WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 10:47 pm BST

PDB ID	:	4AOY
Title	:	Open CtIDH. The complex structures of Isocitrate dehydrogenase from Clostridium thermocellum and Desulfotalea psychrophila, support a new active site locking mechanism
Authors	:	Leiros, H.-K.S.; Fedoy, A.-E.; Leiros, I.; Steen, I.H.
Deposited on	:	2012-03-30
Resolution	:	2.35 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 (i)) were used in the production of this report:

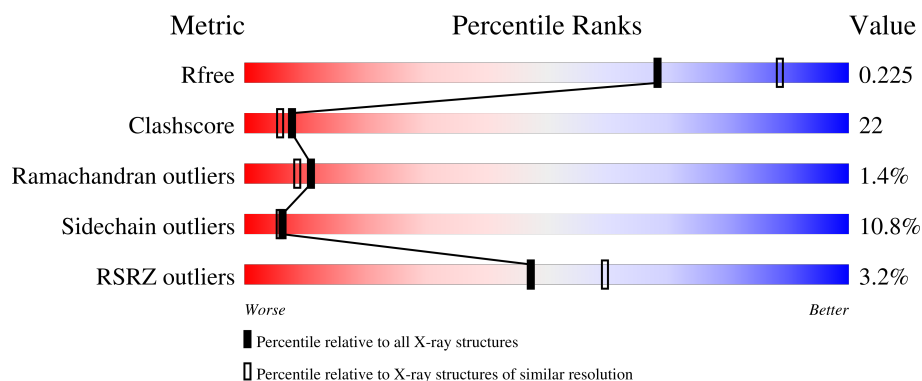|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.35 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	Percentile Ranks	Value
Rfree		0.225
Clashscore		22
Ramachandran outliers		1.4%
Sidechain outliers		10.8%
RSRZ outliers		3.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	402	3% / 61% / 26% / 6% / 6%
1	B	402	3% / 60% / 25% / 7% / 7%
1	C	402	3% / 69% / 19% / · · / 8%
1	D	402	3% / 60% / 27% / 6% / 7%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11678 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 [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2917	1854	488	558	17			
1	B	372	Total	C	N	O	S	0	0	0
			2859	1817	474	552	16			
1	C	371	Total	C	N	O	S	0	0	0
			2884	1837	477	554	16			
1	D	375	Total	C	N	O	S	0	0	0
			2930	1869	485	560	16			

- Molecule 2 is water.

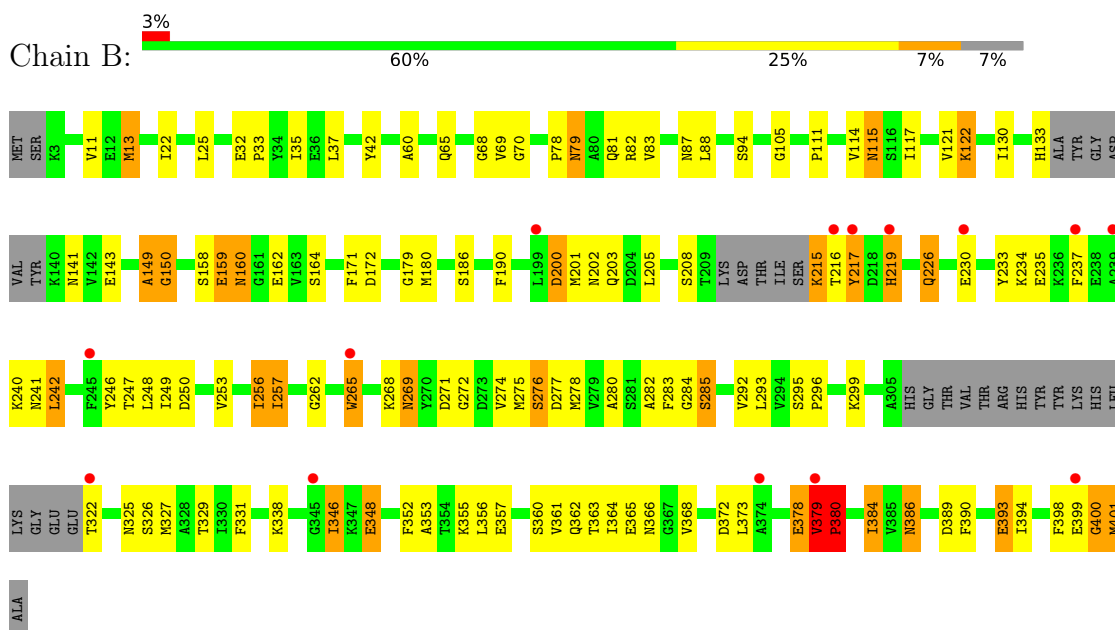| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	15	Total	O	0	0
			15	15		
2	C	22	Total	O	0	0
			22	22		
2	D	30	Total	O	0	0
			30	30		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
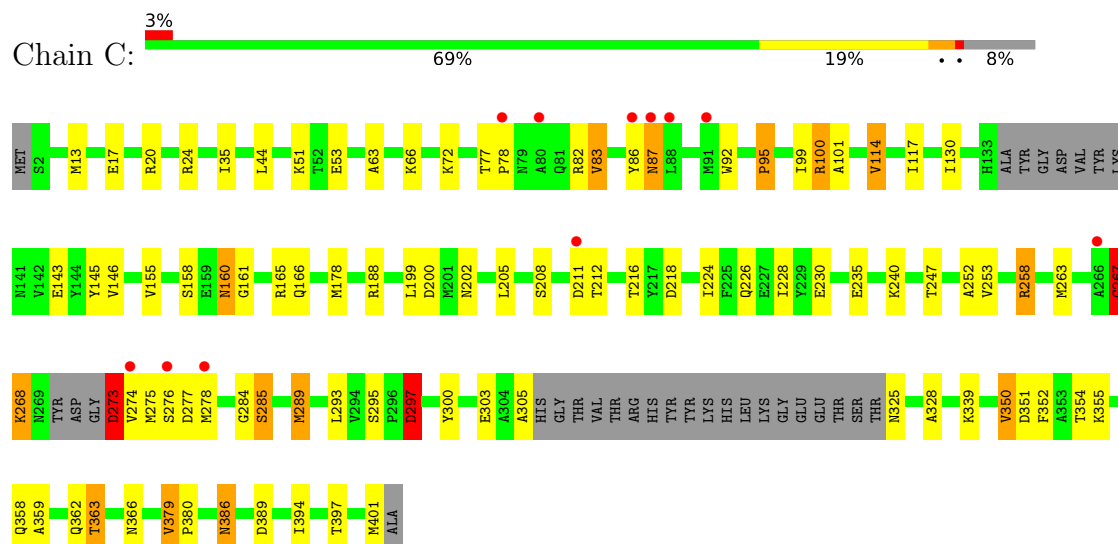
- Molecule 1: ISOCITRATE DEHYDROGENASE [NADP]

