Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 10:30 AM JST

PDB ID	:	5Z16
Title	:	A novel dimeric isocitrate dehydrogenase from Acinetobacter baumannii
Authors	:	Song, P.; Huang, S.P.; Wang, P.; Zhu, G.P.
Deposited on	:	2017-12-25
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

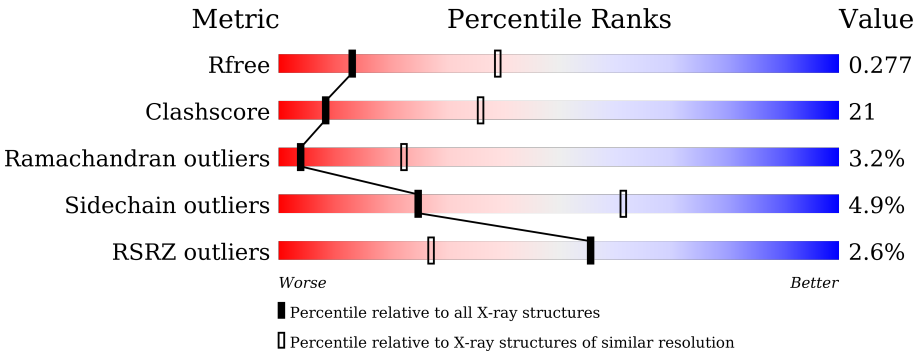
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	751	5% 58% 33% 5% • •
1	B	751	74% 23% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11788 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.

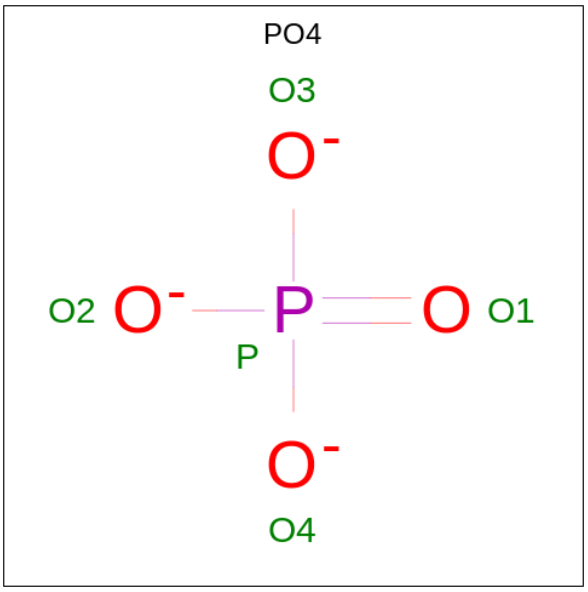
- Molecule 1 is a protein called Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5666	3571	969	1091	35			
1	B	739	Total	C	N	O	S	0	0	0
			5741	3626	978	1102	35			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5VCI0
A	-4	HIS	-	expression tag	UNP V5VCI0
A	-3	HIS	-	expression tag	UNP V5VCI0
A	-2	HIS	-	expression tag	UNP V5VCI0
A	-1	HIS	-	expression tag	UNP V5VCI0
A	0	HIS	-	expression tag	UNP V5VCI0
A	629	THR	ALA	conflict	UNP V5VCI0
B	-5	HIS	-	expression tag	UNP V5VCI0
B	-4	HIS	-	expression tag	UNP V5VCI0
B	-3	HIS	-	expression tag	UNP V5VCI0
B	-2	HIS	-	expression tag	UNP V5VCI0
B	-1	HIS	-	expression tag	UNP V5VCI0
B	0	HIS	-	expression tag	UNP V5VCI0
B	629	THR	ALA	conflict	UNP V5VCI0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

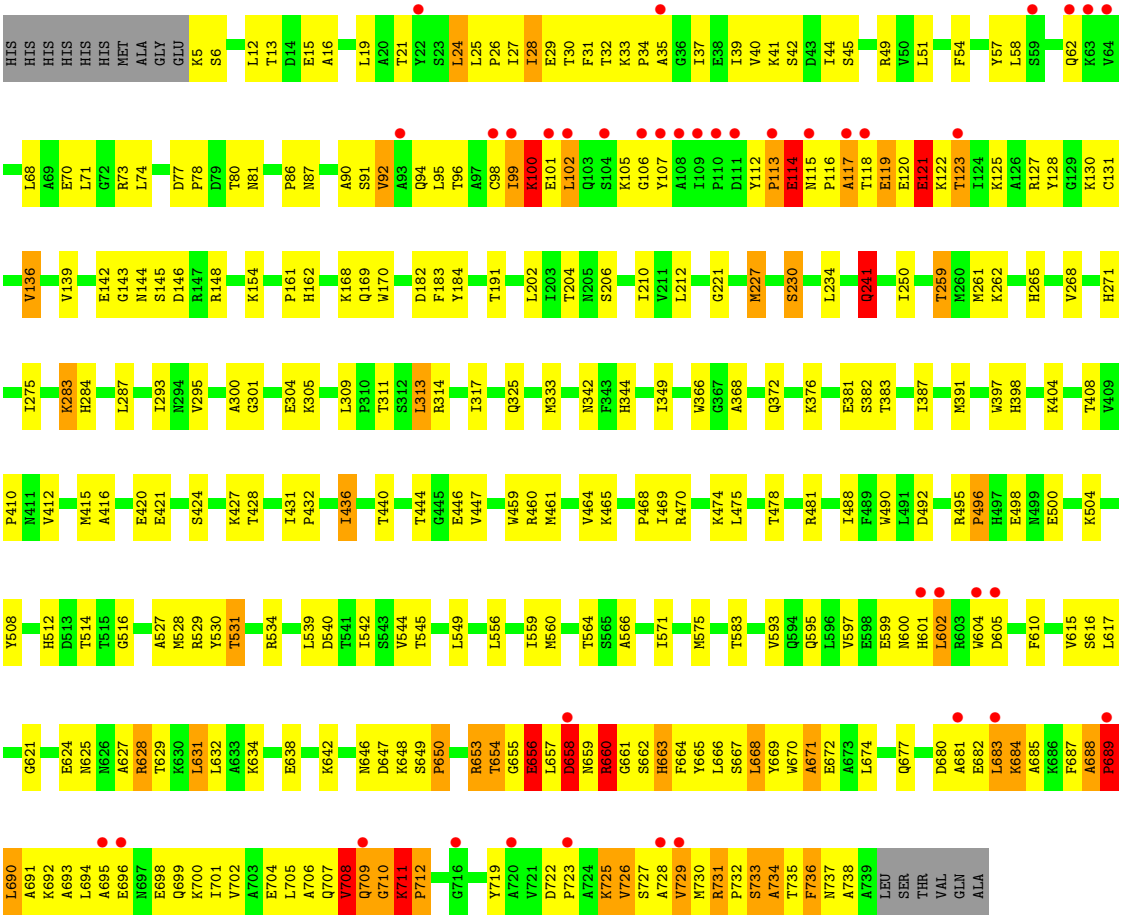
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	201	Total O 201 201	0	0
4	B	168	Total O 168 168	0	0

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.

