HB3	2:C:4494:HOH:O	2.04	0.58
1:D:356:LEU:HD23	1:D:356:LEU:O	2.04	0.57
1:A:40:ALA:HB1	1:A:50:ASN:HB3	1.85	0.57
1:A:128:ASP:HB2	2:A:1649:HOH:O	2.03	0.57
1:D:151:LEU:HD21	1:D:163:ILE:HD13	1.85	0.57
1:B:226:THR:HG21	2:B:3378:HOH:O	2.04	0.57
1:D:277:GLU:HA	1:D:330:ARG:HH12	1.68	0.57
1:A:200:ARG:NH2	1:D:2:HIS:CD2	2.73	0.57
1:B:301:TYR:HB3	1:B:304:ALA:HB3	1.85	0.57
1:B:358:ILE:HG13	1:B:359:SER:N	2.19	0.57
1:B:138:LYS:HE3	2:B:3431:HOH:O	2.05	0.57
1:C:113:VAL:HA	2:C:5187:HOH:O	2.04	0.57
1:B:22:ILE:HG12	1:B:103:VAL:HG21	1.87	0.57
1:B:36:THR:HA	2:B:3423:HOH:O	2.05	0.57
1:B:9:PRO:HB2	2:B:3963:HOH:O	2.03	0.57
1:D:151:LEU:HD13	2:D:6879:HOH:O	2.05	0.57
1:C:168:ASN:O	1:C:172:ARG:HG2	2.04	0.57
1:D:213:TYR:CD2	1:D:216:LEU:HD12	2.40	0.57
1:A:163:ILE:HA	2:A:1582:HOH:O	2.05	0.57
1:C:251:ALA:HB1	2:C:4918:HOH:O	2.05	0.57
1:C:303:ARG:HH11	1:C:303:ARG:HG2	1.69	0.57
1:C:335:SER:O	1:C:339:GLN:HG3	2.05	0.57
1:A:56:ARG:HG3	1:A:85:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG23	2:D:7206:HOH:O	2.03	0.56
1:D:166:ASN:O	1:D:169:VAL:HG12	2.05	0.56
1:C:19:ALA:O	1:C:23:VAL:HG22	2.05	0.56
1:D:39[B]:ILE:HG12	2:D:7167:HOH:O	2.05	0.56
1:C:268:THR:HB	1:C:300:SER:HB2	1.87	0.56
1:B:234:THR:HG23	1:B:235:PRO:HD2	1.86	0.56
1:C:303:ARG:HG2	1:C:303:ARG:NH1	2.21	0.56
1:B:305:LEU:HD21	1:B:334:ASN:HD22	1.70	0.56
1:A:73:ILE:HG13	2:A:1737:HOH:O	2.05	0.56
1:B:276:GLU:HB3	1:B:330:ARG:HD2	1.86	0.56
1:C:46:ILE:HG21	1:C:310:LEU:HG	1.86	0.56
1:C:131:SER:HA	1:C:134:CYS:SG	2.46	0.56
1:A:115:LEU:HD21	1:A:123:THR:HB	1.87	0.56
1:A:206:GLU:HA	2:A:1458:HOH:O	2.06	0.56
1:B:9:PRO:HA	1:B:12:LYS:HE2	1.87	0.56
1:B:52:GLU:HG3	2:B:3750:HOH:O	2.06	0.56
1:B:257:ARG:NH2	1:B:292:LEU:HB3	2.21	0.56
1:C:193:ASP:HB2	2:C:4489:HOH:O	2.05	0.56
1:A:93:PHE:HA	1:A:96:VAL:CG2	2.34	0.56
1:A:115:LEU:HG	1:A:122:THR:HA	1.88	0.56
1:D:304:ALA:HB1	2:D:6532:HOH:O	2.06	0.56
1:D:354:GLU:HG3	1:D:356:LEU:H	1.71	0.56
1:B:63:LEU:HG	2:B:3434:HOH:O	2.06	0.55
1:D:142:ALA:HB2	2:D:6909:HOH:O	2.05	0.55
1:A:272:GLY:HA3	2:A:1978:HOH:O	2.06	0.55
1:D:61:LEU:HB2	2:D:7170:HOH:O	2.06	0.55
1:D:63:LEU:HD21	2:D:6652:HOH:O	2.06	0.55
1:C:190:ILE:HB	1:C:231:ASN:OD1	2.05	0.55
1:D:284:ASN:ND2	1:D:342:TYR:H	2.04	0.55
1:B:308:SER:HA	1:B:311:LYS:CE	2.36	0.55
1:D:152:LYS:HB2	2:D:6612:HOH:O	2.06	0.55
1:B:130:LEU:HB3	1:B:176:ILE:HG21	1.89	0.55
1:D:305:LEU:HD23	1:D:330:ARG:HB3	1.89	0.55
1:A:358:ILE:O	1:A:358:ILE:HG22	2.06	0.55
1:D:42:ARG:HG3	1:D:42:ARG:HH11	1.72	0.55
1:A:229:LYS:HZ3	1:A:270:LEU:HD21	1.71	0.55
1:B:357:PHE:N	1:B:357:PHE:CD1	2.74	0.55
1:A:14:GLU:HG3	2:A:1808:HOH:O	2.07	0.55
1:D:18:ILE:HD12	2:D:6953:HOH:O	2.07	0.55
1:D:41:LYS:O	1:D:45:SER:HB2	2.07	0.55
1:D:114:PRO:HD3	2:D:6893:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HG	2:A:1395:HOH:O	2.06	0.54
1:A:17:ASP:HB3	1:A:21:ARG:HH22	1.72	0.54
1:A:39[B]:ILE:HD13	1:A:42[B]:ARG:HB2	1.90	0.54
1:A:317:LYS:HA	1:A:320:LEU:HB2	1.87	0.54
1:C:27:LYS:HG2	1:C:71:PRO:O	2.07	0.54
1:C:86:LYS:HD3	1:C:90:GLY:O	2.08	0.54
1:A:7:LEU:HD22	1:A:11:GLN:HB3	1.88	0.54
