



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:56 am GMT

PDB ID : 2QG9
Title : Structure of a regulatory subunit mutant D19A of ATCase from E. coli
Authors : Stec, B.; Williams, M.K.; Stieglitz, K.A.; Kantrowitz, E.R.
Deposited on : 2007-06-28
Resolution : 2.70 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

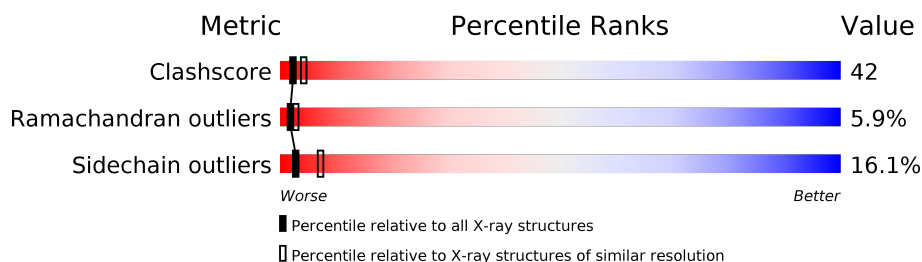
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7436 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1198	751	213	228	6			
2	D	153	Total	C	N	O	S	0	0	0
			1198	751	213	228	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ALA	ASP	ENGINEERED	UNP P0A7F3
D	19	ALA	ASP	ENGINEERED	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		

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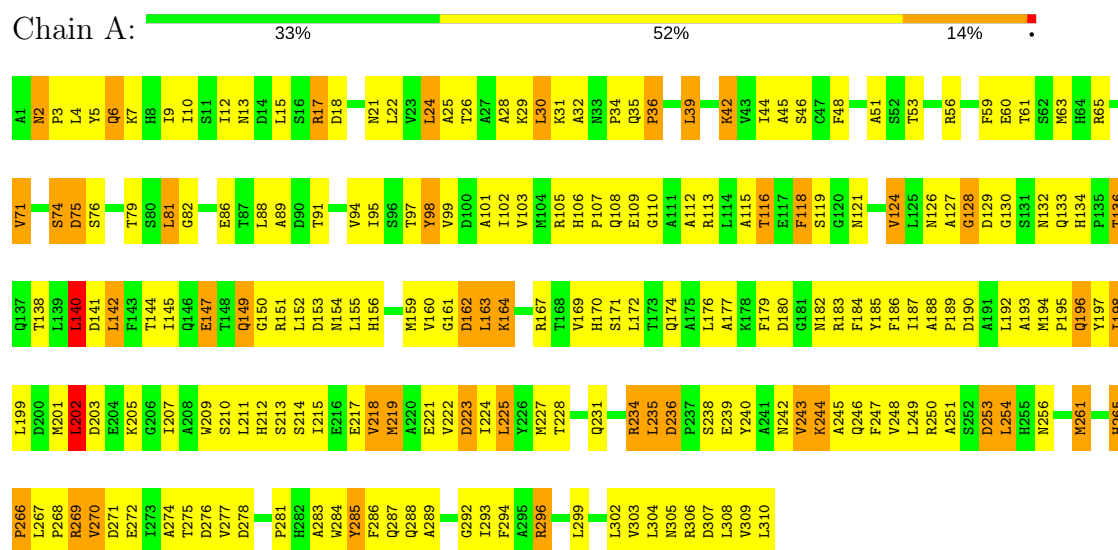
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	23	Total 23	O 23	0	0
4	C	70	Total 70	O 70	0	0
4	D	18	Total 18	O 18	0	0

3 Residue-property plots

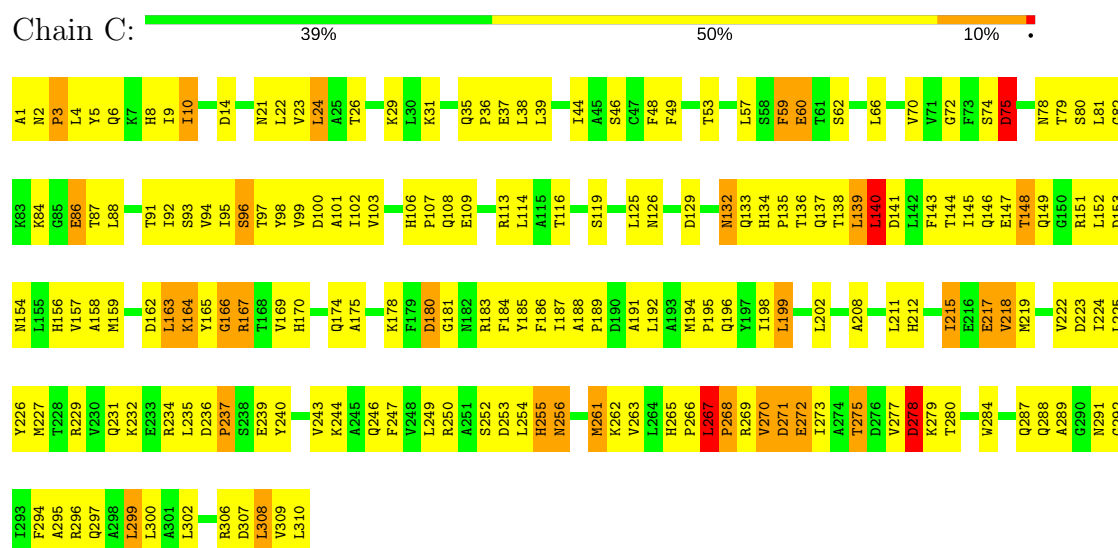
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: Aspartate carbamoyltransferase catalytic chain



• Molecule 1: Aspartate carbamoyltransferase catalytic chain



Chain B: 23% 62% 14%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.29Å 122.29Å 142.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.191 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7436	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.83	2/2461 (0.1%)	1.06	7/3339 (0.2%)
1	C	0.88	2/2461 (0.1%)	1.01	4/3339 (0.1%)
2	B	0.68	0/1216	0.95	2/1643 (0.1%)
2	D	0.75	0/1216	0.98	2/1643 (0.1%)
All	All	0.81	4/7354 (0.1%)	1.01	15/9964 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLU	CD-OE2	8.71	1.35	1.25
1	A	147	GLU	CD-OE2	8.46	1.34	1.25
1	A	60	GLU	CD-OE2	6.49	1.32	1.25
1	C	147	GLU	CD-OE2	6.37	1.32	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	LEU	CA-CB-CG	7.82	133.29	115.30
1	A	140	LEU	CA-CB-CG	7.15	131.75	115.30
2	B	105	ASN	N-CA-C	6.03	127.29	111.00
1	C	267	LEU	CA-CB-CG	-5.86	101.83	115.30
1	A	221	GLU	O-C-N	-5.84	113.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	151	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	119	GLU	N-CA-C	5.48	125.79	111.00
1	A	211	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	82	GLY	N-CA-C	-5.35	99.73	113.10
1	A	202	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	30	LEU	CA-CB-CG	-5.25	103.23	115.30
2	D	45	GLY	N-CA-C	-5.16	100.21	113.10
1	A	39	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	278	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	236	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain

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	2415	0	2422	212	0
1	C	2415	0	2422	186	0
2	B	1198	0	1220	118	0
2	D	1198	0	1220	117	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	97	0	0	6	0
4	B	23	0	0	1	0
4	C	70	0	0	4	0
4	D	18	0	0	2	0
All	All	7436	0	7284	612	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 42.