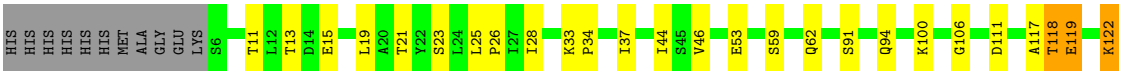
• Molecule 1: Isocitrate dehydrogenase

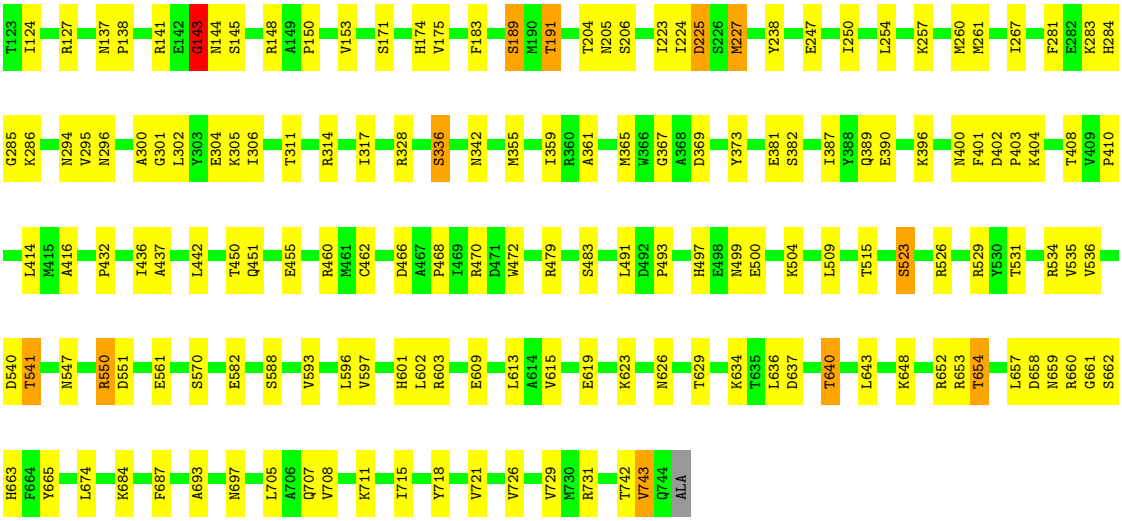
Chain A:



• Molecule 1: Isocitrate dehydrogenase

Chain B:




T123 I124 R127 N137 P138 R141 E142 G143 N144 S145 R148 A149 P150 V153 S171 H174 V175 F183 S189 M190 T191 T204 N205 S206 I223 I224 D225 S226 M227 Y238 E247 I250 L254 K257 M260 M261 I267 F281 E282 K283 H284
G285 K286 N294 V295 N296 A300 G301 L302 Y303 E304 K305 I306 T311 R314 I317 R328 S336 N342 M355 I359 R360 A361 M365 W366 G367 A368 D369 Y373 E381 S382 I387 Y388 Q389 E390 K396 N400 F401 D402 P403 K404 T408 V409 P410
L414 M415 A416 P432 I436 A437 L442 T450 Q451 E455 R460 M461 C462 D466 A467 P468 I469 R470 D471 W472 R479 S483 L491 D492 P493 H497 E498 N499 E500 K504 L509 T515 S523 R526 R529 Y530 T531 R534 V535 V536
D540 T541 N547 R550 D551 E561 S570 E582 S588 V593 L596 V597 H601 L602 R603 E609 L613 A614 V615 E619 K623 N626 T629 K634 T635 L636 D637 T640 L643 K648 R652 R653 T654 L657 D658 N659 R660 G661 S662
H663 F664 Y665 L674 K684 F687 A693 N697 L705 A706 Q707 V708 K711 I715 Y718 V721 V726 V729 M730 R731 T742 V743 Q744 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.16Å 137.16Å 238.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 3.00 48.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-3.00) 100.0 (48.54-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.276 0.209 , 0.277	Depositor DCC
R_{free} test set	2267 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11788	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	0.53	0/5773	0.82	17/7810 (0.2%)
1	B	0.48	0/5855	0.66	1/7923 (0.0%)
All	All	0.51	0/11628	0.74	18/15733 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	722	ASP	C-N-CD	-12.32	93.48	120.60
1	A	102	LEU	CA-CB-CG	9.56	137.28	115.30
1	A	683	LEU	CA-CB-CG	-8.43	95.91	115.30
1	A	689	PRO	N-CA-C	-7.31	93.08	112.10
1	A	709	GLN	N-CA-C	7.31	130.74	111.00
1	A	689	PRO	CA-C-N	-7.13	101.52	117.20
1	A	102	LEU	CB-CG-CD2	7.08	123.03	111.00
1	A	660	ARG	CB-CG-CD	7.07	129.98	111.60
1	A	668	LEU	CA-CB-CG	6.93	131.25	115.30
1	A	710	GLY	N-CA-C	-6.72	96.30	113.10
1	A	119	GLU	N-CA-C	6.61	128.86	111.00
1	A	24	LEU	CA-CB-CG	5.55	128.08	115.30
1	B	143	GLY	N-CA-C	5.26	126.26	113.10
1	A	241	GLN	CA-CB-CG	-5.23	101.89	113.40
1	A	99	ILE	N-CA-C	-5.23	96.89	111.00
1	A	660	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	711	LYS	C-N-CA	-5.08	100.65	122.00
1	A	666	LEU	CA-CB-CG	5.01	126.83	115.30