1:B:8:THR:OG1	1:B:11:GLN:HG3	2.08	0.54
1:A:250:MET:HE2	1:A:289:CYS:SG	2.47	0.54
1:C:146[A]:LYS:HE3	1:C:229:LYS:HE2	1.89	0.54
1:A:66:ASP:O	1:A:69:VAL:HG22	2.07	0.54
1:A:194:GLY:HA3	2:A:1666:HOH:O	2.08	0.54
1:D:257:ARG:HD3	1:D:291:LEU:HD13	1.89	0.54
1:A:158:PRO:HD2	2:A:1365:HOH:O	2.07	0.54
1:A:298:THR:HG22	1:A:299:PHE:CD1	2.43	0.54
1:C:296:ALA:HB2	2:C:5051:HOH:O	2.07	0.54
1:B:296:ALA:HB1	2:B:3786:HOH:O	2.08	0.54
1:B:361:HIS:ND1	1:B:361:HIS:N	2.56	0.54
1:C:232:MET:HG3	2:C:4487:HOH:O	2.07	0.54
1:A:345:SER:HB3	2:A:1550:HOH:O	2.07	0.54
1:D:97:ILE:HG13	2:D:6578:HOH:O	2.07	0.54
1:A:357:PHE:N	1:A:357:PHE:CD1	2.72	0.54
1:B:316:LYS:HA	2:B:3860:HOH:O	2.08	0.54
1:C:65:ALA:HB3	2:C:5080:HOH:O	2.08	0.54
1:C:321:LYS:HG2	2:C:4967:HOH:O	2.08	0.54
1:A:190:ILE:HG21	2:A:1679:HOH:O	2.08	0.54
1:C:152:LYS:HB3	1:C:191:LEU:HD22	1.90	0.54
1:D:60:GLN:HG3	2:D:6428:HOH:O	2.06	0.54
1:D:172:ARG:O	1:D:176:ILE:HG12	2.08	0.54
1:D:18:ILE:O	1:D:22:ILE:HG13	2.09	0.53
1:D:356:LEU:HD12	2:D:6414:HOH:O	2.08	0.53
1:A:7:LEU:HD23	1:A:11:GLN:HB3	1.90	0.53
1:A:115:LEU:HD22	2:A:1383:HOH:O	2.08	0.53
1:C:71:PRO:HG3	2:C:4629:HOH:O	2.07	0.53
1:D:242:LYS:HE2	1:D:352:ALA:CB	2.39	0.53
1:C:172:ARG:HB3	1:C:172:ARG:NH2	2.22	0.53
1:A:223:LEU:HD23	1:A:263:ALA:HB3	1.90	0.53
1:B:41:LYS:HE2	2:B:3614:HOH:O	2.08	0.53
1:B:29:ILE:HD12	2:B:3705:HOH:O	2.08	0.53
1:D:157:THR:HG23	2:D:6486:HOH:O	2.07	0.53
1:D:318:GLU:HG3	2:D:6927:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:O	1:A:274:GLN:HG2	2.08	0.53
1:B:76:VAL:HB	2:B:3529:HOH:O	2.09	0.53
1:D:139:LYS:HG3	2:D:6993:HOH:O	2.08	0.53
1:D:155:GLU:HA	2:D:6453:HOH:O	2.08	0.53
1:D:213:TYR:CE1	1:D:260:VAL:HG13	2.44	0.53
1:D:103:VAL:CG1	1:D:143:ASP:HB2	2.39	0.53
1:A:81:GLU:O	1:A:85:GLN:HG3	2.09	0.52
1:C:25:PRO:HD3	2:C:4891:HOH:O	2.08	0.52
1:A:329:LYS:HD2	2:A:1586:HOH:O	2.10	0.52
1:B:22:ILE:CG2	1:B:29:ILE:HD11	2.39	0.52
1:D:64:THR:HG21	2:D:7114:HOH:O	2.09	0.52
1:D:103:VAL:HG13	1:D:143:ASP:HB2	1.92	0.52
1:B:65:ALA:HB2	1:B:327:TYR:HE1	1.73	0.52
1:D:39[A]:ILE:HG12	2:D:7167:HOH:O	2.09	0.52
1:D:229[A]:LYS:HA	1:D:268:THR:O	2.08	0.52
1:D:242:LYS:HD3	2:D:6437:HOH:O	2.10	0.52
1:B:173:TYR:CE1	1:B:177:CYS:SG	3.02	0.52
1:C:93:PHE:N	1:C:94:PRO:HD2	2.24	0.52
1:C:113:VAL:HG12	2:C:5187:HOH:O	2.09	0.52
1:C:216:LEU:HD22	1:C:221:ILE:HG13	1.92	0.52
1:D:320:LEU:CD1	1:D:324:GLN:HE21	2.23	0.52
1:D:363:TYR:HE2	2:D:7242:HOH:O	1.92	0.52
1:C:127:LEU:O	1:C:130:LEU:HB2	2.10	0.52
1:D:284:ASN:ND2	1:D:340:GLY:HA2	2.24	0.52
1:A:208:VAL:O	1:A:212:VAL:HG23	2.10	0.52
1:A:316:LYS:HG2	1:A:317:LYS:H	1.75	0.52
1:B:78:LEU:O	1:B:106[A]:ILE:HD12	2.10	0.52
1:B:91:ARG:HD2	2:B:3412:HOH:O	2.09	0.52
1:B:78:LEU:O	1:B:106[B]:ILE:HD12	2.10	0.52
1:B:131:SER:HB3	2:B:4053:HOH:O	2.10	0.52
1:C:8:THR:HB	1:C:9:PRO:HD2	1.92	0.52
1:D:290:PRO:HB2	2:D:6503:HOH:O	2.11	0.51
1:A:229:LYS:HB3	1:A:229:LYS:HZ3	1.75	0.51
1:B:73:ILE:HB	2:B:4058:HOH:O	2.11	0.51
1:C:92:PRO:O	1:C:95:GLN:HB2	2.11	0.51
1:B:161:LEU:HA	2:B:3626:HOH:O	2.10	0.51
1:D:58:TYR:HE2	2:D:6854:HOH:O	1.94	0.51
1:C:320:LEU:HD13	2:C:4580:HOH:O	2.11	0.51
