WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 12:14 AM EST

PDB ID	:	4HPQ
Title	:	Crystal Structure of the Atg17-Atg31-Atg29 Complex
Authors	:	Stanley, R.E.; Ragusa, M.J.; Hurley, J.H.
Deposited on	:	2012-10-24
Resolution	:	3.06 Å(reported)

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

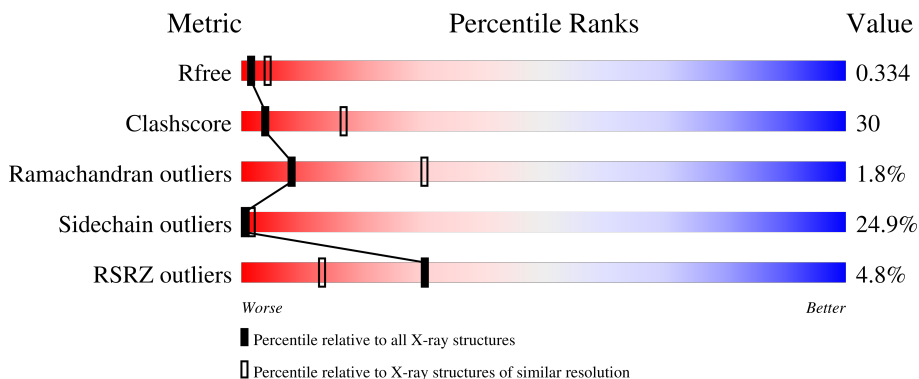|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 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.
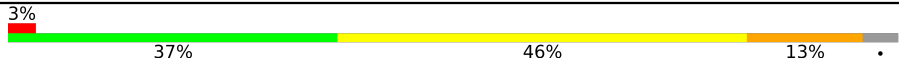
Metric	Percentile Ranks	Value
Rfree		0.334
Clashscore		30
Ramachandran outliers		1.8%
Sidechain outliers		24.9%
RSRZ outliers		4.8%

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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	69	4% 65% 28% 6% •
1	D	69	3% 62% 29% 7% •
2	B	159	% 39% 26% 8% 28%
2	E	159	37% 26% 9% 28%
3	C	413	8% 37% 44% 14% •

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Mol	Chain	Length	Quality of chain
3	F	413	3% 37% 46% 13%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9220 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 Atg29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			429	266	82	80	1			
1	D	69	Total	C	N	O	S	0	0	0
			429	266	82	80	1			

- Molecule 2 is a protein called Atg31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			932	587	156	185	4			
2	E	115	Total	C	N	O	S	0	0	0
			932	587	156	185	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MET	LEU	engineered mutation	UNP C5DEB9
B	110	MET	LEU	engineered mutation	UNP C5DEB9
B	146	ALA	-	expression tag	UNP C5DEB9
B	147	GLY	-	expression tag	UNP C5DEB9
B	148	GLN	-	expression tag	UNP C5DEB9
B	149	PHE	-	expression tag	UNP C5DEB9
B	150	TYR	-	expression tag	UNP C5DEB9
B	151	LEU	-	expression tag	UNP C5DEB9
B	152	ASN	-	expression tag	UNP C5DEB9
B	153	ALA	-	expression tag	UNP C5DEB9
B	154	HIS	-	expression tag	UNP C5DEB9
B	155	HIS	-	expression tag	UNP C5DEB9
B	156	HIS	-	expression tag	UNP C5DEB9
B	157	HIS	-	expression tag	UNP C5DEB9
B	158	HIS	-	expression tag	UNP C5DEB9
B	159	HIS	-	expression tag	UNP C5DEB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	87	MET	LEU	engineered mutation	UNP C5DEB9
E	110	MET	LEU	engineered mutation	UNP C5DEB9
E	146	ALA	-	expression tag	UNP C5DEB9
E	147	GLY	-	expression tag	UNP C5DEB9
E	148	GLN	-	expression tag	UNP C5DEB9
E	149	PHE	-	expression tag	UNP C5DEB9
E	150	TYR	-	expression tag	UNP C5DEB9
E	151	LEU	-	expression tag	UNP C5DEB9
E	152	ASN	-	expression tag	UNP C5DEB9
E	153	ALA	-	expression tag	UNP C5DEB9
E	154	HIS	-	expression tag	UNP C5DEB9
E	155	HIS	-	expression tag	UNP C5DEB9
E	156	HIS	-	expression tag	UNP C5DEB9
E	157	HIS	-	expression tag	UNP C5DEB9
E	158	HIS	-	expression tag	UNP C5DEB9
E	159	HIS	-	expression tag	UNP C5DEB9

- Molecule 3 is a protein called Atg17.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	396	Total 3249	C 2036	N 565	O 635	S 13	0	0	0
3	F	396	Total 3249	C 2036	N 565	O 635	S 13	0	0	0

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.
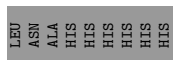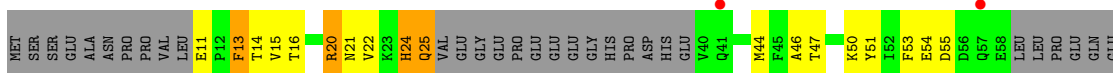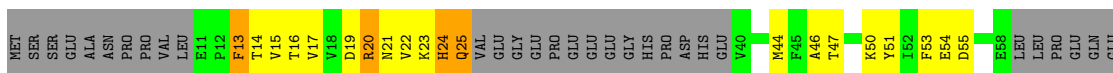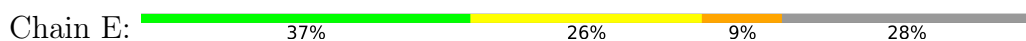
- Molecule 1: Atg29

Chain A:

- Molecule 1: Atg29

Chain D:

- Molecule 2: Atg31

Chain B:

- Molecule 2: Atg31

Chain E:
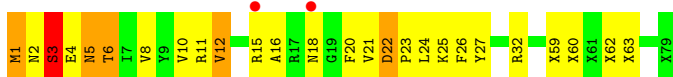
PHE TYR LEU ASN ALA HIS HIS HIS HIS HIS

• Molecule 3: Atg17

Chain C:

