



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID : 2IED
Title : CRYSTAL STRUCTURE of ISONIAZID-RESISTANT S94A ENOYL-ACP(COA) REDUCTASE MUTANT ENZYME FROM MYCOBACTERIUM TUBERCULOSIS UNCOMPLEXED
Authors : Dias, M.V.B.; Prado, A.M.X.; Vasconcelos, I.B.; Fadel, V.; Basso, L.A.; Santos, D.S.; Azevedo Jr., W.F.
Deposited on : 2006-09-18
Resolution : 2.14 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

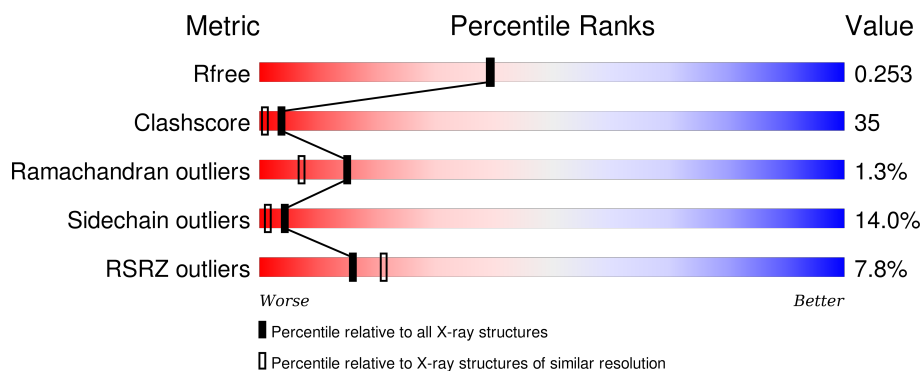
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	<div> <div>9%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>9%</div> </div> </div>
1	B	268	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>35%</div> <div>10%</div> </div> </div>
1	C	268	<div> <div>7%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>10%</div> </div> </div>
1	D	268	<div> <div>10%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8673 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total 1993	C 1263	N 348	O 372	S 10	0	0	0
1	B	268	Total 1993	C 1263	N 348	O 372	S 10	0	0	0
1	C	268	Total 1993	C 1263	N 348	O 372	S 10	0	0	0
1	D	268	Total 1993	C 1263	N 348	O 372	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	SER	ENGINEERED	UNP P0A5Y6
B	94	ALA	SER	ENGINEERED	UNP P0A5Y6
C	94	ALA	SER	ENGINEERED	UNP P0A5Y6
D	94	ALA	SER	ENGINEERED	UNP P0A5Y6

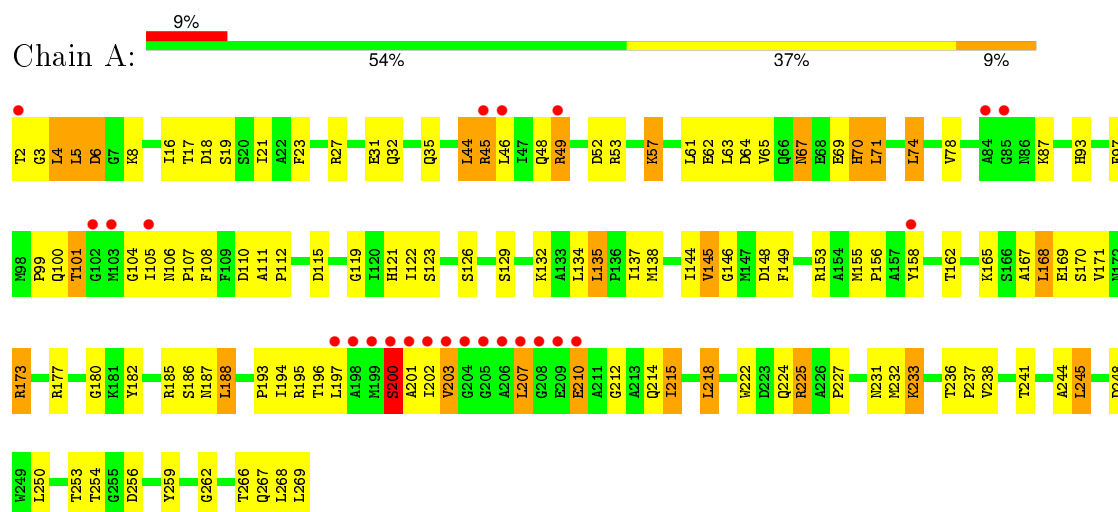
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	185	Total 185	O 185	0	0
2	B	169	Total 169	O 169	0	0
2	C	185	Total 185	O 185	0	0
2	D	162	Total 162	O 162	0	0

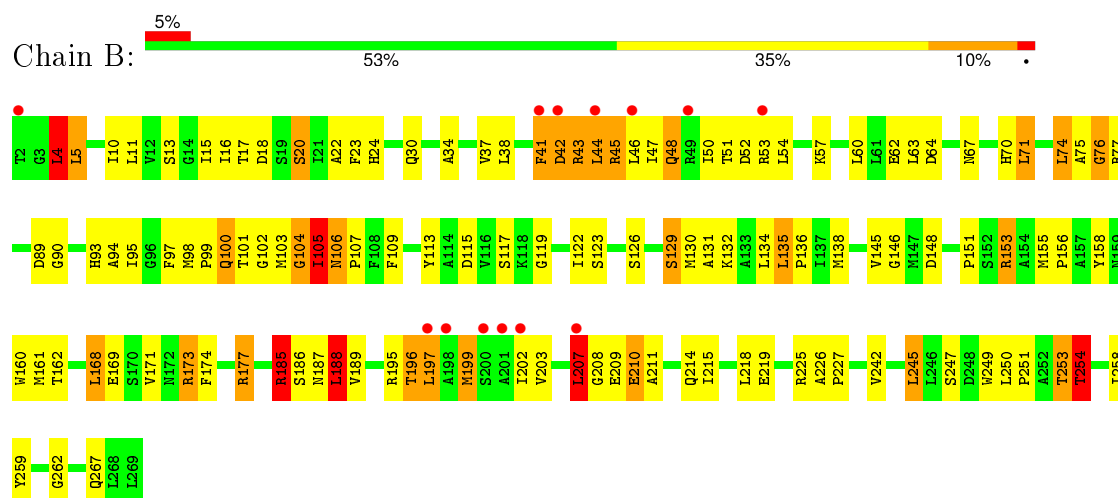
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Enoyl-[acyl-carrier-protein] reductase [NADH]