1:B:159:SER:HB2	2:B:3748:HOH:O	2.09	0.51
1:C:286:ILE:CG2	1:C:297:LEU:HD13	2.40	0.51
1:A:24:ALA:HB3	1:A:27:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.92	0.51
1:B:58:TYR:O	1:B:61:LEU:HB3	2.10	0.51
1:D:250:MET:HG2	2:D:6886:HOH:O	2.10	0.51
1:B:41:LYS:HE3	1:B:363:TYR:HB3	1.93	0.51
1:C:245:HIS:HA	1:C:248:ILE:HD12	1.92	0.51
1:D:355:SER:HA	1:D:358:ILE:HG12	1.92	0.51
1:A:98:LYS:HE3	2:A:1781:HOH:O	2.11	0.50
1:B:7:LEU:N	1:B:7:LEU:HD12	2.26	0.50
1:C:91:ARG:NH2	1:C:96:VAL:HA	2.26	0.50
1:B:176:ILE:HG12	2:B:3722:HOH:O	2.10	0.50
1:B:208:VAL:HG22	2:B:3515:HOH:O	2.12	0.50
2:B:5188:HOH:O	1:C:263:ALA:HB2	2.11	0.50
1:C:141:GLY:HA3	2:C:5198:HOH:O	2.11	0.50
1:C:292:LEU:HD12	1:C:293:LYS:N	2.26	0.50
1:B:42:ARG:HG3	2:B:3950:HOH:O	2.11	0.50
1:A:163:ILE:HD12	2:A:1794:HOH:O	2.11	0.50
1:C:333:ALA:HB2	2:C:4577:HOH:O	2.12	0.50
1:A:200:ARG:NH1	1:D:2:HIS:HA	2.27	0.50
1:A:250:MET:CE	1:A:289:CYS:SG	2.99	0.50
1:A:207:LYS:HE3	1:A:207:LYS:HA	1.94	0.50
1:C:311:LYS:HE2	2:C:4823:HOH:O	2.11	0.50
1:D:151:LEU:HB2	2:D:6879:HOH:O	2.12	0.50
1:B:357:PHE:HD1	1:B:357:PHE:N	2.06	0.49
1:A:51:THR:O	1:A:54:ASN:HB2	2.12	0.49
1:B:268:THR:HB	1:B:300:SER:HB2	1.94	0.49
1:C:274:GLN:HB3	1:C:278:GLU:HG3	1.94	0.49
1:B:24:ALA:HB3	1:B:27:LYS:HD2	1.93	0.49
1:C:318:GLU:HG2	2:C:5009:HOH:O	2.12	0.49
1:B:83:LEU:HD12	2:B:3369:HOH:O	2.11	0.49
1:C:30:LEU:HD23	1:C:76:VAL:HG13	1.95	0.49
1:A:310[B]:LEU:HA	2:A:1994:HOH:O	2.11	0.49
1:B:104:VAL:HB	1:B:142:ALA:HA	1.94	0.49
1:C:138:LYS:HA	1:C:142:ALA:O	2.12	0.49
1:D:27:LYS:HE3	2:D:7064:HOH:O	2.12	0.49
1:D:127:LEU:HD22	1:D:147:TRP:CH2	2.47	0.49
1:B:39:ILE:HD11	2:B:3374:HOH:O	2.13	0.49
1:C:62:LEU:HD13	2:C:4466:HOH:O	2.12	0.49
1:D:11:GLN:HG3	2:D:6497:HOH:O	2.12	0.49
1:D:313:TRP:HH2	2:D:7209:HOH:O	1.95	0.49
1:A:114:PRO:HA	1:A:122:THR:HG22	1.95	0.49
1:B:221:ILE:HB	2:B:3691:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7192:HOH:O	1:D:223:LEU:HD11	2.13	0.48
1:D:8:THR:HB	1:D:9:PRO:HD2	1.95	0.48
1:D:124:THR:HB	2:D:6632:HOH:O	2.12	0.48
1:B:103:VAL:HG23	1:B:144:PHE:CE2	2.47	0.48
1:B:168:ASN:HB2	2:B:3920:HOH:O	2.13	0.48
1:D:46:ILE:HG23	2:D:6661:HOH:O	2.12	0.48
1:D:242:LYS:HE2	1:D:352:ALA:HB2	1.94	0.48
1:A:319:ASN:N	1:A:319:ASN:HD22	2.12	0.48
1:B:183:VAL:HG23	2:B:3804:HOH:O	2.12	0.48
1:C:166:ASN:O	1:C:169:VAL:HG12	2.14	0.48
1:C:260:VAL:HG13	1:C:264:VAL:HG21	1.95	0.48
1:D:229[B]:LYS:HA	1:D:268:THR:O	2.12	0.48
1:B:277:GLU:O	1:B:281:ILE:HG13	2.14	0.48
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.94	0.48
1:B:133:ARG:HG3	2:B:3588:HOH:O	2.13	0.48
1:B:151:LEU:HD13	2:B:3467:HOH:O	2.13	0.48
1:B:310:LEU:HG	2:B:3992:HOH:O	2.13	0.48
1:D:324:GLN:O	1:D:328:VAL:HG23	2.14	0.48
1:A:119:ASN:OD1	1:B:4:HIS:NE2	2.47	0.48
1:A:39[B]:ILE:O	1:A:43[B]:LEU:HD23	2.13	0.48
1:D:260:VAL:HG11	2:D:6720:HOH:O	2.13	0.48
1:A:274:GLN:OE1	1:A:279:ALA:HA	2.14	0.48
1:B:9:PRO:HA	1:B:12:LYS:HE3	1.96	0.48
1:B:1:PRO:HG2	1:C:203:TYR:HE2	1.78	0.48
1:B:205:THR:O	1:B:209:LEU:HG	2.14	0.48
1:B:234:THR:HG22	1:B:235:PRO:O	2.14	0.48
1:C:138:LYS:HB2	1:C:182:ILE:HD11	1.94	0.48