• Molecule 3: Atg17

Chain F:
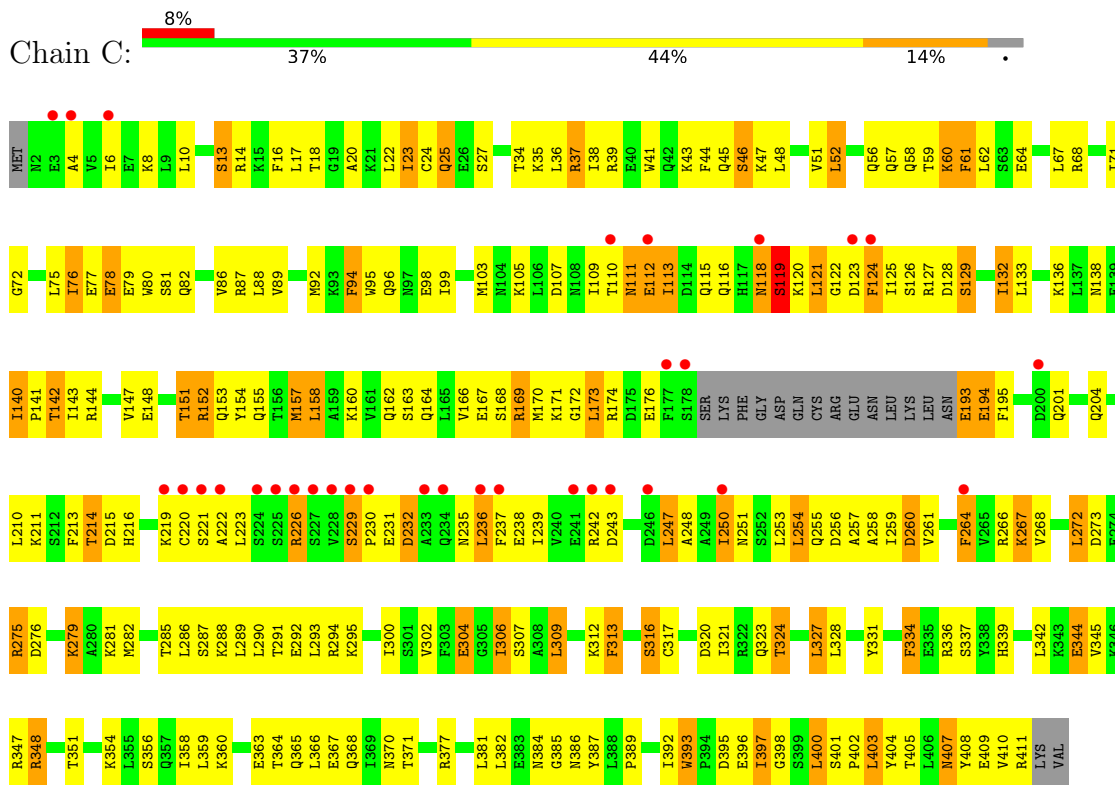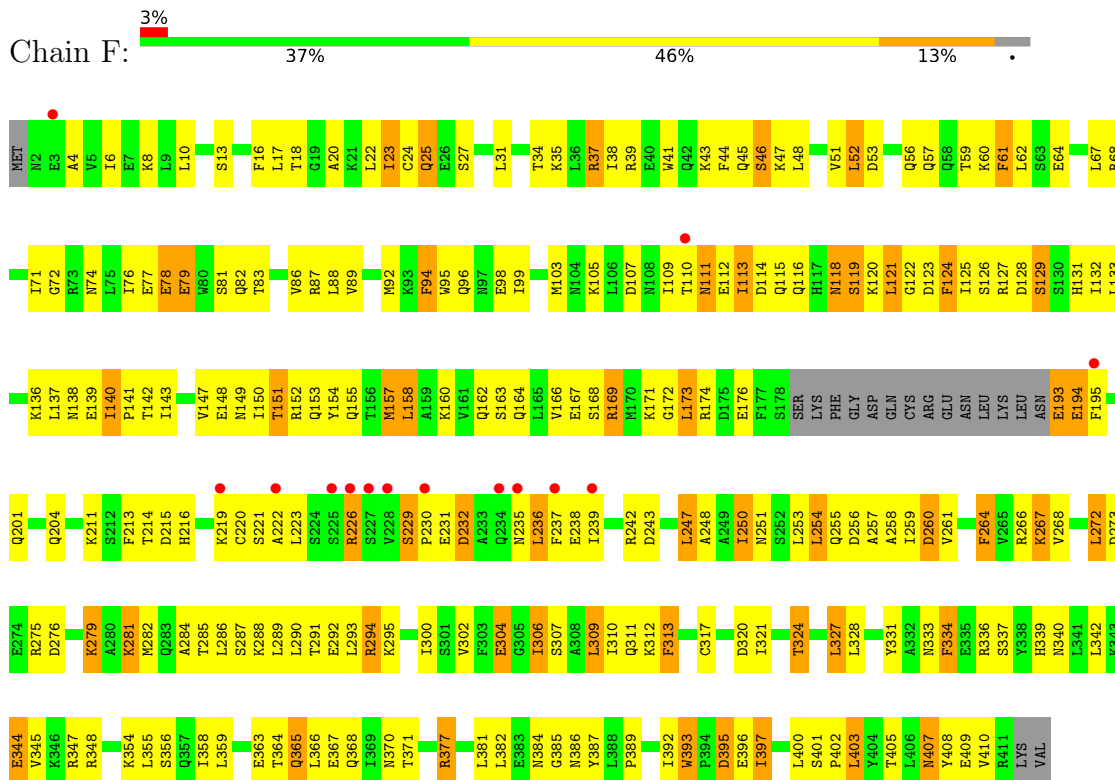
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.37Å 64.20Å 184.21Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	46.56 – 3.06 46.51 – 3.06	Depositor EDS
% Data completeness (in resolution range)	75.4 (46.56-3.06) 75.6 (46.51-3.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.303 , 0.336 0.302 , 0.334	Depositor DCC
R_{free} test set	2329 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9220	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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	0.44	0/288	0.69	0/391
1	D	0.53	0/288	0.73	0/391
2	B	0.50	0/944	0.75	0/1276
2	E	0.66	0/944	0.85	0/1276
3	C	0.50	0/3292	0.73	1/4426 (0.0%)
3	F	0.63	0/3292	0.77	0/4426
All	All	0.57	0/9048	0.76	1/12186 (0.0%)

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
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	152	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	SER	Peptide
2	E	111	SER	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	429	0	278	38	0
1	D	429	0	280	42	0
2	B	932	0	911	60	0
2	E	932	0	911	64	0
3	C	3249	0	3253	224	0
3	F	3249	0	3253	223	0
All	All	9220	0	8886	552	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 30.