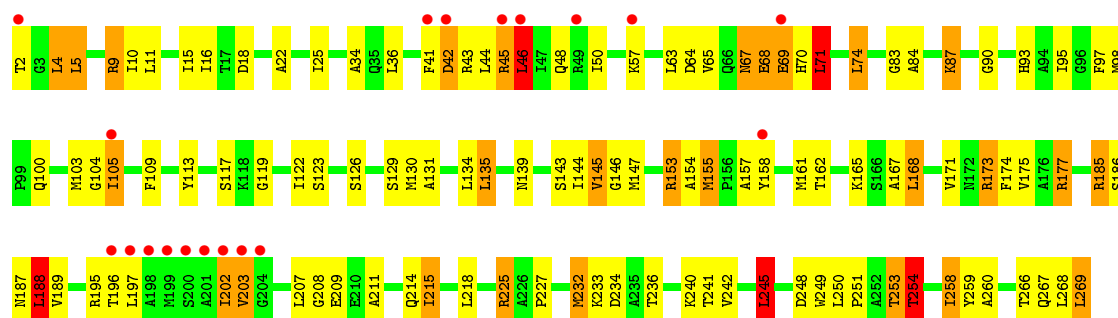


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

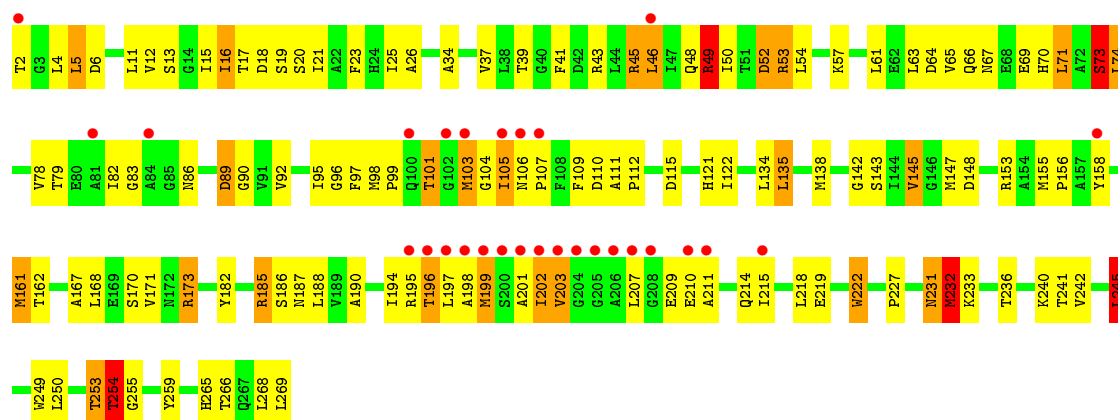


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.69Å 63.52Å 65.18Å 97.21° 85.81° 102.87°	Depositor
Resolution (Å)	42.26 – 2.14 42.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.26-2.14) 91.7 (42.24-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.162 , 0.255 0.161 , 0.253	Depositor DCC
R_{free} test set	2234 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44052 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8673	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	1/2031 (0.0%)	0.99	2/2757 (0.1%)
1	B	1.07	5/2031 (0.2%)	1.24	15/2757 (0.5%)
1	C	1.09	0/2031	1.16	18/2757 (0.7%)
1	D	1.01	1/2031 (0.0%)	1.09	12/2757 (0.4%)
All	All	1.05	7/8124 (0.1%)	1.12	47/11028 (0.4%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	ARG	CB-CG	-6.79	1.34	1.52
1	B	210	GLU	CG-CD	6.59	1.61	1.51
1	B	171	VAL	CB-CG1	5.85	1.65	1.52
1	B	210	GLU	CB-CG	5.66	1.62	1.52
1	B	129	SER	CB-OG	-5.45	1.35	1.42
1	D	145	VAL	CB-CG2	-5.35	1.41	1.52
1	A	108	PHE	CB-CG	-5.04	1.42	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ARG	NE-CZ-NH2	-22.58	109.01	120.30
1	B	173	ARG	NE-CZ-NH1	13.06	126.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	D	173	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	C	153	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	49	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	B	173	ARG	CG-CD-NE	-7.93	95.14	111.80
1	B	173	ARG	CD-NE-CZ	7.80	134.52	123.60
1	C	153	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	185	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	188	LEU	CB-CG-CD1	6.93	122.77	111.00
1	B	104	GLY	N-CA-C	-6.90	95.85	113.10
1	A	225	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	C	245	LEU	CB-CG-CD1	6.77	122.50	111.00
1	C	173	ARG	CG-CD-NE	-6.75	97.62	111.80
1	D	49	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	D	96	GLY	N-CA-C	-6.47	96.92	113.10
1	C	173	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	188	LEU	CB-CG-CD1	6.35	121.79	111.00
1	C	68	GLU	N-CA-C	6.30	128.02	111.00
1	C	254	THR	CB-CA-C	-6.25	94.73	111.60
1	A	173	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	C	225	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	C	9	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	52	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	B	254	THR	CB-CA-C	-5.86	95.78	111.60
1	B	76	GLY	N-CA-C	-5.80	98.59	113.10
1	D	254	THR	CB-CA-C	-5.79	95.96	111.60
1	B	89	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	B	185	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	173	ARG	CG-CD-NE	-5.63	99.98	111.80
1	D	185	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	185	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	68	GLU	C-N-CA	-5.55	107.83	121.70
1	B	207	LEU	N-CA-C	-5.54	96.04	111.00
1	B	153	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	71	LEU	CB-CG-CD1	5.49	120.33	111.00
1	B	185	ARG	CG-CD-NE	-5.46	100.33	111.80
1	D	89	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	C	234	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	D	173	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	46	LEU	CB-CG-CD2	5.22	119.88	111.00
1	B	4	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	185	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	87	LYS	CD-CE-NZ	5.05	123.31	111.70
1	D	245	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	LEU	Peptide
1	C	83	GLY	Peptide
1	D	199	MET	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	1993	0	2008	144	0
1	B	1993	0	2008	148	0
1	C	1993	0	2008	155	0
1	D	1993	0	2008	151	0
2	A	185	0	0	32	2
2	B	169	0	0	25	0
2	C	185	0	0	33	1
2	D	162	0	0	36	1
All	All	8673	0	8032	564	2

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 35.