1:A:245:HIS:HB3	2:A:1423:HOH:O	2.14	0.47
1:C:96:VAL:O	1:C:100:LYS:HG3	2.13	0.47
1:D:20:HIS:HE1	2:D:6638:HOH:O	1.95	0.47
1:A:155:GLU:HB2	2:A:1683:HOH:O	2.13	0.47
1:B:229[A]:LYS:HG3	1:B:268:THR:O	2.14	0.47
1:D:36:THR:HG23	1:D:55:ARG:NH1	2.28	0.47
1:D:191:LEU:HB3	1:D:193:ASP:OD1	2.14	0.47
1:D:321:LYS:HE3	2:D:6942:HOH:O	2.13	0.47
1:B:91:ARG:HH11	1:B:95:GLN:HG2	1.79	0.47
1:B:98:LYS:HB2	2:B:3594:HOH:O	2.12	0.47
1:B:184:PRO:HG2	1:B:226:THR:HG22	1.95	0.47
1:C:313:TRP:HA	1:C:319:ASN:ND2	2.28	0.47
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.49	0.47
1:B:244:SER:HB3	1:B:247:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HB2	2:C:4705:HOH:O	2.14	0.47
1:C:190:ILE:HB	1:C:231:ASN:CG	2.34	0.47
1:C:84:TYR:HB2	2:C:4776:HOH:O	2.14	0.47
1:C:190:ILE:HG13	2:C:4936:HOH:O	2.15	0.47
1:D:274:GLN:OE1	1:D:279:ALA:HA	2.15	0.47
1:B:78:LEU:HG	2:B:3369:HOH:O	2.14	0.47
1:D:242:LYS:HE3	1:D:358:ILE:HG13	1.95	0.47
1:A:310[A]:LEU:HA	2:A:1994:HOH:O	2.14	0.47
1:B:69:VAL:HG13	1:B:328:VAL:HG13	1.97	0.47
1:B:91:ARG:HA	2:B:3995:HOH:O	2.15	0.47
1:B:210:ALA:HB2	2:C:3441:HOH:O	2.15	0.47
1:D:191:LEU:HD13	2:D:7079:HOH:O	2.14	0.47
1:A:19:ALA:O	1:A:23:VAL:HG22	2.14	0.47
1:D:115:LEU:HD13	2:D:6972:HOH:O	2.15	0.47
1:D:136:GLN:HE22	1:D:139:LYS:HE2	1.79	0.47
1:D:34:GLU:HA	2:D:6454:HOH:O	2.14	0.46
1:A:285:ALA:HB3	2:A:1423:HOH:O	2.15	0.46
1:B:229[A]:LYS:HE2	1:B:270:LEU:HB3	1.97	0.46
1:C:133:ARG:HG3	2:C:4425:HOH:O	2.14	0.46
1:D:113:VAL:HG13	1:D:125:GLN:NE2	2.30	0.46
1:A:43[A]:LEU:HD12	1:A:48:THR:HB	1.98	0.46
1:A:170:LEU:HD22	1:A:186:VAL:HG13	1.96	0.46
1:A:314:GLY:N	1:A:319:ASN:OD1	2.47	0.46
1:D:182:ILE:HD12	2:D:6617:HOH:O	2.14	0.46
1:D:320:LEU:HD22	2:D:6747:HOH:O	2.14	0.46
1:A:82:THR:HA	1:A:85:GLN:OE1	2.16	0.46
1:A:229:LYS:CE	1:A:270:LEU:HD21	2.45	0.46
1:B:161:LEU:HD12	1:B:164:MET:HE2	1.96	0.46
1:B:198:LEU:HD11	1:B:233:VAL:HG12	1.96	0.46
1:C:229:LYS:HA	1:C:268:THR:O	2.16	0.46
1:D:13:LYS:HG2	1:D:17:ASP:OD1	2.15	0.46
1:D:58:TYR:HB2	2:D:7071:HOH:O	2.16	0.46
1:D:228[B]:LEU:HB3	1:D:267:VAL:HG22	1.98	0.46
1:D:240:THR:O	1:D:358:ILE:HG23	2.14	0.46
1:A:29:ILE:CD1	1:A:268:THR:HG21	2.45	0.46
1:B:192:PRO:HB2	2:B:3421:HOH:O	2.16	0.46
1:B:288:LYS:HB3	2:B:3875:HOH:O	2.16	0.46
1:C:39:ILE:HD11	1:C:59:ARG:NH1	2.31	0.46
1:B:70:ASN:HA	2:B:3694:HOH:O	2.16	0.46
1:D:198:LEU:HD23	1:D:199:LYS:HZ2	1.79	0.46
1:A:34:GLU:HB2	1:A:39[B]:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:O	1:A:227:LEU:HD12	2.16	0.46
1:B:6:ALA:HB3	1:B:7:LEU:HD12	1.98	0.46
1:B:286:ILE:HG22	1:B:297:LEU:HD13	1.96	0.46
1:C:153:ILE:HD12	2:C:4505:HOH:O	2.14	0.46
1:B:21:ARG:HD2	2:B:3890:HOH:O	2.15	0.46
1:C:69:VAL:HG11	1:C:328:VAL:HA	1.98	0.46
1:C:187:ALA:CB	1:C:229:LYS:HB3	2.37	0.46
1:C:191:LEU:HD23	2:C:4489:HOH:O	2.16	0.46
1:A:27:LYS:HB3	1:A:74:GLY:HA3	1.98	0.46
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.51	0.46
1:A:153:ILE:HD11	2:A:1679:HOH:O	2.15	0.46
1:B:15:LEU:HA	2:B:3804:HOH:O	2.15	0.46
1:B:305:LEU:HD22	2:B:3712:HOH:O	2.15	0.46
1:C:269:PHE:HB3	2:C:4487:HOH:O	2.15	0.46