All (552) 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)
3:C:109:ILE:HG21	3:C:121:LEU:HD22	1.17	1.14
3:F:109:ILE:HG21	3:F:121:LEU:HD22	1.18	1.13
1:D:1:MET:HB3	2:E:44:MET:SD	2.11	0.90
3:F:110:THR:O	3:F:111:ASN:CB	2.19	0.89
3:C:393:TRP:CZ2	3:F:345:VAL:HG23	2.08	0.88
3:C:109:ILE:HG21	3:C:121:LEU:CD2	2.04	0.88
3:F:109:ILE:HG21	3:F:121:LEU:CD2	2.02	0.88
3:C:110:THR:O	3:C:111:ASN:CB	2.21	0.87
3:F:109:ILE:HG22	3:F:120:LYS:HB3	1.57	0.86
2:E:22:VAL:HG11	2:E:130:LEU:HD22	1.56	0.86
3:C:110:THR:O	3:C:111:ASN:HB2	1.77	0.84
2:B:22:VAL:HG11	2:B:130:LEU:HD22	1.58	0.83
3:C:109:ILE:HG22	3:C:120:LYS:HB3	1.62	0.82
3:F:109:ILE:CG2	3:F:121:LEU:HD22	2.08	0.81
3:C:147:VAL:O	3:C:151:THR:HG22	1.79	0.81
3:F:193:GLU:OE2	3:F:193:GLU:N	2.12	0.81
3:F:110:THR:O	3:F:111:ASN:HB2	1.78	0.81
1:A:25:LYS:O	2:B:47:THR:HG21	1.80	0.80
3:F:57:GLN:HA	3:F:57:GLN:OE1	1.80	0.80
1:D:25:LYS:O	2:E:47:THR:HG21	1.82	0.79
3:C:193:GLU:OE2	3:C:193:GLU:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:PHE:HE2	3:C:279:LYS:CG	1.96	0.78
3:F:276:ASP:HA	3:F:279:LYS:HD3	1.65	0.78
3:F:147:VAL:O	3:F:151:THR:HG22	1.84	0.78
3:F:44:PHE:HE2	3:F:279:LYS:CG	1.97	0.78
3:C:57:GLN:OE1	3:C:57:GLN:HA	1.85	0.77
3:C:359:LEU:HD21	3:F:366:LEU:HD11	1.66	0.76
3:C:393:TRP:HZ2	3:F:345:VAL:HG23	1.47	0.75
3:C:276:ASP:HA	3:C:279:LYS:HD3	1.68	0.75
1:D:5:ASN:O	1:D:5:ASN:ND2	2.19	0.75
2:B:93:LYS:HZ3	3:C:47:LYS:HD3	1.50	0.74
3:C:10:LEU:HA	3:C:220:CYS:SG	2.26	0.74
3:C:387:TYR:CD2	3:F:333:ASN:HB3	2.22	0.74
3:C:72:GLY:O	3:C:76:ILE:HB	1.87	0.74
3:C:334:PHE:CD1	3:C:334:PHE:C	2.61	0.74
3:F:119:SER:OG	3:F:123:ASP:HB2	1.88	0.73
3:F:223:LEU:HD21	3:F:236:LEU:HD12	1.69	0.73
1:D:16:ALA:HA	2:E:53:PHE:CD2	2.24	0.73
3:C:223:LEU:HD21	3:C:236:LEU:HD12	1.71	0.73
3:F:389:PRO:O	3:F:392:ILE:HG22	1.89	0.72
1:A:1:MET:HB3	2:B:44:MET:SD	2.30	0.71
1:A:5:ASN:ND2	1:A:5:ASN:O	2.23	0.71
3:C:109:ILE:CG2	3:C:121:LEU:HD22	2.08	0.71
1:D:1:MET:HB3	2:E:44:MET:CG	2.20	0.70
1:D:21:VAL:HG12	1:D:23:PRO:HD3	1.71	0.70
1:A:21:VAL:HG12	1:A:23:PRO:HD3	1.72	0.70
1:D:16:ALA:HA	2:E:53:PHE:HD2	1.56	0.70
3:F:10:LEU:HA	3:F:220:CYS:SG	2.31	0.70
3:F:23:ILE:C	3:F:23:ILE:HD13	2.12	0.70
1:D:10:VAL:HG11	2:E:51:TYR:CD2	2.26	0.70
2:B:93:LYS:NZ	3:C:47:LYS:HD3	2.06	0.69
1:A:24:LEU:HD11	1:A:26:PHE:CE2	2.27	0.69
3:F:78:GLU:O	3:F:82:GLN:HG2	1.92	0.69
1:A:11:ARG:HB2	2:B:75:GLU:HG3	1.75	0.69
3:C:124:PHE:HD2	3:F:392:ILE:HD12	1.56	0.69
1:D:24:LEU:HD11	1:D:26:PHE:CE2	2.28	0.69
3:F:334:PHE:CD1	3:F:334:PHE:C	2.65	0.69
3:F:344:GLU:O	3:F:344:GLU:OE1	2.10	0.69
3:C:44:PHE:HE2	3:C:279:LYS:HG3	1.58	0.69
3:C:119:SER:OG	3:C:123:ASP:HB2	1.92	0.68
3:C:136:LYS:HE2	3:C:317:CYS:SG	2.33	0.68
3:F:72:GLY:O	3:F:76:ILE:HB	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:LYS:HZ2	3:C:47:LYS:HA	1.59	0.68
1:D:5:ASN:O	1:D:5:ASN:CG	2.33	0.67
3:F:44:PHE:HE2	3:F:279:LYS:HG3	1.60	0.67
3:F:367:GLU:O	3:F:371:THR:HG23	1.94	0.67
3:C:78:GLU:O	3:C:82:GLN:HG2	1.95	0.66
2:B:15:VAL:HB	2:B:46:ALA:HB3	1.77	0.66
3:C:381:LEU:O	3:C:384:ASN:O	2.13	0.66
3:C:94:PHE:CE1	3:C:98:GLU:HG3	2.30	0.66
2:B:113:PHE:O	3:C:57:GLN:HG3	1.94	0.66
1:A:5:ASN:O	1:A:5:ASN:CG	2.33	0.66
3:F:44:PHE:HE2	3:F:279:LYS:HG2	1.60	0.66
1:D:25:LYS:H	2:E:47:THR:CG2	2.09	0.65
3:C:99:ILE:HA	3:C:328:LEU:HD21	1.79	0.65
1:D:1:MET:CB	2:E:44:MET:SD	2.84	0.65
3:F:110:THR:O	3:F:111:ASN:HB3	1.96	0.65
1:A:27:TYR:OH	1:A:32:ARG:HA	1.96	0.65
3:C:334:PHE:C	3:C:334:PHE:HD1	2.00	0.65
3:F:111:ASN:OD1	3:F:118:ASN:ND2	2.28	0.65
3:F:136:LYS:HE2	3:F:317:CYS:SG	2.37	0.65
1:D:27:TYR:OH	1:D:32:ARG:HA	1.96	0.64
3:C:162:GLN:O	3:C:166:VAL:HG22	1.98	0.64
3:C:44:PHE:HE2	3:C:279:LYS:HG2	1.60	0.64
3:C:320:ASP:O	3:C:324:THR:OG1	2.14	0.64
1:A:20:PHE:CE1	2:B:53:PHE:CE2	2.86	0.64
2:B:93:LYS:NZ	3:C:46:SER:HB3	2.13	0.64
3:F:393:TRP:HB3	3:F:397:ILE:HG13	1.79	0.64
3:C:193:GLU:N	3:C:194:GLU:OE2	2.31	0.64
1:D:62:UNK:O	1:D:63:UNK:C	2.46	0.64
3:C:41:TRP:HD1	3:C:279:LYS:HZ1	1.42	0.63
3:F:342:LEU:O	3:F:345:VAL:HG12	1.98	0.63
3:C:264:PHE:HE1	3:C:268:VAL:HG21	1.63	0.63
3:C:393:TRP:HB3	3:C:397:ILE:HG13	1.79	0.63
3:F:136:LYS:HD3	3:F:317:CYS:SG	2.39	0.63
3:C:136:LYS:HD3	3:C:317:CYS:SG	2.38	0.62
3:C:94:PHE:CD1	3:C:94:PHE:C	2.71	0.62
1:A:25:LYS:O	2:B:47:THR:CG2	2.47	0.62
3:F:162:GLN:O	3:F:166:VAL:HG22	1.99	0.62
3:C:238:GLU:O	3:C:242:ARG:HG3	2.00	0.62
1:A:10:VAL:HG11	2:B:51:TYR:CD2	2.35	0.61
3:C:94:PHE:C	3:C:94:PHE:HD1	2.03	0.61
3:C:16:PHE:CE2	3:C:248:ALA:HA	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:LEU:O	3:C:345:VAL:HG12	2.00	0.61
3:C:366:LEU:HD11	3:F:359:LEU:HD21	1.83	0.61
3:C:358:ILE:HG21	3:F:365:GLN:HG2	1.82	0.61
3:F:193:GLU:N	3:F:194:GLU:OE2	2.33	0.61
2:B:124:LEU:HD12	3:C:71:ILE:HG12	1.81	0.61
3:F:264:PHE:HE1	3:F:268:VAL:HG21	1.65	0.61
3:C:23:ILE:C	3:C:23:ILE:HD13	2.22	0.61
3:F:334:PHE:C	3:F:334:PHE:HD1	2.04	0.60
1:A:24:LEU:HD13	1:A:24:LEU:C	2.21	0.60
3:C:110:THR:O	3:C:111:ASN:HB3	2.01	0.60
3:F:264:PHE:O	3:F:267:LYS:HG2	2.00	0.60
3:C:344:GLU:O	3:C:344:GLU:OE1	2.18	0.60
1:A:16:ALA:HA	2:B:53:PHE:CD2	2.36	0.60
2:E:15:VAL:HB	2:E:46:ALA:HB3	1.82	0.60
3:C:94:PHE:HE1	3:C:98:GLU:HG3	1.67	0.60
3:F:94:PHE:CE1	3:F:98:GLU:HG3	2.36	0.60
3:F:37:ARG:NH2	3:F:273:ASP:OD1	2.35	0.60
3:F:41:TRP:HD1	3:F:279:LYS:HZ1	1.42	0.60
3:F:320:ASP:O	3:F:324:THR:OG1	2.20	0.60
3:F:359:LEU:HD12	3:F:410:VAL:CG2	2.32	0.60
2:E:85:VAL:HG21	2:E:97:TYR:CD1	2.37	0.60
2:B:115:THR:HG21	3:C:60:LYS:HD2	1.84	0.59
1:D:10:VAL:HG12	2:E:51:TYR:HA	1.83	0.59
1:D:24:LEU:HD13	1:D:24:LEU:C	2.23	0.59
2:E:75:GLU:O	2:E:82:VAL:HA	2.02	0.59
3:F:111:ASN:HA	3:F:120:LYS:HA	1.83	0.59
3:C:96:GLN:O	3:C:99:ILE:HG22	2.02	0.59
3:C:111:ASN:OD1	3:C:118:ASN:ND2	2.31	0.59
3:F:44:PHE:CE2	3:F:279:LYS:HG2	2.37	0.59
3:C:403:LEU:HB2	3:F:355:LEU:CD1	2.33	0.59
3:F:238:GLU:O	3:F:242:ARG:HG3	2.03	0.59
3:C:387:TYR:HB3	3:F:334:PHE:HA	1.86	0.58
3:F:16:PHE:CE2	3:F:248:ALA:HA	2.37	0.58
3:C:112:GLU:O	3:C:113:ILE:HG22	2.03	0.58
3:C:264:PHE:O	3:C:267:LYS:HG2	2.02	0.58
3:C:64:GLU:O	3:C:68:ARG:HB3	2.04	0.58
3:C:309:LEU:C	3:C:309:LEU:HD12	2.23	0.58
3:C:367:GLU:O	3:C:371:THR:HG23	2.03	0.58
2:E:21:ASN:OD1	2:E:22:VAL:N	2.36	0.58
3:F:99:ILE:HA	3:F:328:LEU:HD21	1.85	0.58
3:C:44:PHE:CE2	3:C:279:LYS:HG2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:LEU:HD11	3:C:236:LEU:HD12	1.86	0.58
2:B:75:GLU:O	2:B:82:VAL:HA	2.03	0.58
3:C:387:TYR:CE2	3:F:333:ASN:HB3	2.39	0.58
3:F:24:CYS:O	3:F:25:GLN:C	2.40	0.58
3:F:313:PHE:CE1	3:F:317:CYS:SG	2.97	0.58
3:C:76:ILE:O	3:C:81:SER:HB2	2.04	0.57
3:F:138:ASN:O	3:F:141:PRO:HD2	2.04	0.57
2:B:124:LEU:CD1	3:C:71:ILE:HG12	2.34	0.57
3:C:389:PRO:O	3:C:392:ILE:HG22	2.03	0.57
2:E:112:ARG:O	2:E:113:PHE:C	2.42	0.57
3:C:384:ASN:C	3:C:385:GLY:O	2.41	0.57
3:C:359:LEU:HD12	3:C:410:VAL:CG2	2.35	0.57
3:C:393:TRP:CE3	3:C:396:GLU:HB3	2.39	0.57
2:E:85:VAL:CG2	2:E:97:TYR:CD1	2.88	0.57
3:C:111:ASN:HA	3:C:120:LYS:HA	1.86	0.57
3:F:112:GLU:HG3	3:F:118:ASN:ND2	2.19	0.57
2:B:93:LYS:HZ1	3:C:46:SER:HB3	1.70	0.57
1:D:2:ASN:O	1:D:3:SER:C	2.43	0.57
3:C:124:PHE:CD1	3:C:124:PHE:N	2.72	0.57
3:F:112:GLU:O	3:F:113:ILE:HG22	2.05	0.57
1:A:25:LYS:H	2:B:47:THR:CG2	2.18	0.56
3:F:264:PHE:CD1	3:F:264:PHE:C	2.79	0.56
1:A:2:ASN:O	1:A:3:SER:C	2.43	0.56
3:F:61:PHE:CD1	3:F:61:PHE:C	2.76	0.56
3:C:96:GLN:HE21	3:C:133:LEU:HB2	1.68	0.56
3:C:23:ILE:HD11	3:C:258:ALA:HB2	1.87	0.56
3:F:172:GLY:O	3:F:176:GLU:HG2	2.06	0.56
3:C:112:GLU:HG3	3:C:118:ASN:ND2	2.20	0.56
2:B:85:VAL:HG21	2:B:97:TYR:CD1	2.41	0.56
3:F:293:LEU:HD23	3:F:293:LEU:N	2.21	0.56
3:F:407:ASN:OD1	3:F:407:ASN:N	2.39	0.55
3:C:138:ASN:O	3:C:141:PRO:HD2	2.06	0.55
3:F:43:LYS:HB3	3:F:47:LYS:HE3	1.88	0.55
2:E:124:LEU:HD22	3:F:304:GLU:HG2	1.89	0.55
3:F:96:GLN:HE21	3:F:133:LEU:HB2	1.71	0.55
1:A:20:PHE:HE1	2:B:53:PHE:CE2	2.24	0.55
3:F:223:LEU:HD11	3:F:236:LEU:HD12	1.87	0.55
3:C:334:PHE:HD1	3:C:334:PHE:O	1.90	0.55
3:C:407:ASN:N	3:C:407:ASN:OD1	2.39	0.55
1:D:25:LYS:O	2:E:47:THR:CG2	2.54	0.55
3:C:61:PHE:CD1	3:C:61:PHE:C	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:ASP:O	3:C:129:SER:HB3	2.07	0.55
3:F:381:LEU:O	3:F:384:ASN:O	2.25	0.55
2:B:21:ASN:OD1	2:B:22:VAL:N	2.40	0.55
3:C:210:LEU:O	3:C:214:THR:OG1	2.25	0.55
3:F:109:ILE:O	3:F:120:LYS:HD2	2.06	0.55