All (564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:O	1:B:43:ARG:N	1.62	1.31
1:C:67:ASN:HD22	1:C:68:GLU:N	1.31	1.27
1:A:253:THR:HB	2:A:273:HOH:O	1.10	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:HB1	2:C:358:HOH:O	1.29	1.24
1:D:26:ALA:HB2	2:D:364:HOH:O	1.08	1.20
1:B:145:VAL:HB	2:B:411:HOH:O	1.04	1.19
1:C:68:GLU:C	1:C:70:HIS:H	1.48	1.15
1:C:68:GLU:O	1:C:70:HIS:N	1.79	1.15
1:A:254:THR:HB	2:A:318:HOH:O	0.97	1.13
1:C:232:MET:CB	2:C:404:HOH:O	1.97	1.11
1:D:15:ILE:HD11	2:D:364:HOH:O	1.52	1.09
1:C:147:MET:SD	2:C:313:HOH:O	2.12	1.07
1:D:218:LEU:HG	2:D:330:HOH:O	1.55	1.06
1:C:232:MET:HB2	2:C:404:HOH:O	1.56	1.06
1:A:17:THR:HG22	1:A:19:SER:H	1.17	1.05
1:B:254:THR:HG21	2:B:270:HOH:O	1.55	1.05
1:B:185:ARG:HB2	1:B:254:THR:HG23	1.39	1.05
1:C:254:THR:HG21	2:C:291:HOH:O	1.56	1.03
1:C:68:GLU:C	1:C:70:HIS:N	2.10	1.02
1:A:248:ASP:OD1	2:A:453:HOH:O	1.79	1.00
1:C:87:LYS:HD3	2:C:397:HOH:O	1.60	1.00
1:C:68:GLU:OE1	1:C:68:GLU:N	1.94	1.00
1:C:202:ILE:HA	1:C:207:LEU:HD13	1.45	0.99
1:A:145:VAL:CG1	2:A:391:HOH:O	2.10	0.99
1:B:101:THR:HG21	1:B:115:ASP:OD2	1.63	0.99
1:B:218:LEU:HD23	1:D:269:LEU:HG	1.45	0.99
1:D:98:MET:HE2	2:D:376:HOH:O	1.63	0.98
1:D:101:THR:HG21	1:D:112:PRO:HD2	1.45	0.97
1:B:158:TYR:HD1	1:B:162:THR:HG1	0.98	0.97
1:D:145:VAL:HG21	1:D:242:VAL:HG13	1.45	0.96
1:C:45:ARG:HH11	1:C:45:ARG:HB3	1.29	0.95
1:C:233:LYS:CE	2:C:392:HOH:O	2.14	0.95
1:C:186:SER:H	1:C:254:THR:HG22	1.31	0.95
1:A:145:VAL:HG12	2:A:391:HOH:O	1.65	0.95
1:B:199:MET:HG2	2:B:351:HOH:O	1.65	0.94
1:B:41:PHE:C	1:B:43:ARG:H	1.71	0.94
1:A:145:VAL:HB	2:A:391:HOH:O	1.66	0.93
1:C:67:ASN:ND2	1:C:68:GLU:N	2.15	0.93
1:C:196:THR:HB	2:C:441:HOH:O	1.68	0.93
1:A:253:THR:HG23	2:D:286:HOH:O	1.69	0.93
1:D:46:LEU:HB3	2:D:339:HOH:O	1.65	0.92
1:D:101:THR:HG21	1:D:115:ASP:OD1	1.68	0.92
1:B:129:SER:HB3	2:B:308:HOH:O	1.70	0.91
1:A:200:SER:HA	1:A:203:VAL:HB	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:THR:HG21	2:D:288:HOH:O	1.70	0.90
1:C:104:GLY:HA2	1:C:157:ALA:HA	1.52	0.90
1:B:16:ILE:HB	2:B:435:HOH:O	1.71	0.89
1:A:158:TYR:HD1	1:A:162:THR:HG1	0.93	0.89
1:A:101:THR:HG21	1:A:112:PRO:HD2	1.52	0.88
1:D:99:PRO:HD3	2:D:426:HOH:O	1.72	0.87
1:B:186:SER:H	1:B:254:THR:CG2	1.87	0.87
1:D:147:MET:SD	2:D:296:HOH:O	2.31	0.87
1:C:68:GLU:HG2	2:C:416:HOH:O	1.73	0.86
1:C:232:MET:HB3	2:C:404:HOH:O	1.64	0.86
1:A:64:ASP:H	1:A:70:HIS:HD2	1.23	0.86
1:D:97:PHE:CD2	2:D:426:HOH:O	2.28	0.86
1:C:45:ARG:HH11	1:C:45:ARG:CB	1.87	0.85
1:A:173:ARG:NE	2:A:275:HOH:O	1.99	0.85
1:C:45:ARG:NH1	1:C:45:ARG:HB3	1.91	0.85
1:B:185:ARG:CB	1:B:254:THR:HG23	2.06	0.84
1:A:16:ILE:HB	2:A:416:HOH:O	1.76	0.84
1:A:269:LEU:HD11	1:C:218:LEU:HA	1.59	0.84
1:D:186:SER:H	1:D:254:THR:HG22	1.43	0.84
1:C:174:PHE:HA	1:C:177:ARG:HD2	1.60	0.83
1:A:185:ARG:NH2	2:A:282:HOH:O	2.04	0.83
1:D:64:ASP:H	1:D:70:HIS:HD2	1.24	0.83
1:B:186:SER:H	1:B:254:THR:HG22	1.41	0.83
1:B:64:ASP:H	1:B:70:HIS:CD2	1.97	0.82
1:C:68:GLU:O	1:C:69:GLU:C	2.15	0.82
1:A:254:THR:CB	2:A:318:HOH:O	1.75	0.82
1:D:101:THR:CG2	1:D:115:ASP:OD1	2.28	0.81
1:C:41:PHE:O	1:C:42:ASP:HB3	1.80	0.81
1:D:203:VAL:CG2	1:D:215:ILE:HB	2.10	0.81
1:A:185:ARG:NE	2:A:282:HOH:O	2.04	0.81
1:D:63:LEU:HD11	1:D:71:LEU:HD13	1.62	0.81
1:B:153:ARG:HG3	2:D:424:HOH:O	1.81	0.81
1:A:254:THR:HG21	2:A:302:HOH:O	1.79	0.80
1:A:253:THR:HG22	1:D:259:TYR:O	1.81	0.80
1:C:67:ASN:C	1:C:67:ASN:HD22	1.83	0.79
1:A:203:VAL:HG22	1:A:215:ILE:HD11	1.64	0.79
1:B:132:LYS:HE3	2:B:432:HOH:O	1.83	0.79
1:B:202:ILE:HG21	1:B:215:ILE:HD13	1.65	0.78
1:D:158:TYR:CZ	1:D:161:MET:HG3	2.17	0.78
1:A:153:ARG:NH1	1:C:153:ARG:NH2	2.31	0.77
1:D:26:ALA:CB	2:D:364:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASP:H	1:D:70:HIS:CD2	2.03	0.77
1:B:145:VAL:HG11	1:B:242:VAL:HG13	1.66	0.77
1:D:2:THR:O	1:D:6:ASP:HB2	1.85	0.77
1:C:63:LEU:HD11	1:C:71:LEU:HD13	1.66	0.77
1:A:203:VAL:HG22	1:A:215:ILE:CD1	2.15	0.76
1:B:210:GLU:HB3	2:B:415:HOH:O	1.86	0.76
1:D:185:ARG:NH2	2:D:294:HOH:O	2.15	0.76
1:A:186:SER:H	1:A:254:THR:HG23	1.51	0.76
1:C:147:MET:HE3	1:C:242:VAL:HG21	1.67	0.76
1:C:67:ASN:HD22	1:C:68:GLU:H	1.31	0.75
1:A:250:LEU:HD23	1:D:241:THR:HG23	1.67	0.75
1:B:75:ALA:O	2:B:299:HOH:O	2.03	0.75
1:D:185:ARG:NE	2:D:294:HOH:O	2.04	0.75
1:D:186:SER:H	1:D:254:THR:CG2	1.98	0.75
1:A:74:LEU:HD13	1:A:134:LEU:HD21	1.68	0.75
1:B:63:LEU:HD11	1:B:71:LEU:HD13	1.69	0.75
1:C:104:GLY:CA	1:C:157:ALA:HA	2.17	0.75
1:D:231:ASN:ND2	1:D:233:LYS:H	1.84	0.74
1:C:9:ARG:NE	2:C:325:HOH:O	1.96	0.74
1:C:155:MET:SD	2:C:341:HOH:O	2.44	0.74
1:A:231:ASN:OD1	1:A:233:LYS:HG2	1.88	0.74
1:A:101:THR:HG23	1:A:111:ALA:HA	1.69	0.74
1:B:196:THR:OG1	1:B:197:LEU:N	2.22	0.73
1:A:145:VAL:CB	2:A:391:HOH:O	2.22	0.73
1:D:185:ARG:HA	1:D:254:THR:HG23	1.70	0.73
1:A:17:THR:HG22	1:A:19:SER:N	1.99	0.72
1:D:74:LEU:HD13	1:D:134:LEU:HD21	1.69	0.72
1:D:203:VAL:HG23	1:D:215:ILE:HB	1.71	0.72
1:B:64:ASP:H	1:B:70:HIS:HD2	1.34	0.72
1:C:248:ASP:OD1	2:C:408:HOH:O	2.06	0.72
1:A:64:ASP:H	1:A:70:HIS:CD2	2.08	0.71
1:A:158:TYR:HD1	1:A:162:THR:OG1	1.70	0.71
1:C:9:ARG:NH2	2:C:325:HOH:O	2.17	0.71
1:D:155:MET:HG3	1:D:218:LEU:HD11	1.72	0.70
1:B:245:LEU:HD13	1:B:250:LEU:HD22	1.73	0.70
1:B:202:ILE:CG2	1:B:215:ILE:HD13	2.21	0.70
1:C:202:ILE:CG2	1:C:215:ILE:HD13	2.21	0.70
1:D:218:LEU:HD23	1:D:222:TRP:HZ3	1.56	0.70
1:C:16:ILE:CD1	2:C:399:HOH:O	2.40	0.69
1:B:174:PHE:HA	1:B:177:ARG:HD2	1.75	0.69
1:C:232:MET:CE	2:C:344:HOH:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:HA3	1:A:202:ILE:HG13	1.75	0.69
1:D:236:THR:O	1:D:240:LYS:HG3	1.92	0.69
1:C:67:ASN:O	1:C:70:HIS:HB2	1.93	0.69
1:D:158:TYR:HB2	2:D:397:HOH:O	1.94	0.68
1:C:44:LEU:HD13	2:C:377:HOH:O	1.92	0.68
1:B:99:PRO:HB2	1:B:101:THR:HG22	1.74	0.68
1:A:104:GLY:HA3	1:A:202:ILE:CG1	2.23	0.68
1:A:4:LEU:HB3	1:A:5:LEU:HD13	1.76	0.68
1:C:74:LEU:HD13	1:C:134:LEU:HD21	1.76	0.68
1:C:68:GLU:CG	2:C:416:HOH:O	2.36	0.67
1:A:63:LEU:HD11	1:A:71:LEU:HD13	1.76	0.67
1:B:41:PHE:HA	1:B:63:LEU:O	1.94	0.67
1:D:158:TYR:HD1	1:D:162:THR:OG1	1.78	0.67
1:C:155:MET:HE1	2:C:274:HOH:O	1.95	0.67
1:A:17:THR:CG2	1:A:19:SER:H	2.02	0.67