1:A:86:LYS:HA	1:A:92:PRO:HA	1.98	0.46
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.46
1:A:257:ARG:O	1:D:262:PRO:HD2	2.15	0.46
1:B:198:LEU:CD1	1:B:233:VAL:HG12	2.46	0.46
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.98	0.45
1:B:252:THR:HA	2:B:3513:HOH:O	2.16	0.45
1:C:92:PRO:HD2	1:C:95:GLN:HG3	1.97	0.45
1:C:313:TRP:HA	1:C:319:ASN:HD22	1.81	0.45
1:D:78:LEU:HD22	2:D:6652:HOH:O	2.15	0.45
1:D:86:LYS:HA	1:D:92:PRO:HA	1.97	0.45
1:B:63:LEU:HD13	1:B:63:LEU:HA	1.78	0.45
1:C:78:LEU:HD13	1:C:79:PHE:O	2.17	0.45
1:B:59:ARG:HB3	2:B:3551:HOH:O	2.15	0.45
1:A:42[A]:ARG:HG3	1:A:42[A]:ARG:HH11	1.82	0.45
1:C:172:ARG:HB3	1:C:172:ARG:HH21	1.81	0.45
1:A:39[A]:ILE:HD12	1:A:43[A]:LEU:CD2	2.46	0.45
1:A:116:ALA:HB2	1:B:175:SER:OG	2.17	0.45
1:B:49:GLU:HB3	2:B:3834:HOH:O	2.16	0.45
1:C:163:ILE:HG12	2:C:5028:HOH:O	2.16	0.45
1:D:163:ILE:HD12	1:D:208:VAL:HG22	1.96	0.45
1:D:334:ASN:HA	1:D:337:ALA:HB3	1.98	0.45
1:A:72:CYS:SG	1:A:332:LEU:HD23	2.57	0.45
1:B:43:LEU:HD13	1:B:49:GLU:O	2.16	0.45
1:A:311[A]:LYS:HB3	2:A:1611:HOH:O	2.17	0.45
1:C:42:ARG:HD2	1:C:303:ARG:HH12	1.82	0.45
1:C:222:TYR:CZ	1:C:224:GLU:HB2	2.52	0.45
1:A:351:ALA:HB3	2:A:1861:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:THR:HB	1:C:235:PRO:HD2	1.99	0.45
1:C:261:PRO:O	1:C:264:VAL:HG23	2.17	0.45
1:D:58:TYR:HA	2:D:7170:HOH:O	2.15	0.45
1:A:39[A]:ILE:HD13	1:A:42[A]:ARG:HB2	1.99	0.45
1:B:200:ARG:HD3	2:B:3607:HOH:O	2.17	0.45
1:D:178:GLN:HE22	1:D:222:TYR:HB3	1.82	0.45
1:C:185:ILE:HG12	1:C:227:LEU:HB2	1.98	0.44
1:A:185:ILE:HG21	1:A:229:LYS:CD	2.47	0.44
1:A:287:ASN:ND2	1:A:338:CYS:HA	2.32	0.44
1:B:16:SER:O	1:B:20:HIS:ND1	2.51	0.44
1:A:131:SER:O	1:A:180:ASN:ND2	2.51	0.44
1:C:9:PRO:HG2	1:C:10:GLU:OE1	2.16	0.44
1:A:311[B]:LYS:HB3	2:A:1611:HOH:O	2.18	0.44
1:B:292:LEU:HG	2:B:3609:HOH:O	2.17	0.44
1:D:320:LEU:C	1:D:320:LEU:HD12	2.38	0.44
1:B:310:LEU:HD13	2:B:3835:HOH:O	2.16	0.44
1:C:36:THR:HG23	2:C:4954:HOH:O	2.17	0.44
1:C:195:ASP:HB3	2:C:5058:HOH:O	2.17	0.44
1:C:228:LEU:HG	1:C:230:PRO:HD3	2.00	0.44
2:C:4569:HOH:O	1:D:176:ILE:HD13	2.16	0.44
1:D:295:TRP:O	1:D:297:LEU:HD22	2.16	0.44
1:A:18:ILE:HD11	2:A:1769:HOH:O	2.17	0.44
1:D:77:ILE:HG21	1:D:146:LYS:HG2	1.99	0.44
1:A:41[A]:LYS:HG2	2:A:1982:HOH:O	2.18	0.44
1:A:42[A]:ARG:HG3	1:A:42[A]:ARG:NH1	2.32	0.44
1:A:110:LYS:HG2	2:A:1757:HOH:O	2.18	0.44
1:B:38:SER:HB3	2:B:3799:HOH:O	2.18	0.44
1:B:279:ALA:HB1	1:B:301:TYR:CZ	2.53	0.44
1:C:110:LYS:HB2	1:C:125:GLN:HG3	2.00	0.44
1:C:190:ILE:HG23	2:C:4936:HOH:O	2.17	0.44
1:A:17:ASP:HB3	1:A:21:ARG:NH2	2.32	0.43
1:A:41[A]:LYS:HG3	2:A:1691:HOH:O	2.16	0.43
1:A:213:TYR:HB3	2:A:2054:HOH:O	2.17	0.43
1:B:209:LEU:HD11	2:B:4019:HOH:O	2.18	0.43
1:B:288:LYS:HG3	2:B:3730:HOH:O	2.18	0.43
1:C:353:SER:HB3	2:C:4996:HOH:O	2.17	0.43
1:D:155:GLU:HG2	1:D:156:HIS:N	2.33	0.43
1:D:248:ILE:HG23	2:D:6906:HOH:O	2.17	0.43
1:A:41[B]:LYS:HG2	2:A:1982:HOH:O	2.18	0.43
1:A:41[B]:LYS:HG3	2:A:1691:HOH:O	2.16	0.43
1:A:121:GLU:HB3	2:A:1382:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CD2	1:A:216:LEU:HD12	2.53	0.43