3:C:354:LYS:O	3:C:358:ILE:HG12	2.07	0.54
3:F:384:ASN:C	3:F:385:GLY:O	2.45	0.54
1:A:10:VAL:HG12	2:B:51:TYR:HA	1.89	0.54
2:E:136:ASP:OD1	3:F:294:ARG:NH2	2.41	0.54
3:F:107:ASP:OD1	3:F:122:GLY:HA3	2.08	0.54
2:E:13:PHE:HB2	2:E:51:TYR:OH	2.09	0.53
2:E:124:LEU:CD2	3:F:304:GLU:HG2	2.38	0.53
2:B:85:VAL:CG2	2:B:97:TYR:CD1	2.91	0.53
3:C:215:ASP:O	3:C:219:LYS:HG2	2.08	0.53
3:F:140:ILE:HG22	3:F:141:PRO:HD3	1.91	0.53
3:F:94:PHE:CD1	3:F:94:PHE:C	2.82	0.53
1:A:3:SER:HB2	2:B:47:THR:OG1	2.09	0.53
3:F:96:GLN:O	3:F:99:ILE:HG22	2.07	0.53
3:F:267:LYS:HG3	3:F:268:VAL:N	2.23	0.53
3:C:124:PHE:CD2	3:F:392:ILE:HD12	2.41	0.53
3:F:17:LEU:HA	3:F:213:PHE:HD2	1.73	0.53
3:C:409:GLU:HB2	3:F:405:THR:OG1	2.09	0.53
3:F:23:ILE:HD11	3:F:258:ALA:HB2	1.91	0.53
3:F:393:TRP:CE3	3:F:396:GLU:HB3	2.44	0.53
3:C:44:PHE:CE2	3:C:279:LYS:CG	2.86	0.52
3:C:238:GLU:O	3:C:242:ARG:CG	2.58	0.52
3:F:64:GLU:O	3:F:68:ARG:HB3	2.09	0.52
3:F:154:TYR:O	3:F:158:LEU:HB2	2.09	0.52
1:A:1:MET:HB3	2:B:44:MET:CG	2.40	0.52
2:B:13:PHE:HB2	2:B:51:TYR:OH	2.10	0.52
3:C:313:PHE:CE1	3:C:317:CYS:SG	3.03	0.52
3:F:41:TRP:CD1	3:F:279:LYS:NZ	2.72	0.52
3:F:122:GLY:O	3:F:125:ILE:HG22	2.10	0.52
3:C:172:GLY:O	3:C:176:GLU:HG2	2.09	0.52
3:C:344:GLU:OE1	3:C:344:GLU:C	2.48	0.52
1:D:1:MET:N	1:D:6:THR:HG21	2.25	0.52
3:F:107:ASP:O	3:F:120:LYS:HG3	2.10	0.52
3:F:356:SER:OG	3:F:410:VAL:HG11	2.10	0.52
3:F:370:ASN:OD1	3:F:402:PRO:HB3	2.10	0.52
3:C:17:LEU:HA	3:C:213:PHE:HD2	1.75	0.52
3:C:148:GLU:HA	3:C:151:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:ASP:OD1	3:C:216:HIS:N	2.43	0.52
3:C:291:THR:O	3:C:295:LYS:HG3	2.10	0.52
1:D:1:MET:SD	2:E:17:VAL:HG21	2.50	0.52
3:C:385:GLY:O	3:C:386:ASN:HB2	2.09	0.51
3:F:38:ILE:HG13	3:F:39:ARG:N	2.25	0.51
3:C:94:PHE:HD1	3:C:95:TRP:N	2.08	0.51
3:C:140:ILE:HG22	3:C:141:PRO:HD3	1.92	0.51
1:A:56:UNK:O	1:A:60:UNK:N	2.43	0.51
3:C:405:THR:OG1	3:F:409:GLU:HB2	2.09	0.51
3:F:223:LEU:HD11	3:F:236:LEU:CD1	2.41	0.51
1:D:2:ASN:O	1:D:4:GLU:N	2.43	0.51
2:B:124:LEU:HD22	3:C:304:GLU:HG2	1.93	0.51
3:C:86:VAL:HG12	3:C:87:ARG:N	2.26	0.51
1:D:2:ASN:H	1:D:6:THR:HG21	1.74	0.51
3:F:41:TRP:CH2	3:F:45:GLN:HG3	2.46	0.51
3:F:124:PHE:N	3:F:124:PHE:CD1	2.75	0.51
3:F:167:GLU:O	3:F:171:LYS:HG2	2.10	0.51
3:F:285:THR:HA	3:F:288:LYS:HD3	1.93	0.51
3:F:385:GLY:O	3:F:386:ASN:HB2	2.10	0.51
1:D:10:VAL:CG1	2:E:51:TYR:CD2	2.94	0.51
3:F:302:VAL:O	3:F:306:ILE:HG23	2.11	0.51
1:D:1:MET:HB3	2:E:44:MET:CB	2.40	0.51
3:C:384:ASN:HD21	3:F:340:ASN:HB3	1.76	0.51
1:D:11:ARG:HB2	2:E:75:GLU:HG3	1.91	0.51
3:C:327:LEU:HD13	3:C:331:TYR:CE1	2.47	0.50
3:F:136:LYS:NZ	3:F:320:ASP:OD2	2.44	0.50
2:B:115:THR:HG22	3:C:61:PHE:HB2	1.92	0.50
3:C:89:VAL:CG2	3:C:140:ILE:HD12	2.41	0.50
3:C:285:THR:HA	3:C:288:LYS:HD3	1.92	0.50
3:F:94:PHE:HE1	3:F:98:GLU:HG3	1.77	0.50
3:C:174:ARG:HB2	3:C:174:ARG:CZ	2.40	0.50
3:F:86:VAL:HG12	3:F:87:ARG:N	2.27	0.50
1:A:2:ASN:H	1:A:6:THR:HG21	1.75	0.50
3:F:61:PHE:O	3:F:62:LEU:C	2.49	0.50
3:C:223:LEU:HD11	3:C:236:LEU:CD1	2.41	0.50
3:F:354:LYS:O	3:F:358:ILE:HG12	2.11	0.50
3:C:13:SER:OG	3:C:14:ARG:N	2.44	0.50
3:C:264:PHE:CD1	3:C:264:PHE:C	2.85	0.50
3:C:43:LYS:HB3	3:C:47:LYS:HE3	1.92	0.50
3:C:122:GLY:O	3:C:125:ILE:HG22	2.12	0.50
3:F:119:SER:OG	3:F:123:ASP:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:128:ASP:O	3:F:129:SER:HB3	2.11	0.50
3:C:267:LYS:HG3	3:C:268:VAL:N	2.27	0.49
3:C:403:LEU:HD22	3:C:403:LEU:N	2.27	0.49
3:F:257:ALA:O	3:F:260:ASP:N	2.45	0.49
3:C:107:ASP:OD1	3:C:122:GLY:HA3	2.12	0.49
3:C:356:SER:OG	3:C:410:VAL:HG11	2.10	0.49
3:C:377:ARG:HG3	3:F:347:ARG:HH22	1.77	0.49
2:E:19:ASP:OD2	2:E:111:SER:OG	2.31	0.49
3:C:229:SER:HB2	3:C:232:ASP:HB2	1.93	0.49
3:F:27:SER:HB3	3:F:261:VAL:HG11	1.95	0.49
3:F:43:LYS:O	3:F:44:PHE:C	2.50	0.49
3:F:223:LEU:HD13	3:F:237:PHE:CE1	2.48	0.49
3:F:344:GLU:OE2	3:F:347:ARG:NH2	2.46	0.49
2:E:145:LEU:CD2	3:F:47:LYS:HB2	2.43	0.49
3:F:76:ILE:O	3:F:81:SER:HB2	2.11	0.49
3:F:174:ARG:HB2	3:F:174:ARG:CZ	2.41	0.49
1:D:8:VAL:HG21	2:E:46:ALA:HB1	1.93	0.49
3:F:148:GLU:HA	3:F:151:THR:CG2	2.43	0.49
3:C:37:ARG:NH2	3:C:273:ASP:OD1	2.45	0.49
3:F:215:ASP:OD1	3:F:216:HIS:N	2.46	0.49
1:D:25:LYS:H	2:E:47:THR:HG23	1.78	0.49
3:C:23:ILE:HD12	3:C:254:LEU:HD11	1.95	0.49
3:C:119:SER:OG	3:C:123:ASP:N	2.46	0.49
1:D:2:ASN:O	1:D:4:GLU:O	2.30	0.49
3:F:403:LEU:N	3:F:403:LEU:HD22	2.28	0.49
3:F:89:VAL:CG2	3:F:140:ILE:HD12	2.43	0.49
3:F:94:PHE:C	3:F:94:PHE:HD1	2.16	0.49
3:F:34:THR:O	3:F:35:LYS:C	2.50	0.48
3:C:230:PRO:HD2	3:C:232:ASP:OD2	2.12	0.48
3:F:52:LEU:O	3:F:53:ASP:C	2.51	0.48
3:F:67:LEU:HD11	3:F:157:MET:CE	2.43	0.48
3:F:167:GLU:CG	3:F:168:SER:N	2.77	0.48
3:F:230:PRO:HD2	3:F:232:ASP:OD2	2.13	0.48
2:E:124:LEU:CD2	3:F:304:GLU:CG	2.92	0.48
3:F:113:ILE:HG23	3:F:113:ILE:O	2.12	0.48
3:F:229:SER:HB2	3:F:232:ASP:HB2	1.95	0.48
1:A:16:ALA:HA	2:B:53:PHE:HD2	1.77	0.48
3:F:119:SER:OG	3:F:123:ASP:N	2.46	0.48
3:F:223:LEU:HD13	3:F:237:PHE:HE1	1.78	0.48
3:F:238:GLU:O	3:F:242:ARG:CG	2.61	0.48
3:C:167:GLU:O	3:C:171:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:6:THR:HG21	2.27	0.48
3:C:111:ASN:O	3:C:112:GLU:C	2.52	0.48
3:C:119:SER:OG	3:C:119:SER:O	2.30	0.48
3:C:154:TYR:O	3:C:158:LEU:HB2	2.13	0.48
3:F:44:PHE:CE2	3:F:279:LYS:CG	2.87	0.48
3:C:27:SER:HB3	3:C:261:VAL:HG11	1.95	0.48
3:C:77:GLU:O	3:C:81:SER:HB3	2.14	0.48
3:F:89:VAL:HG22	3:F:140:ILE:HD12	1.96	0.48
3:F:152:ARG:HA	3:F:155:GLN:HG3	1.96	0.48
2:B:112:ARG:O	2:B:113:PHE:C	2.50	0.48
3:C:41:TRP:CH2	3:C:45:GLN:HG3	2.49	0.48
3:C:113:ILE:HG23	3:C:113:ILE:O	2.13	0.48
3:C:302:VAL:O	3:C:306:ILE:HG23	2.14	0.48
3:C:344:GLU:OE2	3:C:347:ARG:NH2	2.47	0.48
2:B:77:ASP:HB2	2:B:81:ARG:H	1.79	0.48
1:D:12:VAL:HG23	2:E:53:PHE:HA	1.96	0.48
3:F:140:ILE:N	3:F:141:PRO:HD2	2.29	0.48
3:C:48:LEU:HG	3:C:52:LEU:CD2	2.44	0.48
3:C:61:PHE:O	3:C:62:LEU:C	2.52	0.47
3:C:293:LEU:HD23	3:C:293:LEU:N	2.29	0.47
3:C:89:VAL:HG22	3:C:140:ILE:HD12	1.94	0.47
3:C:167:GLU:CG	3:C:168:SER:N	2.78	0.47
2:E:76:ALA:HB1	2:E:80:LEU:HA	1.96	0.47
1:A:8:VAL:HG21	2:B:46:ALA:HB1	1.96	0.47
3:C:44:PHE:CE2	3:C:279:LYS:HG3	2.44	0.47
3:F:359:LEU:HD12	3:F:410:VAL:HG21	1.95	0.47
3:C:41:TRP:CD1	3:C:279:LYS:NZ	2.76	0.47
1:A:59:UNK:O	1:A:60:UNK:CB	2.63	0.47
2:B:125:GLU:O	2:B:128:VAL:HG12	2.15	0.47
3:C:366:LEU:HD21	3:F:358:ILE:HB	1.96	0.47
1:D:8:VAL:CG2	2:E:46:ALA:HB1	2.44	0.47
3:F:111:ASN:O	3:F:112:GLU:C	2.53	0.47
2:B:124:LEU:CD2	3:C:304:GLU:HG2	2.43	0.47
3:C:24:CYS:O	3:C:25:GLN:C	2.52	0.47
3:C:223:LEU:HD13	3:C:237:PHE:HE1	1.80	0.47
3:C:393:TRP:CD2	3:C:396:GLU:HB3	2.50	0.47
2:E:77:ASP:HB2	2:E:81:ARG:H	1.78	0.47
1:A:2:ASN:O	1:A:4:GLU:N	2.47	0.47
1:A:25:LYS:H	2:B:47:THR:HG23	1.80	0.47
3:F:44:PHE:CE2	3:F:279:LYS:HG3	2.47	0.47
1:A:25:LYS:C	2:B:47:THR:HG21	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ALA:HB1	2:B:80:LEU:HA	1.97	0.46
3:C:141:PRO:O	3:C:144:ARG:N	2.48	0.46
3:C:223:LEU:HD13	3:C:237:PHE:CE1	2.50	0.46
3:C:152:ARG:HA	3:C:155:GLN:HG3	1.97	0.46
3:C:169:ARG:O	3:C:173:LEU:HD22	2.15	0.46
3:F:20:ALA:HA	3:F:23:ILE:HG22	1.97	0.46
3:F:48:LEU:HG	3:F:52:LEU:CD2	2.45	0.46
2:E:20:ARG:HA	2:E:20:ARG:HD3	1.75	0.46
2:E:124:LEU:CD1	3:F:71:ILE:HG12	2.46	0.46
3:F:239:ILE:O	3:F:243:ASP:N	2.40	0.46
3:C:37:ARG:NH1	3:C:272:LEU:HB3	2.31	0.46
3:C:38:ILE:HG13	3:C:39:ARG:N	2.31	0.46
3:F:344:GLU:OE1	3:F:344:GLU:C	2.54	0.46
3:C:67:LEU:HD11	3:C:157:MET:CE	2.44	0.46
3:C:359:LEU:HD13	3:C:408:TYR:CG	2.51	0.46
2:E:122:LEU:HD23	2:E:122:LEU:N	2.31	0.46
2:E:124:LEU:HD12	3:F:71:ILE:HG12	1.96	0.46
2:E:53:PHE:N	2:E:53:PHE:CD1	2.84	0.46
3:F:94:PHE:HD1	3:F:95:TRP:N	2.12	0.46
3:F:309:LEU:C	3:F:309:LEU:HD12	2.36	0.46
3:F:213:PHE:HE1	3:F:250:ILE:HD11	1.80	0.46
2:B:145:LEU:HD22	3:C:44:PHE:CE1	2.51	0.45
3:C:148:GLU:HA	3:C:151:THR:HG22	1.98	0.45
3:C:384:ASN:HD21	3:F:340:ASN:CB	2.29	0.45
1:D:15:ARG:HG3	2:E:53:PHE:CE2	2.51	0.45
3:C:109:ILE:O	3:C:120:LYS:HD2	2.16	0.45
2:B:53:PHE:CD1	2:B:53:PHE:N	2.84	0.45
2:B:81:ARG:C	2:B:82:VAL:HG23	2.36	0.45
3:C:47:LYS:O	3:C:51:VAL:HG23	2.17	0.45
3:C:359:LEU:HD13	3:C:408:TYR:CB	2.47	0.45
3:F:23:ILE:HD12	3:F:254:LEU:HD11	1.99	0.45
3:C:118:ASN:O	3:C:120:LYS:N	2.49	0.45
3:F:291:THR:O	3:F:295:LYS:HG3	2.17	0.45
3:C:132:ILE:HD12	3:C:132:ILE:HA	1.90	0.45