All (612) 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:109:GLU:HG3	1:A:130:GLY:HA3	1.39	1.04
2:D:30:LEU:HA	2:D:35:LEU:HD12	1.47	0.96
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.46	0.96
1:C:10:ILE:CD1	1:C:113:ARG:HA	1.97	0.94
2:B:105:ASN:HA	2:B:123:SER:OG	1.68	0.93
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.49	0.93
1:A:219:MET:HG3	1:A:256:ASN:HB3	1.49	0.92
2:D:55:ARG:HG3	2:D:55:ARG:HH11	1.34	0.91
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.50	0.90
2:D:77:TYR:O	2:D:79:PRO:HD3	1.70	0.90
1:C:81:LEU:HD22	1:C:84:LYS:HB2	1.54	0.89
2:B:12:ILE:HA	2:B:41:ARG:HH22	1.39	0.87
2:B:85:ARG:HH11	2:B:85:ARG:HB3	1.37	0.87
1:A:187:ILE:HG22	1:A:247:PHE:CE1	2.10	0.86
1:A:156:HIS:HB3	1:A:185:TYR:HE1	1.40	0.86
1:C:185:TYR:CD2	1:C:218:VAL:HG21	2.11	0.85
1:A:9:ILE:HG21	1:A:299:LEU:HD21	1.58	0.84
1:A:145:ILE:HG23	1:A:224:ILE:HG13	1.59	0.84
2:D:27:PHE:HA	2:D:30:LEU:HG	1.60	0.82
1:C:163:LEU:HD12	1:C:194:MET:HB2	1.60	0.82
1:A:151:ARG:HE	1:A:154:ASN:HB2	1.44	0.82
2:B:80:GLN:HA	2:B:96:ARG:HH12	1.45	0.81
2:B:110:PRO:HD2	2:B:145:PHE:CD1	2.14	0.81
1:A:243:VAL:HG23	1:A:246:GLN:HB2	1.60	0.81
1:C:137:GLN:O	1:C:140:LEU:HB3	1.81	0.81
1:A:187:ILE:HD12	1:A:187:ILE:H	1.44	0.81
1:C:60:GLU:HG2	1:C:70:VAL:HG11	1.64	0.80
1:C:10:ILE:HD13	1:C:113:ARG:HA	1.64	0.80
2:D:102:ARG:HA	2:D:125:PHE:O	1.82	0.80
2:B:18:ILE:HG12	2:B:83:VAL:HG13	1.62	0.80
2:D:91:VAL:HG12	2:D:93:GLY:H	1.48	0.79
1:C:187:ILE:HG22	1:C:247:PHE:HE1	1.47	0.79
1:A:184:PHE:CD1	1:A:202:LEU:HD21	2.19	0.78
1:A:160:VAL:HG12	1:A:161:GLY:N	1.99	0.78
1:C:108:GLN:HA	2:D:113:ASN:HD21	1.48	0.77
1:A:243:VAL:HA	1:A:246:GLN:HG2	1.65	0.77
2:D:21:ILE:O	2:D:53:MET:HE1	1.85	0.76
2:B:12:ILE:HA	2:B:41:ARG:NH2	2.00	0.76
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.68	0.75
2:B:18:ILE:HA	2:B:82:THR:O	1.86	0.75
1:A:218:VAL:HG22	1:A:222:VAL:HG13	1.69	0.74
1:C:31:LYS:HE3	1:C:294:PHE:HE2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:SER:O	2:D:71:VAL:HG23	1.87	0.74
1:A:113:ARG:O	1:A:116:THR:HB	1.88	0.74
2:B:44:ILE:HG23	2:B:59:ILE:HD13	1.70	0.74
1:C:252:SER:O	1:C:255:HIS:HB2	1.88	0.73
2:B:76:LEU:HD12	2:B:76:LEU:H	1.52	0.73
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.24	0.73
1:A:187:ILE:HG22	1:A:247:PHE:HE1	1.53	0.73
2:D:24:GLN:NE2	2:D:24:GLN:HA	2.04	0.73
1:C:39:LEU:HD12	1:C:66:LEU:HD13	1.70	0.72
2:B:28:LYS:O	2:B:32:LEU:HB2	1.89	0.72
1:A:95:ILE:O	1:A:99:VAL:HG22	1.89	0.72
1:A:3:PRO:O	1:A:7:LYS:HE3	1.90	0.72
1:A:236:ASP:O	1:A:239:GLU:HG2	1.90	0.71
1:C:59:PHE:CZ	1:C:136:THR:HG21	2.25	0.71
1:C:141:ASP:O	1:C:144:THR:HG22	1.90	0.71
2:D:129:LYS:HG3	2:D:134:ILE:CD1	2.19	0.71
2:D:91:VAL:HG12	2:D:93:GLY:N	2.04	0.71
2:D:55:ARG:HG3	2:D:55:ARG:NH1	2.04	0.71
2:B:110:PRO:HD3	2:B:150:VAL:HG22	1.73	0.71
1:A:17:ARG:HH11	1:A:179:PHE:HA	1.56	0.71
1:A:308:LEU:HD13	1:A:310:LEU:HD11	1.70	0.71
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.72	0.71
2:D:24:GLN:HE21	2:D:24:GLN:HA	1.55	0.71
1:A:4:LEU:HD23	1:A:7:LYS:HD2	1.72	0.71
1:C:235:LEU:HD12	1:C:240:TYR:HA	1.72	0.71
1:C:189:PRO:CG	1:C:192:LEU:HB2	2.19	0.70
2:D:20:HIS:O	2:D:81:ALA:HA	1.90	0.70
2:B:17:VAL:O	2:B:83:VAL:HA	1.91	0.70
2:B:85:ARG:NH1	2:B:85:ARG:HB3	2.06	0.70
1:C:208:ALA:HA	4:C:314:HOH:O	1.90	0.70
2:D:5:ASN:HA	2:D:8:GLN:HG3	1.74	0.69
1:A:205:LYS:HB2	1:A:207:ILE:HG13	1.73	0.69
1:C:31:LYS:HE3	1:C:294:PHE:CE2	2.27	0.69
1:C:183:ARG:CZ	1:C:208:ALA:HB1	2.22	0.69
1:A:160:VAL:HG12	1:A:161:GLY:H	1.55	0.69
2:B:8:GLN:HB3	2:D:8:GLN:HB2	1.73	0.69
2:D:129:LYS:HG3	2:D:134:ILE:HD11	1.73	0.69
1:A:184:PHE:CE1	1:A:202:LEU:HD21	2.28	0.68
1:A:26:THR:HG23	1:A:310:LEU:HD11	1.74	0.68
2:D:143:LYS:HB2	2:D:145:PHE:CE1	2.28	0.68
1:A:28:ALA:O	1:A:31:LYS:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HB	4:A:347:HOH:O	1.93	0.68
2:B:11:ALA:H	2:D:7:LEU:HD22	1.58	0.68
1:A:5:TYR:CE1	1:A:6:GLN:HG2	2.28	0.68
1:A:184:PHE:O	1:A:209:TRP:HA	1.94	0.68
1:C:10:ILE:HD11	1:C:113:ARG:HA	1.76	0.67
1:C:134:HIS:HB2	1:C:167:ARG:HE	1.60	0.67
1:C:88:LEU:HD23	1:C:114:LEU:HD22	1.74	0.67
2:D:127:VAL:HG22	2:D:136:LEU:HB3	1.75	0.67
2:D:24:GLN:HE21	2:D:24:GLN:CA	2.07	0.67
1:A:245:ALA:HA	1:A:248:VAL:HG13	1.76	0.67
2:B:47:ASN:HB2	2:D:40:GLN:O	1.95	0.66
2:B:84:ASN:HB3	2:B:91:VAL:HG13	1.76	0.66
1:C:163:LEU:HD23	1:C:188:ALA:HB2	1.75	0.66
2:B:48:LEU:O	2:B:55:ARG:HA	1.95	0.66
1:C:183:ARG:HA	1:C:208:ALA:O	1.94	0.66
1:C:151:ARG:HH21	1:C:151:ARG:HG2	1.61	0.65
1:A:108:GLN:HA	2:B:113:ASN:ND2	2.10	0.65
1:A:202:LEU:HA	1:A:207:ILE:HD12	1.78	0.65
1:A:292:GLY:O	1:A:296:ARG:HB2	1.96	0.65
2:B:146:SER:HG	2:B:149:VAL:HG23	1.61	0.65
2:D:13:LYS:NZ	4:D:169:HOH:O	2.29	0.65
1:A:234:ARG:HD3	4:A:352:HOH:O	1.94	0.65
1:C:229:ARG:HD2	1:C:270:VAL:HG11	1.78	0.65
2:D:72:ASP:O	2:D:100:PRO:HD3	1.96	0.65
1:C:187:ILE:HG22	1:C:247:PHE:CE1	2.29	0.65
1:A:108:GLN:HA	2:B:113:ASN:HD21	1.62	0.65
2:B:71:VAL:O	2:B:74:LEU:HG	1.97	0.64
2:D:22:PRO:HG2	2:D:25:ILE:HG13	1.77	0.64
1:C:39:LEU:HD12	1:C:66:LEU:HB3	1.79	0.64
2:D:109:CYS:SG	2:D:111:ASN:HB3	2.38	0.64
1:C:79:THR:HG22	1:C:80:SER:N	2.11	0.64
1:C:183:ARG:NE	1:C:208:ALA:HB1	2.12	0.64
2:D:38:THR:HG23	2:D:42:ILE:HD11	1.80	0.64
2:D:18:ILE:HG12	2:D:83:VAL:HG22	1.79	0.64
1:A:284:TRP:O	1:A:287:GLN:HB2	1.98	0.64
2:B:30:LEU:HB3	2:D:27:PHE:CE1	2.33	0.64
1:A:187:ILE:HG22	1:A:247:PHE:CD1	2.33	0.64
1:A:4:LEU:HD12	1:A:22:LEU:HD23	1.80	0.63
1:A:239:GLU:HA	1:A:242:ASN:HB2	1.79	0.63
2:D:12:ILE:O	2:D:12:ILE:HD12	1.98	0.63
2:B:59:ILE:HG22	2:B:61:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD23	1:A:207:ILE:CD1	2.29	0.63
1:C:81:LEU:HD12	1:C:86:GLU:HB2	1.81	0.63
2:D:19:ALA:HB1	2:D:56:LYS:HZ1	1.64	0.63
1:A:163:LEU:HD11	1:A:186:PHE:HB3	1.81	0.63
1:C:141:ASP:O	1:C:145:ILE:HG13	1.99	0.63
1:C:79:THR:HG22	1:C:80:SER:H	1.63	0.63
1:C:232:LYS:HA	1:C:240:TYR:CD2	2.33	0.62
1:C:243:VAL:HA	1:C:246:GLN:HG3	1.79	0.62
1:C:35:GLN:O	1:C:66:LEU:HD23	1.99	0.62
1:A:302:LEU:CD2	1:A:308:LEU:HD12	2.30	0.62
1:C:199:LEU:O	1:C:202:LEU:HB2	1.99	0.62
1:A:132:ASN:OD1	2:B:142:GLU:HB2	1.99	0.62
1:C:308:LEU:HB3	1:C:310:LEU:HD23	1.79	0.62
1:A:155:LEU:HB2	1:A:182:ASN:OD1	1.98	0.62
1:A:194:MET:SD	1:A:195:PRO:HD3	2.39	0.62
1:C:169:VAL:HG23	1:C:170:HIS:N	2.15	0.62
1:A:133:GLN:O	1:A:167:ARG:NH2	2.33	0.62
1:A:202:LEU:HD23	1:A:207:ILE:HD12	1.82	0.62
2:B:87:ASP:HB3	2:B:92:VAL:HG21	1.80	0.62
1:A:156:HIS:HD2	1:A:183:ARG:HD3	1.65	0.62
1:A:195:PRO:O	1:A:197:TYR:N	2.33	0.62
1:C:24:LEU:HD13	1:C:143:PHE:HA	1.82	0.62
1:C:166:GLY:O	1:C:169:VAL:HG22	2.00	0.62
1:A:285:TYR:HA	1:A:288:GLN:HG2	1.82	0.62
1:C:196:GLN:HA	1:C:199:LEU:HD12	1.82	0.61
1:A:136:THR:HB	1:A:296:ARG:HE	1.64	0.61
1:C:91:THR:HG22	1:C:95:ILE:HD11	1.83	0.61
2:B:84:ASN:OD1	2:B:94:LYS:HA	2.00	0.61