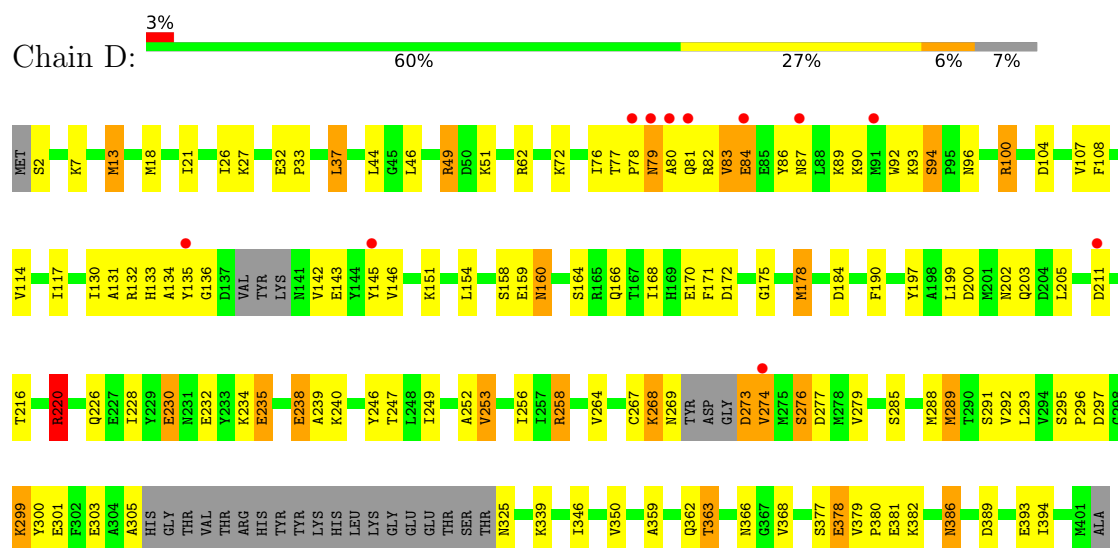- Molecule 1: ISOCITRATE DEHYDROGENASE [NADP]

• Molecule 1: ISOCITRATE DEHYDROGENASE [NADP]

Chain C:

• Molecule 1: ISOCITRATE DEHYDROGENASE [NADP]

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	56.13Å 106.84Å 154.50Å 90.00° 93.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 48.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.35) 99.7 (48.02-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.258 0.211 , 0.225	Depositor DCC
R_{free} test set	2280 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11678	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.70	0/2970	0.80	0/4011
1	B	0.64	0/2913	0.81	5/3936 (0.1%)
1	C	0.76	1/2938 (0.0%)	0.81	3/3966 (0.1%)
1	D	0.75	1/2985 (0.0%)	0.80	4/4029 (0.1%)
All	All	0.71	2/11806 (0.0%)	0.80	12/15942 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	CYS	CB-SG	-7.07	1.70	1.82
1	D	297	ASP	CB-CG	-5.26	1.40	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	150	GLY	N-CA-C	7.74	132.45	113.10
1	B	379	VAL	C-N-CA	-7.08	92.28	122.00
1	C	297	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	B	13	MET	CG-SD-CE	-6.59	89.66	100.20
1	B	149	ALA	N-CA-C	6.43	128.37	111.00
1	B	400	GLY	N-CA-C	-6.23	97.52	113.10
1	C	293	LEU	CB-CG-CD2	-5.63	101.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	293	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	220	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	49	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	297	ASP	N-CA-CB	-5.07	101.48	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	VAL	Peptide
1	B	380	PRO	Peptide
1	C	273	ASP	Peptide

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	2917	0	2820	144	0
1	B	2859	0	2723	149	0
1	C	2884	0	2788	81	0
1	D	2930	0	2855	132	0
2	A	21	0	0	2	0
2	B	15	0	0	0	0
2	C	22	0	0	3	0
2	D	30	0	0	4	0
All	All	11678	0	11186	492	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 22.