3:F:169:ARG:O	3:F:173:LEU:HD22	2.17	0.45
3:C:34:THR:O	3:C:35:LYS:C	2.54	0.45
3:F:215:ASP:O	3:F:219:LYS:HG2	2.16	0.45
3:C:20:ALA:HA	3:C:23:ILE:HG22	1.99	0.45
1:D:10:VAL:CG1	2:E:51:TYR:HA	2.47	0.45
1:A:24:LEU:HD13	1:A:24:LEU:O	2.17	0.45
3:C:257:ALA:O	3:C:260:ASP:N	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:139:GLU:O	3:F:143:ILE:HD13	2.17	0.45
2:B:115:THR:HG21	3:C:60:LYS:CD	2.47	0.44
3:F:359:LEU:HD13	3:F:408:TYR:CG	2.53	0.44
2:B:77:ASP:OD2	2:B:81:ARG:HG3	2.17	0.44
3:F:222:ALA:HA	3:F:226:ARG:HG2	1.99	0.44
3:F:67:LEU:HD11	3:F:157:MET:HE2	1.98	0.44
3:F:258:ALA:O	3:F:261:VAL:HG12	2.17	0.44
3:C:75:LEU:HB3	3:C:80:TRP:CH2	2.53	0.44
3:C:107:ASP:O	3:C:120:LYS:HG3	2.17	0.44
3:C:256:ASP:O	3:C:259:ILE:HB	2.17	0.44
3:C:231:GLU:O	3:C:231:GLU:HG2	2.18	0.44
3:C:286:LEU:O	3:C:289:LEU:N	2.49	0.44
3:C:327:LEU:HD22	3:C:327:LEU:HA	1.84	0.44
2:E:94:GLN:HA	2:E:109:ALA:HA	1.99	0.44
2:B:93:LYS:HZ2	3:C:47:LYS:CA	2.29	0.44
3:C:16:PHE:CZ	3:C:248:ALA:HA	2.53	0.44
3:C:366:LEU:HD21	3:F:358:ILE:CB	2.47	0.44
3:F:136:LYS:HE2	3:F:317:CYS:HA	1.99	0.44
1:A:2:ASN:O	1:A:4:GLU:O	2.35	0.44
1:D:4:GLU:OE2	1:D:4:GLU:HA	2.17	0.44
3:F:96:GLN:OE1	3:F:131:HIS:CD2	2.70	0.44
3:C:163:SER:OG	3:C:164:GLN:N	2.51	0.44
3:C:309:LEU:HD12	3:C:309:LEU:O	2.18	0.44
3:C:370:ASN:OD1	3:C:402:PRO:HB3	2.18	0.44
3:F:230:PRO:O	3:F:231:GLU:HB3	2.18	0.44
2:E:24:HIS:C	2:E:24:HIS:CD2	2.91	0.44
2:E:128:VAL:HG23	3:F:300:ILE:HG21	2.00	0.44
1:A:1:MET:CB	2:B:44:MET:SD	3.05	0.43
3:C:44:PHE:CD1	3:C:44:PHE:C	2.90	0.43
3:C:403:LEU:HB2	3:F:355:LEU:HD12	2.00	0.43
2:E:25:GLN:OE1	2:E:25:GLN:HA	2.18	0.43
3:F:74:ASN:N	3:F:74:ASN:HD22	2.16	0.43
3:C:216:HIS:CD2	3:C:216:HIS:C	2.91	0.43
3:F:79:GLU:OE2	3:F:79:GLU:HA	2.17	0.43
3:C:76:ILE:O	3:C:81:SER:CB	2.66	0.43
3:F:281:LYS:O	3:F:284:ALA:N	2.51	0.43
3:C:10:LEU:CA	3:C:220:CYS:SG	3.04	0.43
3:C:387:TYR:CE2	3:F:333:ASN:CB	3.01	0.43
2:E:85:VAL:HG22	2:E:97:TYR:CE1	2.54	0.43
3:F:125:ILE:HD12	3:F:125:ILE:HA	1.84	0.43
3:C:201:GLN:O	3:C:204:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:359:LEU:HD12	3:C:410:VAL:HG21	1.99	0.43
3:C:403:LEU:N	3:C:403:LEU:CD2	2.81	0.43
2:E:93:LYS:HZ3	3:F:47:LYS:HD3	1.83	0.43
3:F:393:TRP:CD2	3:F:396:GLU:HB3	2.53	0.43
1:D:25:LYS:C	2:E:47:THR:HG21	2.38	0.43
2:E:139:HIS:HD1	2:E:139:HIS:C	2.22	0.43
3:C:119:SER:OG	3:C:123:ASP:CB	2.63	0.43
3:C:222:ALA:HA	3:C:226:ARG:HG2	2.00	0.43
2:E:93:LYS:NZ	3:F:47:LYS:HD3	2.34	0.43
2:E:115:THR:HG22	3:F:61:PHE:HB2	2.00	0.43
3:C:407:ASN:OD1	3:F:407:ASN:O	2.36	0.43
3:C:141:PRO:O	3:C:142:THR:C	2.57	0.43
3:F:216:HIS:CD2	3:F:216:HIS:C	2.91	0.43
3:F:359:LEU:HD13	3:F:408:TYR:CB	2.49	0.43
3:F:61:PHE:C	3:F:61:PHE:HD1	2.23	0.43
3:F:327:LEU:HD13	3:F:331:TYR:CE1	2.53	0.43
3:C:48:LEU:HG	3:C:52:LEU:HD21	2.01	0.42
3:C:213:PHE:HE1	3:C:250:ILE:HD11	1.83	0.42
3:C:230:PRO:O	3:C:231:GLU:HB3	2.19	0.42
1:D:22:ASP:N	1:D:23:PRO:CD	2.82	0.42
3:F:247:LEU:HG	3:F:248:ALA:N	2.33	0.42
2:B:94:GLN:HA	2:B:109:ALA:HA	1.99	0.42
3:C:404:TYR:HA	3:F:410:VAL:HA	2.01	0.42
3:F:385:GLY:O	3:F:387:TYR:N	2.46	0.42
2:B:25:GLN:HA	2:B:25:GLN:OE1	2.20	0.42
2:B:117:ARG:O	2:B:119:LEU:O	2.37	0.42
3:C:94:PHE:CD1	3:C:95:TRP:N	2.87	0.42
3:C:239:ILE:O	3:C:243:ASP:N	2.43	0.42
2:E:136:ASP:OD1	2:E:136:ASP:N	2.52	0.42
3:F:118:ASN:O	3:F:120:LYS:N	2.51	0.42
2:B:24:HIS:C	2:B:24:HIS:CD2	2.92	0.42
3:C:75:LEU:HD13	3:C:80:TRP:CZ2	2.55	0.42
3:C:275:ARG:HD3	3:C:275:ARG:HA	1.81	0.42
1:D:8:VAL:HG21	2:E:46:ALA:CB	2.49	0.42
3:F:256:ASP:O	3:F:259:ILE:HB	2.19	0.42
3:C:48:LEU:HD21	3:C:282:MET:HG2	2.01	0.42
3:C:136:LYS:HE2	3:C:317:CYS:CA	2.49	0.42
1:D:24:LEU:HD13	1:D:24:LEU:O	2.20	0.42
2:E:117:ARG:O	2:E:119:LEU:O	2.37	0.42
2:B:21:ASN:ND2	2:B:111:SER:O	2.53	0.42
3:C:411:ARG:NH1	3:F:396:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:LYS:HZ2	3:F:47:LYS:HA	1.84	0.42
3:F:4:ALA:O	3:F:8:LYS:HG3	2.20	0.42
1:A:10:VAL:CG1	2:B:51:TYR:CD2	3.03	0.42
3:F:20:ALA:HA	3:F:23:ILE:CG2	2.50	0.42
3:F:37:ARG:NH1	3:F:272:LEU:HB3	2.35	0.42
3:F:119:SER:CB	3:F:123:ASP:HB2	2.49	0.42
1:A:5:ASN:O	2:B:68:ILE:O	2.37	0.42
2:B:93:LYS:HZ3	3:C:46:SER:HB3	1.85	0.42
2:E:85:VAL:HG22	2:E:97:TYR:CD1	2.55	0.42
3:C:140:ILE:N	3:C:141:PRO:HD2	2.34	0.42
3:F:344:GLU:OE1	3:F:344:GLU:CA	2.68	0.42
3:F:385:GLY:C	3:F:387:TYR:N	2.73	0.42
1:A:18:ASN:HA	1:A:20:PHE:CE1	2.55	0.42
2:B:138:LEU:O	2:B:139:HIS:C	2.58	0.42
3:F:31:LEU:HD23	3:F:31:LEU:HA	1.82	0.42
3:F:35:LYS:O	3:F:38:ILE:HG12	2.19	0.42
3:F:148:GLU:HA	3:F:151:THR:HG22	2.01	0.42
3:F:334:PHE:HD1	3:F:334:PHE:O	2.02	0.42
2:B:133:LEU:O	2:B:137:GLN:HG3	2.20	0.41
1:D:22:ASP:N	1:D:23:PRO:HD3	2.35	0.41
3:C:48:LEU:HD12	3:C:48:LEU:HA	1.92	0.41
1:D:59:UNK:O	1:D:60:UNK:CB	2.68	0.41
2:E:133:LEU:O	2:E:137:GLN:HG3	2.21	0.41
2:E:141:LEU:HD23	2:E:141:LEU:HA	1.94	0.41
3:F:48:LEU:HD21	3:F:282:MET:HG2	2.02	0.41
3:F:232:ASP:O	3:F:236:LEU:HB2	2.20	0.41
3:F:286:LEU:O	3:F:289:LEU:N	2.53	0.41
3:F:359:LEU:HD13	3:F:408:TYR:HB2	2.02	0.41
3:C:348:ARG:NH2	3:F:377:ARG:HG2	2.35	0.41
3:C:398:GLY:O	3:C:400:LEU:HB2	2.20	0.41
3:F:77:GLU:O	3:F:81:SER:HB3	2.20	0.41
3:F:231:GLU:O	3:F:231:GLU:HG2	2.20	0.41
1:A:22:ASP:N	1:A:23:PRO:CD	2.83	0.41
2:B:128:VAL:HG23	3:C:300:ILE:HG21	2.03	0.41
2:E:81:ARG:C	2:E:82:VAL:HG23	2.41	0.41
3:F:149:ASN:O	3:F:150:ILE:C	2.56	0.41
3:C:136:LYS:HE2	3:C:317:CYS:HA	2.01	0.41
3:F:47:LYS:O	3:F:51:VAL:HG23	2.20	0.41
3:F:137:LEU:O	3:F:140:ILE:HG22	2.19	0.41
3:C:58:GLN:O	3:C:58:GLN:HG3	2.21	0.41
1:D:2:ASN:ND2	1:D:4:GLU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:TYR:HB3	2:E:53:PHE:HE1	1.86	0.41
3:F:310:ILE:O	3:F:311:GLN:C	2.58	0.41
3:C:136:LYS:CD	3:C:317:CYS:SG	3.08	0.41
3:F:82:GLN:CG	3:F:83:THR:N	2.84	0.41
3:F:136:LYS:HE2	3:F:317:CYS:CA	2.50	0.41
3:F:163:SER:OG	3:F:164:GLN:N	2.54	0.41
1:A:22:ASP:N	1:A:23:PRO:HD3	2.36	0.41
3:C:61:PHE:C	3:C:61:PHE:HD1	2.24	0.41
3:C:67:LEU:HD11	3:C:157:MET:HE2	2.02	0.41
1:D:4:GLU:HB2	1:D:26:PHE:CE1	2.56	0.41
2:E:21:ASN:ND2	2:E:23:LYS:HD2	2.36	0.41
2:E:128:VAL:HG23	3:F:300:ILE:CG2	2.50	0.41
3:F:89:VAL:CG2	3:F:140:ILE:CD1	2.98	0.41
3:F:96:GLN:OE1	3:F:131:HIS:HD2	2.04	0.41
1:A:8:VAL:CG2	2:B:46:ALA:HB1	2.50	0.41
3:C:136:LYS:NZ	3:C:316:SER:OG	2.40	0.41
3:C:247:LEU:HG	3:C:248:ALA:N	2.36	0.41
3:F:393:TRP:O	3:F:395:ASP:N	2.54	0.41
1:D:18:ASN:HA	1:D:20:PHE:CE1	2.56	0.40
2:E:138:LEU:HD23	2:E:138:LEU:HA	1.98	0.40
3:F:113:ILE:C	3:F:114:ASP:OD1	2.60	0.40
3:F:403:LEU:N	3:F:403:LEU:CD2	2.84	0.40
2:B:20:ARG:HD3	2:B:20:ARG:HA	1.74	0.40
3:C:89:VAL:CG2	3:C:140:ILE:CD1	2.99	0.40
3:C:123:ASP:HB3	3:C:124:PHE:CD1	2.56	0.40
3:C:250:ILE:HA	3:C:253:LEU:HD23	2.03	0.40
2:B:124:LEU:CD2	3:C:304:GLU:CG	2.99	0.40
3:C:136:LYS:CE	3:C:317:CYS:SG	3.05	0.40
2:E:93:LYS:NZ	3:F:46:SER:HB3	2.36	0.40
3:F:119:SER:O	3:F:120:LYS:C	2.59	0.40
3:F:128:ASP:OD1	3:F:128:ASP:N	2.54	0.40
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.22	0.40
3:F:201:GLN:O	3:F:204:GLN:HB3	2.21	0.40
3:F:250:ILE:HA	3:F:253:LEU:HD23	2.03	0.40
3:C:4:ALA:O	3:C:8:LYS:HG3	2.21	0.40
3:C:143:ILE:O	3:C:147:VAL:HG23	2.21	0.40
3:C:359:LEU:HD13	3:C:408:TYR:HB2	2.03	0.40
3:C:393:TRP:CZ2	3:F:345:VAL:CG2	2.93	0.40
3:F:294:ARG:HD2	3:F:294:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	38/69 (55%)	31 (82%)	6 (16%)	1 (3%)	5	22
1	D	38/69 (55%)	30 (79%)	7 (18%)	1 (3%)	5	22
2	B	109/159 (69%)	94 (86%)	10 (9%)	5 (5%)	2	12
2	E	109/159 (69%)	94 (86%)	9 (8%)	6 (6%)	2	9
3	C	392/413 (95%)	339 (86%)	49 (12%)	4 (1%)	15	45
3	F	392/413 (95%)	340 (87%)	50 (13%)	2 (0%)	29	60
All	All	1078/1282 (84%)	928 (86%)	131 (12%)	19 (2%)	8	30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	111	ASN
3	F	111	ASN
2	B	77	ASP
2	B	113	PHE
3	C	113	ILE
2	E	77	ASP
2	E	113	PHE
3	F	113	ILE
2	B	54	GLU
2	B	66	PRO
1	D	3	SER
2	E	54	GLU
2	E	66	PRO
1	A	3	SER
2	E	97	TYR
3	C	119	SER
3	C	112	GLU
2	B	82	VAL
2	E	82	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	23/36 (64%)	17 (74%)	6 (26%)	0	1
1	D	23/36 (64%)	17 (74%)	6 (26%)	0	1
2	B	107/145 (74%)	87 (81%)	20 (19%)	1	5
2	E	107/145 (74%)	87 (81%)	20 (19%)	1	5
3	C	367/383 (96%)	266 (72%)	101 (28%)	0	1
3	F	367/383 (96%)	272 (74%)	95 (26%)	0	1
All	All	994/1128 (88%)	746 (75%)	248 (25%)	0	2