1:C:78:LEU:HB3	2:C:4374:HOH:O	2.17	0.43
1:D:213:TYR:HB3	2:D:6533:HOH:O	2.18	0.43
1:D:330:ARG:HA	1:D:330:ARG:HD3	1.62	0.43
1:A:121:GLU:OE1	1:A:158:PRO:HA	2.18	0.43
1:B:1:PRO:HG2	1:C:203:TYR:CE2	2.53	0.43
1:B:86:LYS:HE2	1:B:92:PRO:HG3	2.00	0.43
1:B:294:PRO:HG3	2:B:3575:HOH:O	2.19	0.43
1:B:326:GLU:HA	1:B:329:LYS:HE2	2.00	0.43
1:C:154:GLY:HA3	2:C:4728:HOH:O	2.17	0.43
1:D:141:GLY:HA2	2:D:6501:HOH:O	2.18	0.43
1:A:319:ASN:N	1:A:319:ASN:ND2	2.66	0.43
1:C:69:VAL:HG11	1:C:331:ALA:HB3	1.99	0.43
1:C:84:TYR:HE1	1:C:140:ASP:OD2	2.01	0.43
1:C:91:ARG:HH22	1:C:96:VAL:HA	1.84	0.43
1:A:27:LYS:HB3	1:A:74:GLY:CA	2.49	0.43
1:D:301:TYR:HB3	1:D:304:ALA:HB3	2.01	0.43
1:C:193:ASP:O	1:C:196:HIS:HE1	2.01	0.43
1:C:276:GLU:HB3	1:C:330:ARG:CZ	2.48	0.43
1:A:18:ILE:HG13	1:A:21:ARG:NH1	2.34	0.43
1:B:164:MET:HG2	2:B:4009:HOH:O	2.18	0.43
1:B:233:VAL:HG11	1:B:251:ALA:HB1	2.00	0.43
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.77	0.43
1:D:184:PRO:HG2	2:D:6955:HOH:O	2.19	0.43
1:D:205:THR:O	1:D:209:LEU:HG	2.18	0.43
1:D:360:ASN:OD1	1:D:361:HIS:N	2.52	0.43
1:A:160:ALA:HB1	2:A:1747:HOH:O	2.19	0.43
1:A:35:SER:HA	1:A:79:PHE:CE2	2.54	0.42
2:B:5201:HOH:O	1:C:292:LEU:HD13	2.18	0.42
1:C:77:ILE:HG12	1:C:144:PHE:HE1	1.84	0.42
1:D:289:CYS:O	1:D:291:LEU:N	2.52	0.42
1:A:139:LYS:HA	2:A:1496:HOH:O	2.18	0.42
1:C:23:VAL:HG21	1:C:265:THR:HG22	2.01	0.42
1:D:101:GLY:HA2	2:D:6581:HOH:O	2.17	0.42
1:D:198:LEU:HD23	1:D:199:LYS:HZ1	1.81	0.42
1:B:18:ILE:HD11	2:B:3816:HOH:O	2.20	0.42
1:B:159:SER:HB3	2:B:3779:HOH:O	2.17	0.42
1:C:67:ASP:HB3	1:C:70:ASN:ND2	2.34	0.42
1:D:69:VAL:HG22	1:D:328:VAL:HG13	2.02	0.42
1:D:297:LEU:HD22	1:D:297:LEU:N	2.33	0.42
1:A:293:LYS:HB2	1:A:293:LYS:HE2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LYS:HE2	2:B:3625:HOH:O	2.19	0.42
1:B:182:ILE:O	1:B:184:PRO:HD3	2.19	0.42
1:D:21:ARG:HB2	2:D:7100:HOH:O	2.20	0.42
1:D:161:LEU:HA	2:D:7252:HOH:O	2.20	0.42
1:D:114:PRO:HB3	2:D:6496:HOH:O	2.20	0.42
1:A:48:THR:HG22	1:A:54:ASN:HD22	1.84	0.42
1:B:160:ALA:O	1:B:164:MET:HB2	2.19	0.42
1:B:324:GLN:O	1:B:328:VAL:HG23	2.19	0.42
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.93	0.42
1:A:27:LYS:HG2	1:A:71:PRO:O	2.20	0.42
1:A:293:LYS:HD2	1:A:297:LEU:HD12	2.01	0.42
1:B:95:GLN:O	1:B:98:LYS:HB3	2.20	0.42
1:C:190:ILE:HG21	2:C:4583:HOH:O	2.20	0.42
1:D:8:THR:O	1:D:12:LYS:HG3	2.20	0.42
1:D:127:LEU:HD13	1:D:130:LEU:HD22	2.01	0.42
1:A:34:GLU:HB2	1:A:39[A]:ILE:HG12	2.02	0.42
1:A:234:THR:HB	1:A:235:PRO:HD2	2.02	0.42
1:B:92:PRO:O	1:B:96:VAL:HG23	2.19	0.42
2:B:4957:HOH:O	1:C:291:LEU:HD21	2.19	0.42
1:D:12:LYS:HE2	2:D:6960:HOH:O	2.19	0.42
1:D:54:ASN:HB3	2:D:7209:HOH:O	2.20	0.42
1:A:86:LYS:HB2	2:A:1960:HOH:O	2.19	0.42
1:A:161:LEU:HD22	1:B:220:HIS:CE1	2.55	0.42
1:B:226:THR:HB	2:B:3916:HOH:O	2.20	0.42
1:B:330:ARG:HG2	2:B:3884:HOH:O	2.18	0.42
1:A:39[B]:ILE:HG23	1:A:43[B]:LEU:HD23	2.02	0.42
1:D:115:LEU:HD12	2:D:6938:HOH:O	2.20	0.42
1:A:246:GLU:HB2	2:A:1836:HOH:O	2.19	0.41
1:B:29:ILE:O	1:B:300:SER:HA	2.19	0.41
1:B:256:LEU:HD11	1:B:267:VAL:HG11	2.02	0.41
1:C:95:GLN:HG2	2:C:5133:HOH:O	2.19	0.41