All (492) 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:379:VAL:HG12	1:A:380:PRO:CB	1.38	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG12	1:A:380:PRO:CG	1.10	1.52
1:A:379:VAL:CG1	1:A:380:PRO:CG	1.97	1.43
1:A:379:VAL:CG1	1:A:380:PRO:CB	2.00	1.38
1:A:379:VAL:CG1	1:A:380:PRO:HB3	1.54	1.36
1:B:13:MET:CE	1:B:60:ALA:HB1	1.58	1.32
1:A:379:VAL:CG1	1:A:380:PRO:HG3	1.58	1.29
1:A:355:LYS:HD3	1:A:398:PHE:CE1	1.68	1.28
1:D:273:ASP:O	1:D:274:VAL:HG23	1.16	1.25
1:B:13:MET:HE3	1:B:60:ALA:CB	1.69	1.21
1:A:118:LYS:HD3	1:A:378:GLU:OE2	1.36	1.21
1:B:115:ASN:H	1:B:115:ASN:ND2	1.34	1.19
1:B:241:ASN:C	1:B:242:LEU:HD23	1.66	1.16
1:B:115:ASN:HD22	1:B:115:ASN:N	1.37	1.15
1:A:355:LYS:HD3	1:A:398:PHE:CZ	1.82	1.13
1:A:379:VAL:HG13	1:A:380:PRO:HB3	1.16	1.12
1:A:148:SER:O	1:A:149:ALA:CB	1.96	1.11
1:D:258:ARG:HH11	1:D:258:ARG:HG2	1.07	1.09
1:D:273:ASP:O	1:D:274:VAL:CG2	2.01	1.09
1:D:130:ILE:HG21	1:D:276:SER:HB2	1.29	1.09
1:A:148:SER:O	1:A:149:ALA:HB3	1.46	1.08
1:A:379:VAL:HG12	1:A:380:PRO:CD	1.84	1.07
1:B:379:VAL:O	1:B:379:VAL:HG13	1.48	1.07
1:C:130:ILE:HG21	1:C:276:SER:HB3	1.34	1.06
1:D:258:ARG:HH11	1:D:258:ARG:CG	1.69	1.05
1:B:13:MET:CE	1:B:60:ALA:CB	2.27	1.05
1:A:379:VAL:HG12	1:A:380:PRO:HG3	1.17	1.02
1:B:242:LEU:HD23	1:B:242:LEU:N	1.62	1.01
1:A:202:ASN:OD1	1:A:240:LYS:NZ	1.95	1.00
1:D:363:THR:HG21	1:D:394:ILE:HA	1.44	0.99
1:D:107:VAL:HG22	1:D:293:LEU:CD1	1.92	0.97
1:A:274:VAL:O	1:A:277:ASP:HB2	1.66	0.96
1:D:107:VAL:HG22	1:D:293:LEU:HD13	1.48	0.95
1:A:355:LYS:CD	1:A:398:PHE:CE1	2.50	0.94
1:B:203:GLN:HG2	1:B:262:GLY:O	1.69	0.93
1:B:79:ASN:ND2	1:B:82:ARG:HG2	1.83	0.93
1:C:247:THR:HG21	1:C:252:ALA:HB2	1.50	0.93
1:B:380:PRO:HD2	1:B:380:PRO:O	1.69	0.93
1:B:379:VAL:O	1:B:379:VAL:CG1	2.16	0.91
1:C:258:ARG:HG2	1:C:258:ARG:HH11	1.33	0.89
1:D:258:ARG:HG2	1:D:258:ARG:NH1	1.85	0.89
1:A:363:THR:HG22	1:A:368:VAL:HG22	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG11	1:A:380:PRO:HG3	1.53	0.88
1:B:386:ASN:C	1:B:386:ASN:HD22	1.75	0.88
1:D:132:ARG:NH1	1:D:267:CYS:HB3	1.87	0.88
1:D:381:GLU:HB3	2:D:2028:HOH:O	1.73	0.88
1:A:188:ARG:HG2	1:A:228:ILE:HD11	1.55	0.88
1:C:208:SER:HB3	1:C:247:THR:HG23	1.54	0.88
1:B:105:GLY:HA3	1:B:293:LEU:HD11	1.57	0.87
1:B:158:SER:OG	1:B:160:ASN:ND2	2.07	0.86
1:B:149:ALA:O	1:B:171:PHE:O	1.93	0.86
1:B:79:ASN:H	1:B:79:ASN:HD22	1.20	0.86
1:D:160:ASN:ND2	1:D:160:ASN:H	1.70	0.86
1:A:327:MET:HE3	1:A:327:MET:HA	1.58	0.85
1:A:380:PRO:HG2	1:A:382:LYS:HG3	1.58	0.84
1:B:363:THR:CG2	1:B:368:VAL:CG2	2.55	0.84
1:D:51:LYS:HB3	1:D:51:LYS:NZ	1.93	0.83
1:C:208:SER:HB3	1:C:247:THR:CG2	2.07	0.83
1:B:202:ASN:CG	1:B:240:LYS:HZ1	1.82	0.83
1:B:242:LEU:N	1:B:242:LEU:CD2	2.41	0.83
1:D:378:GLU:OE1	1:D:378:GLU:HA	1.76	0.83
1:C:267:CYS:HB2	2:C:2012:HOH:O	1.79	0.81
1:C:289:MET:HB3	1:C:305:ALA:HB3	1.62	0.81
1:C:51:LYS:HB3	1:C:51:LYS:HZ2	1.45	0.81
1:A:327:MET:HA	1:A:327:MET:CE	2.10	0.80
1:A:362:GLN:NE2	1:A:366:ASN:OD1	2.15	0.80
1:B:215:LYS:O	1:B:219:HIS:ND1	2.14	0.79
1:A:253:VAL:HG12	1:A:265:TRP:HH2	1.47	0.79
1:C:284:GLY:O	1:C:285:SER:HB2	1.82	0.79
1:D:379:VAL:O	1:D:382:LYS:HE2	1.84	0.78
1:C:386:ASN:HD22	1:C:386:ASN:C	1.87	0.78
1:A:355:LYS:CD	1:A:398:PHE:CZ	2.65	0.77
1:B:386:ASN:ND2	1:B:389:ASP:H	1.83	0.77
1:A:274:VAL:HG12	1:A:275:MET:N	1.98	0.77
1:C:273:ASP:HB2	1:C:275:MET:H	1.50	0.76
1:B:130:ILE:HD13	1:B:265:TRP:HB3	1.67	0.76
1:B:208:SER:OG	1:B:265:TRP:CH2	2.38	0.76
1:D:79:ASN:O	1:D:80:ALA:C	2.24	0.76
1:D:386:ASN:ND2	1:D:389:ASP:H	1.83	0.76
1:A:215:LYS:O	1:A:219:HIS:HB3	1.85	0.75
1:D:83:VAL:O	1:D:87:ASN:N	2.19	0.75
1:B:79:ASN:HD21	1:B:82:ARG:HG2	1.48	0.74
1:D:107:VAL:CG2	1:D:293:LEU:CD1	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:MET:HE3	1:B:60:ALA:HB1	0.79	0.74
1:B:380:PRO:O	1:B:380:PRO:CD	2.35	0.74
1:D:362:GLN:HE21	1:D:366:ASN:HD21	1.34	0.74
1:B:363:THR:HG23	1:B:368:VAL:CG2	2.17	0.74
1:B:217:TYR:CE2	1:D:178:MET:HB2	2.23	0.73
1:B:274:VAL:O	1:B:277:ASP:N	2.20	0.73
1:D:21:ILE:HD12	1:D:21:ILE:H	1.53	0.73
1:D:114:VAL:HG22	1:D:117:ILE:HG13	1.71	0.73
1:A:3:LYS:HE2	1:A:32:GLU:O	1.88	0.73
1:B:384:ILE:HG13	1:B:384:ILE:O	1.86	0.73
1:B:348:GLU:OE1	1:B:348:GLU:N	2.21	0.73
1:D:132:ARG:CZ	1:D:267:CYS:HB3	2.19	0.72
1:D:104:ASP:O	1:D:104:ASP:OD1	2.07	0.72
1:D:291:SER:HB3	1:D:303:GLU:HG3	1.70	0.72
1:A:3:LYS:CE	1:A:32:GLU:O	2.38	0.72
1:C:284:GLY:O	1:C:285:SER:CB	2.39	0.71
1:D:51:LYS:HB3	1:D:51:LYS:HZ1	1.55	0.71
1:B:117:ILE:HG22	1:B:117:ILE:O	1.90	0.71
1:B:233:TYR:O	1:B:234:LYS:C	2.27	0.71
1:A:253:VAL:HG21	1:C:277:ASP:HB3	1.71	0.70
1:B:325:ASN:HB2	1:B:372:ASP:OD2	1.91	0.70
1:C:386:ASN:ND2	1:C:389:ASP:H	1.90	0.69
1:B:241:ASN:C	1:B:242:LEU:CD2	2.56	0.69
1:C:247:THR:CG2	1:C:252:ALA:HB2	2.21	0.69
1:B:363:THR:HG22	1:B:368:VAL:CG2	2.22	0.69
1:D:146:VAL:CG2	1:D:175:GLY:H	2.07	0.69
1:D:386:ASN:C	1:D:386:ASN:HD22	1.96	0.69
1:B:208:SER:OG	1:B:265:TRP:HH2	1.74	0.68
1:D:51:LYS:NZ	1:D:51:LYS:CB	2.54	0.68
1:B:253:VAL:O	1:B:256:ILE:HG22	1.94	0.68
1:D:160:ASN:H	1:D:160:ASN:HD22	1.38	0.68
1:A:188:ARG:HG2	1:A:228:ILE:CD1	2.23	0.68
1:A:379:VAL:H	1:A:380:PRO:HD3	1.58	0.68
1:C:363:THR:HG21	1:C:394:ILE:HA	1.74	0.67
1:D:386:ASN:HD21	1:D:389:ASP:H	1.41	0.67
1:C:258:ARG:HH11	1:C:258:ARG:CG	2.08	0.67
1:A:251:ASP:O	1:A:255:ARG:HG2	1.95	0.67
1:A:379:VAL:HG12	1:A:380:PRO:N	2.04	0.66