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	SER
1	A	5	ASN
1	A	6	THR
1	A	12	VAL
1	A	22	ASP
2	B	11	GLU
2	B	13	PHE
2	B	14	THR
2	B	16	THR
2	B	20	ARG
2	B	24	HIS
2	B	25	GLN
2	B	50	LYS
2	B	55	ASP
2	B	68	ILE
2	B	79	SER
2	B	80	LEU
2	B	86	GLU
2	B	90	ASP
2	B	94	GLN
2	B	106	CYS

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Mol	Chain	Res	Type
2	B	108	ASP
2	B	118	GLN
2	B	119	LEU
2	B	122	LEU
3	C	6	ILE
3	C	13	SER
3	C	18	THR
3	C	22	LEU
3	C	23	ILE
3	C	25	GLN
3	C	36	LEU
3	C	37	ARG
3	C	46	SER
3	C	52	LEU
3	C	56	GLN
3	C	59	THR
3	C	60	LYS
3	C	61	PHE
3	C	76	ILE
3	C	78	GLU
3	C	79	GLU
3	C	88	LEU
3	C	92	MET
3	C	94	PHE
3	C	103	MET
3	C	105	LYS
3	C	115	GLN
3	C	116	GLN
3	C	118	ASN
3	C	119	SER
3	C	121	LEU
3	C	124	PHE
3	C	126	SER
3	C	127	ARG
3	C	129	SER
3	C	132	ILE
3	C	140	ILE
3	C	142	THR
3	C	151	THR
3	C	153	GLN
3	C	157	MET
3	C	158	LEU