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	5666	0	5620	356	0
1	B	5741	0	5699	120	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	201	0	0	22	0
4	B	168	0	0	21	0
All	All	11788	0	11319	474	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 21.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:CD2	1:A:663:HIS:ND1	1.81	1.43
1:A:24:LEU:HD23	1:A:663:HIS:ND1	1.14	1.40
1:A:96:THR:HA	1:A:99:ILE:CG2	1.56	1.35
1:A:688:ALA:C	1:A:690:LEU:H	1.04	1.35
1:A:96:THR:O	1:A:100:LYS:HD2	1.25	1.31
1:A:731:ARG:HG3	1:A:736:PHE:CE1	1.66	1.29
1:A:725:LYS:CE	1:A:726:VAL:HG13	1.63	1.28
1:A:659:ASN:O	1:A:663:HIS:CB	1.83	1.24
1:A:659:ASN:O	1:A:663:HIS:HB2	1.33	1.24
1:A:96:THR:CA	1:A:99:ILE:HG22	1.67	1.23
1:A:24:LEU:HD23	1:A:663:HIS:CE1	1.76	1.21
1:A:24:LEU:HD11	1:A:659:ASN:OD1	1.42	1.20
1:A:96:THR:O	1:A:100:LYS:CD	1.91	1.18
1:A:688:ALA:C	1:A:690:LEU:N	1.83	1.16
1:A:725:LYS:HE2	1:A:726:VAL:HG13	1.15	1.15
1:A:705:LEU:HA	1:A:708:VAL:HG13	1.35	1.07
1:A:725:LYS:HE2	1:A:726:VAL:CG1	1.85	1.06
1:A:729:VAL:HG13	1:A:730:MET:H	1.18	1.06
1:A:101:GLU:OE1	1:A:719:TYR:HB2	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:CG	1:A:736:PHE:HE1	1.70	1.04
1:A:24:LEU:HD23	1:A:663:HIS:CG	1.93	1.03
1:A:96:THR:HA	1:A:99:ILE:HG22	1.04	1.02
1:A:24:LEU:CD2	1:A:663:HIS:CG	2.43	1.01
1:A:729:VAL:O	1:A:732:PRO:HD3	1.60	1.00
1:A:657:LEU:O	1:A:658:ASP:O	1.79	0.99
1:B:117:ALA:O	1:B:118:THR:HB	1.61	0.99
1:A:729:VAL:HG13	1:A:730:MET:N	1.73	0.99
1:A:725:LYS:NZ	1:A:726:VAL:HG13	1.80	0.97
1:A:687:PHE:C	1:A:689:PRO:HD2	1.84	0.97
1:A:729:VAL:CG1	1:A:730:MET:H	1.77	0.96
1:A:655:GLY:H	1:A:656:GLU:HB3	1.31	0.96
1:B:254:LEU:H	1:B:342:ASN:HD21	1.13	0.94
1:A:659:ASN:O	1:A:663:HIS:HB3	1.68	0.94
1:A:101:GLU:CD	1:A:719:TYR:HB2	1.88	0.93
1:A:101:GLU:OE1	1:A:719:TYR:CD2	2.21	0.93
1:A:101:GLU:OE1	1:A:719:TYR:HD2	1.52	0.91
1:A:24:LEU:HD21	1:A:663:HIS:HA	1.52	0.91
1:A:96:THR:HA	1:A:99:ILE:HG21	1.52	0.91
1:B:534:ARG:NH2	1:B:540:ASP:O	2.04	0.90
1:A:24:LEU:CD1	1:A:659:ASN:OD1	2.21	0.89
1:A:25:LEU:HD23	1:A:41:LYS:HE3	1.55	0.89
1:A:695:ALA:HA	1:A:698:GLU:HB3	1.54	0.87
1:A:101:GLU:OE1	1:A:719:TYR:CB	2.23	0.86
1:A:24:LEU:HD21	1:A:663:HIS:CB	2.06	0.86
1:A:24:LEU:HD21	1:A:663:HIS:CA	2.05	0.85
1:A:688:ALA:N	1:A:689:PRO:CD	2.38	0.85
1:A:628:ARG:HD3	1:A:683:LEU:HD11	1.59	0.84
1:A:99:ILE:CD1	4:A:954:HOH:O	2.26	0.84
1:A:705:LEU:CA	1:A:708:VAL:HG13	2.07	0.84
1:A:631:LEU:HD12	1:A:632:LEU:H	1.43	0.83
1:A:96:THR:C	1:A:99:ILE:HG22	1.97	0.83
1:A:115:ASN:N	1:A:116:PRO:HD3	1.93	0.82
1:A:731:ARG:O	4:A:901:HOH:O	1.95	0.82
1:A:564:THR:HG22	1:A:566:ALA:H	1.45	0.82
1:A:24:LEU:HD21	1:A:663:HIS:CG	2.13	0.81
1:B:19:LEU:HD13	1:B:596:LEU:HD22	1.61	0.81
1:A:655:GLY:N	1:A:656:GLU:HB3	1.95	0.81
1:A:688:ALA:O	1:A:690:LEU:N	2.14	0.81
1:A:704:GLU:OE1	1:A:733:SER:OG	1.97	0.81
1:A:725:LYS:CE	1:A:726:VAL:CG1	2.50	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:H	1:A:464:VAL:HG22	1.46	0.79
1:A:731:ARG:HG3	1:A:736:PHE:HE1	0.74	0.79
1:A:631:LEU:HD21	1:A:683:LEU:HD13	1.67	0.77
1:B:117:ALA:O	1:B:118:THR:CB	2.33	0.77
1:A:725:LYS:HD3	1:A:725:LYS:N	2.00	0.77
1:A:118:THR:N	1:A:121:GLU:OE2	2.18	0.76
1:A:96:THR:CA	1:A:99:ILE:CG2	2.41	0.76
1:A:687:PHE:C	1:A:689:PRO:CD	2.54	0.75
1:A:658:ASP:HB2	1:A:660:ARG:NH2	2.02	0.74
1:B:119:GLU:OE2	4:B:901:HOH:O	2.04	0.74
1:A:99:ILE:HG12	4:A:954:HOH:O	1.88	0.74
1:B:204:THR:HG22	1:B:206:SER:H	1.53	0.74
1:A:668:LEU:HG	1:A:669:TYR:CE1	2.23	0.73
1:A:28:ILE:O	1:A:30:THR:N	2.22	0.73
1:A:99:ILE:C	1:A:100:LYS:HD3	2.10	0.72
1:A:692:LYS:HA	1:A:695:ALA:HB3	1.72	0.72
1:A:729:VAL:O	1:A:732:PRO:CD	2.37	0.72
1:A:77:ASP:HB3	1:A:80:THR:HG23	1.72	0.72
1:B:15:GLU:OE2	1:B:718:TYR:OH	2.05	0.71
1:A:102:LEU:O	1:A:106:GLY:N	2.23	0.71
1:A:182:ASP:OD2	1:A:382:SER:HB3	1.91	0.71
1:A:51:LEU:HD21	1:A:102:LEU:HD11	1.72	0.71
1:B:402:ASP:OD1	1:B:404:LYS:HD3	1.89	0.71
1:A:646:ASN:HD22	1:A:648:LYS:NZ	1.89	0.70
1:A:646:ASN:O	1:A:648:LYS:N	2.21	0.70
1:A:481:ARG:HH22	1:A:516:GLY:H	1.40	0.70
1:B:191:THR:HG22	1:B:500:GLU:HG3	1.74	0.69
1:A:96:THR:O	1:A:100:LYS:HD3	1.89	0.68
1:A:293:ILE:HG13	4:A:968:HOH:O	1.93	0.68
1:A:100:LYS:HD3	1:A:100:LYS:N	2.09	0.68
1:A:99:ILE:H	1:A:100:LYS:HD3	1.58	0.68
1:A:96:THR:C	1:A:100:LYS:HD2	2.14	0.68
1:A:123:THR:O	1:A:127:ARG:HB2	1.94	0.68
1:A:656:GLU:CD	1:A:660:ARG:HH21	1.97	0.68
1:B:254:LEU:H	1:B:342:ASN:ND2	1.89	0.68
1:A:527:ALA:O	1:A:531:THR:HG23	1.94	0.67
1:A:693:ALA:HA	1:A:696:GLU:HG2	1.77	0.67
1:B:436:ILE:HG23	1:B:450:THR:HG23	1.76	0.67
1:B:37:ILE:HD11	1:B:629:THR:HG22	1.76	0.67
1:B:416:ALA:HB3	1:B:468:PRO:HB3	1.76	0.67
1:A:99:ILE:HD11	4:A:954:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:PHE:HE1	1:A:694:LEU:HB3	1.59	0.67
1:B:150:PRO:HG2	1:B:153:VAL:HG23	1.76	0.67
1:A:692:LYS:O	1:A:696:GLU:N	2.28	0.66
1:B:44:ILE:HG12	4:B:946:HOH:O	1.95	0.66
1:A:62:GLN:NE2	1:A:106:GLY:O	2.29	0.66
1:A:601:HIS:HA	1:A:660:ARG:NH2	2.11	0.65
1:A:688:ALA:N	1:A:689:PRO:HD2	2.06	0.65
1:A:685:ALA:HA	1:A:687:PHE:H	1.62	0.65
1:A:96:THR:O	1:A:99:ILE:HG22	1.96	0.65
1:A:646:ASN:HD22	1:A:648:LYS:HZ1	1.45	0.64
1:B:653:ARG:O	1:B:654:THR:CB	2.45	0.64
1:A:729:VAL:CG1	1:A:730:MET:N	2.40	0.64
1:A:727:SER:O	1:A:729:VAL:N	2.28	0.64
1:A:26:PRO:HB2	1:A:731:ARG:HH12	1.62	0.63
1:A:169:GLN:HB2	1:B:174:HIS:CD2	2.33	0.63
1:A:685:ALA:CA	1:A:687:PHE:H	2.11	0.63
1:B:148:ARG:HB3	1:B:410:PRO:HB3	1.81	0.63
1:B:191:THR:CG2	1:B:500:GLU:HG3	2.28	0.63
1:A:704:GLU:OE1	1:A:735:THR:OG1	2.16	0.62
1:A:112:TYR:HE1	1:A:125:LYS:HG3	1.62	0.62
1:A:602:LEU:CB	1:A:658:ASP:OD2	2.47	0.62
1:A:311:THR:HG22	1:A:314:ARG:NH1	2.15	0.62
1:A:113:PRO:O	1:A:114:GLU:O	2.17	0.61
1:A:101:GLU:HG3	1:A:101:GLU:O	1.99	0.61
1:A:112:TYR:HD1	1:A:125:LYS:HD2	1.63	0.61
1:A:127:ARG:O	1:A:128:TYR:CD1	2.53	0.61
1:A:685:ALA:HA	1:A:687:PHE:N	2.15	0.61
1:A:733:SER:OG	1:A:734:ALA:N	2.32	0.61
1:A:688:ALA:C	1:A:690:LEU:CA	2.68	0.61
1:A:344:HIS:ND1	2:A:801:PO4:O4	2.24	0.61
1:A:305:LYS:HD2	4:A:968:HOH:O	2.00	0.61
1:B:301:GLY:O	1:B:305:LYS:HG3	2.01	0.61
1:A:96:THR:O	1:A:99:ILE:CG2	2.48	0.61
1:A:631:LEU:HD12	1:A:632:LEU:N	2.14	0.61
1:A:127:ARG:C	1:A:130:LYS:HD3	2.21	0.60
1:A:148:ARG:HB3	1:A:410:PRO:HB3	1.82	0.60
1:A:655:GLY:H	1:A:656:GLU:CB	2.09	0.60
1:B:531:THR:O	1:B:535:VAL:HG23	2.00	0.60
1:A:342:ASN:OD1	1:A:349:ILE:HD12	2.01	0.60
1:A:731:ARG:HD2	1:A:736:PHE:HD1	1.65	0.60
1:A:99:ILE:CG1	4:A:954:HOH:O	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ASN:O	1:B:629:THR:OG1	2.19	0.59
1:A:687:PHE:O	1:A:689:PRO:HD2	2.01	0.59
1:A:736:PHE:CG	1:A:737:ASN:N	2.70	0.59
1:A:24:LEU:CD2	1:A:663:HIS:HA	2.29	0.59
1:B:707:GLN:O	1:B:711:LYS:NZ	2.35	0.59
1:A:27:ILE:HD11	1:A:667:SER:CB	2.32	0.59
1:A:664:PHE:CE1	1:A:694:LEU:HB3	2.37	0.59
1:A:731:ARG:HD2	1:A:736:PHE:CD1	2.38	0.59
1:A:101:GLU:OE1	1:A:719:TYR:CG	2.55	0.59
1:A:705:LEU:HB2	1:A:708:VAL:HG11	1.85	0.59
1:A:120:GLU:HA	1:A:123:THR:HG22	1.85	0.58
1:B:653:ARG:O	1:B:654:THR:HB	2.02	0.58
1:A:661:GLY:O	1:A:665:TYR:N	2.25	0.58
1:A:688:ALA:HA	1:A:690:LEU:HA	1.85	0.58