1:A:160:ASN:HD21	1:A:162:GLU:HB2	1.60	0.66
1:D:200:ASP:OD2	1:D:339:LYS:NZ	2.17	0.66
1:C:35:ILE:HD11	1:C:352:PHE:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:CG2	1:C:117:ILE:HG13	2.27	0.65
1:D:81:GLN:O	1:D:84:GLU:HG2	1.96	0.65
1:D:362:GLN:HE21	1:D:366:ASN:ND2	1.93	0.65
1:A:274:VAL:O	1:A:277:ASP:N	2.30	0.65
1:D:359:ALA:O	1:D:363:THR:HG23	1.97	0.65
1:B:79:ASN:HD22	1:B:79:ASN:N	1.94	0.64
1:B:362:GLN:NE2	1:B:366:ASN:OD1	2.30	0.64
1:B:378:GLU:O	1:B:380:PRO:HG3	1.96	0.64
1:A:147:PRO:O	1:A:148:SER:HB3	1.97	0.64
1:A:386:ASN:C	1:A:386:ASN:HD22	2.00	0.64
1:A:115:ASN:N	1:A:115:ASN:HD22	1.96	0.64
1:B:240:LYS:O	1:B:242:LEU:HD21	1.97	0.64
1:D:258:ARG:HH11	1:D:258:ARG:CB	2.10	0.64
1:A:327:MET:HE1	1:A:360:SER:HB3	1.78	0.64
1:B:327:MET:CE	1:B:331:PHE:CE1	2.81	0.64
1:B:121:VAL:O	1:B:122:LYS:C	2.36	0.63
1:D:234:LYS:O	1:D:238:GLU:HG2	1.98	0.63
1:A:274:VAL:O	1:A:277:ASP:CB	2.43	0.63
1:D:377:SER:O	1:D:382:LYS:NZ	2.32	0.63
1:A:114:VAL:O	1:A:114:VAL:CG2	2.46	0.63
1:B:159:GLU:N	1:B:159:GLU:OE1	2.32	0.63
1:D:46:LEU:HD12	1:D:49:ARG:NH2	2.14	0.63
1:D:203:GLN:NE2	2:D:2014:HOH:O	2.19	0.63
1:A:295:SER:HB2	1:A:296:PRO:HD2	1.80	0.63
1:D:13:MET:HE3	1:D:72:LYS:HD2	1.81	0.62
1:A:363:THR:CG2	1:A:368:VAL:HG22	2.28	0.62
1:D:114:VAL:CG2	1:D:117:ILE:HG13	2.29	0.62
1:B:368:VAL:HG23	1:B:368:VAL:O	1.98	0.62
1:C:218:ASP:OD1	1:C:268:LYS:HD3	2.00	0.62
1:C:226:GLN:O	1:C:230:GLU:HG2	2.00	0.62
1:D:130:ILE:HG21	1:D:276:SER:CB	2.19	0.62
1:A:295:SER:HB2	1:A:296:PRO:CD	2.30	0.62
1:B:160:ASN:OD1	1:B:162:GLU:HG3	1.99	0.62
1:B:240:LYS:O	1:B:242:LEU:CD2	2.47	0.62
1:A:379:VAL:N	1:A:380:PRO:HD3	2.13	0.61
1:C:355:LYS:HG3	1:C:401:MET:CE	2.30	0.61
1:B:241:ASN:O	1:B:242:LEU:HD23	2.01	0.61
1:D:151:LYS:HE3	1:D:170:GLU:OE2	2.00	0.61
1:A:362:GLN:HE21	1:A:366:ASN:CG	2.03	0.61
1:C:51:LYS:HB3	1:C:51:LYS:NZ	2.14	0.61
1:D:146:VAL:HG22	1:D:175:GLY:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HD11	1:B:373:LEU:CD2	2.30	0.61
1:B:363:THR:HG23	1:B:368:VAL:HG21	1.82	0.61
1:D:258:ARG:CG	1:D:258:ARG:NH1	2.42	0.61
1:D:79:ASN:OD1	1:D:81:GLN:N	2.34	0.61
1:B:348:GLU:CD	1:B:348:GLU:H	2.03	0.60
1:D:300:TYR:CE1	1:D:339:LYS:HE2	2.36	0.60
1:A:13:MET:CG	1:A:72:LYS:HB2	2.32	0.60
1:D:107:VAL:HG22	1:D:293:LEU:HD12	1.82	0.60
1:B:117:ILE:HD11	1:B:373:LEU:HD22	1.84	0.60
1:B:268:LYS:C	1:B:269:ASN:O	2.36	0.60
1:B:13:MET:CE	1:B:60:ALA:HB3	2.29	0.60
1:B:256:ILE:CG2	1:B:257:ILE:N	2.64	0.59
1:B:79:ASN:ND2	1:B:79:ASN:H	1.96	0.59
1:D:82:ARG:O	1:D:83:VAL:C	2.39	0.59
1:D:146:VAL:CG2	1:D:175:GLY:N	2.65	0.59
1:A:133:HIS:HB2	1:A:190:PHE:CD1	2.38	0.59
1:D:108:PHE:HB2	1:D:292:VAL:HG13	1.83	0.59
1:D:154:LEU:C	1:D:154:LEU:HD13	2.22	0.59
1:D:273:ASP:O	1:D:274:VAL:CB	2.49	0.59
1:B:249:ILE:O	1:B:253:VAL:HG13	2.03	0.59
1:C:63:ALA:HA	1:C:66:LYS:HD2	1.85	0.58
1:A:324:THR:O	1:A:370:THR:HG21	2.02	0.58
1:B:386:ASN:C	1:B:386:ASN:ND2	2.49	0.58
1:C:188:ARG:HG2	1:C:228:ILE:HD11	1.84	0.58
1:B:368:VAL:CG2	1:B:368:VAL:O	2.51	0.58
1:C:166:GLN:HG3	2:C:2013:HOH:O	2.03	0.58
1:C:86:TYR:O	1:C:87:ASN:C	2.42	0.58
1:C:258:ARG:HG2	1:C:258:ARG:NH1	2.08	0.58
1:D:252:ALA:O	1:D:256:ILE:HG12	2.03	0.58
1:B:217:TYR:HE2	1:D:178:MET:HB2	1.69	0.58
1:A:115:ASN:HD22	1:A:115:ASN:H	1.51	0.58
1:A:379:VAL:HG12	1:A:380:PRO:CA	2.25	0.58
1:D:79:ASN:OD1	1:D:79:ASN:C	2.41	0.58
1:D:158:SER:OG	1:D:160:ASN:ND2	2.36	0.58
1:B:105:GLY:HA3	1:B:293:LEU:CD1	2.33	0.57
1:B:79:ASN:OD1	1:B:81:GLN:OE1	2.22	0.57
1:B:111:PRO:HG3	1:B:283:PHE:CD2	2.38	0.57
1:B:363:THR:CG2	1:B:368:VAL:HG22	2.35	0.57
1:D:78:PRO:HG2	1:D:92:TRP:O	2.05	0.57
1:A:386:ASN:ND2	1:A:389:ASP:H	2.02	0.57
1:C:359:ALA:O	1:C:363:THR:CG2	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:O	1:A:219:HIS:CB	2.53	0.56
1:A:219:HIS:CE1	1:A:223:ASP:OD2	2.59	0.56
1:C:386:ASN:HD21	1:C:389:ASP:H	1.53	0.56
1:A:32:GLU:N	1:A:33:PRO:CD	2.68	0.56
1:B:159:GLU:OE1	1:B:159:GLU:CA	2.53	0.56
1:B:272:GLY:O	1:B:276:SER:OG	2.24	0.56
1:B:364:ILE:HD13	1:B:373:LEU:HD13	1.88	0.56
1:A:379:VAL:CB	1:A:380:PRO:CD	2.84	0.55
1:B:32:GLU:N	1:B:33:PRO:CD	2.68	0.55
1:B:79:ASN:OD1	1:B:81:GLN:HB2	2.06	0.55
1:A:3:LYS:HE3	1:A:32:GLU:O	2.05	0.55
1:B:276:SER:O	1:B:280:ALA:HB2	2.07	0.55
1:C:289:MET:HB3	1:C:305:ALA:CB	2.36	0.55
1:A:81:GLN:HB2	2:A:2009:HOH:O	2.06	0.55
1:C:158:SER:OG	1:C:160:ASN:ND2	2.40	0.55
1:C:386:ASN:C	1:C:386:ASN:ND2	2.60	0.55
1:D:13:MET:HG3	1:D:72:LYS:HB2	1.88	0.55
1:A:34:TYR:OH	1:A:399:GLU:OE2	2.21	0.55
1:D:18:MET:HA	1:D:21:ILE:HD13	1.89	0.55
1:D:80:ALA:O	1:D:84:GLU:HG2	2.07	0.55
1:A:160:ASN:C	1:A:160:ASN:HD22	2.10	0.54
1:B:216:THR:HG21	1:D:145:TYR:HB2	1.87	0.54
1:C:24:ARG:HG3	1:C:24:ARG:HH11	1.70	0.54
1:B:276:SER:O	1:B:280:ALA:CB	2.55	0.54
1:C:258:ARG:CG	1:C:258:ARG:NH1	2.66	0.54
1:A:363:THR:HG22	1:A:368:VAL:CG2	2.34	0.54
1:D:72:LYS:HE3	1:D:96:ASN:OD1	2.08	0.54
1:D:107:VAL:CG2	1:D:293:LEU:HD13	2.30	0.54
1:C:362:GLN:HE21	1:C:366:ASN:ND2	2.06	0.54
1:A:304:ALA:HB1	1:A:328:ALA:HB1	1.89	0.54
1:D:21:ILE:HD12	1:D:21:ILE:N	2.21	0.54
1:A:216:THR:CG2	1:C:145:TYR:HB2	2.38	0.54
1:B:202:ASN:OD1	1:B:240:LYS:NZ	2.30	0.54
1:C:72:LYS:HB3	1:C:303:GLU:HG3	1.88	0.54
1:A:118:LYS:CD	1:A:378:GLU:OE2	2.31	0.53
1:C:35:ILE:HD11	1:C:352:PHE:CD2	2.43	0.53
1:A:379:VAL:CG1	1:A:380:PRO:CD	2.64	0.53
1:B:226:GLN:CA	1:B:226:GLN:OE1	2.56	0.53
1:D:269:ASN:O	1:D:273:ASP:OD1	2.26	0.53