1:D:45:ARG:HD3	2:D:406:HOH:O	1.95	0.66
1:C:202:ILE:HG23	1:C:215:ILE:HD13	1.77	0.66
1:B:75:ALA:HA	2:B:303:HOH:O	1.94	0.66
1:C:67:ASN:C	1:C:68:GLU:OE1	2.34	0.66
1:C:100:GLN:NE2	1:C:207:LEU:HD11	2.11	0.66
1:D:268:LEU:O	2:D:331:HOH:O	2.14	0.66
1:A:107:PRO:HG2	1:A:110:ASP:OD1	1.94	0.65
1:A:186:SER:H	1:A:254:THR:CG2	2.09	0.65
1:B:104:GLY:O	2:B:416:HOH:O	2.14	0.65
1:A:173:ARG:NH2	2:A:275:HOH:O	2.27	0.65
1:A:132:LYS:HD2	1:B:109:PHE:HB3	1.79	0.65
1:A:3:GLY:HA2	1:A:32:GLN:OE1	1.96	0.65
1:D:203:VAL:HG21	1:D:215:ILE:HB	1.79	0.65
1:D:198:ALA:HA	1:D:201:ALA:HB3	1.79	0.64
1:D:199:MET:SD	1:D:203:VAL:CG1	2.86	0.64
1:D:103:MET:HE2	2:D:400:HOH:O	1.97	0.64
1:A:67:ASN:HD22	1:A:69:GLU:H	1.46	0.63
1:D:199:MET:SD	1:D:203:VAL:HG12	2.39	0.63
1:D:69:GLU:O	1:D:73:SER:HB3	1.98	0.63
1:C:233:LYS:HE2	2:C:392:HOH:O	1.90	0.63
1:D:20:SER:OG	2:D:363:HOH:O	1.75	0.63
1:D:215:ILE:O	1:D:219:GLU:HG3	1.99	0.62
1:A:87:LYS:HE2	2:A:436:HOH:O	1.99	0.62
1:C:232:MET:HE2	2:C:344:HOH:O	1.98	0.62
1:D:109:PHE:HB2	2:D:272:HOH:O	1.98	0.62
1:C:195:ARG:HE	1:C:203:VAL:HG21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:VAL:HG22	1:C:215:ILE:HG21	1.82	0.62
1:C:15:ILE:HG13	2:C:358:HOH:O	1.98	0.62
1:B:42:ASP:HA	1:B:62:GLU:CD	2.20	0.61
1:A:107:PRO:HB3	2:A:326:HOH:O	2.00	0.61
1:D:153:ARG:NE	2:D:425:HOH:O	2.31	0.61
1:A:45:ARG:H	1:A:45:ARG:HE	1.47	0.61
1:C:185:ARG:HA	1:C:254:THR:CG2	2.29	0.61
1:C:43:ARG:HB3	1:C:46:LEU:HB3	1.81	0.61
1:B:259:TYR:O	1:C:253:THR:HB	2.01	0.61
1:D:98:MET:HB3	1:D:103:MET:HG3	1.82	0.61
1:B:199:MET:O	1:B:203:VAL:HG23	2.00	0.61
1:D:185:ARG:HA	1:D:254:THR:CG2	2.31	0.61
1:D:49:ARG:HH11	1:D:49:ARG:HG3	1.65	0.60
1:B:210:GLU:HB2	2:B:397:HOH:O	2.01	0.60
1:A:153:ARG:HH11	1:C:153:ARG:NH2	1.99	0.60
1:B:202:ILE:HG21	1:B:215:ILE:CD1	2.32	0.60
1:D:107:PRO:HB3	2:D:272:HOH:O	2.01	0.60
1:B:134:LEU:O	1:B:138:MET:HG3	2.02	0.60
1:C:214:GLN:HG2	2:C:314:HOH:O	2.02	0.60
1:A:173:ARG:CZ	2:A:275:HOH:O	2.41	0.60
1:C:41:PHE:O	1:C:42:ASP:CB	2.49	0.60
1:C:174:PHE:O	1:C:177:ARG:HG2	2.01	0.59
1:A:201:ALA:HB3	2:A:363:HOH:O	2.02	0.59
1:B:185:ARG:CA	1:B:254:THR:HG23	2.32	0.59
1:B:98:MET:HB3	1:B:103:MET:HG2	1.84	0.59
1:A:153:ARG:NH1	1:C:153:ARG:CZ	2.65	0.59
1:A:259:TYR:O	1:D:253:THR:HB	2.03	0.59
1:B:5:LEU:HB3	1:B:34:ALA:HB2	1.85	0.59
1:D:66:GLN:HE21	1:D:121:HIS:CD2	2.19	0.59
1:A:74:LEU:HD22	1:A:78:VAL:HG23	1.83	0.59
1:D:121:HIS:HD2	2:D:301:HOH:O	1.86	0.58
1:B:158:TYR:CZ	1:B:161:MET:HG3	2.38	0.58
2:C:369:HOH:O	1:D:156:PRO:HG3	2.04	0.58
1:D:17:THR:HG22	1:D:19:SER:H	1.69	0.58
1:A:225:ARG:HD2	1:A:267:GLN:O	2.04	0.58
1:C:225:ARG:HD2	1:C:267:GLN:O	2.02	0.58
1:A:177:ARG:NH1	1:B:156:PRO:HG3	2.19	0.58
1:D:158:TYR:CD1	1:D:162:THR:OG1	2.54	0.58
1:C:122:ILE:O	1:C:126:SER:OG	2.20	0.58
1:D:207:LEU:HB3	1:D:211:ALA:HB3	1.86	0.57
1:B:41:PHE:O	1:B:43:ARG:CA	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:CA	1:D:254:THR:HG23	2.34	0.57
1:A:218:LEU:HD22	1:A:222:TRP:HZ3	1.68	0.57
1:D:53:ARG:HH11	1:D:53:ARG:HG3	1.69	0.57
1:B:253:THR:HB	1:C:259:TYR:O	2.05	0.57
1:B:98:MET:CE	1:B:119:GLY:HA3	2.34	0.57
1:B:101:THR:HG21	1:B:115:ASP:CG	2.24	0.57
1:D:101:THR:HG21	1:D:112:PRO:CD	2.26	0.57
1:A:269:LEU:HD23	2:A:403:HOH:O	2.03	0.57
1:A:253:THR:CB	2:A:273:HOH:O	1.91	0.57
2:A:293:HOH:O	1:D:253:THR:HG22	2.03	0.57
1:B:148:ASP:OD1	1:B:169:GLU:OE2	2.22	0.57
1:C:68:GLU:CA	1:C:70:HIS:H	2.17	0.56
1:B:51:THR:C	1:B:53:ARG:H	2.08	0.56
1:D:16:ILE:HD12	1:D:43:ARG:NH2	2.21	0.56
1:C:113:TYR:CE2	1:C:117:SER:HB2	2.41	0.56
1:D:105:ILE:HG22	1:D:207:LEU:HD13	1.87	0.56
1:A:45:ARG:HA	2:A:427:HOH:O	2.05	0.56
1:B:177:ARG:HA	1:C:227:PRO:HB3	1.88	0.56
2:A:284:HOH:O	1:B:173:ARG:HD2	2.06	0.56
1:B:258:ILE:HD12	1:C:258:ILE:HD13	1.86	0.56
1:A:2:THR:O	1:A:6:ASP:OD1	2.24	0.56
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.87	0.56
1:D:98:MET:HB2	2:D:376:HOH:O	2.07	0.56
1:D:145:VAL:CG2	1:D:242:VAL:HG13	2.30	0.55
1:C:18:ASP:HB3	1:C:50:ILE:HG23	1.88	0.55
1:B:13:SER:HB2	1:B:95:ILE:HD11	1.88	0.55
1:B:97:PHE:O	1:B:119:GLY:HA2	2.07	0.55
1:A:97:PHE:O	1:A:119:GLY:HA2	2.06	0.55
1:B:76:GLY:N	2:B:303:HOH:O	2.10	0.55
1:A:196:THR:HG22	1:A:197:LEU:HG	1.89	0.55
1:C:189:VAL:HG23	1:C:245:LEU:HD23	1.89	0.55
1:C:87:LYS:NZ	2:C:398:HOH:O	2.40	0.55
1:D:195:ARG:HA	1:D:199:MET:HE2	1.88	0.55
1:A:268:LEU:HD13	1:C:155:MET:CE	2.37	0.55
1:B:10:ILE:HG12	1:B:90:GLY:HA3	1.89	0.55
1:C:202:ILE:HG12	1:C:207:LEU:HD11	1.89	0.54
1:B:103:MET:HG3	1:B:103:MET:O	2.07	0.54
1:B:253:THR:HG22	2:C:270:HOH:O	2.05	0.54
1:B:131:ALA:O	1:B:135:LEU:HB2	2.07	0.54
1:A:193:PRO:O	1:A:232:MET:HG3	2.07	0.54
1:C:202:ILE:O	1:C:207:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:THR:HG22	1:D:197:LEU:H	1.73	0.54
1:D:135:LEU:HG	1:D:182:TYR:CD1	2.42	0.54
1:A:67:ASN:ND2	1:A:69:GLU:H	2.05	0.54
1:D:185:ARG:CZ	2:D:294:HOH:O	2.42	0.54
1:B:214:GLN:HG3	2:B:356:HOH:O	2.06	0.54
1:C:207:LEU:HD23	1:C:211:ALA:HB1	1.89	0.54
1:C:147:MET:CE	1:C:242:VAL:HG21	2.37	0.54
1:D:106:ASN:ND2	1:D:110:ASP:HB2	2.23	0.54
1:C:202:ILE:HG21	1:C:215:ILE:HD13	1.90	0.53
1:A:135:LEU:HD13	1:A:144:ILE:HD11	1.91	0.53
1:C:135:LEU:HD13	1:C:144:ILE:HD11	1.89	0.53
1:A:244:ALA:HB2	1:D:249:TRP:HB3	1.89	0.53
1:B:64:ASP:N	1:B:70:HIS:HD2	2.04	0.53
1:D:148:ASP:HB3	1:D:190:ALA:HA	1.90	0.53
1:B:105:ILE:HG22	1:B:211:ALA:CB	2.38	0.53
1:B:63:LEU:HD22	1:B:74:LEU:HD11	1.91	0.53
1:C:105:ILE:HG12	1:C:105:ILE:O	2.08	0.53
1:A:101:THR:CG2	1:A:112:PRO:HD2	2.33	0.53
1:A:245:LEU:HD13	1:A:250:LEU:HD13	1.91	0.53
1:A:202:ILE:HD12	1:A:207:LEU:HD23	1.91	0.53
1:B:186:SER:H	1:B:254:THR:HG23	1.69	0.53
1:C:245:LEU:HD13	1:C:250:LEU:HD13	1.91	0.53
1:C:177:ARG:NH2	2:C:369:HOH:O	2.24	0.52
1:C:145:VAL:HA	1:C:187:ASN:O	2.09	0.52
1:C:69:GLU:N	1:C:69:GLU:OE2	2.42	0.52
1:A:65:VAL:HB	1:A:126:SER:HB2	1.91	0.52
1:D:13:SER:HB2	1:D:95:ILE:HD11	1.90	0.52
1:C:158:TYR:HD1	1:C:162:THR:HG1	1.55	0.52
1:C:158:TYR:CZ	1:C:161:MET:HG3	2.44	0.52
1:C:232:MET:HE1	2:C:344:HOH:O	2.07	0.52
1:C:67:ASN:ND2	1:C:68:GLU:H	1.96	0.52
1:D:195:ARG:NH1	1:D:199:MET:O	2.43	0.52
1:B:60:LEU:HB2	2:B:294:HOH:O	2.08	0.52
1:A:268:LEU:HB3	1:C:155:MET:HE2	1.91	0.52