1:A:130:LYS:H	1:A:130:LYS:HD2	1.69	0.58
1:A:112:TYR:CD1	1:A:125:LYS:HD2	2.38	0.58
1:A:70:GLU:HA	1:A:73:ARG:HH11	1.68	0.57
1:A:144:ASN:HA	1:A:415:MET:HG2	1.85	0.57
1:A:259:THR:O	1:A:262:LYS:HE3	2.04	0.57
1:A:283:LYS:HE2	1:A:284:HIS:NE2	2.19	0.57
1:B:336:SER:OG	1:B:367:GLY:O	2.21	0.57
1:A:81:ASN:OD1	1:A:616:SER:OG	2.21	0.57
1:A:24:LEU:HG	1:A:659:ASN:HD21	1.68	0.57
1:A:130:LYS:HD2	1:A:130:LYS:N	2.18	0.57
1:A:474:LYS:O	1:A:478:THR:HG23	2.04	0.57
1:A:534:ARG:NH2	1:A:540:ASP:O	2.33	0.57
1:A:90:ALA:HB3	1:A:131:CYS:O	2.04	0.57
1:A:736:PHE:H	1:A:736:PHE:HD2	1.52	0.57
1:A:333:MET:HG3	1:A:368:ALA:HA	1.87	0.57
1:B:91:SER:OG	1:B:94:GLN:HG3	2.05	0.57
1:A:726:VAL:HA	1:A:729:VAL:HG12	1.86	0.56
1:A:40:VAL:HG23	4:A:917:HOH:O	2.04	0.56
1:A:5:LYS:N	4:A:915:HOH:O	2.39	0.56
1:A:601:HIS:C	1:A:660:ARG:HH22	2.09	0.56
1:B:596:LEU:HD13	1:B:602:LEU:HB2	1.88	0.56
1:A:115:ASN:N	1:A:116:PRO:CD	2.63	0.56
1:B:311:THR:HG22	1:B:314:ARG:HH11	1.71	0.56
1:B:659:ASN:O	1:B:662:SER:OG	2.22	0.56
1:A:428:THR:HG23	1:A:460:ARG:HB3	1.87	0.56
1:B:387:ILE:HG13	4:B:986:HOH:O	2.06	0.56
1:A:709:GLN:O	1:A:709:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:CG	1:A:736:PHE:CE1	2.58	0.55
1:B:365:MET:HG2	4:B:928:HOH:O	2.05	0.55
1:A:650:PRO:HB3	1:A:658:ASP:HA	1.88	0.55
1:A:99:ILE:N	1:A:100:LYS:HD3	2.21	0.55
1:A:470:ARG:NH1	1:A:508:TYR:OH	2.40	0.55
1:A:688:ALA:O	1:A:690:LEU:HB2	2.06	0.55
1:A:114:GLU:OE1	1:A:114:GLU:N	2.40	0.55
1:A:725:LYS:HZ3	1:A:726:VAL:HG13	1.70	0.55
1:A:122:LYS:HD3	4:A:967:HOH:O	2.06	0.54
1:A:632:LEU:HD22	1:A:670:TRP:CZ2	2.41	0.54
1:A:658:ASP:HB2	1:A:660:ARG:CZ	2.37	0.54
1:A:604:TRP:HA	1:A:650:PRO:HG2	1.90	0.54
1:A:731:ARG:N	1:A:732:PRO:HD3	2.23	0.54
1:A:119:GLU:N	1:A:121:GLU:OE1	2.41	0.54
1:A:730:MET:C	1:A:732:PRO:HD3	2.28	0.54
1:B:191:THR:HG22	1:B:223:ILE:HG12	1.88	0.54
1:B:225:ASP:OD1	1:B:497:HIS:ND1	2.36	0.54
1:B:223:ILE:HD13	1:B:500:GLU:HB3	1.89	0.54
1:B:634:LYS:O	1:B:637:ASP:HB2	2.07	0.54
1:A:669:TYR:O	1:A:672:GLU:HB3	2.08	0.54
1:A:40:VAL:N	4:A:917:HOH:O	2.40	0.53
1:A:705:LEU:HB2	1:A:708:VAL:CG1	2.38	0.53
1:A:102:LEU:HA	1:A:105:LYS:HB2	1.90	0.53
1:B:267:ILE:HA	1:B:296:ASN:ND2	2.22	0.53
1:B:742:THR:OG1	1:B:743:VAL:N	2.38	0.53
1:A:24:LEU:O	1:A:27:ILE:HG22	2.09	0.53
1:A:534:ARG:HB3	1:A:539:LEU:HB2	1.91	0.53
1:B:355:MET:O	1:B:359:ILE:HG13	2.07	0.53
1:A:99:ILE:H	1:A:100:LYS:CD	2.20	0.53
1:A:648:LYS:NZ	1:A:669:TYR:OH	2.36	0.53
1:A:688:ALA:N	1:A:689:PRO:HD3	2.23	0.53
1:A:130:LYS:HB2	1:A:131:CYS:SG	2.49	0.53
1:A:311:THR:HG22	1:A:314:ARG:HH12	1.74	0.53
1:B:175:VAL:HB	1:B:389:GLN:HB2	1.90	0.53
1:B:225:ASP:OD2	1:B:462:CYS:HB2	2.09	0.53
1:B:547:ASN:OD1	1:B:550:ARG:NH1	2.41	0.53
1:A:31:PHE:N	4:A:920:HOH:O	2.42	0.53
1:A:387:ILE:HD13	1:A:490:TRP:HZ3	1.73	0.53
1:A:659:ASN:HA	1:A:662:SER:OG	2.08	0.53
1:A:726:VAL:CA	1:A:729:VAL:HG12	2.39	0.52
1:A:727:SER:C	1:A:729:VAL:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:HB	4:B:997:HOH:O	2.09	0.52
1:B:300:ALA:O	1:B:304:GLU:HG3	2.10	0.52
1:B:369:ASP:OD2	1:B:373:TYR:OH	2.27	0.52
1:A:54:PHE:HA	1:A:127:ARG:NH2	2.24	0.52
1:A:681:ALA:O	1:A:684:LYS:HB3	2.10	0.52
1:A:250:ILE:HG21	4:A:930:HOH:O	2.09	0.52
1:B:281:PHE:O	1:B:285:GLY:N	2.42	0.52
1:B:306:ILE:HD12	4:B:981:HOH:O	2.10	0.52
1:A:733:SER:HB3	1:A:736:PHE:CD2	2.45	0.52
1:A:102:LEU:HB3	1:A:107:TYR:HB2	1.91	0.51
1:A:283:LYS:HG2	1:A:284:HIS:CD2	2.45	0.51
1:A:115:ASN:H	1:A:116:PRO:HD3	1.74	0.51
1:A:397:TRP:CD1	1:A:398:HIS:CD2	2.99	0.51
1:A:120:GLU:N	1:A:121:GLU:HG3	2.26	0.51
1:A:204:THR:HG22	1:A:206:SER:H	1.75	0.51
1:A:653:ARG:O	1:A:654:THR:OG1	2.22	0.51
1:B:660:ARG:NH1	1:B:729:VAL:O	2.44	0.51
1:A:24:LEU:HD22	1:A:663:HIS:ND1	2.10	0.51
1:A:21:THR:HB	4:A:902:HOH:O	2.10	0.50
1:A:658:ASP:CB	1:A:660:ARG:CZ	2.89	0.50
1:B:26:PRO:HG2	1:B:731:ARG:HD2	1.93	0.50
1:A:646:ASN:CB	1:A:648:LYS:HE3	2.41	0.50
1:A:99:ILE:O	1:A:99:ILE:HG13	2.12	0.50
1:A:707:GLN:O	1:A:709:GLN:N	2.43	0.50
1:B:705:LEU:O	1:B:708:VAL:HG22	2.11	0.50
1:A:117:ALA:HB3	1:A:121:GLU:OE2	2.10	0.50
1:A:184:TYR:CE2	1:A:495:ARG:HB2	2.46	0.50
1:A:366:TRP:CZ3	1:A:372:GLN:HG3	2.46	0.50
1:B:15:GLU:OE1	1:B:588:SER:OG	2.27	0.50
1:A:168:LYS:HD2	1:A:170:TRP:CH2	2.47	0.50
1:A:495:ARG:HD3	1:A:498:GLU:HG3	1.94	0.50
1:A:692:LYS:NZ	1:A:696:GLU:OE2	2.33	0.50
1:A:427:LYS:HD2	1:A:461:MET:HE3	1.94	0.50
1:A:230:SER:OG	1:A:230:SER:O	2.30	0.49
1:A:424:SER:HA	1:A:427:LYS:HE2	1.93	0.49
1:A:490:TRP:HB2	1:A:545:THR:HG22	1.93	0.49
1:B:257:LYS:HE2	1:B:260:MET:HG3	1.94	0.49
1:B:257:LYS:HE2	1:B:260:MET:CG	2.42	0.49
1:B:601:HIS:CE1	1:B:658:ASP:HB3	2.47	0.49
1:A:309:LEU:HD13	1:A:313:LEU:HD13	1.93	0.49
1:B:550:ARG:CZ	4:B:961:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:TYR:HB3	1:A:669:TYR:CE2	2.46	0.49
1:B:257:LYS:NZ	1:B:551:ASP:OD2	2.41	0.49
1:A:21:THR:O	4:A:902:HOH:O	2.20	0.49
1:A:412:VAL:HB	1:A:544:VAL:HG13	1.93	0.49
1:B:53:GLU:OE2	1:B:127:ARG:HD2	2.12	0.49
1:A:221:GLY:O	1:A:504:LYS:NZ	2.37	0.49
1:A:112:TYR:HA	1:A:125:LYS:HZ2	1.76	0.49
1:A:440:THR:OG1	1:A:447:VAL:HG22	2.13	0.49
1:A:646:ASN:HB3	1:A:648:LYS:HE3	1.94	0.49
1:A:35:ALA:HA	1:A:628:ARG:HD2	1.93	0.48
1:A:658:ASP:CB	1:A:660:ARG:NH2	2.74	0.48
1:A:162:HIS:CD2	4:A:965:HOH:O	2.66	0.48
1:B:603:ARG:CD	1:B:652:ARG:HG3	2.43	0.48
1:B:603:ARG:HD3	1:B:652:ARG:HG3	1.93	0.48
1:A:627:ALA:O	1:A:631:LEU:HG	2.13	0.48
1:B:25:LEU:HD22	4:B:997:HOH:O	2.13	0.48
1:B:171:SER:HB3	1:B:396:LYS:HE2	1.96	0.48
1:B:328:ARG:HD3	4:B:911:HOH:O	2.12	0.48
1:A:13:THR:O	1:A:45:SER:HB3	2.14	0.48
1:B:250:ILE:HG21	4:B:1044:HOH:O	2.14	0.48
1:B:284:HIS:ND1	4:B:903:HOH:O	2.35	0.48
1:B:294:ASN:OD1	1:B:296:ASN:HB2	2.13	0.48
1:A:146:ASP:HB3	1:A:571:ILE:HB	1.95	0.48
1:A:677:GLN:NE2	1:A:680:ASP:HB3	2.29	0.48
1:A:661:GLY:O	1:A:664:PHE:N	2.47	0.48
1:B:11:THR:HB	4:B:946:HOH:O	2.14	0.48
1:B:534:ARG:HH21	1:B:540:ASP:N	2.11	0.47
1:A:19:LEU:HA	4:A:974:HOH:O	2.14	0.47
1:B:137:ASN:N	1:B:138:PRO:HD2	2.28	0.47
1:B:227:MET:HE1	1:B:460:ARG:HE	1.78	0.47
1:A:101:GLU:OE2	1:A:719:TYR:HB2	2.13	0.47
1:A:387:ILE:HB	4:A:950:HOH:O	2.14	0.47
1:A:128:TYR:HA	1:A:130:LYS:HG2	1.96	0.47
1:B:643:LEU:HD12	1:B:648:LYS:HB2	1.96	0.47
1:A:595:GLN:O	1:A:601:HIS:N	2.47	0.47
1:B:119:GLU:O	1:B:122:LYS:HD3	2.15	0.47
1:B:432:PRO:O	1:B:455:GLU:HG3	2.15	0.47
1:B:597:VAL:HG13	4:B:1014:HOH:O	2.13	0.47
1:A:94:GLN:NE2	1:A:719:TYR:OH	2.47	0.47
1:A:387:ILE:HD13	1:A:490:TRP:CZ3	2.50	0.47
1:A:488:ILE:HD11	1:A:530:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HD3	1:A:68:LEU:HD13	1.97	0.47
1:A:650:PRO:HA	1:A:658:ASP:N	2.30	0.47
1:A:729:VAL:O	1:A:732:PRO:CG	2.63	0.47
1:B:466:ASP:OD2	1:B:470:ARG:HD2	2.15	0.46
1:B:550:ARG:HG2	1:B:551:ASP:N	2.29	0.46
1:A:631:LEU:CD1	1:A:632:LEU:N	2.78	0.46
1:A:699:GLN:OE1	1:A:699:GLN:N	2.48	0.46
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.80	0.46
1:A:465:LYS:O	1:A:469:ILE:HG13	2.15	0.46
1:B:523:SER:HB3	1:B:526:ARG:HG3	1.97	0.46
1:A:287:LEU:HD21	1:A:309:LEU:HD11	1.98	0.46
1:A:444:THR:OG1	1:A:446:GLU:HG3	2.15	0.46