1:C:100:ARG:NH1	1:C:101:ALA:HA	2.24	0.53
1:B:362:GLN:HE21	1:B:366:ASN:CG	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:LYS:HG3	1:C:401:MET:HE1	1.89	0.53
1:B:325:ASN:CB	1:B:372:ASP:OD2	2.57	0.53
1:B:250:ASP:HB3	1:D:277:ASP:OD2	2.09	0.53
1:B:284:GLY:O	1:B:285:SER:CB	2.56	0.53
1:A:256:ILE:CG2	1:A:257:ILE:N	2.72	0.53
1:C:359:ALA:O	1:C:363:THR:HG23	2.09	0.53
1:D:13:MET:HB2	1:D:44:LEU:HD22	1.91	0.53
1:D:81:GLN:O	1:D:84:GLU:N	2.42	0.53
1:A:246:TYR:CD1	1:A:246:TYR:C	2.82	0.53
1:C:100:ARG:C	1:C:100:ARG:HH11	2.11	0.53
1:D:199:LEU:HD22	1:D:240:LYS:HE2	1.91	0.53
1:A:237:PHE:CD2	1:A:242:LEU:HD13	2.44	0.52
1:B:327:MET:CE	1:B:331:PHE:HE1	2.21	0.52
1:D:130:ILE:HD11	1:D:279:VAL:HG21	1.89	0.52
1:A:65:GLN:HG2	2:A:2020:HOH:O	2.08	0.52
1:B:79:ASN:HD22	1:B:82:ARG:HG2	1.70	0.52
1:B:133:HIS:HB2	1:B:190:PHE:CD1	2.44	0.52
1:A:380:PRO:HG2	1:A:382:LYS:CG	2.37	0.52
1:B:346:ILE:HG12	1:B:346:ILE:O	2.09	0.52
1:B:390:PHE:O	1:B:394:ILE:HG13	2.09	0.52
1:B:355:LYS:HE3	1:B:398:PHE:CZ	2.45	0.52
1:D:146:VAL:HG22	1:D:175:GLY:N	2.24	0.52
1:B:327:MET:CE	1:B:360:SER:HB3	2.40	0.52
1:D:226:GLN:O	1:D:230:GLU:HG2	2.08	0.52
1:D:166:GLN:HG3	2:D:2016:HOH:O	2.10	0.52
1:B:390:PHE:CE2	1:B:394:ILE:HD11	2.45	0.52
1:C:53:GLU:HG2	1:C:92:TRP:HH2	1.74	0.52
1:B:208:SER:OG	1:B:265:TRP:CZ3	2.63	0.51
1:D:114:VAL:HG22	1:D:117:ILE:CG1	2.37	0.51
1:A:160:ASN:C	1:A:160:ASN:ND2	2.64	0.51
1:B:141:ASN:ND2	1:B:180:MET:HB3	2.25	0.51
1:C:160:ASN:C	1:C:160:ASN:HD22	2.13	0.51
1:D:7:LYS:HG3	1:D:346:ILE:HD11	1.93	0.51
1:A:114:VAL:O	1:A:114:VAL:HG23	2.09	0.51
1:B:200:ASP:C	1:B:200:ASP:OD1	2.49	0.51
1:B:115:ASN:ND2	1:B:115:ASN:N	2.11	0.51
1:B:241:ASN:O	1:B:242:LEU:CD2	2.58	0.51
1:C:13:MET:HB3	1:C:44:LEU:HD22	1.92	0.51
1:A:385:VAL:HB	1:A:389:ASP:HB3	1.93	0.51
1:D:154:LEU:HD12	2:D:2016:HOH:O	2.11	0.51
1:A:117:ILE:O	1:A:117:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ALA:O	1:D:363:THR:CG2	2.59	0.51
1:A:127:PRO:O	1:A:262:GLY:HA2	2.11	0.51
1:B:143:GLU:OE1	1:D:216:THR:HB	2.10	0.51
1:D:132:ARG:HH12	1:D:267:CYS:HB3	1.74	0.51
1:A:379:VAL:H	1:A:380:PRO:CD	2.23	0.50
1:B:362:GLN:HE21	1:B:366:ASN:ND2	2.07	0.50
1:A:322:THR:O	1:A:386:ASN:HB2	2.11	0.50
1:A:364:ILE:HG23	1:A:369:MET:HE2	1.93	0.50
1:B:160:ASN:H	1:B:160:ASN:HD22	1.59	0.50
1:B:226:GLN:OE1	1:B:226:GLN:O	2.30	0.50
1:C:325:ASN:ND2	1:C:328:ALA:H	2.10	0.50
1:D:108:PHE:CE2	1:D:131:ALA:HB2	2.46	0.50
1:D:258:ARG:NH1	1:D:258:ARG:CB	2.73	0.50
1:A:211:ASP:HB2	1:A:218:ASP:HB3	1.94	0.50
1:A:385:VAL:HB	1:A:389:ASP:CB	2.42	0.50
1:A:143:GLU:OE1	1:C:216:THR:HB	2.12	0.50
1:A:253:VAL:O	1:A:256:ILE:HG22	2.12	0.50
1:D:108:PHE:CD2	1:D:131:ALA:HB2	2.46	0.50
1:D:295:SER:HB2	1:D:296:PRO:HD2	1.93	0.50
1:A:188:ARG:CG	1:A:228:ILE:HD11	2.33	0.50
1:D:235:GLU:CD	1:D:235:GLU:H	2.14	0.50
1:B:130:ILE:HD13	1:B:265:TRP:CB	2.37	0.50
1:B:149:ALA:O	1:B:171:PHE:HB2	2.12	0.50
1:D:146:VAL:HG23	1:D:175:GLY:H	1.75	0.50
1:B:295:SER:HB2	1:B:296:PRO:CD	2.42	0.49
1:A:355:LYS:CE	1:A:398:PHE:CZ	2.96	0.49
1:C:143:GLU:HG2	1:C:178:MET:HG2	1.94	0.49
1:A:386:ASN:HD21	1:A:389:ASP:H	1.58	0.49
1:C:100:ARG:NH1	1:C:100:ARG:O	2.45	0.49
1:D:46:LEU:CD1	1:D:49:ARG:NH2	2.75	0.49
1:A:216:THR:HG21	1:C:145:TYR:HB2	1.94	0.49
1:B:400:GLY:O	1:B:401:MET:O	2.30	0.49
1:B:274:VAL:O	1:B:277:ASP:HB2	2.11	0.49
1:A:256:ILE:HG23	1:A:257:ILE:N	2.27	0.49
1:C:114:VAL:HG22	1:C:117:ILE:HG13	1.95	0.49
1:A:180:MET:HG2	1:A:181:HIS:N	2.28	0.49
1:C:397:THR:O	1:C:401:MET:HG3	2.13	0.49
1:B:219:HIS:CD2	1:B:219:HIS:C	2.86	0.49
1:D:146:VAL:HG21	1:D:171:PHE:CD2	2.48	0.49
1:D:160:ASN:ND2	1:D:160:ASN:N	2.48	0.49
1:A:386:ASN:C	1:A:386:ASN:ND2	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PHE:CE2	1:D:131:ALA:CB	2.95	0.48
1:B:363:THR:HG22	1:B:368:VAL:HG23	1.94	0.48
1:C:355:LYS:HG3	1:C:401:MET:HE3	1.94	0.48
1:D:368:VAL:HG11	1:D:393:GLU:HG3	1.96	0.48
1:A:355:LYS:CE	1:A:398:PHE:CE1	2.96	0.48
1:D:89:LYS:O	1:D:90:LYS:HG3	2.13	0.48
1:D:378:GLU:OE1	1:D:378:GLU:CA	2.55	0.48
1:A:158:SER:OG	1:A:160:ASN:ND2	2.46	0.48
1:A:379:VAL:CB	1:A:380:PRO:HD3	2.43	0.48
1:C:355:LYS:CG	1:C:401:MET:HE1	2.44	0.48
1:A:398:PHE:O	1:A:400:GLY:N	2.44	0.48
1:D:249:ILE:O	1:D:253:VAL:HG13	2.14	0.48
1:A:362:GLN:HE21	1:A:366:ASN:ND2	2.12	0.47
1:B:237:PHE:CD2	1:B:242:LEU:HB2	2.49	0.47
1:B:327:MET:HE2	1:B:331:PHE:CE1	2.49	0.47
1:C:355:LYS:CG	1:C:401:MET:CE	2.93	0.47
1:A:237:PHE:HA	1:A:242:LEU:HD11	1.96	0.47
1:B:78:PRO:HA	1:B:82:ARG:HG3	1.96	0.47
1:B:217:TYR:HB2	1:D:143:GLU:CD	2.35	0.47
1:B:240:LYS:HB3	1:B:240:LYS:HE2	1.43	0.47
1:B:246:TYR:CD1	1:B:247:THR:N	2.83	0.47
1:A:13:MET:HA	1:A:42:TYR:O	2.14	0.47
1:A:220:ARG:HA	1:A:220:ARG:CZ	2.45	0.47
1:B:355:LYS:CE	1:B:398:PHE:CZ	2.98	0.47
1:D:246:TYR:O	1:D:247:THR:HB	2.15	0.47
1:B:149:ALA:HB3	1:D:159:GLU:CG	2.45	0.47
1:A:209:THR:OG1	1:A:211:ASP:HB3	2.15	0.46
1:A:379:VAL:CB	1:A:380:PRO:HG3	2.37	0.46
1:B:83:VAL:HA	1:B:88:LEU:HG	1.97	0.46
1:A:325:ASN:C	1:A:325:ASN:OD1	2.52	0.46
1:C:17:GLU:O	1:C:20:ARG:HB3	2.16	0.46
1:D:199:LEU:CD2	1:D:240:LYS:HE2	2.44	0.46
1:B:226:GLN:OE1	1:B:226:GLN:C	2.54	0.46
1:B:65:GLN:O	1:B:299:LYS:HE3	2.16	0.46
1:A:327:MET:HE3	1:A:330:ILE:HD12	1.98	0.46
1:B:233:TYR:O	1:B:235:GLU:N	2.48	0.46
1:A:160:ASN:ND2	1:A:162:GLU:H	2.14	0.46
1:B:114:VAL:HG22	1:B:117:ILE:HB	1.96	0.46
1:D:81:GLN:O	1:D:82:ARG:C	2.54	0.46