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.83	0.61
1:A:184:PHE:HD1	1:A:202:LEU:HD21	1.66	0.61
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.01	0.61
1:C:49:PHE:O	1:C:75:ASP:HA	2.00	0.61
2:D:14:ARG:HB2	2:D:87:ASP:HA	1.83	0.61
1:C:273:ILE:HD12	1:C:273:ILE:H	1.66	0.61
1:A:140:LEU:CB	1:A:292:GLY:HA2	2.31	0.60
1:C:46:SER:O	1:C:72:GLY:HA3	2.01	0.60
1:C:74:SER:O	1:C:78:ASN:HB2	2.01	0.60
2:B:32:LEU:HD22	2:B:106:VAL:HB	1.83	0.60
1:C:162:ASP:HB2	1:C:192:LEU:HD13	1.83	0.60
1:C:244:LYS:HD2	1:C:271:ASP:OD2	2.02	0.60
2:D:65:PHE:HB3	2:D:85:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:PRO:HG2	1:C:22:LEU:CD2	2.32	0.59
1:A:89:ALA:HB1	1:A:118:PHE:CE2	2.37	0.59
1:A:128:GLY:C	1:A:167:ARG:HH22	2.06	0.59
1:A:187:ILE:HD12	1:A:187:ILE:N	2.14	0.59
1:C:170:HIS:O	1:C:174:GLN:HG3	2.03	0.59
2:B:29:LEU:HD23	2:B:33:PHE:CE1	2.38	0.59
1:C:1:ALA:HB2	1:C:306:ARG:NH2	2.18	0.59
1:A:136:THR:HB	1:A:296:ARG:NE	2.18	0.59
2:D:24:GLN:NE2	2:D:24:GLN:CA	2.65	0.59
2:B:110:PRO:HG3	2:B:153:ASN:HD21	1.68	0.58
1:A:277:VAL:O	1:A:283:ALA:HB2	2.03	0.58
1:A:283:ALA:O	1:A:284:TRP:HE3	1.85	0.58
2:D:105:ASN:HB3	2:D:122:SER:HB2	1.86	0.58
2:B:134:ILE:HB	2:B:147:HIS:HB3	1.85	0.58
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.84	0.58
2:B:29:LEU:HD23	2:B:33:PHE:HE1	1.69	0.58
2:B:150:VAL:HG12	2:B:150:VAL:O	2.04	0.58
1:C:23:VAL:HG11	1:C:139:LEU:HG	1.86	0.58
1:A:196:GLN:HA	1:A:199:LEU:HD12	1.85	0.58
2:B:40:GLN:NE2	2:B:63:ASN:HB2	2.18	0.58
1:C:250:ARG:HB2	1:C:253:ASP:OD1	2.04	0.58
2:B:110:PRO:CD	2:B:150:VAL:HG22	2.33	0.58
1:C:225:LEU:HD23	1:C:263:VAL:HG22	1.84	0.58
1:C:24:LEU:N	1:C:24:LEU:HD23	2.18	0.58
1:A:153:ASP:HA	1:A:182:ASN:HD21	1.69	0.57
1:C:235:LEU:HD22	1:C:239:GLU:OE1	2.04	0.57
1:A:140:LEU:HB3	1:A:292:GLY:HA2	1.85	0.57
2:B:44:ILE:HD12	2:D:44:ILE:HB	1.86	0.57
2:B:62:GLU:HG2	2:B:63:ASN:N	2.19	0.57
2:B:18:ILE:HG23	2:B:83:VAL:HG22	1.87	0.57
2:D:24:GLN:N	2:D:24:GLN:HE21	2.02	0.57
1:A:201:MET:C	1:A:201:MET:SD	2.83	0.57
1:C:154:ASN:ND2	1:C:181:GLY:HA3	2.18	0.57
2:B:30:LEU:HB3	2:D:27:PHE:HE1	1.70	0.57
1:A:35:GLN:N	1:A:36:PRO:HD3	2.18	0.57
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.70	0.56
1:C:164:LYS:HD2	1:C:191:ALA:O	2.05	0.56
1:C:59:PHE:HZ	1:C:136:THR:HG21	1.70	0.56
2:D:76:LEU:HD11	2:D:103:ILE:HD12	1.87	0.56
2:D:136:LEU:HD13	2:D:150:VAL:HG21	1.87	0.56
1:C:196:GLN:O	1:C:199:LEU:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ASP:O	1:C:308:LEU:HG	2.05	0.56
1:A:79:THR:HG21	4:A:359:HOH:O	2.05	0.56
1:A:170:HIS:CG	4:A:394:HOH:O	2.58	0.56
1:A:239:GLU:O	1:A:242:ASN:HB2	2.05	0.56
1:A:82:GLY:HA2	1:A:86:GLU:HB3	1.88	0.56
1:C:169:VAL:CG2	1:C:170:HIS:N	2.69	0.56
1:C:5:TYR:CZ	1:C:6:GLN:HG2	2.41	0.56
1:A:152:LEU:HD12	1:A:176:LEU:HD21	1.88	0.55
1:A:156:HIS:CD2	1:A:183:ARG:HD3	2.41	0.55
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.35	0.55
2:B:68:GLU:HA	2:B:71:VAL:CG2	2.36	0.55
1:A:177:ALA:HB1	1:A:207:ILE:CD1	2.36	0.55
1:A:202:LEU:HD23	1:A:207:ILE:HB	1.88	0.55
1:A:243:VAL:CA	1:A:246:GLN:HG2	2.33	0.55
2:B:99:LEU:HD12	2:B:100:PRO:CD	2.27	0.55
1:A:5:TYR:CD1	1:A:6:GLN:HG2	2.42	0.55
2:B:33:PHE:HZ	2:B:77:TYR:CE2	2.25	0.55
1:C:188:ALA:HB1	1:C:189:PRO:HD2	1.87	0.55
1:C:249:LEU:HD23	1:C:273:ILE:HG13	1.88	0.55
2:D:10:GLU:OE2	2:D:12:ILE:HG23	2.07	0.55
1:A:189:PRO:HA	4:A:313:HOH:O	2.05	0.55
2:B:110:PRO:HG3	2:B:153:ASN:ND2	2.22	0.55
1:C:81:LEU:HD13	1:C:86:GLU:H	1.72	0.55
2:B:125:PHE:CE2	2:B:138:CYS:HB2	2.42	0.55
1:A:10:ILE:HD12	1:A:112:ALA:HB1	1.89	0.54
1:A:26:THR:HG23	1:A:310:LEU:CD1	2.36	0.54
1:A:239:GLU:HA	1:A:242:ASN:HD22	1.72	0.54
1:C:108:GLN:HA	2:D:113:ASN:ND2	2.20	0.54
1:C:109:GLU:HB3	2:D:141:CYS:HA	1.88	0.54
1:C:158:ALA:HB2	1:C:222:VAL:HG11	1.89	0.54
1:C:39:LEU:CD1	1:C:66:LEU:HD13	2.35	0.54
1:A:193:ALA:HB3	4:A:346:HOH:O	2.08	0.54
1:C:2:ASN:HB2	1:C:3:PRO:HD2	1.90	0.54
1:A:218:VAL:HG22	1:A:222:VAL:CG1	2.38	0.54
1:A:243:VAL:HG22	1:A:244:LYS:N	2.21	0.54
1:C:162:ASP:OD2	1:C:192:LEU:HD22	2.07	0.54
1:C:5:TYR:CE1	1:C:6:GLN:HG2	2.43	0.54
1:A:214:SER:O	1:A:217:GLU:HB2	2.06	0.54
2:D:4:ASP:O	2:D:8:GLN:HA	2.08	0.54
1:A:205:LYS:HB2	1:A:207:ILE:CG1	2.38	0.54
1:C:148:THR:HB	1:C:149:GLN:HE21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:ARG:HD3	2:D:65:PHE:HZ	1.72	0.54
1:A:9:ILE:HD13	1:A:15:LEU:HD21	1.90	0.53
2:D:43:THR:HB	2:D:60:LYS:HB2	1.89	0.53
2:B:52:GLU:HG2	2:B:53:MET:N	2.24	0.53
2:B:15:GLY:HA3	2:B:61:ILE:O	2.08	0.53
1:C:187:ILE:HG12	1:C:212:HIS:HB2	1.89	0.53
1:A:302:LEU:HD21	1:A:308:LEU:HD12	1.91	0.53
1:C:185:TYR:CE2	1:C:218:VAL:HG21	2.43	0.53
2:B:25:ILE:HG21	2:B:77:TYR:O	2.09	0.53
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.43	0.53
1:A:25:ALA:O	1:A:29:LYS:HG3	2.08	0.53
2:B:121:VAL:HB	2:B:140:TYR:OH	2.09	0.53
1:C:98:TYR:HB2	1:C:99:VAL:HG13	1.91	0.53
2:D:103:ILE:HG21	2:D:107:LEU:HD11	1.91	0.53
2:D:44:ILE:HG22	2:D:46:LEU:HD21	1.90	0.53
1:C:227:MET:HG3	1:C:273:ILE:HD11	1.91	0.53
2:B:109:CYS:HB2	2:B:125:PHE:HZ	1.74	0.52
2:B:76:LEU:HD12	2:B:76:LEU:N	2.23	0.52
1:C:246:GLN:HB2	1:C:247:PHE:CE2	2.45	0.52
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.91	0.52
1:A:182:ASN:HB3	1:A:184:PHE:CE2	2.44	0.52
1:A:160:VAL:CG1	1:A:161:GLY:H	2.22	0.52
1:A:34:PRO:C	1:A:36:PRO:HD3	2.30	0.52
1:A:159:MET:O	1:A:163:LEU:HD22	2.10	0.52
1:A:128:GLY:HA2	1:A:167:ARG:HH22	1.75	0.52
1:A:199:LEU:HD22	1:A:209:TRP:CZ3	2.45	0.52
1:A:265:HIS:C	1:A:265:HIS:ND1	2.62	0.52
2:B:114:CYS:SG	2:B:141:CYS:HB3	2.50	0.52
2:B:14:ARG:O	2:B:63:ASN:HA	2.10	0.52
2:D:127:VAL:HG13	2:D:134:ILE:HG23	1.92	0.52
2:D:86:ILE:CG2	2:D:87:ASP:N	2.73	0.52
1:A:160:VAL:CG1	1:A:161:GLY:N	2.69	0.52
1:A:149:GLN:NE2	1:A:224:ILE:HD11	2.25	0.52
1:A:288:GLN:HG3	1:A:289:ALA:N	2.23	0.52
2:D:76:LEU:CD1	2:D:103:ILE:HD12	2.40	0.52
2:D:68:GLU:CD	2:D:68:GLU:H	2.13	0.52
1:A:129:ASP:N	1:A:167:ARG:HH22	2.08	0.52
1:A:17:ARG:NH1	1:A:179:PHE:HA	2.25	0.52
1:A:209:TRP:CE3	1:A:209:TRP:O	2.63	0.52
2:B:25:ILE:HG21	2:B:77:TYR:HB3	1.91	0.52
1:C:8:HIS:ND1	1:C:116:THR:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LEU:CD2	2:B:33:PHE:HE1	2.22	0.51
2:B:62:GLU:HG2	2:B:63:ASN:H	1.76	0.51
1:C:273:ILE:N	1:C:273:ILE:HD12	2.25	0.51
2:D:19:ALA:HB1	2:D:56:LYS:NZ	2.25	0.51
1:C:109:GLU:HG2	1:C:132:ASN:HB2	1.93	0.51
1:C:199:LEU:O	1:C:202:LEU:N	2.44	0.51
1:C:26:THR:O	1:C:29:LYS:N	2.40	0.51
1:C:96:SER:OG	1:C:119:SER:HA	2.10	0.51
1:A:61:THR:HB	1:A:293:ILE:HD11	1.92	0.51
2:B:50:SER:O	2:B:52:GLU:N	2.44	0.51
2:B:14:ARG:HG2	2:B:87:ASP:OD2	2.10	0.51
2:D:13:LYS:O	2:D:13:LYS:HG2	2.08	0.51
2:D:77:TYR:CE1	2:D:151:LEU:HD12	2.46	0.51
1:A:156:HIS:HB3	1:A:185:TYR:CE1	2.32	0.51
2:B:126:ALA:HB3	2:B:137:LYS:HB3	1.93	0.51
2:D:129:LYS:HG3	2:D:134:ILE:HD12	1.92	0.51
1:C:231:GLN:O	1:C:235:LEU:HG	2.11	0.51
2:D:21:ILE:HG22	2:D:25:ILE:HB	1.92	0.51