1:B:62:GLN:NE2	1:B:106:GLY:O	2.47	0.46
1:B:284:HIS:CE1	1:B:317:ILE:HG12	2.50	0.46
1:A:112:TYR:CE1	1:A:125:LYS:HG3	2.47	0.46
1:A:420:GLU:HG2	1:A:464:VAL:HG21	1.98	0.46
1:A:26:PRO:HD2	1:A:731:ARG:HH11	1.81	0.46
1:A:100:LYS:CD	1:A:100:LYS:N	2.78	0.46
1:A:410:PRO:HG2	1:A:542:ILE:HA	1.97	0.46
1:A:665:TYR:O	1:A:668:LEU:HB3	2.16	0.46
1:A:700:LYS:O	1:A:704:GLU:N	2.34	0.46
1:B:23:SER:O	1:B:731:ARG:NH2	2.48	0.46
1:B:189:SER:HB2	1:B:224:ILE:O	2.15	0.46
1:A:12:LEU:HD11	1:A:41:LYS:HD3	1.97	0.46
1:A:701:ILE:O	1:A:705:LEU:HG	2.16	0.46
1:A:731:ARG:HA	1:A:731:ARG:HD3	1.62	0.46
1:B:15:GLU:HB3	1:B:593:VAL:HG21	1.97	0.46
1:A:92:VAL:HG23	4:A:1047:HOH:O	2.16	0.45
1:A:212:LEU:HD12	1:A:459:TRP:HZ3	1.81	0.45
1:B:227:MET:CE	1:B:460:ARG:HE	2.29	0.45
1:A:677:GLN:NE2	1:A:680:ASP:H	2.14	0.45
1:A:26:PRO:HD2	1:A:731:ARG:NH1	2.32	0.45
1:A:77:ASP:HB3	1:A:80:THR:CG2	2.44	0.45
1:A:87:ASN:ND2	1:A:136:VAL:HG21	2.31	0.45
1:A:154:LYS:HE2	1:A:408:THR:HG23	1.97	0.45
1:A:599:GLU:OE1	4:A:903:HOH:O	2.21	0.45
1:B:143:GLY:O	1:B:144:ASN:HB2	2.17	0.45
1:B:479:ARG:HH21	1:B:483:SER:HB3	1.80	0.45
1:A:621:GLY:HA2	1:A:629:THR:OG1	2.16	0.45
1:B:183:PHE:HB2	1:B:381:GLU:OE2	2.17	0.45
1:A:736:PHE:CD2	1:A:736:PHE:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:LEU:O	1:B:640:THR:OG1	2.32	0.45
1:A:300:ALA:O	1:A:304:GLU:HG3	2.16	0.45
1:A:130:LYS:H	1:A:130:LYS:CD	2.29	0.45
1:A:461:MET:HE3	1:A:461:MET:HB3	1.82	0.45
1:A:481:ARG:HA	1:A:481:ARG:HD3	1.80	0.45
1:A:656:GLU:OE2	1:A:660:ARG:NE	2.50	0.45
1:A:671:ALA:HA	1:A:674:LEU:HB2	1.98	0.45
1:A:683:LEU:C	1:A:685:ALA:H	2.18	0.45
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.81	0.45
1:A:690:LEU:CD2	1:A:692:LYS:HD3	2.47	0.45
1:A:733:SER:HB3	1:A:736:PHE:CG	2.52	0.45
1:A:736:PHE:CZ	1:A:737:ASN:HB2	2.52	0.45
1:B:693:ALA:O	1:B:697:ASN:ND2	2.43	0.44
1:A:71:LEU:HD23	1:A:74:LEU:HD22	1.98	0.44
1:A:301:GLY:O	1:A:305:LYS:HG3	2.17	0.44
1:A:725:LYS:HD3	1:A:725:LYS:H	1.77	0.44
1:B:466:ASP:OD1	1:B:504:LYS:NZ	2.47	0.44
1:A:412:VAL:HG13	1:A:475:LEU:HD23	1.99	0.44
1:A:734:ALA:HA	1:A:736:PHE:HE2	1.82	0.44
1:A:25:LEU:HD11	1:A:39:ILE:HG21	2.00	0.44
1:A:142:GLU:O	1:A:575:MET:HG2	2.18	0.44
1:B:657:LEU:HD11	1:B:661:GLY:HA3	1.99	0.44
1:A:37:ILE:HD11	1:A:629:THR:CG2	2.46	0.44
1:A:529:ARG:HH12	1:B:390:GLU:CD	2.20	0.44
1:A:731:ARG:N	1:A:732:PRO:CD	2.81	0.44
1:B:408:THR:HA	1:B:561:GLU:OE1	2.18	0.44
1:A:161:PRO:HG3	1:A:404:LYS:HE2	2.00	0.44
1:A:512:HIS:O	1:A:514:THR:HG23	2.18	0.44
1:A:600:ASN:N	1:A:710:GLY:HA2	2.32	0.44
1:A:690:LEU:HD23	1:A:692:LYS:HB3	2.00	0.44
1:A:325:GLN:OE1	4:A:904:HOH:O	2.21	0.44
1:A:726:VAL:HA	1:A:729:VAL:CG1	2.46	0.44
1:B:124:ILE:HA	4:B:905:HOH:O	2.18	0.44
1:B:414:LEU:HB2	1:B:472:TRP:CE2	2.53	0.43
1:A:95:LEU:O	1:A:99:ILE:N	2.51	0.43
1:A:202:LEU:HB3	1:A:210:ILE:HB	2.00	0.43
1:A:261:MET:CE	1:A:421:GLU:HB3	2.48	0.43
1:B:122:LYS:H	1:B:122:LYS:HG3	1.57	0.43
1:A:191:THR:OG1	1:A:500:GLU:HG3	2.17	0.43
1:A:692:LYS:O	1:A:696:GLU:HG2	2.18	0.43
1:B:314:ARG:HB2	4:B:981:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:O	1:A:58:LEU:HD23	2.18	0.43
1:A:241:GLN:CA	1:A:241:GLN:HE21	2.32	0.43
1:B:261:MET:HE1	4:B:920:HOH:O	2.19	0.43
1:A:391:MET:HB2	1:A:528:MET:CE	2.48	0.43
1:A:492:ASP:HB2	1:A:498:GLU:OE1	2.18	0.43
1:A:495:ARG:HA	1:A:496:PRO:HD2	1.76	0.43
1:A:27:ILE:HG21	1:A:663:HIS:CE1	2.54	0.43
1:A:634:LYS:O	1:A:638:GLU:HG3	2.19	0.43
1:A:33:LYS:N	1:A:34:PRO:HD2	2.34	0.43
1:A:120:GLU:C	1:A:121:GLU:HG3	2.38	0.43
1:B:137:ASN:CG	1:B:141:ARG:HH21	2.21	0.43
1:A:32:THR:HB	1:A:37:ILE:HB	2.01	0.43
1:A:661:GLY:HA2	1:A:664:PHE:HB3	2.01	0.43
1:A:617:LEU:HD13	1:A:632:LEU:HB3	2.00	0.42
1:B:491:LEU:O	1:B:493:PRO:HD3	2.19	0.42
1:B:509:LEU:HD12	4:B:1060:HOH:O	2.18	0.42
1:A:683:LEU:C	1:A:685:ALA:N	2.72	0.42
1:A:726:VAL:C	1:A:729:VAL:HG12	2.39	0.42
1:A:431:ILE:HA	1:A:432:PRO:HD3	1.69	0.42
1:A:669:TYR:HA	1:A:672:GLU:HB2	2.02	0.42
1:B:401:PHE:O	1:B:403:PRO:HD3	2.19	0.42
1:B:404:LYS:HE2	4:B:1035:HOH:O	2.19	0.42
1:B:674:LEU:HD13	1:B:687:PHE:CE2	2.54	0.42
1:B:715:ILE:HB	1:B:726:VAL:HG22	2.01	0.42
1:A:77:ASP:HA	1:A:78:PRO:HD3	1.76	0.42
1:A:86:PRO:HD3	1:A:583:THR:OG1	2.20	0.42
1:A:664:PHE:O	1:A:667:SER:N	2.52	0.42
1:B:665:TYR:HD1	4:B:1038:HOH:O	2.02	0.42
1:A:98:CYS:HB2	1:A:719:TYR:CD2	2.55	0.42
1:A:416:ALA:HB3	1:A:468:PRO:HB3	2.02	0.42
1:A:27:ILE:HG21	1:A:27:ILE:HD13	1.83	0.42
1:A:284:HIS:ND1	1:A:317:ILE:HG12	2.35	0.42
1:B:183:PHE:HD2	1:B:381:GLU:CG	2.33	0.42
1:B:283:LYS:HG2	1:B:284:HIS:CD2	2.55	0.42
1:A:488:ILE:HD11	1:A:530:TYR:CD2	2.55	0.41
1:A:705:LEU:CB	1:A:708:VAL:HG13	2.48	0.41
1:B:437:ALA:HB3	1:B:451:GLN:HB2	2.02	0.41
1:B:570:SER:HB3	1:B:582:GLU:HB2	2.01	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.87	0.41
1:A:690:LEU:CD2	1:A:692:LYS:HB3	2.50	0.41
1:B:28:ILE:HG23	1:B:613:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HA	1:B:296:ASN:HD21	1.83	0.41
1:A:102:LEU:HD22	1:A:107:TYR:CZ	2.56	0.41
1:A:733:SER:HB3	1:A:736:PHE:HB3	2.03	0.41
1:B:400:ASN:OD1	1:B:401:PHE:N	2.50	0.41
1:A:96:THR:O	1:A:99:ILE:HG23	2.21	0.41
1:A:729:VAL:C	1:A:732:PRO:HD3	2.37	0.41
1:A:271:HIS:O	1:A:275:ILE:HG12	2.21	0.41
1:A:659:ASN:O	1:A:663:HIS:N	2.54	0.41
1:A:688:ALA:CA	1:A:690:LEU:H	2.12	0.41
1:A:729:VAL:HG13	1:A:730:MET:HG2	2.02	0.41
1:B:33:LYS:N	1:B:34:PRO:HD2	2.36	0.41
1:A:24:LEU:HA	1:A:663:HIS:CE1	2.56	0.41
1:B:657:LEU:HD12	1:B:657:LEU:HA	1.96	0.41
1:A:15:GLU:HB3	1:A:16:ALA:H	1.54	0.41
1:A:44:ILE:HD11	4:A:1064:HOH:O	2.20	0.41
1:A:68:LEU:HD21	1:A:139:VAL:HG21	2.02	0.41
1:A:91:SER:OG	1:A:94:GLN:HB2	2.21	0.41
1:A:183:PHE:HB2	1:A:381:GLU:CD	2.42	0.41
1:A:234:LEU:HD21	1:A:268:VAL:HG13	2.03	0.41
1:A:261:MET:HG3	1:A:265:HIS:CE1	2.55	0.41
1:A:301:GLY:HA2	1:A:304:GLU:HG3	2.02	0.41
1:A:420:GLU:HG2	1:A:464:VAL:CG2	2.50	0.41
1:A:642:LYS:HE3	1:A:669:TYR:CG	2.56	0.41
1:A:702:VAL:O	1:A:706:ALA:HB2	2.21	0.41
1:B:284:HIS:ND1	1:B:317:ILE:HG12	2.35	0.41
1:B:551:ASP:HA	4:B:961:HOH:O	2.20	0.41
1:B:711:LYS:NZ	4:B:919:HOH:O	2.53	0.41
1:A:376:LYS:HB2	1:A:376:LYS:HE2	1.76	0.41
1:A:660:ARG:C	1:A:663:HIS:HB3	2.41	0.41
1:B:619:GLU:O	1:B:623:LYS:HG2	2.20	0.41
1:A:24:LEU:HD13	1:A:610:PHE:HE1	1.87	0.40
1:A:559:ILE:HD13	1:A:559:ILE:HA	1.95	0.40
1:A:650:PRO:CB	1:A:658:ASP:HA	2.50	0.40
1:A:699:GLN:OE1	1:A:700:LYS:HE2	2.21	0.40
1:A:102:LEU:HD22	1:A:107:TYR:CE1	2.55	0.40
1:A:227:MET:CE	1:A:460:ARG:HE	2.33	0.40
1:B:23:SER:HG	1:B:663:HIS:CE1	2.28	0.40
1:B:534:ARG:NE	1:B:541:THR:HG23	2.36	0.40
1:A:241:GLN:HE21	1:A:241:GLN:N	2.19	0.40
1:A:556:LEU:O	1:A:560:MET:HG2	2.21	0.40
1:A:628:ARG:C	1:A:631:LEU:HD11	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:SER:C	1:A:729:VAL:N	2.75	0.40
1:A:711:LYS:HB3	1:A:712:PRO:CD	2.52	0.40
1:B:302:LEU:HD23	1:B:306:ILE:HD13	2.03	0.40
1:A:184:TYR:HB2	1:A:383:THR:OG1	2.22	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	733/751 (98%)	626 (85%)	70 (10%)	37 (5%)	2 12
1	B	737/751 (98%)	673 (91%)	54 (7%)	10 (1%)	11 43
All	All	1470/1502 (98%)	1299 (88%)	124 (8%)	47 (3%)	4 22