1:B:156:PRO:HB3	1:B:214:GLN:HE21	1.74	0.52
1:D:16:ILE:HD12	1:D:43:ARG:HH21	1.73	0.52
1:C:93:HIS:O	1:C:146:GLY:HA2	2.09	0.52
1:D:218:LEU:HD23	1:D:222:TRP:CZ3	2.40	0.52
1:B:155:MET:HB2	1:B:218:LEU:HD21	1.91	0.52
1:D:41:PHE:CD1	1:D:64:ASP:HB2	2.44	0.52
1:B:105:ILE:HG22	1:B:211:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ALA:HB1	1:B:262:GLY:O	2.10	0.52
1:C:195:ARG:HH11	1:C:195:ARG:HG3	1.75	0.51
1:A:126:SER:HA	1:A:129:SER:HB2	1.93	0.51
1:A:104:GLY:HA3	1:A:202:ILE:HG12	1.91	0.51
1:D:173:ARG:NH2	2:D:300:HOH:O	2.30	0.51
1:D:12:VAL:HG11	2:D:364:HOH:O	2.10	0.51
1:A:101:THR:O	1:A:106:ASN:ND2	2.42	0.51
1:D:231:ASN:C	1:D:231:ASN:HD22	2.13	0.51
1:A:67:ASN:HD22	1:A:67:ASN:C	2.14	0.51
1:B:10:ILE:HD12	1:B:34:ALA:HB1	1.93	0.51
1:A:210:GLU:HB2	2:A:418:HOH:O	2.09	0.51
1:A:18:ASP:HA	1:A:23:PHE:CG	2.46	0.51
1:B:15:ILE:HD12	1:B:38:LEU:HD22	1.93	0.51
1:C:87:LYS:NZ	1:C:139:ASN:HD22	2.09	0.51
1:C:41:PHE:CG	1:C:64:ASP:HB2	2.45	0.51
1:B:202:ILE:CG2	1:B:215:ILE:CD1	2.89	0.50
1:D:39:THR:HA	1:D:61:LEU:O	2.11	0.50
1:C:233:LYS:HE3	2:C:392:HOH:O	1.93	0.50
1:C:158:TYR:CZ	1:C:161:MET:CG	2.94	0.50
1:C:154:ALA:HB2	1:D:173:ARG:HB3	1.92	0.50
1:A:62:GLU:OE2	2:A:448:HOH:O	2.19	0.50
1:D:11:LEU:HA	1:D:37:VAL:O	2.10	0.50
1:A:134:LEU:O	1:A:138:MET:HG3	2.12	0.50
1:C:232:MET:HG3	1:C:233:LYS:HG3	1.93	0.50
1:C:161:MET:CE	1:C:165:LYS:HE2	2.42	0.50
1:C:105:ILE:HA	1:C:211:ALA:HB2	1.94	0.50
1:A:203:VAL:HG22	1:A:215:ILE:HD12	1.91	0.50
1:D:49:ARG:O	1:D:52:ASP:HB2	2.12	0.50
1:A:180:GLY:HA3	1:D:227:PRO:O	2.12	0.50
1:A:107:PRO:HG3	2:A:434:HOH:O	2.12	0.49
1:B:97:PHE:CE2	1:B:99:PRO:HD3	2.48	0.49
1:A:200:SER:CA	1:A:203:VAL:HB	2.34	0.49
1:B:102:GLY:O	1:B:160:TRP:HB2	2.11	0.49
1:D:158:TYR:HB3	1:D:162:THR:OG1	2.12	0.49
1:D:64:ASP:HB3	1:D:70:HIS:CD2	2.47	0.49
1:D:97:PHE:HD2	2:D:426:HOH:O	1.83	0.49
1:D:20:SER:HB3	1:D:23:PHE:H	1.78	0.49
1:B:135:LEU:N	1:B:136:PRO:CD	2.76	0.49
1:D:195:ARG:NH2	1:D:203:VAL:HG13	2.27	0.49
1:A:21:ILE:HD13	1:A:238:VAL:HG11	1.93	0.49
1:B:158:TYR:CE1	1:B:161:MET:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ALA:O	1:C:135:LEU:HB2	2.13	0.49
1:A:148:ASP:OD1	1:A:169:GLU:OE2	2.30	0.49
1:D:196:THR:HG21	2:D:379:HOH:O	2.13	0.49
1:A:61:LEU:HD11	1:A:78:VAL:HA	1.95	0.49
1:B:250:LEU:HB3	1:B:253:THR:HG23	1.95	0.49
1:B:156:PRO:CB	1:B:214:GLN:HE21	2.26	0.48
1:C:203:VAL:HG22	1:C:215:ILE:CG2	2.43	0.48
1:C:41:PHE:CD1	1:C:64:ASP:HB2	2.48	0.48
1:D:101:THR:CG2	1:D:112:PRO:HD2	2.31	0.48
1:B:41:PHE:CZ	1:B:42:ASP:HB2	2.49	0.48
1:C:147:MET:CE	1:C:242:VAL:CG2	2.91	0.48
1:A:266:THR:HB	1:D:173:ARG:HG2	1.94	0.48
1:A:93:HIS:O	1:A:146:GLY:HA2	2.14	0.48
1:B:76:GLY:HA3	2:B:301:HOH:O	2.13	0.48
1:D:161:MET:SD	2:D:376:HOH:O	2.61	0.48
1:B:126:SER:HA	1:B:129:SER:OG	2.13	0.48
1:B:77:ARG:NH1	2:B:346:HOH:O	2.45	0.48
1:B:45:ARG:HD2	2:B:404:HOH:O	2.13	0.48
1:C:46:LEU:O	1:C:46:LEU:HD12	2.13	0.48
1:C:202:ILE:HG12	1:C:207:LEU:CD1	2.43	0.48
1:D:46:LEU:O	1:D:50:ILE:HG12	2.13	0.48
1:B:41:PHE:HE2	1:B:43:ARG:NE	2.12	0.47
1:B:100:GLN:HB3	1:B:207:LEU:HD21	1.95	0.47
1:A:268:LEU:HD23	1:A:269:LEU:HG	1.96	0.47
1:D:65:VAL:O	1:D:71:LEU:HD21	2.14	0.47
2:A:293:HOH:O	1:D:253:THR:CG2	2.59	0.47
1:C:249:TRP:C	1:C:251:PRO:HD3	2.34	0.47
1:B:145:VAL:CG1	2:B:411:HOH:O	2.44	0.47
1:D:145:VAL:HA	1:D:187:ASN:O	2.13	0.47
1:B:202:ILE:HG12	1:B:207:LEU:HD22	1.96	0.47
1:A:170:SER:HA	1:A:173:ARG:NH1	2.29	0.47
1:D:20:SER:CB	1:D:23:PHE:H	2.27	0.47
1:A:156:PRO:HD2	1:A:218:LEU:HG	1.96	0.47
1:B:22:ALA:HB2	1:B:94:ALA:HB3	1.96	0.47
1:A:201:ALA:CB	2:A:363:HOH:O	2.61	0.47
1:C:161:MET:HE2	1:C:165:LYS:HE2	1.96	0.47
1:C:123:SER:O	1:C:168:LEU:HG	2.13	0.47
1:B:186:SER:N	1:B:254:THR:CG2	2.68	0.47
1:A:250:LEU:HB2	2:A:313:HOH:O	2.14	0.47
1:D:83:GLY:O	1:D:86:ASN:HB2	2.15	0.47
1:B:153:ARG:NH2	2:D:425:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:HD21	1:A:69:GLU:HB3	1.80	0.47
1:A:218:LEU:HA	1:C:269:LEU:HD13	1.95	0.47
1:B:48:GLN:O	1:B:52:ASP:OD2	2.32	0.47
1:A:27:ARG:O	1:A:31:GLU:HG3	2.14	0.47
1:A:63:LEU:HD11	1:A:71:LEU:CD1	2.45	0.47
1:B:259:TYR:N	1:B:259:TYR:CD1	2.83	0.47
1:A:148:ASP:HB2	1:A:188:LEU:HG	1.97	0.47
1:C:241:THR:HG21	1:C:260:ALA:HB2	1.97	0.47
1:B:145:VAL:HA	1:B:187:ASN:O	2.15	0.47
1:C:87:LYS:HZ3	1:C:139:ASN:HD22	1.62	0.47
1:D:202:ILE:HA	1:D:207:LEU:HG	1.97	0.47
1:B:4:LEU:HD13	1:B:247:SER:HB3	1.96	0.47
1:B:153:ARG:CZ	1:D:265:HIS:O	2.64	0.46
1:B:42:ASP:HA	1:B:62:GLU:CG	2.45	0.46
1:D:103:MET:HE1	2:D:401:HOH:O	2.16	0.46
1:A:241:THR:HG23	1:D:250:LEU:HD23	1.96	0.46
1:C:250:LEU:N	1:C:251:PRO:HD3	2.31	0.46
1:A:57:LYS:CB	1:A:57:LYS:NZ	2.78	0.46
1:D:78:VAL:O	1:D:82:ILE:HG12	2.15	0.46
1:B:98:MET:O	1:B:99:PRO:C	2.51	0.46
1:D:21:ILE:O	1:D:25:ILE:HG13	2.15	0.46
1:B:18:ASP:HA	1:B:23:PHE:CG	2.50	0.46
1:B:185:ARG:HA	1:B:254:THR:HG23	1.97	0.46
1:B:45:ARG:CD	2:B:404:HOH:O	2.63	0.46
1:B:20:SER:O	1:B:24:HIS:HD2	1.98	0.46
1:A:49:ARG:O	1:A:52:ASP:HB2	2.15	0.46
1:C:185:ARG:HA	1:C:254:THR:HG23	1.96	0.46
1:D:106:ASN:O	1:D:107:PRO:C	2.52	0.46
1:B:10:ILE:HD12	1:B:34:ALA:CB	2.46	0.46
1:C:167:ALA:O	1:C:171:VAL:HG23	2.16	0.46
1:B:126:SER:O	1:B:130:MET:HG3	2.16	0.46
1:A:173:ARG:HG2	1:D:266:THR:HB	1.98	0.46
1:B:145:VAL:CB	2:B:411:HOH:O	1.92	0.45
1:C:195:ARG:NH1	1:C:232:MET:SD	2.86	0.45
1:D:197:LEU:C	1:D:199:MET:H	2.19	0.45
1:D:199:MET:SD	1:D:203:VAL:HG11	2.55	0.45
1:A:67:ASN:HD22	1:A:69:GLU:N	2.12	0.45
1:D:92:VAL:HG22	1:D:145:VAL:HG22	1.98	0.45
1:D:64:ASP:N	1:D:70:HIS:HD2	2.03	0.45
1:B:199:MET:HA	1:B:202:ILE:HD12	1.96	0.45
1:A:268:LEU:CB	1:C:155:MET:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HD2	1:B:267:GLN:O	2.16	0.45
1:A:46:LEU:O	1:A:46:LEU:HD23	2.16	0.45
1:D:101:THR:HG23	1:D:111:ALA:HA	1.99	0.45
1:A:101:THR:HG21	1:A:115:ASP:OD2	2.16	0.45
1:D:158:TYR:CE2	1:D:161:MET:HG3	2.50	0.45
1:B:227:PRO:HB3	1:C:177:ARG:HA	1.98	0.45
1:A:135:LEU:HG	1:A:182:TYR:CD1	2.51	0.45
1:D:2:THR:O	1:D:6:ASP:CB	2.61	0.45
1:B:195:ARG:HA	1:B:199:MET:HB3	1.98	0.45
1:D:54:LEU:HA	1:D:54:LEU:HD23	1.85	0.45
1:B:62:GLU:HG2	1:B:70:HIS:NE2	2.32	0.45
1:C:87:LYS:NZ	1:C:139:ASN:ND2	2.65	0.45
1:D:39:THR:HB	1:D:63:LEU:HB3	1.99	0.45