1:A:153:ASP:O	1:A:154:ASN:HB2	2.11	0.51
2:B:34:LYS:HB3	2:B:37:GLU:OE1	2.11	0.51
1:C:1:ALA:HB2	1:C:306:ARG:HH22	1.75	0.51
1:C:187:ILE:HD12	1:C:215:ILE:HG23	1.92	0.51
1:C:79:THR:CG2	1:C:80:SER:H	2.23	0.51
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.26	0.51
2:B:25:ILE:CG2	2:B:77:TYR:HB3	2.41	0.51
1:C:113:ARG:HG2	2:D:139:LYS:O	2.11	0.51
2:D:17:VAL:HG13	2:D:58:LEU:HD21	1.93	0.51
2:B:119:GLU:HB3	2:B:120:PRO:HD2	1.92	0.50
1:C:9:ILE:HG13	1:C:299:LEU:HD21	1.92	0.50
2:B:27:PHE:CE1	2:D:30:LEU:HB2	2.46	0.50
1:C:243:VAL:HG12	1:C:246:GLN:OE1	2.12	0.50
1:C:92:ILE:HD12	1:C:102:ILE:HD13	1.93	0.50
2:D:20:HIS:C	2:D:80:GLN:HE22	2.15	0.50
1:A:177:ALA:HB1	1:A:207:ILE:HD13	1.91	0.50
2:B:110:PRO:HD2	2:B:145:PHE:HD1	1.70	0.50
2:D:16:THR:HG23	2:D:83:VAL:HG13	1.94	0.50
2:D:8:GLN:CD	2:D:8:GLN:H	2.15	0.50
1:A:118:PHE:N	1:A:118:PHE:CD1	2.79	0.50
2:D:107:LEU:HB2	2:D:125:PHE:CE1	2.47	0.50
1:A:110:GLY:O	1:A:113:ARG:N	2.44	0.50
2:D:41:ARG:HB3	2:D:62:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LYS:N	2:D:6:LYS:HD2	2.26	0.50
1:A:156:HIS:CD2	1:A:183:ARG:HB3	2.47	0.50
1:A:245:ALA:HB1	1:A:250:ARG:HH12	1.76	0.50
2:B:61:ILE:HG22	2:B:64:THR:HB	1.94	0.50
1:A:48:PHE:O	1:A:74:SER:HA	2.11	0.50
2:B:134:ILE:HG22	2:B:135:ALA:N	2.27	0.49
2:B:110:PRO:HD2	2:B:145:PHE:CE1	2.46	0.49
1:A:194:MET:SD	1:A:195:PRO:CD	3.00	0.49
1:A:177:ALA:CB	1:A:207:ILE:HD13	2.42	0.49
1:C:229:ARG:CZ	1:C:268:PRO:HG2	2.42	0.49
2:D:19:ALA:O	2:D:20:HIS:HB2	2.12	0.49
1:C:109:GLU:HA	1:C:129:ASP:O	2.13	0.49
1:C:79:THR:CG2	1:C:80:SER:N	2.75	0.49
2:B:67:SER:O	2:B:69:ASP:N	2.46	0.49
1:C:229:ARG:HD2	1:C:270:VAL:CG1	2.42	0.49
2:D:76:LEU:HD11	2:D:103:ILE:CD1	2.42	0.49
1:A:266:PRO:HA	1:A:288:GLN:HE22	1.77	0.49
2:B:111:ASN:HB3	2:B:114:CYS:HB2	1.94	0.49
2:B:44:ILE:HG23	2:B:59:ILE:CD1	2.38	0.49
2:B:27:PHE:CD1	2:D:36:THR:HG21	2.48	0.49
1:A:201:MET:O	1:A:205:LYS:HG2	2.12	0.49
2:B:25:ILE:O	2:B:29:LEU:HG	2.13	0.49
2:D:24:GLN:H	2:D:24:GLN:HE21	1.61	0.49
1:A:138:THR:O	1:A:141:ASP:HB2	2.13	0.49
1:A:223:ASP:O	1:A:261:MET:HG2	2.13	0.49
2:B:84:ASN:HB3	2:B:91:VAL:CG1	2.43	0.49
1:C:231:GLN:HB2	1:C:234:ARG:HB2	1.94	0.49
1:C:154:ASN:N	1:C:180:ASP:O	2.43	0.49
1:A:45:ALA:HA	1:A:71:VAL:O	2.13	0.48
1:C:145:ILE:HG23	1:C:224:ILE:HG13	1.95	0.48
1:C:81:LEU:CD1	1:C:86:GLU:HB2	2.42	0.48
1:A:243:VAL:O	1:A:245:ALA:N	2.46	0.48
1:A:251:ALA:O	1:A:254:LEU:HB2	2.13	0.48
1:A:265:HIS:O	1:A:267:LEU:HG	2.13	0.48
2:D:69:ASP:O	2:D:72:ASP:N	2.46	0.48
1:C:186:PHE:HB2	1:C:211:LEU:HD23	1.95	0.48
1:A:265:HIS:HE2	1:A:269:ARG:HA	1.78	0.48
1:A:199:LEU:O	1:A:202:LEU:HB2	2.14	0.48
2:D:147:HIS:CG	2:D:148:ASN:N	2.80	0.48
1:C:292:GLY:HA2	1:C:295:ALA:HB3	1.95	0.48
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HB3	1:A:152:LEU:HD11	1.95	0.48
1:A:187:ILE:H	1:A:187:ILE:CD1	2.22	0.48
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.66	0.47
1:C:253:ASP:C	1:C:255:HIS:N	2.66	0.47
1:C:254:LEU:O	1:C:256:ASN:N	2.47	0.47
1:A:170:HIS:CD2	1:A:170:HIS:H	2.32	0.47
2:B:124:SER:HB3	2:B:139:LYS:HD3	1.96	0.47
2:D:124:SER:HB3	2:D:139:LYS:HD3	1.95	0.47
2:B:46:LEU:HD12	2:D:42:ILE:HB	1.95	0.47
2:B:70:GLN:O	2:B:73:GLN:HB2	2.15	0.47
1:A:244:LYS:HD3	1:A:245:ALA:N	2.28	0.47
1:A:265:HIS:CD2	1:A:269:ARG:HB3	2.50	0.47
1:A:307:ASP:OD2	1:A:309:VAL:HG23	2.14	0.47
1:A:151:ARG:O	1:A:155:LEU:HD11	2.14	0.47
2:B:150:VAL:HA	2:B:153:ASN:ND2	2.29	0.47
1:C:236:ASP:O	1:C:239:GLU:N	2.47	0.47
1:C:272:GLU:HG2	1:C:273:ILE:H	1.79	0.47
1:A:197:TYR:CE1	1:A:198:ILE:HD12	2.49	0.47
1:A:218:VAL:O	1:A:222:VAL:HG22	2.15	0.47
1:C:21:ASN:N	1:C:21:ASN:HD22	2.13	0.47
2:D:14:ARG:HG2	2:D:15:GLY:N	2.30	0.47
1:A:51:ALA:HB3	1:A:75:ASP:HB2	1.97	0.47
2:B:109:CYS:SG	2:B:111:ASN:HB3	2.55	0.47
1:C:277:VAL:O	1:C:280:THR:HG23	2.15	0.47
2:B:7:LEU:N	2:B:7:LEU:HD22	2.31	0.46
1:C:59:PHE:CD2	1:C:296:ARG:HD3	2.50	0.46
2:D:86:ILE:HG22	2:D:87:ASP:N	2.29	0.46
1:A:44:ILE:HG12	1:A:101:ALA:HB3	1.96	0.46
2:B:109:CYS:O	2:B:117:HIS:NE2	2.46	0.46
1:C:39:LEU:HD12	1:C:66:LEU:CB	2.44	0.46
2:D:115:ILE:HA	2:D:115:ILE:HD12	1.73	0.46
1:A:149:GLN:O	1:A:151:ARG:HG2	2.15	0.46
1:A:128:GLY:CA	1:A:167:ARG:HH22	2.29	0.46
1:A:164:LYS:O	1:A:170:HIS:CE1	2.68	0.46
1:A:196:GLN:O	1:A:199:LEU:N	2.48	0.46
2:B:88:ASN:ND2	4:B:174:HOH:O	2.48	0.46
1:C:308:LEU:C	1:C:310:LEU:H	2.18	0.46
1:A:112:ALA:CB	1:A:126:ASN:HB2	2.46	0.46
2:B:89:TYR:O	2:B:90:GLU:HG2	2.16	0.46
1:C:183:ARG:CG	1:C:208:ALA:HB3	2.34	0.46
2:B:27:PHE:HE1	2:D:30:LEU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:HA	1:A:183:ARG:O	2.15	0.46
1:C:246:GLN:HB2	1:C:247:PHE:CD2	2.51	0.46
1:C:8:HIS:N	1:C:8:HIS:CD2	2.84	0.46
2:D:139:LYS:NZ	2:D:140:TYR:OH	2.40	0.46
1:C:175:ALA:O	1:C:178:LYS:HB2	2.16	0.46
1:A:126:ASN:HD21	1:A:129:ASP:H	1.64	0.45
1:A:24:LEU:HA	1:A:24:LEU:HD22	1.56	0.45
1:A:272:GLU:H	1:A:272:GLU:CD	2.18	0.45
1:A:275:THR:HA	1:A:278:ASP:OD2	2.17	0.45
2:B:16:THR:HG21	2:B:66:LEU:H	1.81	0.45
1:C:265:HIS:HA	1:C:266:PRO:HD3	1.81	0.45
1:C:275:THR:HB	4:C:366:HOH:O	2.16	0.45
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.56	0.45
2:B:119:GLU:HB3	2:B:120:PRO:CD	2.45	0.45
2:D:65:PHE:HB3	2:D:85:ARG:HH11	1.81	0.45
1:A:12:ILE:HA	1:A:12:ILE:HD12	1.64	0.45
1:A:32:ALA:O	1:A:34:PRO:HD3	2.15	0.45
1:A:9:ILE:HG22	1:A:9:ILE:O	2.17	0.45
2:B:67:SER:C	2:B:69:ASP:H	2.19	0.45
1:C:9:ILE:HG13	1:C:299:LEU:HD11	1.97	0.45
1:A:160:VAL:HG22	1:A:187:ILE:HD13	1.98	0.45
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.64	0.45
1:C:202:LEU:HA	1:C:202:LEU:HD23	1.64	0.45
1:C:284:TRP:CD1	1:C:287:GLN:HB2	2.51	0.45
2:D:42:ILE:HG22	2:D:43:THR:N	2.32	0.45
1:C:267:LEU:HD23	1:C:267:LEU:HA	1.41	0.45
1:A:31:LYS:HD2	1:A:294:PHE:CE2	2.52	0.45
2:B:14:ARG:NH1	2:B:14:ARG:HB2	2.32	0.45
2:D:23:ALA:HA	2:D:57:ASP:OD2	2.15	0.45
2:D:47:ASN:HB3	2:D:55:ARG:HG2	1.98	0.45
1:A:128:GLY:HA2	1:A:167:ARG:NH2	2.31	0.45
1:C:244:LYS:HB3	1:C:244:LYS:HE3	1.89	0.45
1:C:252:SER:O	1:C:255:HIS:CB	2.63	0.45
1:A:153:ASP:CB	1:A:180:ASP:O	2.65	0.45
1:A:170:HIS:N	1:A:170:HIS:CD2	2.84	0.45
1:A:219:MET:HG3	1:A:256:ASN:CB	2.33	0.45
1:A:270:VAL:HG13	1:A:271:ASP:N	2.32	0.45
2:B:68:GLU:HA	2:B:71:VAL:HG23	1.98	0.45
1:A:115:ALA:O	1:A:119:SER:HB3	2.17	0.44
1:A:132:ASN:ND2	1:A:133:GLN:HG2	2.32	0.44
1:A:205:LYS:HG3	1:A:207:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASN:HD21	1:C:129:ASP:CG	2.20	0.44
1:A:225:LEU:HD12	1:A:225:LEU:C	2.37	0.44
1:A:74:SER:O	1:A:75:ASP:C	2.55	0.44
1:C:151:ARG:NH2	1:C:151:ARG:HG2	2.30	0.44
1:A:215:ILE:C	1:A:217:GLU:H	2.20	0.44
2:B:107:LEU:HD11	2:B:136:LEU:HD13	1.99	0.44
1:C:94:VAL:HG12	1:C:95:ILE:N	2.32	0.44
2:D:14:ARG:HA	2:D:86:ILE:HG22	1.99	0.44
2:D:58:LEU:HD23	2:D:59:ILE:N	2.31	0.44
1:A:163:LEU:HG	1:A:188:ALA:HB2	2.00	0.44
1:A:202:LEU:CD2	1:A:207:ILE:HB	2.46	0.44