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	117	ALA
1	A	647	ASP
1	A	654	THR
1	A	658	ASP
1	A	690	LEU
1	A	691	ALA
1	A	711	LYS
1	A	728	ALA
1	A	729	VAL
1	A	733	SER
1	B	118	THR
1	A	29	GLU
1	A	92	VAL

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Mol	Chain	Res	Type
1	A	602	LEU
1	A	625	ASN
1	A	663	HIS
1	A	671	ALA
1	A	723	PRO
1	A	726	VAL
1	A	738	ALA
1	B	143	GLY
1	B	654	THR
1	A	28	ILE
1	A	100	LYS
1	A	113	PRO
1	A	605	ASP
1	A	650	PRO
1	A	656	GLU
1	A	684	LYS
1	A	712	PRO
1	A	734	ALA
1	B	119	GLU
1	B	361	ALA
1	B	523	SER
1	A	283	LYS
1	A	496	PRO
1	A	708	VAL
1	B	13	THR
1	B	111	ASP
1	B	743	VAL
1	A	121	GLU
1	A	143	GLY
1	A	688	ALA
1	B	46	VAL
1	A	597	VAL
1	A	689	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	601/628 (96%)	569 (95%)	32 (5%)	22 58
1	B	614/628 (98%)	587 (96%)	27 (4%)	28 65
All	All	1215/1256 (97%)	1156 (95%)	59 (5%)	25 61