1:C:4:LEU:HD13	1:C:5:LEU:HD13	1.99	0.45
1:B:196:THR:HG1	1:B:197:LEU:H	1.61	0.45
1:B:15:ILE:O	1:B:47:ILE:HG12	2.17	0.45
1:A:169:GLU:HG2	1:A:188:LEU:HD23	1.99	0.45
1:B:63:LEU:HD12	1:B:70:HIS:HB3	1.99	0.44
1:A:158:TYR:CD1	1:A:162:THR:OG1	2.55	0.44
1:B:95:ILE:HG22	1:B:122:ILE:HG22	1.99	0.44
1:D:145:VAL:HG11	1:D:245:LEU:HB3	1.98	0.44
1:B:146:GLY:HA3	1:B:188:LEU:HD12	1.99	0.44
1:B:98:MET:CG	1:B:103:MET:HG2	2.47	0.44
1:B:67:ASN:ND2	1:B:70:HIS:ND1	2.65	0.44
1:A:185:ARG:HA	1:A:254:THR:HG23	1.98	0.44
1:A:250:LEU:CD2	1:D:241:THR:HG23	2.42	0.44
1:A:87:LYS:HB3	1:A:137:ILE:O	2.16	0.44
1:A:63:LEU:HD13	1:A:74:LEU:HG	1.99	0.44
1:A:231:ASN:HD21	1:A:233:LYS:HD2	1.82	0.44
1:D:79:THR:O	1:D:83:GLY:N	2.45	0.44
1:B:247:SER:HB2	2:B:391:HOH:O	2.18	0.44
1:C:173:ARG:NH1	2:C:444:HOH:O	1.65	0.44
1:B:113:TYR:CE2	1:B:117:SER:HB2	2.52	0.44
1:C:90:GLY:HA2	1:C:143:SER:O	2.17	0.44
1:A:65:VAL:O	1:A:71:LEU:HD21	2.18	0.44
1:B:106:ASN:HD22	1:B:107:PRO:HD2	1.83	0.44
1:D:63:LEU:HD13	1:D:74:LEU:HG	2.00	0.44
1:B:249:TRP:C	1:B:251:PRO:HD3	2.38	0.44
1:A:167:ALA:O	1:A:171:VAL:HG23	2.18	0.44
1:A:222:TRP:HZ2	2:A:340:HOH:O	2.00	0.43
1:B:215:ILE:O	1:B:219:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:THR:O	1:C:240:LYS:HG2	2.18	0.43
1:C:126:SER:HA	1:C:129:SER:HB2	2.00	0.43
1:C:157:ALA:HB1	1:C:215:ILE:HD12	2.00	0.43
1:A:268:LEU:HD13	1:C:155:MET:HE2	1.99	0.43
1:B:44:LEU:HD12	1:B:60:LEU:HD13	1.98	0.43
1:A:17:THR:CG2	1:A:18:ASP:N	2.82	0.43
1:D:101:THR:HG22	1:D:115:ASP:OD1	2.14	0.43
1:D:106:ASN:HD21	1:D:110:ASP:CB	2.31	0.43
1:C:155:MET:HE2	1:C:155:MET:HB3	1.70	0.43
1:A:165:LYS:O	1:A:169:GLU:HG3	2.18	0.43
1:D:134:LEU:O	1:D:138:MET:HG3	2.18	0.43
1:D:231:ASN:HD22	1:D:233:LYS:H	1.63	0.43
1:C:202:ILE:HG23	1:C:207:LEU:HD22	2.00	0.43
1:B:30:GLN:OE1	1:B:54:LEU:HB3	2.19	0.43
1:C:95:ILE:HG22	1:C:122:ILE:HG22	2.00	0.43
1:A:21:ILE:HD11	1:A:194:ILE:HG13	2.01	0.43
1:A:169:GLU:HA	1:A:188:LEU:CD2	2.49	0.43
1:D:186:SER:O	1:D:255:GLY:N	2.42	0.43
1:C:98:MET:HB3	1:C:103:MET:SD	2.59	0.43
1:A:135:LEU:HD23	1:B:109:PHE:HE2	1.84	0.42
1:C:146:GLY:HA3	1:C:188:LEU:HD12	2.01	0.42
1:C:207:LEU:HD23	1:C:211:ALA:CB	2.48	0.42
1:B:259:TYR:O	1:C:253:THR:HG22	2.19	0.42
1:A:186:SER:N	1:A:254:THR:HG23	2.26	0.42
1:A:170:SER:HA	1:A:173:ARG:CZ	2.49	0.42
1:C:109:PHE:HE2	1:D:135:LEU:HD23	1.83	0.42
1:C:5:LEU:HA	1:C:5:LEU:HD12	1.91	0.42
1:D:231:ASN:ND2	1:D:231:ASN:C	2.73	0.42
1:D:106:ASN:HD21	1:D:110:ASP:HB2	1.83	0.42
1:C:171:VAL:O	1:C:175:VAL:HG23	2.20	0.42
1:B:11:LEU:HA	1:B:37:VAL:O	2.19	0.42
1:B:63:LEU:HD11	1:B:71:LEU:CD1	2.46	0.42
1:B:215:ILE:HG23	1:B:219:GLU:CD	2.39	0.42
1:C:268:LEU:HD12	1:C:268:LEU:HA	1.83	0.42
1:C:68:GLU:HA	1:C:71:LEU:H	1.85	0.42
1:D:106:ASN:HB2	2:D:378:HOH:O	2.19	0.42
1:D:53:ARG:CG	1:D:53:ARG:HH11	2.33	0.42
1:C:65:VAL:O	1:C:71:LEU:HD21	2.20	0.42
1:D:64:ASP:CB	1:D:70:HIS:HD2	2.33	0.42
1:D:202:ILE:O	1:D:215:ILE:HD12	2.20	0.42
1:C:225:ARG:HG3	2:C:390:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HG22	2:B:431:HOH:O	2.20	0.42
2:B:281:HOH:O	1:C:253:THR:HG23	2.20	0.42
1:B:41:PHE:CE1	1:B:42:ASP:HB2	2.55	0.42
1:C:65:VAL:HB	1:C:126:SER:HB2	2.02	0.42
1:C:100:GLN:HE21	1:C:207:LEU:HD11	1.83	0.41
1:D:103:MET:CE	2:D:400:HOH:O	2.60	0.41
1:B:93:HIS:HD2	1:B:130:MET:HG3	1.85	0.41
1:C:46:LEU:O	1:C:50:ILE:HD12	2.20	0.41
1:B:15:ILE:HG21	1:B:51:THR:CG2	2.50	0.41
1:B:123:SER:O	1:B:168:LEU:HG	2.19	0.41
1:D:145:VAL:HG21	1:D:242:VAL:CG1	2.33	0.41
1:B:189:VAL:HG23	1:B:245:LEU:HD23	2.02	0.41
2:B:281:HOH:O	1:C:253:THR:CG2	2.68	0.41
1:A:214:GLN:HG2	2:A:352:HOH:O	2.20	0.41
1:C:11:LEU:CD2	1:C:130:MET:HE1	2.50	0.41
1:C:208:GLY:O	1:C:209:GLU:C	2.58	0.41
1:A:212:GLY:O	1:A:215:ILE:HG22	2.20	0.41
1:D:198:ALA:HB1	1:D:202:ILE:HG13	2.03	0.41
1:A:202:ILE:CD1	1:A:207:LEU:HD23	2.49	0.41
1:A:5:LEU:O	1:A:8:LYS:HB2	2.20	0.41
1:A:97:PHE:CE2	1:A:99:PRO:HD3	2.55	0.41
1:A:149:PHE:HD1	1:A:158:TYR:CE1	2.38	0.41
1:C:5:LEU:HB3	1:C:34:ALA:HB2	2.02	0.41
1:B:46:LEU:HD23	2:B:343:HOH:O	2.20	0.41
1:C:147:MET:HE1	1:C:242:VAL:HG22	2.01	0.41
1:B:98:MET:CB	1:B:103:MET:HG2	2.50	0.41
1:B:151:PRO:HA	1:B:162:THR:HG23	2.02	0.41
1:A:155:MET:HB2	1:A:218:LEU:HD11	2.03	0.41
1:C:158:TYR:HD1	1:C:162:THR:OG1	2.03	0.41
1:D:103:MET:SD	1:D:161:MET:HB2	2.60	0.41
1:B:15:ILE:CD1	1:B:38:LEU:HD22	2.51	0.41
1:B:106:ASN:HD22	1:B:106:ASN:HA	1.66	0.41
1:D:218:LEU:CD2	1:D:222:TRP:HZ3	2.31	0.41
1:A:156:PRO:HG2	1:A:214:GLN:HB3	2.02	0.41
1:B:173:ARG:HG2	1:C:266:THR:HB	2.03	0.41
1:A:121:HIS:CD2	1:B:113:TYR:CD2	3.09	0.41
1:B:186:SER:N	1:B:254:THR:HG23	2.34	0.41
1:B:47:ILE:HG22	1:B:60:LEU:HD11	2.03	0.41
1:A:97:PHE:HB3	1:A:122:ILE:HG21	2.03	0.41
1:D:214:GLN:HB3	2:D:394:HOH:O	2.19	0.41
1:C:97:PHE:O	1:C:119:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD13	1:D:250:LEU:HD13	2.03	0.41
1:B:18:ASP:N	1:B:18:ASP:OD2	2.53	0.41
1:C:147:MET:HE3	1:C:242:VAL:CG2	2.41	0.40
1:B:101:THR:CG2	1:B:115:ASP:CB	3.00	0.40
1:D:17:THR:HG22	1:D:18:ASP:N	2.36	0.40
1:D:89:ASP:O	1:D:142:GLY:HA2	2.20	0.40
1:A:227:PRO:HD2	1:A:262:GLY:O	2.21	0.40
1:B:101:THR:HG21	1:B:115:ASP:CB	2.52	0.40
1:A:101:THR:HG23	1:A:111:ALA:CA	2.45	0.40
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.86	0.40
1:B:44:LEU:CD1	1:B:60:LEU:HB3	2.51	0.40
1:A:123:SER:O	1:A:168:LEU:HG	2.20	0.40
1:A:256:ASP:OD2	1:D:259:TYR:HB2	2.21	0.40
1:C:25:ILE:CD1	1:C:147:MET:HE3	2.51	0.40
1:D:64:ASP:HB3	1:D:70:HIS:HD2	1.85	0.40
1:C:16:ILE:HD13	2:C:399:HOH:O	2.17	0.40
1:D:95:ILE:HG22	1:D:122:ILE:CG2	2.52	0.40
1:A:57:LYS:HB2	1:A:57:LYS:NZ	2.36	0.40
1:D:90:GLY:HA2	1:D:143:SER:O	2.21	0.40
1:C:63:LEU:HD12	1:C:70:HIS:HB3	2.03	0.40
1:B:185:ARG:HA	1:B:254:THR:CG2	2.50	0.40
1:A:44:LEU:HD13	2:A:448:HOH:O	2.20	0.40
1:D:167:ALA:O	1:D:171:VAL:HG23	2.21	0.40
1:C:10:ILE:O	1:C:36:LEU:HA	2.21	0.40
1:A:236:THR:HB	1:A:237:PRO:HD3	2.03	0.40
1:A:145:VAL:HA	1:A:187:ASN:O	2.22	0.40
1:D:232:MET:HB2	2:D:416:HOH:O	2.21	0.40
1:C:2:THR:HA	2:C:362:HOH:O	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:HOH:O	2:C:439:HOH:O[1_655]	1.91	0.29
2:A:425:HOH:O	2:D:402:HOH:O[1_665]	2.19	0.01