1:A:269:ARG:O	1:A:270:VAL:HB	2.17	0.44
2:B:50:SER:N	2:B:54:GLY:O	2.50	0.44
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.63	0.44
2:B:70:GLN:O	2:B:73:GLN:N	2.51	0.44
1:C:165:TYR:CD2	1:C:234:ARG:NE	2.85	0.44
1:C:81:LEU:CD2	1:C:84:LYS:HB2	2.36	0.44
2:D:110:PRO:CG	2:D:150:VAL:HG22	2.48	0.44
2:B:14:ARG:HH11	2:B:14:ARG:HB2	1.82	0.44
1:C:103:VAL:HG22	1:C:125:LEU:HB2	1.99	0.44
1:C:156:HIS:HB3	1:C:222:VAL:HA	1.99	0.44
2:D:104:ASP:O	2:D:106:VAL:N	2.50	0.44
1:A:286:PHE:HA	1:A:289:ALA:HB3	1.99	0.44
2:B:21:ILE:HA	2:B:81:ALA:HB2	1.99	0.44
2:B:36:THR:HG21	2:D:27:PHE:CE1	2.53	0.44
2:B:20:HIS:O	2:B:81:ALA:HA	2.17	0.44
2:B:85:ARG:C	2:B:86:ILE:HD12	2.38	0.44
1:C:194:MET:SD	1:C:198:ILE:HG21	2.58	0.44
1:C:217:GLU:H	1:C:217:GLU:HG2	1.61	0.44
1:C:39:LEU:HD12	1:C:66:LEU:CD1	2.43	0.44
1:C:273:ILE:HG23	1:C:277:VAL:HG21	2.00	0.44
1:A:39:LEU:C	1:A:42:LYS:HG2	2.38	0.43
2:B:79:PRO:HG2	2:B:80:GLN:H	1.82	0.43
1:C:269:ARG:NH1	1:C:278:ASP:OD1	2.51	0.43
1:A:169:VAL:HG12	1:A:228:THR:HG21	1.99	0.43
2:B:13:LYS:HD3	2:B:62:GLU:OE1	2.17	0.43
2:B:35:LEU:H	2:B:35:LEU:HD12	1.82	0.43
1:C:138:THR:O	1:C:139:LEU:C	2.56	0.43
1:A:39:LEU:O	1:A:42:LYS:HG2	2.17	0.43
2:B:129:LYS:HE3	2:B:129:LYS:HB3	1.74	0.43
2:B:36:THR:HG21	2:D:27:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:NE	1:C:208:ALA:CB	2.80	0.43
1:C:192:LEU:HD23	1:C:192:LEU:HA	1.71	0.43
1:C:292:GLY:HA2	1:C:295:ALA:CB	2.47	0.43
2:D:20:HIS:O	2:D:81:ALA:CA	2.64	0.43
2:D:48:LEU:O	2:D:55:ARG:HA	2.18	0.43
1:A:56:ARG:HH21	1:A:56:ARG:HG2	1.84	0.43
1:C:256:ASN:HB2	4:C:349:HOH:O	2.18	0.43
2:D:146:SER:OG	2:D:147:HIS:N	2.50	0.43
1:A:153:ASP:HA	1:A:182:ASN:ND2	2.34	0.43
1:A:39:LEU:HD22	1:A:304:LEU:HB2	1.99	0.43
1:C:255:HIS:HB3	1:C:256:ASN:OD1	2.18	0.43
1:C:3:PRO:CG	1:C:22:LEU:HD22	2.49	0.43
1:C:95:ILE:C	1:C:97:THR:H	2.21	0.43
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.48	0.43
1:A:81:LEU:HD23	1:A:82:GLY:H	1.83	0.43
1:C:158:ALA:HB2	1:C:222:VAL:CG1	2.48	0.43
1:C:3:PRO:CG	1:C:22:LEU:CD2	2.96	0.43
1:C:31:LYS:HG3	1:C:294:PHE:CE2	2.53	0.43
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.34	0.43
1:A:17:ARG:HH11	1:A:179:PHE:CA	2.30	0.43
1:A:164:LYS:HB2	1:A:193:ALA:O	2.19	0.43
2:B:23:ALA:O	2:B:24:GLN:HB2	2.19	0.43
2:B:61:ILE:CG2	2:B:64:THR:HB	2.49	0.43
2:D:55:ARG:CG	2:D:55:ARG:NH1	2.75	0.43
1:C:24:LEU:N	1:C:24:LEU:CD2	2.82	0.43
1:C:272:GLU:CG	1:C:273:ILE:H	2.32	0.43
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.88	0.43
1:C:8:HIS:H	1:C:8:HIS:CD2	2.36	0.43
2:D:33:PHE:O	2:D:34:LYS:HB2	2.18	0.43
2:D:38:THR:CG2	2:D:42:ILE:HD11	2.47	0.43
1:A:265:HIS:HA	1:A:266:PRO:HD2	1.69	0.43
1:A:95:ILE:HG22	1:A:99:VAL:HG22	2.01	0.43
1:C:289:ALA:O	1:C:291:ASN:N	2.52	0.43
1:C:278:ASP:N	1:C:278:ASP:OD2	2.52	0.42
2:B:67:SER:C	2:B:69:ASP:N	2.71	0.42
1:C:163:LEU:HB3	1:C:194:MET:HA	2.00	0.42
1:C:265:HIS:H	1:C:288:GLN:HE22	1.66	0.42
1:A:187:ILE:HA	1:A:212:HIS:O	2.20	0.42
1:A:184:PHE:CE1	1:A:207:ILE:HG21	2.53	0.42
1:C:108:GLN:HG2	4:D:174:HOH:O	2.19	0.42
1:C:198:ILE:O	1:C:202:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:NH1	4:C:376:HOH:O	2.42	0.42
2:D:22:PRO:HG2	2:D:25:ILE:CG1	2.48	0.42
2:D:80:GLN:OE1	2:D:81:ALA:N	2.52	0.42
1:A:164:LYS:HD3	1:A:192:LEU:HD23	2.00	0.42
1:A:51:ALA:HB2	1:A:75:ASP:H	1.84	0.42
1:C:140:LEU:O	1:C:143:PHE:N	2.53	0.42
1:C:148:THR:HB	1:C:149:GLN:NE2	2.34	0.42
1:C:227:MET:CG	1:C:273:ILE:HD11	2.49	0.42
1:A:274:ALA:O	1:A:277:VAL:HB	2.19	0.42
1:C:35:GLN:HA	1:C:36:PRO:HD2	1.88	0.42
1:A:105:ARG:HD2	1:A:127:ALA:O	2.19	0.42
2:B:75:ALA:O	2:B:79:PRO:HB3	2.20	0.42
2:D:77:TYR:N	2:D:77:TYR:CD2	2.88	0.42
1:A:31:LYS:NZ	1:A:147:GLU:OE1	2.52	0.42
2:B:25:ILE:HG22	2:B:25:ILE:O	2.20	0.42
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.61	0.42
1:C:270:VAL:N	1:C:272:GLU:OE2	2.53	0.42
2:D:25:ILE:HG22	2:D:29:LEU:HD21	2.02	0.42
1:A:162:ASP:O	1:A:162:ASP:CG	2.59	0.42
1:A:253:ASP:N	1:A:253:ASP:OD2	2.53	0.42
1:A:302:LEU:HD23	1:A:308:LEU:HD12	2.02	0.42
1:C:125:LEU:CD2	1:C:300:LEU:HD23	2.50	0.42
2:D:49:PRO:HA	2:D:54:GLY:O	2.20	0.42
1:A:239:GLU:CA	1:A:242:ASN:HB2	2.49	0.41
2:B:11:ALA:O	2:D:7:LEU:HD13	2.19	0.41
1:C:22:LEU:O	1:C:22:LEU:HG	2.20	0.41
1:A:106:HIS:HA	1:A:107:PRO:HD3	1.85	0.41
1:A:231:GLN:H	1:A:234:ARG:HE	1.67	0.41
1:A:243:VAL:O	1:A:246:GLN:HG2	2.19	0.41
1:C:44:ILE:HG23	1:C:101:ALA:O	2.20	0.41
1:C:159:MET:HE3	1:C:184:PHE:HD2	1.85	0.41
1:C:48:PHE:O	1:C:74:SER:HA	2.20	0.41
2:D:110:PRO:HG2	2:D:150:VAL:HG22	2.02	0.41
2:D:4:ASP:OD1	2:D:7:LEU:HB2	2.20	0.41
2:B:96:ARG:HA	2:B:97:PRO:HD3	1.69	0.41
2:D:14:ARG:CB	2:D:87:ASP:HA	2.49	0.41
1:A:61:THR:O	1:A:65:ARG:HG2	2.21	0.41
1:A:129:ASP:OD1	1:A:133:GLN:HB2	2.21	0.41
1:A:177:ALA:HB1	1:A:207:ILE:HD11	2.02	0.41
1:A:244:LYS:O	1:A:248:VAL:HG13	2.20	0.41
1:C:185:TYR:CE2	1:C:218:VAL:CG2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASP:H	1:C:239:GLU:HB3	1.85	0.41
2:D:29:LEU:HD22	2:D:33:PHE:HE2	1.86	0.41
1:A:269:ARG:HH12	1:A:278:ASP:CG	2.24	0.41
2:B:128:ARG:HH21	2:B:144:GLU:CD	2.22	0.41
2:B:83:VAL:O	2:B:95:SER:HB2	2.21	0.41
1:C:223:ASP:O	1:C:261:MET:HA	2.20	0.41
2:D:30:LEU:CA	2:D:35:LEU:HD12	2.34	0.41
2:D:21:ILE:C	2:D:53:MET:HE1	2.41	0.41
1:A:261:MET:SD	1:A:261:MET:C	2.99	0.41
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.21	0.41
1:A:293:ILE:HD12	1:A:293:ILE:HA	1.87	0.41
1:A:2:ASN:OD1	1:A:2:ASN:C	2.59	0.41
2:B:104:ASP:O	2:B:106:VAL:HG13	2.20	0.41
2:B:127:VAL:HG13	2:B:134:ILE:CG2	2.51	0.41
2:B:24:GLN:NE2	2:B:24:GLN:HA	2.36	0.41
1:C:162:ASP:CB	1:C:192:LEU:HD13	2.50	0.41
1:A:126:ASN:ND2	1:A:129:ASP:OD1	2.53	0.41
1:C:157:VAL:O	1:C:184:PHE:HA	2.20	0.41
2:D:20:HIS:N	2:D:56:LYS:HZ1	2.19	0.41
2:B:41:ARG:O	2:B:62:GLU:HB3	2.22	0.40
1:C:187:ILE:CD1	1:C:215:ILE:HG23	2.50	0.40
1:C:250:ARG:NH2	1:C:252:SER:HB2	2.36	0.40
1:C:299:LEU:O	1:C:302:LEU:N	2.53	0.40
1:A:102:ILE:O	1:A:124:VAL:HA	2.20	0.40
1:A:153:ASP:HB2	1:A:180:ASP:O	2.21	0.40
1:A:140:LEU:HB2	1:A:292:GLY:HA2	2.03	0.40
1:A:12:ILE:CG2	1:A:13:ASN:N	2.84	0.40
1:A:140:LEU:CB	1:A:292:GLY:CA	2.98	0.40
2:B:107:LEU:HD22	2:B:150:VAL:HG12	2.02	0.40
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.81	0.40
2:D:83:VAL:O	2:D:95:SER:N	2.54	0.40
1:A:149:GLN:O	1:A:151:ARG:N	2.55	0.40
1:A:94:VAL:O	1:A:97:THR:HG23	2.21	0.40
2:B:107:LEU:CD1	2:B:136:LEU:HD13	2.51	0.40
1:C:194:MET:HA	1:C:195:PRO:HD3	1.93	0.40
2:D:40:GLN:NE2	2:D:63:ASN:OD1	2.54	0.40
2:D:21:ILE:HG23	2:D:78:ALA:CB	2.52	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	308/310 (99%)	246 (80%)	44 (14%)	18 (6%)	2	3
1	C	308/310 (99%)	243 (79%)	47 (15%)	18 (6%)	2	3
2	B	151/153 (99%)	124 (82%)	15 (10%)	12 (8%)	1	1
2	D	151/153 (99%)	118 (78%)	27 (18%)	6 (4%)	3	7
All	All	918/926 (99%)	731 (80%)	133 (14%)	54 (6%)	2	3