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	42	SER
1	A	100	LYS
1	A	114	GLU
1	A	121	GLU
1	A	123	THR
1	A	136	VAL
1	A	145	SER
1	A	227	MET
1	A	230	SER
1	A	241	GLN
1	A	259	THR
1	A	295	VAL
1	A	313	LEU
1	A	436	ILE
1	A	531	THR
1	A	593	VAL
1	A	615	VAL
1	A	624	GLU
1	A	628	ARG
1	A	631	LEU
1	A	649	SER
1	A	653	ARG
1	A	656	GLU
1	A	658	ASP
1	A	660	ARG
1	A	682	GLU
1	A	708	VAL
1	A	711	LYS
1	A	725	LYS
1	A	731	ARG
1	A	736	PHE
1	B	59	SER
1	B	100	LYS
1	B	122	LYS

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Mol	Chain	Res	Type
1	B	145	SER
1	B	189	SER
1	B	191	THR
1	B	205	ASN
1	B	225	ASP
1	B	227	MET
1	B	238	TYR
1	B	247	GLU
1	B	286	LYS
1	B	295	VAL
1	B	336	SER
1	B	382	SER
1	B	442	LEU
1	B	499	ASN
1	B	515	THR
1	B	529	ARG
1	B	536	VAL
1	B	541	THR
1	B	550	ARG
1	B	609	GLU
1	B	615	VAL
1	B	640	THR
1	B	684	LYS
1	B	721	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	160	HIS
1	A	241	GLN
1	A	646	ASN
1	A	677	GLN
1	B	296	ASN
1	B	342	ASN