1:C:185:ILE:HD12	2:C:4860:HOH:O	2.20	0.41
1:A:151:LEU:HD12	1:A:158:PRO:CB	2.49	0.41
1:C:292:LEU:HG	1:C:294:PRO:HD3	2.02	0.41
1:D:11:GLN:HA	2:D:7067:HOH:O	2.21	0.41
1:D:113:VAL:HA	2:D:6893:HOH:O	2.19	0.41
1:D:289:CYS:HA	1:D:290:PRO:HD2	1.83	0.41
2:A:1454:HOH:O	1:D:2:HIS:CE1	2.73	0.41
1:C:237:HIS:O	1:C:237:HIS:ND1	2.53	0.41
1:D:181:GLY:HA3	2:D:6907:HOH:O	2.19	0.41
1:D:213:TYR:HD2	1:D:216:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:O	1:A:59:ARG:HD3	2.20	0.41
1:A:66:ASP:HB2	2:A:1533:HOH:O	2.20	0.41
1:D:42:ARG:HG3	1:D:42:ARG:NH1	2.34	0.41
1:D:317:LYS:HD3	2:D:7196:HOH:O	2.20	0.41
1:B:104:VAL:HA	2:B:3529:HOH:O	2.21	0.41
1:B:239:CYS:SG	1:B:240:THR:N	2.93	0.41
1:C:59:ARG:HD2	1:C:59:ARG:N	2.36	0.41
1:D:114:PRO:HA	1:D:122:THR:HG22	2.01	0.41
1:A:67:ASP:HA	1:A:70:ASN:OD1	2.20	0.41
1:A:356:LEU:HD22	1:A:356:LEU:HA	1.83	0.41
1:B:344:PRO:HG3	2:B:3769:HOH:O	2.20	0.41
1:A:146[B]:LYS:HZ2	1:A:229:LYS:HE3	1.82	0.41
1:B:18:ILE:HB	2:B:3804:HOH:O	2.20	0.41
1:C:240:THR:HG22	1:C:357:PHE:O	2.20	0.41
1:D:7:LEU:HG	2:D:6998:HOH:O	2.21	0.41
1:B:18:ILE:HD12	2:B:3804:HOH:O	2.20	0.41
1:B:27:LYS:HA	1:B:72:CYS:O	2.21	0.41
1:B:256:LEU:HD22	1:B:260:VAL:HG21	2.03	0.41
1:B:271:SER:HB3	1:B:304:ALA:HB2	2.02	0.41
1:B:274:GLN:OE1	1:B:282:ASN:ND2	2.53	0.41
1:B:280:SER:HB3	1:B:330:ARG:HH12	1.85	0.41
1:C:106:ILE:O	1:C:145[B]:ALA:HA	2.20	0.41
1:D:14:GLU:HG3	2:D:6866:HOH:O	2.21	0.41
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.38	0.41
1:B:127:LEU:HD13	1:B:172:ARG:HD2	2.02	0.41
1:C:49:GLU:HG2	2:C:4711:HOH:O	2.21	0.41
1:C:132:GLU:HB3	2:C:4680:HOH:O	2.20	0.41
1:A:29:ILE:HD12	1:A:268:THR:HG21	2.03	0.40
1:A:43[A]:LEU:HD11	1:A:313:TRP:HZ3	1.85	0.40
1:A:316:LYS:HG2	1:A:317:LYS:N	2.36	0.40
1:B:316:LYS:HE2	1:B:316:LYS:HB3	1.91	0.40
1:C:356:LEU:HB3	2:C:4742:HOH:O	2.20	0.40
1:C:358:ILE:O	1:C:358:ILE:HG22	2.21	0.40
1:D:207:LYS:HB2	2:D:6844:HOH:O	2.21	0.40
1:D:320:LEU:HG	1:D:321:LYS:N	2.36	0.40
1:A:317:LYS:HB3	2:A:1470:HOH:O	2.21	0.40
1:B:273:GLY:HA2	1:B:303:ARG:NH2	2.36	0.40
1:C:70:ASN:HB2	1:C:71:PRO:HD3	2.03	0.40
1:C:72:CYS:SG	1:C:332:LEU:HD23	2.61	0.40
1:C:113:VAL:HG11	2:C:6792:HOH:O	2.21	0.40
1:C:192:PRO:O	1:C:236:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:O	1:C:212:VAL:HG23	2.22	0.40
1:D:136:GLN:O	1:D:140:ASP:HB2	2.20	0.40
1:B:10:GLU:HG3	2:B:3649:HOH:O	2.20	0.40
1:D:320:LEU:HD11	1:D:324:GLN:HE21	1.86	0.40
1:A:1:PRO:HD3	2:D:1455:HOH:O	2.21	0.40
1:A:298:THR:HG23	1:A:338:CYS:CB	2.51	0.40
1:C:202:GLN:HB2	1:C:233:VAL:HG11	2.04	0.40
1:C:249:ALA:HB1	1:C:286:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	376/363 (104%)	322 (86%)	43 (11%)	11 (3%)	4 2
1	B	372/363 (102%)	327 (88%)	39 (10%)	6 (2%)	9 7
1	C	364/363 (100%)	326 (90%)	33 (9%)	5 (1%)	11 8
1	D	367/363 (101%)	327 (89%)	34 (9%)	6 (2%)	9 7
All	All	1479/1452 (102%)	1302 (88%)	149 (10%)	28 (2%)	8 5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	PHE
1	B	3	SER
1	B	307	ALA
1	B	355	SER
1	A	89	ASP
1	A	362	ALA
1	D	3	SER

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Mol	Chain	Res	Type