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	244	LYS
1	A	270	VAL
2	B	51	GLY
2	B	63	ASN
2	B	75	ALA
2	B	105	ASN
1	C	132	ASN
1	C	255	HIS
1	C	270	VAL
1	C	272	GLU
2	D	105	ASN
2	D	131	ALA
2	D	152	ALA
1	A	75	ASP
1	A	150	GLY
1	A	218	VAL
1	A	219	MET
2	B	6	LYS
2	B	47	ASN
2	B	68	GLU
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	166	GLY
1	C	219	MET
2	D	54	GLY
1	A	121	ASN
1	A	128	GLY
1	A	164	LYS
1	A	234	ARG
1	A	235	LEU
2	B	32	LEU
1	C	4	LEU
1	C	96	SER
1	C	271	ASP
1	C	299	LEU
1	A	266	PRO
1	A	306	ARG
2	B	54	GLY
1	A	6	GLN
1	A	76	SER
2	B	31	SER
1	C	75	ASP
1	C	199	LEU
2	D	20	HIS
1	A	281	PRO
2	D	78	ALA
2	B	12	ILE
1	C	309	VAL
1	C	3	PRO
1	C	237	PRO
1	A	36	PRO
1	C	267	LEU
2	B	120	PRO
1	C	135	PRO

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	261/261 (100%)	208 (80%)	53 (20%)	1	4
1	C	261/261 (100%)	228 (87%)	33 (13%)	5	12
2	B	136/136 (100%)	115 (85%)	21 (15%)	3	8
2	D	136/136 (100%)	115 (85%)	21 (15%)	3	8
All	All	794/794 (100%)	666 (84%)	128 (16%)	3	7