5.3.3 RNA

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	801	-	4,4,4	0.87	0	6,6,6	0.64	0
2	PO4	B	801	-	4,4,4	0.97	0	6,6,6	0.64	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	735/751 (97%)	-0.13	39 (5%) 26 10	28, 50, 130, 141	0
1	B	739/751 (98%)	-0.61	0 100 100	22, 38, 64, 100	0
All	All	1474/1502 (98%)	-0.37	39 (2%) 56 27	22, 42, 125, 141	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	728	ALA	8.2
1	A	108	ALA	4.2
1	A	113	PRO	4.2
1	A	709	GLN	4.0
1	A	689	PRO	3.8
1	A	123	THR	3.3
1	A	109	ILE	3.2
1	A	22	TYR	3.2
1	A	681	ALA	3.1
1	A	63	LYS	3.0
1	A	62	GLN	2.9
1	A	696	GLU	2.9
1	A	115	ASN	2.9
1	A	104	SER	2.8
1	A	604	TRP	2.8
1	A	658	ASP	2.8
1	A	720	ALA	2.7
1	A	64	VAL	2.7
1	A	99	ILE	2.7
1	A	716	GLY	2.6
1	A	101	GLU	2.6
1	A	605	ASP	2.5
1	A	106	GLY	2.5
1	A	118	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	110	PRO	2.5
1	A	723	PRO	2.4
1	A	107	TYR	2.4
1	A	729	VAL	2.4
1	A	111	ASP	2.4
1	A	102	LEU	2.3
1	A	35	ALA	2.3
1	A	602	LEU	2.3
1	A	601	HIS	2.2
1	A	93	ALA	2.1
1	A	683	LEU	2.1
1	A	98	CYS	2.1
1	A	695	ALA	2.0
1	A	59	SER	2.0
1	A	117	ALA	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	802	1/1	0.94	0.33	38,38,38,38	0
3	MG	A	802	1/1	0.96	0.42	27,27,27,27	0
2	PO4	A	801	5/5	0.97	0.08	52,53,59,66	0
2	PO4	B	801	5/5	0.98	0.14	41,41,49,53	0

6.5 Other polymers (i)

There are no such residues in this entry.