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	266/268 (99%)	243 (91%)	21 (8%)	2 (1%)	24	14
1	B	266/268 (99%)	244 (92%)	19 (7%)	3 (1%)	17	9
1	C	266/268 (99%)	242 (91%)	20 (8%)	4 (2%)	13	5
1	D	266/268 (99%)	239 (90%)	22 (8%)	5 (2%)	10	3
All	All	1064/1072 (99%)	968 (91%)	82 (8%)	14 (1%)	15	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	VAL
1	B	42	ASP
1	C	42	ASP
1	C	69	GLU
1	D	73	SER
1	A	200	SER
1	C	84	ALA
1	D	203	VAL
1	B	208	GLY
1	C	232	MET
1	D	232	MET
1	D	104	GLY
1	D	202	ILE
1	B	105	ILE

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	202/203 (100%)	172 (85%)	30 (15%)	4	1
1	B	202/203 (100%)	174 (86%)	28 (14%)	4	1
1	C	202/203 (100%)	177 (88%)	25 (12%)	6	2
1	D	202/203 (100%)	172 (85%)	30 (15%)	4	1
All	All	808/812 (100%)	695 (86%)	113 (14%)	4	1

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	6	ASP
1	A	35	GLN
1	A	44	LEU
1	A	45	ARG
1	A	48	GLN
1	A	49	ARG
1	A	53	ARG
1	A	57	LYS
1	A	67	ASN
1	A	70	HIS
1	A	71	LEU
1	A	74	LEU
1	A	100	GLN
1	A	101	THR
1	A	105	ILE
1	A	135	LEU
1	A	145	VAL
1	A	168	LEU
1	A	188	LEU
1	A	195	ARG
1	A	200	SER
1	A	207	LEU
1	A	210	GLU
1	A	215	ILE
1	A	218	LEU
1	A	224	GLN
1	A	233	LYS
1	A	245	LEU
1	B	4	LEU
1	B	5	LEU
1	B	17	THR