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	17	ARG
1	A	18	ASP
1	A	21	ASN
1	A	24	LEU
1	A	42	LYS
1	A	46	SER
1	A	63	MET
1	A	71	VAL
1	A	74	SER
1	A	81	LEU
1	A	88	LEU
1	A	91	THR
1	A	98	TYR
1	A	103	VAL
1	A	116	THR
1	A	118	PHE
1	A	124	VAL
1	A	134	HIS
1	A	136	THR
1	A	140	LEU
1	A	142	LEU
1	A	144	THR
1	A	149	GLN
1	A	162	ASP
1	A	163	LEU
1	A	171	SER
1	A	174	GLN
1	A	190	ASP
1	A	198	ILE
1	A	202	LEU
1	A	203	ASP
1	A	210	SER

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Mol	Chain	Res	Type
1	A	213	SER
1	A	223	ASP
1	A	225	LEU
1	A	227	MET
1	A	235	LEU
1	A	238	SER
1	A	240	TYR
1	A	243	VAL
1	A	249	LEU
1	A	253	ASP
1	A	254	LEU
1	A	261	MET
1	A	265	HIS
1	A	268	PRO
1	A	269	ARG
1	A	276	ASP
1	A	285	TYR
1	A	296	ARG
1	A	303	VAL
1	A	305	ASN
2	B	2	THR
2	B	5	ASN
2	B	7	LEU
2	B	16	THR
2	B	18	ILE
2	B	20	HIS
2	B	31	SER
2	B	35	LEU
2	B	38	THR
2	B	43	THR
2	B	50	SER
2	B	52	GLU
2	B	53	MET
2	B	68	GLU
2	B	76	LEU
2	B	80	GLN
2	B	85	ARG
2	B	102	ARG
2	B	122	SER
2	B	148	ASN
2	B	153	ASN
1	C	10	ILE