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Mol	Chain	Res	Type
3	C	160	LYS
3	C	169	ARG
3	C	170	MET
3	C	173	LEU
3	C	193	GLU
3	C	194	GLU
3	C	195	PHE
3	C	211	LYS
3	C	214	THR
3	C	221	SER
3	C	226	ARG
3	C	229	SER
3	C	232	ASP
3	C	235	ASN
3	C	236	LEU
3	C	247	LEU
3	C	250	ILE
3	C	251	ASN
3	C	254	LEU
3	C	255	GLN
3	C	260	ASP
3	C	264	PHE
3	C	266	ARG
3	C	267	LYS
3	C	272	LEU
3	C	275	ARG
3	C	279	LYS
3	C	281	LYS
3	C	287	SER
3	C	290	LEU
3	C	292	GLU
3	C	294	ARG
3	C	304	GLU
3	C	306	ILE
3	C	307	SER
3	C	309	LEU
3	C	312	LYS
3	C	313	PHE
3	C	316	SER
3	C	321	ILE
3	C	323	GLN
3	C	324	THR

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Mol	Chain	Res	Type
3	C	327	LEU
3	C	334	PHE
3	C	336	ARG
3	C	337	SER
3	C	339	HIS
3	C	344	GLU
3	C	348	ARG
3	C	351	THR
3	C	360	LYS
3	C	363	GLU
3	C	364	THR
3	C	365	GLN
3	C	368	GLN
3	C	382	LEU
3	C	393	TRP
3	C	395	ASP
3	C	397	ILE
3	C	400	LEU
3	C	401	SER
3	C	403	LEU
3	C	407	ASN
1	D	1	MET
1	D	3	SER
1	D	5	ASN
1	D	6	THR
1	D	12	VAL
1	D	22	ASP
2	E	13	PHE
2	E	14	THR
2	E	16	THR
2	E	20	ARG
2	E	24	HIS
2	E	25	GLN
2	E	50	LYS
2	E	55	ASP
2	E	68	ILE
2	E	79	SER
2	E	80	LEU
2	E	86	GLU
2	E	90	ASP
2	E	94	GLN
2	E	106	CYS