1	D	290	PRO
1	A	307	ALA
1	A	321	LYS
1	B	349	GLY
1	C	344	PRO
1	D	66	ASP
1	D	238	ALA
1	A	347	GLN
1	C	347	GLN
1	A	304	ALA
1	A	360	ASN
1	C	64	THR
1	A	188	PRO
1	B	23	VAL
1	A	315	GLY
1	A	235	PRO
1	C	46	ILE
1	C	23	VAL
1	B	358	ILE
1	D	230[A]	PRO
1	D	230[B]	PRO

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	302/290 (104%)	283 (94%)	19 (6%)	18 20
1	B	300/290 (103%)	283 (94%)	17 (6%)	20 24
1	C	292/290 (101%)	273 (94%)	19 (6%)	17 19
1	D	295/290 (102%)	271 (92%)	24 (8%)	11 12
All	All	1189/1160 (102%)	1110 (93%)	79 (7%)	16 19

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	39[A]	ILE
1	A	39[B]	ILE
1	A	51	THR
1	A	56	ARG
1	A	59	ARG
1	A	80	HIS
1	A	82	THR
1	A	91	ARG
1	A	98	LYS
1	A	173	TYR
1	A	207	LYS
1	A	242	LYS
1	A	295	TRP
1	A	320	LEU
1	A	325	GLU
1	A	327	TYR
1	A	356	LEU
1	A	357	PHE
1	B	59	ARG
1	B	66	ASP
1	B	67	ASP
1	B	148	ARG
1	B	157	THR
1	B	165	GLU
1	B	172	ARG
1	B	173	TYR
1	B	200	ARG
1	B	240	THR
1	B	295	TRP
1	B	311	LYS
1	B	327	TYR
1	B	330	ARG
1	B	354	GLU
1	B	357	PHE
1	B	361	HIS
1	C	4	HIS
1	C	41	LYS
1	C	48	THR
1	C	59	ARG
1	C	66	ASP
1	C	67	ASP
1	C	82	THR

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Mol	Chain	Res	Type
1	C	140	ASP
1	C	150	VAL
1	C	173	TYR
1	C	183	VAL
1	C	193	ASP
1	C	198	LEU
1	C	200	ARG
1	C	226	THR
1	C	227	LEU
1	C	295	TRP
1	C	318	GLU
1	C	319	ASN
1	D	33	ASP
1	D	49	GLU
1	D	51	THR
1	D	59	ARG
1	D	61	LEU
1	D	77	ILE
1	D	78	LEU
1	D	109	ASP
1	D	110	LYS
1	D	131	SER
1	D	140	ASP
1	D	146	LYS
1	D	155	GLU
1	D	173	TYR
1	D	237	HIS
1	D	270	LEU
1	D	271	SER
1	D	293	LYS
1	D	295	TRP
1	D	316	LYS
1	D	320	LEU
1	D	343	THR
1	D	345	SER
1	D	358	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	GLN

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Mol	Chain	Res	Type
1	A	287	ASN
1	B	2	HIS
1	B	95	GLN
1	B	136	GLN
1	B	324	GLN
1	B	334	ASN
1	C	4	HIS
1	C	156	HIS
1	C	178	GLN
1	C	179	GLN
1	C	306	GLN
1	C	339	GLN
1	C	361	HIS
1	D	2	HIS
1	D	20	HIS
1	D	125	GLN
1	D	196	HIS
1	D	202	GLN
1	D	241	GLN
1	D	284	ASN
1	D	306	GLN
1	D	324	GLN
1	D	361	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	363/363 (100%)	-0.29	11 (3%)	50	48	2, 3, 21, 43	0
1	B	363/363 (100%)	-0.35	8 (2%)	62	59	2, 3, 20, 41	0
1	C	363/363 (100%)	-0.36	8 (2%)	62	59	2, 3, 14, 30	0
1	D	363/363 (100%)	-0.40	2 (0%)	89	88	2, 3, 15, 26	0
All	All	1452/1452 (100%)	-0.35	29 (1%)	65	63	2, 3, 17, 43	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	10.2
1	A	355	SER	5.6
1	C	351	ALA	5.2
1	A	358	ILE	4.8
1	B	361	HIS	4.7
1	C	348	ALA	4.6
1	B	356	LEU	4.3
1	C	349	GLY	4.2
1	A	357	PHE	4.1
1	C	344	PRO	3.9
1	C	350	ALA	3.6
1	B	349	GLY	3.3
1	B	348	ALA	3.3
1	B	353	SER	3.2
1	D	352	ALA	3.2
1	A	347	GLN	3.2
1	A	359	SER	3.1
1	B	359	SER	2.9
1	A	40	ALA	2.9
1	B	363	TYR	2.8
1	D	345	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	353	SER	2.5
1	A	348	ALA	2.4
1	A	314	GLY	2.2
1	C	347	GLN	2.2
1	C	354	GLU	2.2
1	B	360	ASN	2.1
1	C	346	GLY	2.0
1	A	363	TYR	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 monosaccharides 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.