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Mol	Chain	Res	Type
1	C	14	ASP
1	C	24	LEU
1	C	37	GLU
1	C	38	LEU
1	C	53	THR
1	C	59	PHE
1	C	62	SER
1	C	75	ASP
1	C	86	GLU
1	C	87	THR
1	C	93	SER
1	C	100	ASP
1	C	139	LEU
1	C	140	LEU
1	C	146	GLN
1	C	148	THR
1	C	153	ASP
1	C	163	LEU
1	C	167	ARG
1	C	180	ASP
1	C	215	ILE
1	C	217	GLU
1	C	218	VAL
1	C	237	PRO
1	C	256	ASN
1	C	261	MET
1	C	268	PRO
1	C	275	THR
1	C	278	ASP
1	C	279	LYS
1	C	297	GLN
1	C	308	LEU
2	D	3	HIS
2	D	6	LYS
2	D	8	GLN
2	D	24	GLN
2	D	31	SER
2	D	35	LEU
2	D	55	ARG
2	D	57	ASP
2	D	63	ASN
2	D	77	TYR

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Mol	Chain	Res	Type
2	D	80	GLN
2	D	92	VAL
2	D	96	ARG
2	D	99	LEU
2	D	101	GLU
2	D	112	SER
2	D	122	SER
2	D	132	ASN
2	D	136	LEU
2	D	149	VAL
2	D	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	149	GLN
1	A	154	ASN
1	A	156	HIS
1	A	242	ASN
1	A	288	GLN
2	B	8	GLN
2	B	24	GLN
2	B	40	GLN
2	B	47	ASN
2	B	113	ASN
2	B	148	ASN
2	B	153	ASN
1	C	13	ASN
1	C	21	ASN
1	C	64	HIS
1	C	146	GLN
1	C	149	GLN
1	C	154	ASN
1	C	288	GLN
2	D	5	ASN
2	D	8	GLN
2	D	20	HIS
2	D	24	GLN
2	D	70	GLN
2	D	113	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.