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Mol	Chain	Res	Type
1	B	20	SER
1	B	41	PHE
1	B	43	ARG
1	B	44	LEU
1	B	45	ARG
1	B	48	GLN
1	B	50	ILE
1	B	57	LYS
1	B	71	LEU
1	B	74	LEU
1	B	100	GLN
1	B	105	ILE
1	B	106	ASN
1	B	135	LEU
1	B	168	LEU
1	B	177	ARG
1	B	185	ARG
1	B	188	LEU
1	B	196	THR
1	B	197	LEU
1	B	199	MET
1	B	209	GLU
1	B	245	LEU
1	B	253	THR
1	B	254	THR
1	C	4	LEU
1	C	5	LEU
1	C	45	ARG
1	C	46	LEU
1	C	48	GLN
1	C	57	LYS
1	C	67	ASN
1	C	71	LEU
1	C	74	LEU
1	C	105	ILE
1	C	135	LEU
1	C	145	VAL
1	C	155	MET
1	C	168	LEU
1	C	177	ARG
1	C	188	LEU
1	C	197	LEU

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Mol	Chain	Res	Type
1	C	202	ILE
1	C	203	VAL
1	C	215	ILE
1	C	245	LEU
1	C	253	THR
1	C	254	THR
1	C	258	ILE
1	C	269	LEU
1	D	4	LEU
1	D	5	LEU
1	D	16	ILE
1	D	45	ARG
1	D	48	GLN
1	D	49	ARG
1	D	53	ARG
1	D	57	LYS
1	D	67	ASN
1	D	71	LEU
1	D	73	SER
1	D	74	LEU
1	D	101	THR
1	D	103	MET
1	D	105	ILE
1	D	135	LEU
1	D	161	MET
1	D	168	LEU
1	D	170	SER
1	D	188	LEU
1	D	194	ILE
1	D	196	THR
1	D	209	GLU
1	D	210	GLU
1	D	222	TRP
1	D	231	ASN
1	D	232	MET
1	D	245	LEU
1	D	253	THR
1	D	254	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	66	GLN
1	A	67	ASN
1	A	70	HIS
1	A	121	HIS
1	B	70	HIS
1	B	106	ASN
1	B	121	HIS
1	B	214	GLN
1	C	67	ASN
1	C	100	GLN
1	C	121	HIS
1	C	139	ASN
1	D	67	ASN
1	D	70	HIS
1	D	106	ASN
1	D	121	HIS
1	D	231	ASN

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 carbohydrates 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 ⓘ

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	268/268 (100%)	0.40	24 (8%)	12 17	13, 25, 61, 95	0
1	B	268/268 (100%)	0.21	13 (4%)	33 43	11, 23, 52, 67	0
1	C	268/268 (100%)	0.26	19 (7%)	19 25	10, 22, 57, 85	0
1	D	268/268 (100%)	0.53	28 (10%)	8 12	13, 24, 77, 93	0
All	All	1072/1072 (100%)	0.35	84 (7%)	16 21	10, 23, 59, 95	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ALA	13.5
1	C	201	ALA	11.9
1	A	200	SER	9.6
1	C	197	LEU	9.1
1	C	203	VAL	8.5
1	B	2	THR	8.4
1	C	202	ILE	8.4
1	A	207	LEU	8.1
1	D	197	LEU	8.0
1	A	206	ALA	7.7
1	A	203	VAL	7.6
1	A	202	ILE	7.5
1	D	200	SER	7.3
1	D	206	ALA	7.1
1	A	198	ALA	7.0
1	A	204	GLY	7.0
1	D	198	ALA	6.7
1	D	211	ALA	6.7
1	D	202	ILE	6.5
1	A	105	ILE	6.0
1	C	2	THR	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	199	MET	5.7
1	D	208	GLY	5.7
1	B	42	ASP	5.7
1	D	205	GLY	5.7
1	C	198	ALA	5.5
1	B	197	LEU	5.4
1	A	205	GLY	5.4
1	B	202	ILE	5.2
1	D	207	LEU	5.2
1	D	203	VAL	5.1
1	D	196	THR	5.0
1	D	105	ILE	4.9
1	B	200	SER	4.6
1	C	204	GLY	4.5
1	C	200	SER	4.3
1	A	210	GLU	4.2
1	A	208	GLY	4.2
1	B	201	ALA	4.2
1	D	2	THR	4.1
1	B	198	ALA	4.0
1	A	197	LEU	4.0
1	D	106	ASN	3.9
1	A	209	GLU	3.9
1	A	2	THR	3.9
1	A	199	MET	3.8
1	D	102	GLY	3.7
1	B	41	PHE	3.6
1	D	204	GLY	3.5
1	D	46	LEU	3.5
1	B	49	ARG	3.4
1	C	69	GLU	3.2
1	A	201	ALA	3.2
1	C	196	THR	3.1
1	C	49	ARG	2.9
1	C	199	MET	2.9
1	D	210	GLU	2.8
1	D	84	ALA	2.7
1	B	207	LEU	2.7
1	C	46	LEU	2.7
1	A	84	ALA	2.6
1	A	158	TYR	2.5
1	D	103	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	103	MET	2.4
1	C	45	ARG	2.4
1	A	102	GLY	2.4
1	C	105	ILE	2.3
1	D	215	ILE	2.3
1	D	195	ARG	2.3
1	D	81	ALA	2.3
1	A	46	LEU	2.3
1	D	158	TYR	2.2
1	C	42	ASP	2.2
1	D	100	GLN	2.1
1	B	44	LEU	2.1
1	A	85	GLY	2.1
1	A	45	ARG	2.0
1	D	107	PRO	2.0
1	B	46	LEU	2.0
1	C	41	PHE	2.0
1	A	49	ARG	2.0
1	C	57	LYS	2.0
1	B	53	ARG	2.0
1	C	158	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.