1:B:35:ILE:HD11	1:B:352:PHE:CE2	2.51	0.46
1:B:115:ASN:H	1:B:115:ASN:HD22	0.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:CB	1:A:380:PRO:CG	2.86	0.45
1:B:256:ILE:HG22	1:B:257:ILE:N	2.31	0.45
1:B:363:THR:HG22	1:B:368:VAL:HG22	1.94	0.45
1:D:37:LEU:HD12	1:D:37:LEU:HA	1.40	0.45
1:D:72:LYS:CE	1:D:96:ASN:OD1	2.63	0.45
1:A:363:THR:CG2	1:A:368:VAL:CG2	2.94	0.45
1:C:362:GLN:HE21	1:C:366:ASN:HD21	1.62	0.45
1:C:258:ARG:HD3	2:C:2020:HOH:O	2.15	0.45
1:A:338:LYS:HE3	1:A:338:LYS:HB2	1.30	0.45
1:B:247:THR:OG1	1:B:248:LEU:N	2.50	0.45
1:A:371:LYS:O	1:A:374:ALA:HB3	2.15	0.45
1:A:323:SER:OG	1:A:371:LYS:CB	2.65	0.45
1:A:355:LYS:HE2	1:A:398:PHE:CE2	2.52	0.45
1:C:208:SER:HA	1:C:247:THR:O	2.16	0.45
1:A:293:LEU:HB3	1:A:301:GLU:HB3	1.99	0.45
1:C:224:ILE:O	1:C:228:ILE:HG12	2.16	0.45
1:A:155:VAL:HG21	1:C:155:VAL:HG21	1.98	0.45
1:B:216:THR:HA	1:B:219:HIS:CE1	2.52	0.45
1:B:275:MET:HA	1:B:278:MET:HB3	1.98	0.45
1:D:133:HIS:O	1:D:134:ALA:HB2	2.17	0.45
1:B:130:ILE:CD1	1:B:265:TRP:HB3	2.43	0.45
1:C:354:THR:HG22	1:C:358:GLN:NE2	2.32	0.45
1:A:23:TRP:HH2	1:A:71:VAL:HG22	1.83	0.44
1:B:355:LYS:HD2	1:B:401:MET:CE	2.47	0.44
1:D:197:TYR:CE1	1:D:292:VAL:HG11	2.52	0.44
1:A:91:MET:O	1:A:92:TRP:C	2.55	0.44
1:C:77:THR:HA	1:C:78:PRO:HD3	1.76	0.44
1:C:295:SER:OG	1:C:297:ASP:HB3	2.18	0.44
1:D:203:GLN:HG3	1:D:264:VAL:HG23	2.00	0.44
1:D:268:LYS:HE2	1:D:268:LYS:HB3	1.60	0.44
1:C:82:ARG:O	1:C:83:VAL:C	2.55	0.44
1:D:132:ARG:HG3	1:D:135:TYR:CD1	2.52	0.44
1:D:379:VAL:HA	1:D:380:PRO:HD3	1.65	0.44
1:A:13:MET:HG3	1:A:72:LYS:HB2	1.99	0.44
1:A:368:VAL:HA	1:A:383:LYS:O	2.17	0.44
1:D:247:THR:HG23	1:D:252:ALA:HB2	1.99	0.44
1:A:116:SER:CB	1:A:379:VAL:HG23	2.48	0.44
1:A:99:ILE:HG21	1:A:301:GLU:OE2	2.18	0.44
1:A:7:LYS:HB2	1:A:346:ILE:HD11	1.99	0.43
1:A:100:ARG:O	1:A:104:ASP:N	2.50	0.43
1:A:195:PHE:O	1:A:196:ASN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:O	1:B:242:LEU:HD23	2.16	0.43
1:B:363:THR:CG2	1:B:368:VAL:HG23	2.45	0.43
1:C:160:ASN:ND2	1:C:160:ASN:C	2.70	0.43
1:D:228:ILE:O	1:D:232:GLU:HB2	2.17	0.43
1:A:116:SER:HB3	1:A:379:VAL:HG23	1.99	0.43
1:C:95:PRO:O	1:C:99:ILE:HD12	2.17	0.43
1:A:211:ASP:OD1	1:A:211:ASP:C	2.56	0.43
1:B:352:PHE:O	1:B:353:ALA:C	2.56	0.43
1:B:368:VAL:HG21	1:B:393:GLU:HG2	2.00	0.43
1:C:379:VAL:HA	1:C:380:PRO:HD3	1.53	0.43
1:B:363:THR:HG23	1:B:368:VAL:HG22	1.97	0.43
1:B:68:GLY:C	1:B:69:VAL:HG23	2.39	0.43
1:A:380:PRO:HB2	1:A:381:GLU:H	1.11	0.43
1:D:295:SER:OG	1:D:299:LYS:HB2	2.18	0.43
1:B:398:PHE:O	1:B:400:GLY:O	2.36	0.42
1:A:352:PHE:CD1	1:A:352:PHE:C	2.92	0.42
1:C:202:ASN:HD21	1:C:240:LYS:HD3	1.85	0.42
1:D:21:ILE:H	1:D:21:ILE:CD1	2.28	0.42
1:A:15:GLY:O	1:A:20:ARG:HD2	2.18	0.42
1:B:149:ALA:O	1:B:171:PHE:C	2.56	0.42
1:B:278:MET:O	1:B:282:ALA:HB2	2.19	0.42
1:C:202:ASN:ND2	1:C:240:LYS:HD3	2.34	0.42
1:D:13:MET:HG3	1:D:72:LYS:CB	2.49	0.42
1:A:13:MET:HG2	1:A:72:LYS:HB2	2.01	0.42
1:D:184:ASP:OD1	1:D:220:ARG:HD3	2.20	0.42
1:A:242:LEU:HD12	1:A:242:LEU:O	2.19	0.42
1:D:100:ARG:HG3	1:D:293:LEU:HD11	2.02	0.42
1:D:238:GLU:O	1:D:239:ALA:C	2.58	0.42
1:D:246:TYR:CD2	1:D:246:TYR:C	2.93	0.42
1:B:22:ILE:HG21	1:B:326:SER:HB3	2.02	0.42
1:B:179:GLY:HA2	1:D:178:MET:O	2.19	0.42
1:C:275:MET:O	1:C:278:MET:HB3	2.19	0.42
1:D:77:THR:HA	1:D:78:PRO:HD2	1.60	0.42
1:A:7:LYS:HB3	1:A:8:VAL:H	1.58	0.42
1:A:208:SER:HA	1:A:247:THR:O	2.20	0.42
1:C:208:SER:HB3	1:C:247:THR:HG22	1.93	0.42
1:A:17:GLU:O	1:A:21:ILE:HD12	2.20	0.41
1:A:160:ASN:HD22	1:A:161:GLY:N	2.18	0.41
1:B:11:VAL:O	1:B:70:GLY:HA2	2.19	0.41
1:C:350:VAL:CG2	1:C:351:ASP:N	2.82	0.41
1:B:246:TYR:CD1	1:B:246:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:OD1	1:A:303:GLU:OE2	2.38	0.41
1:B:226:GLN:OE1	1:B:226:GLN:HA	2.20	0.41
1:B:361:VAL:CG1	1:B:365:GLU:OE2	2.69	0.41
1:A:115:ASN:N	1:A:115:ASN:ND2	2.67	0.41
1:D:295:SER:HB2	1:D:296:PRO:CD	2.51	0.41
1:A:18:MET:O	1:A:21:ILE:HB	2.20	0.41
1:A:114:VAL:HG22	1:A:117:ILE:HB	2.02	0.41
1:A:211:ASP:O	1:A:211:ASP:CG	2.58	0.41
1:C:24:ARG:HG3	1:C:24:ARG:NH1	2.34	0.41
1:C:114:VAL:HG22	1:C:117:ILE:CG1	2.51	0.41
1:D:32:GLU:N	1:D:33:PRO:CD	2.83	0.41
1:D:104:ASP:OD1	1:D:104:ASP:C	2.59	0.41
1:A:108:PHE:CE2	1:A:131:ALA:HB2	2.56	0.41
1:A:384:ILE:O	1:A:384:ILE:HG13	2.18	0.41
1:B:111:PRO:HG3	1:B:283:PHE:CE2	2.56	0.41
1:B:355:LYS:HE3	1:B:398:PHE:CE2	2.54	0.41
1:C:268:LYS:HB3	1:C:268:LYS:HE2	1.79	0.41
1:D:133:HIS:HB2	1:D:190:PHE:CD1	2.56	0.41
1:D:154:LEU:HB2	1:D:168:ILE:HD11	2.03	0.41
1:A:380:PRO:CG	1:A:381:GLU:N	2.74	0.41
1:B:216:THR:CG2	1:D:145:TYR:HB2	2.51	0.41
1:A:23:TRP:CE3	1:A:73:CYS:HB2	2.56	0.41
1:A:126:LYS:O	1:A:127:PRO:C	2.57	0.41
1:A:245:PHE:HE2	1:A:255:ARG:HD2	1.87	0.41
1:C:235:GLU:N	1:C:235:GLU:CD	2.75	0.41
1:D:82:ARG:O	1:D:86:TYR:N	2.39	0.41
1:B:356:LEU:O	1:B:357:GLU:C	2.58	0.40
1:D:230:GLU:HG2	1:D:230:GLU:H	1.63	0.40
1:D:289:MET:HB3	1:D:305:ALA:CB	2.51	0.40
1:B:13:MET:HA	1:B:42:TYR:O	2.21	0.40
1:B:208:SER:HB3	1:B:247:THR:O	2.22	0.40
1:B:355:LYS:HD2	1:B:401:MET:HE3	2.02	0.40
1:C:160:ASN:HD22	1:C:161:GLY:N	2.19	0.40
1:C:359:ALA:O	1:C:363:THR:HG22	2.21	0.40
1:D:77:THR:OG1	1:D:94:SER:HB2	2.22	0.40
1:D:151:LYS:CE	1:D:170:GLU:OE2	2.69	0.40
1:A:104:ASP:O	1:A:104:ASP:CG	2.58	0.40
1:B:68:GLY:C	1:B:69:VAL:CG2	2.90	0.40
1:D:26:ILE:O	1:D:27:LYS:C	2.59	0.40
1:C:300:TYR:CE1	1:C:339:LYS:HE2	2.56	0.40