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Mol	Chain	Res	Type
2	E	108	ASP
2	E	118	GLN
2	E	119	LEU
2	E	122	LEU
2	E	128	VAL
3	F	6	ILE
3	F	13	SER
3	F	18	THR
3	F	22	LEU
3	F	23	ILE
3	F	25	GLN
3	F	37	ARG
3	F	46	SER
3	F	52	LEU
3	F	56	GLN
3	F	59	THR
3	F	60	LYS
3	F	61	PHE
3	F	78	GLU
3	F	79	GLU
3	F	88	LEU
3	F	92	MET
3	F	94	PHE
3	F	103	MET
3	F	105	LYS
3	F	115	GLN
3	F	116	GLN
3	F	118	ASN
3	F	119	SER
3	F	121	LEU
3	F	124	PHE
3	F	126	SER
3	F	127	ARG
3	F	129	SER
3	F	132	ILE
3	F	140	ILE
3	F	142	THR
3	F	151	THR
3	F	153	GLN
3	F	157	MET
3	F	158	LEU
3	F	160	LYS

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Mol	Chain	Res	Type
3	F	169	ARG
3	F	173	LEU
3	F	193	GLU
3	F	194	GLU
3	F	195	PHE
3	F	211	LYS
3	F	214	THR
3	F	221	SER
3	F	226	ARG
3	F	229	SER
3	F	232	ASP
3	F	235	ASN
3	F	236	LEU
3	F	247	LEU
3	F	250	ILE
3	F	251	ASN
3	F	254	LEU
3	F	255	GLN
3	F	260	ASP
3	F	264	PHE
3	F	266	ARG
3	F	267	LYS
3	F	272	LEU
3	F	275	ARG
3	F	279	LYS
3	F	281	LYS
3	F	287	SER
3	F	290	LEU
3	F	292	GLU
3	F	294	ARG
3	F	304	GLU
3	F	306	ILE
3	F	307	SER
3	F	309	LEU
3	F	312	LYS
3	F	313	PHE
3	F	321	ILE
3	F	324	THR
3	F	327	LEU
3	F	334	PHE
3	F	336	ARG
3	F	337	SER

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Mol	Chain	Res	Type
3	F	339	HIS
3	F	344	GLU
3	F	348	ARG
3	F	363	GLU
3	F	364	THR
3	F	365	GLN
3	F	368	GLN
3	F	377	ARG
3	F	382	LEU
3	F	393	TRP
3	F	395	ASP
3	F	397	ILE
3	F	400	LEU
3	F	401	SER
3	F	403	LEU
3	F	407	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	ASN
2	B	24	HIS
2	B	91	GLN
3	C	25	GLN
3	C	56	GLN
3	C	74	ASN
3	C	82	GLN
3	C	96	GLN
3	C	115	GLN
3	C	131	HIS
3	C	162	GLN
3	C	216	HIS
3	C	251	ASN
3	C	283	GLN
3	C	311	GLN
3	C	326	ASN
1	D	2	ASN
1	D	5	ASN
2	E	24	HIS
2	E	91	GLN
3	F	25	GLN

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Mol	Chain	Res	Type
3	F	74	ASN
3	F	82	GLN
3	F	96	GLN
3	F	131	HIS
3	F	216	HIS
3	F	251	ASN
3	F	283	GLN
3	F	311	GLN
3	F	326	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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	40:VAL	C	51:UNK	N	15.44
1	D	40:VAL	C	51:UNK	N	14.58

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(Å²)	Q<0.9
1	A	40/69 (57%)	0.03	3 (7%)	14	5	59, 94, 148, 158	0
1	D	40/69 (57%)	0.31	2 (5%)	28	12	53, 69, 117, 161	0
2	B	115/159 (72%)	-0.12	2 (1%)	70	46	45, 78, 111, 126	0
2	E	115/159 (72%)	-0.10	0	100	100	23, 50, 94, 115	0
3	C	396/413 (95%)	0.28	32 (8%)	12	4	31, 72, 148, 189	0
3	F	396/413 (95%)	0.13	14 (3%)	44	22	22, 52, 126, 165	0
All	All	1102/1282 (85%)	0.14	53 (4%)	30	13	22, 67, 135, 189	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	233	ALA	8.4
3	C	237	PHE	6.8
3	C	226	ARG	6.4
3	C	228	VAL	5.8
3	C	178	SER	4.7
3	F	230	PRO	4.4
3	F	195	PHE	4.3
1	D	15	ARG	4.3
3	C	225	SER	4.0
3	F	222	ALA	3.8
3	C	177	PHE	3.8
3	F	237	PHE	3.6
3	F	110	THR	3.5
3	C	227	SER	3.4
3	C	220	CYS	3.4
3	C	243	ASP	3.3
3	C	221	SER	3.1
3	F	235	ASN	3.0
3	C	236	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	226	ARG	3.0
3	F	239	ILE	3.0
3	C	234	GLN	3.0
3	C	118	ASN	2.9
3	C	229	SER	2.9
3	C	230	PRO	2.9
2	B	57	GLN	2.9
3	F	3	GLU	2.9
3	C	123	ASP	2.9
3	C	219	LYS	2.8
3	C	124	PHE	2.8
3	C	241	GLU	2.8
3	F	219	LYS	2.8
1	A	15	ARG	2.7
3	C	250	ILE	2.7
3	C	224	SER	2.6
3	C	4	ALA	2.6
3	C	3	GLU	2.6
3	F	225	SER	2.5
3	C	110	THR	2.4
3	C	246	ASP	2.4
1	D	18	ASN	2.4
3	F	234	GLN	2.3
3	C	200	ASP	2.3
3	C	264	PHE	2.3
3	C	6	ILE	2.2
2	B	41	GLN	2.2
1	A	3	SER	2.2
3	C	112	GLU	2.2
3	F	227	SER	2.2
1	A	1	MET	2.1
3	C	222	ALA	2.1
3	F	228	VAL	2.0
3	C	242	ARG	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.