There are no symmetry-related clashes.

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	368/402 (92%)	338 (92%)	24 (6%)	6 (2%)	9	8
1	B	364/402 (90%)	329 (90%)	28 (8%)	7 (2%)	8	6
1	C	363/402 (90%)	342 (94%)	16 (4%)	5 (1%)	11	9
1	D	367/402 (91%)	347 (95%)	17 (5%)	3 (1%)	19	20
All	All	1462/1608 (91%)	1356 (93%)	85 (6%)	21 (1%)	11	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	A	380	PRO
1	B	122	LYS
1	B	150	GLY
1	B	285	SER
1	B	380	PRO
1	C	274	VAL
1	C	285	SER
1	D	274	VAL
1	A	149	ALA
1	C	297	ASP
1	D	83	VAL
1	A	379	VAL
1	B	399	GLU
1	A	399	GLU
1	B	269	ASN
1	B	378	GLU
1	C	87	ASN
1	D	136	GLY
1	A	400	GLY
1	C	83	VAL

5.3.2　Protein sidechains　ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/347 (87%)	270 (89%)	32 (11%)	6	6
1	B	291/347 (84%)	254 (87%)	37 (13%)	4	4
1	C	299/347 (86%)	276 (92%)	23 (8%)	13	12
1	D	306/347 (88%)	269 (88%)	37 (12%)	5	4
All	All	1198/1388 (86%)	1069 (89%)	129 (11%)	6	6

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	13	MET
1	A	18	MET
1	A	37	LEU
1	A	114	VAL
1	A	115	ASN
1	A	118	LYS
1	A	125	LYS
1	A	159	GLU
1	A	160	ASN
1	A	162	GLU
1	A	164	SER
1	A	186	SER
1	A	205	LEU
1	A	210	LYS
1	A	211	ASP
1	A	242	LEU
1	A	255	ARG
1	A	256	ILE
1	A	269	ASN
1	A	292	VAL
1	A	322	THR
1	A	327	MET
1	A	329	THR

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Mol	Chain	Res	Type
1	A	338	LYS
1	A	368	VAL
1	A	377	SER
1	A	379	VAL
1	A	384	ILE
1	A	386	ASN
1	A	393	GLU
1	A	401	MET
1	B	25	LEU
1	B	37	LEU
1	B	79	ASN
1	B	87	ASN
1	B	94	SER
1	B	115	ASN
1	B	159	GLU
1	B	160	ASN
1	B	164	SER
1	B	172	ASP
1	B	186	SER
1	B	200	ASP
1	B	201	MET
1	B	205	LEU
1	B	215	LYS
1	B	217	TYR
1	B	219	HIS
1	B	226	GLN
1	B	230	GLU
1	B	242	LEU
1	B	256	ILE
1	B	257	ILE
1	B	265	TRP
1	B	271	ASP
1	B	276	SER
1	B	292	VAL
1	B	322	THR
1	B	329	THR
1	B	338	LYS
1	B	346	ILE
1	B	348	GLU
1	B	379	VAL
1	B	380	PRO
1	B	384	ILE

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Mol	Chain	Res	Type
1	B	386	ASN
1	B	393	GLU
1	B	401	MET
1	C	95	PRO
1	C	100	ARG
1	C	114	VAL
1	C	146	VAL
1	C	160	ASN
1	C	165	ARG
1	C	199	LEU
1	C	200	ASP
1	C	205	LEU
1	C	211	ASP
1	C	212	THR
1	C	253	VAL
1	C	258	ARG
1	C	263	MET
1	C	267	CYS
1	C	268	LYS
1	C	273	ASP
1	C	289	MET
1	C	297	ASP
1	C	350	VAL
1	C	363	THR
1	C	379	VAL
1	C	386	ASN
1	D	2	SER
1	D	13	MET
1	D	37	LEU
1	D	62	ARG
1	D	76	ILE
1	D	79	ASN
1	D	84	GLU
1	D	93	LYS
1	D	94	SER
1	D	100	ARG
1	D	142	VAL
1	D	160	ASN
1	D	164	SER
1	D	172	ASP
1	D	178	MET
1	D	202	ASN

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Mol	Chain	Res	Type
1	D	205	LEU
1	D	211	ASP
1	D	220	ARG
1	D	230	GLU
1	D	235	GLU
1	D	238	GLU
1	D	253	VAL
1	D	258	ARG
1	D	268	LYS
1	D	273	ASP
1	D	276	SER
1	D	285	SER
1	D	288	MET
1	D	289	MET
1	D	299	LYS
1	D	301	GLU
1	D	325	ASN
1	D	350	VAL
1	D	363	THR
1	D	378	GLU
1	D	386	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	160	ASN
1	A	241	ASN
1	A	362	GLN
1	A	386	ASN
1	B	79	ASN
1	B	87	ASN
1	B	115	ASN
1	B	141	ASN
1	B	160	ASN
1	B	362	GLN
1	B	386	ASN
1	C	160	ASN
1	C	325	ASN
1	C	358	GLN
1	C	366	ASN
1	C	386	ASN

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Mol	Chain	Res	Type
1	D	160	ASN
1	D	182	ASN
1	D	231	ASN
1	D	325	ASN
1	D	366	ASN
1	D	386	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	376/402 (93%)	0.27	12 (3%)	47	59	31, 50, 80, 121	0
1	B	372/402 (92%)	0.32	14 (3%)	40	53	33, 53, 86, 104	0
1	C	371/402 (92%)	0.18	11 (2%)	50	61	26, 42, 75, 97	0
1	D	375/402 (93%)	0.19	11 (2%)	51	62	27, 44, 75, 100	0
All	All	1494/1608 (92%)	0.24	48 (3%)	47	59	26, 47, 81, 121	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	ASP	5.3
1	A	212	THR	4.9
1	B	217	TYR	4.5
1	D	84	GLU	3.8
1	D	91	MET	3.5
1	D	135	TYR	3.4
1	A	213	ILE	3.4
1	A	384	ILE	3.4
1	D	211	ASP	3.4
1	A	322	THR	3.4
1	B	379	VAL	3.3
1	A	399	GLU	3.2
1	C	86	TYR	3.2
1	D	274	VAL	3.0
1	D	80	ALA	3.0
1	D	78	PRO	3.0
1	D	87	ASN	2.9
1	A	216	THR	2.9
1	B	216	THR	2.8
1	C	211	ASP	2.7
1	C	87	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	271	ASP	2.6
1	C	78	PRO	2.5
1	C	91	MET	2.5
1	A	323	SER	2.5
1	A	180	MET	2.5
1	B	237	PHE	2.5
1	B	219	HIS	2.4
1	B	230	GLU	2.4
1	B	345	GLY	2.4
1	C	266	ALA	2.3
1	B	239	ALA	2.2
1	C	88	LEU	2.2
1	B	265	TRP	2.2
1	A	380	PRO	2.2
1	C	80	ALA	2.2
1	C	276	SER	2.2
1	B	245	PHE	2.1
1	D	79	ASN	2.1
1	C	274	VAL	2.1
1	D	81	GLN	2.1
1	B	374	ALA	2.1
1	B	399	GLU	2.1
1	D	145	TYR	2.1
1	A	81	GLN	2.0
1	B	199	LEU	2.0
1	C	278	MET	2.0
1	B	322	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.